



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:19 pm GMT

PDB ID : 6EM4
EMDB ID : EMD-3889
Title : State B architectural model (Nsa1-TAP Flag-Ytm1) - Visualizing the assembly pathway of nucleolar pre-60S ribosomes
Authors : Kater, L.; Cheng, J.; Barrio-Garcia, C.; Hurt, E.; Beckmann, R.
Deposited on : 2017-10-01
Resolution : 4.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

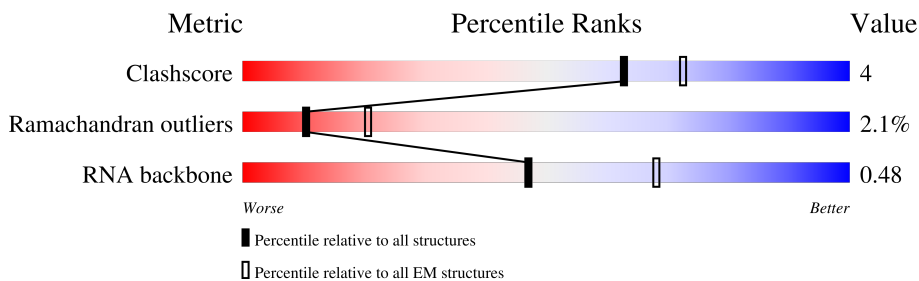
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.




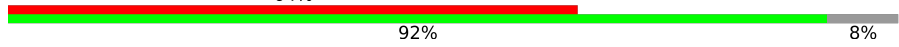

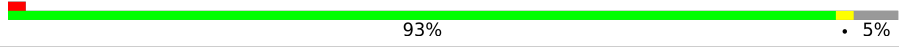
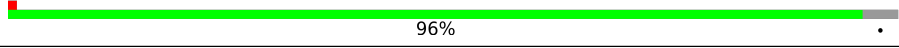

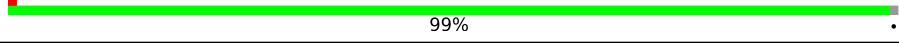
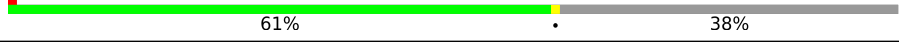
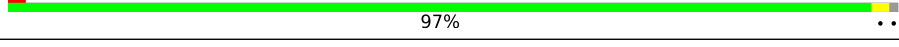



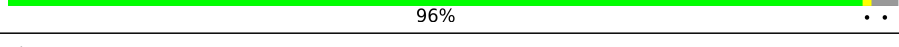

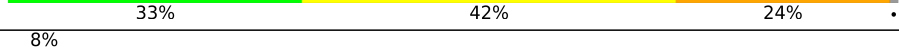
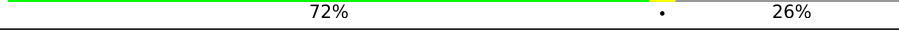
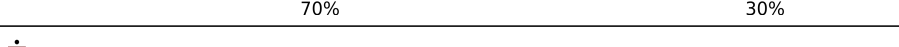
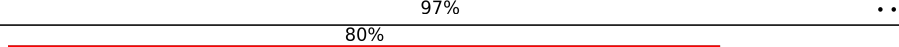
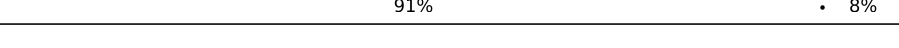
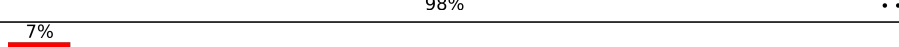
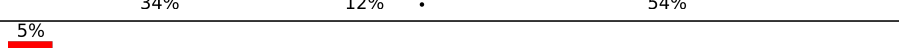




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | x | 295 | |
| 2 | F | 244 | |
| 3 | 3 | 306 | |
| 4 | 4 | 278 | |
| 5 | 5 | 463 | |
| 6 | A | 291 | |
| 7 | J | 427 | |
| 8 | u | 199 | |





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 9 | v | 231 |  56% 44% |
| 10 | y | 245 |  64% 92% 8% |
| 11 | B | 387 |  23% 82% 14% |
| 12 | C | 362 |  93% 5% |
| 13 | e | 130 |  96% |
| 14 | E | 176 |  86% 14% |
| 15 | f | 107 |  99% |
| 16 | G | 256 |  61% 38% |
| 17 | h | 120 |  97% |
| 18 | i | 100 |  72% 26% |
| 19 | j | 88 |  81% 19% |
| 20 | L | 199 |  53% 46% |
| 21 | M | 138 |  96% |
| 22 | N | 204 |  86% 13% |
| 23 | O | 199 |  6% 33% 42% 24% |
| 24 | P | 184 |  8% 72% 26% |
| 25 | Q | 186 |  70% 30% |
| 26 | S | 172 |  97% |
| 27 | V | 137 |  80% 91% 8% |
| 28 | Y | 127 |  98% |
| 29 | 1 | 3396 |  7% 34% 12% 54% |
| 30 | 2 | 158 |  5% 76% 22% |
| 31 | D | 505 |  37% 62% |
| 32 | K | 376 |  64% 35% |
| 33 | n | 605 |  52% 48% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 34 | o | 220 |  53% 47% |
| 35 | t | 322 |  76% 23% |
| 36 | 6 | 232 |  14% 12% 72% |
| 37 | H | 807 |  17% 82% |

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 45400 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 protein called Ribosome production factor 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 1 | x | 267 | 1068 | 534 | 267 | 267 | 0 | 0 |

- Molecule 2 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 2 | F | 241 | 964 | 482 | 241 | 241 | 0 | 0 |

- Molecule 3 is a protein called Protein MAK16.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 3 | 3 | 173 | 692 | 346 | 173 | 173 | 0 | 0 |

- Molecule 4 is a protein called Ribosomal RNA-processing protein 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 4 | 4 | 220 | 880 | 440 | 220 | 220 | 0 | 0 |

- Molecule 5 is a protein called Ribosome biogenesis protein NSA1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 5 | 5 | 385 | 1540 | 770 | 385 | 385 | 0 | 0 |

- Molecule 6 is a protein called Ribosome biogenesis protein BRX1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 6 | A | 145 | 580 | 290 | 145 | 145 | 0 | 0 |

- Molecule 7 is a protein called rRNA-processing protein EBP2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 7 | J | 66 | 264 | 132 | 66 | 66 | 0 | 0 |

- Molecule 8 is a protein called Ribosome biogenesis protein RLP24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 8 | u | 116 | 464 | 232 | 116 | 116 | 0 | 0 |

- Molecule 9 is a protein called Nucleolar protein 16.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 9 | v | 130 | 520 | 260 | 130 | 130 | 0 | 0 |

- Molecule 10 is a protein called Eukaryotic translation initiation factor 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 10 | y | 225 | 900 | 450 | 225 | 225 | 0 | 0 |

- Molecule 11 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 11 | B | 333 | 1332 | 666 | 333 | 333 | 0 | 0 |

- Molecule 12 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 12 | C | 343 | 1372 | 686 | 343 | 343 | 0 | 0 |

- Molecule 13 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 13 | e | 125 | 500 | 250 | 125 | 125 | 0 | 0 |

- Molecule 14 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 14 | E | 151 | Total | C | N | O | 0 | 0 |
| | | | 604 | 302 | 151 | 151 | | |

- Molecule 15 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 15 | f | 106 | Total | C | N | O | 0 | 0 |
| | | | 424 | 212 | 106 | 106 | | |

- Molecule 16 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 16 | G | 159 | Total | C | N | O | 0 | 0 |
| | | | 636 | 318 | 159 | 159 | | |

- Molecule 17 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 17 | h | 119 | Total | C | N | O | 0 | 0 |
| | | | 476 | 238 | 119 | 119 | | |

- Molecule 18 is a protein called 60S ribosomal protein L36-B.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|----|---------|-------|---|
| 18 | i | 74 | Total | C | N | O | 0 | 0 |
| | | | 296 | 148 | 74 | 74 | | |

- Molecule 19 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|----|---------|-------|---|
| 19 | j | 71 | Total | C | N | O | 0 | 0 |
| | | | 284 | 142 | 71 | 71 | | |

- Molecule 20 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 20 | L | 108 | Total | C | N | O | 0 | 0 |
| | | | 432 | 216 | 108 | 108 | | |

- Molecule 21 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 21 | M | 134 | Total | C | N | O | 0 | 0 |
| | | | 536 | 268 | 134 | 134 | | |

- Molecule 22 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 22 | N | 177 | Total | C | N | O | 0 | 0 |
| | | | 708 | 354 | 177 | 177 | | |

- Molecule 23 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 23 | O | 197 | Total | C | N | O | 0 | 0 |
| | | | 788 | 394 | 197 | 197 | | |

- Molecule 24 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 24 | P | 137 | Total | C | N | O | 0 | 0 |
| | | | 548 | 274 | 137 | 137 | | |

- Molecule 25 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 25 | Q | 131 | Total | C | N | O | 0 | 0 |
| | | | 524 | 262 | 131 | 131 | | |

- Molecule 26 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 26 | S | 170 | Total | C | N | O | 0 | 0 |
| | | | 680 | 340 | 170 | 170 | | |

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 27 | V | 126 | Total | C | N | O | 0 | 0 |
| | | | 504 | 252 | 126 | 126 | | |

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 28 | Y | 125 | Total | C | N | O | 0 | 0 |
| | | | 500 | 250 | 125 | 125 | | |

- Molecule 29 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 29 | 1 | 1556 | Total | C | O | P | 0 | 0 |
| | | | 18672 | 7780 | 9336 | 1556 | | |

- Molecule 30 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 30 | 2 | 158 | Total | C | O | P | 0 | 0 |
| | | | 1896 | 790 | 948 | 158 | | |

- Molecule 31 is a protein called ATP-dependent RNA helicase HAS1.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 31 | D | 194 | Total | C | N | O | 0 | 0 |
| | | | 776 | 388 | 194 | 194 | | |

- Molecule 32 is a protein called Proteasome-interacting protein CIC1.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 32 | K | 246 | Total | C | N | O | 0 | 0 |
| | | | 984 | 492 | 246 | 246 | | |

- Molecule 33 is a protein called Pescadillo homolog.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 33 | n | 312 | Total | C | N | O | 0 | 0 |
| | | | 1248 | 624 | 312 | 312 | | |

- Molecule 34 is a protein called Ribosome biogenesis protein 15.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| 34 | o | 116 | Total | C | N | O | 0 | 0 |
| | | | 464 | 232 | 116 | 116 | | |

- Molecule 35 is a protein called Ribosome biogenesis protein RLP7.

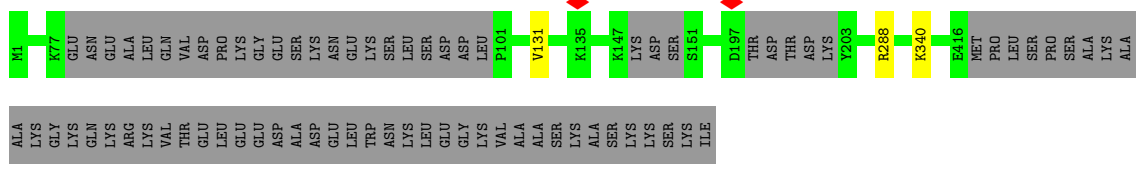
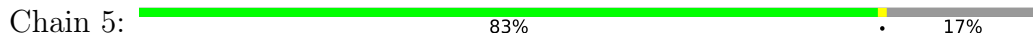
| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| | | | Total | C | N | | | O |
| 35 | t | 248 | 992 | 496 | 248 | 248 | 0 | 0 |

- Molecule 36 is a RNA chain called internal transcribed spacer 1.

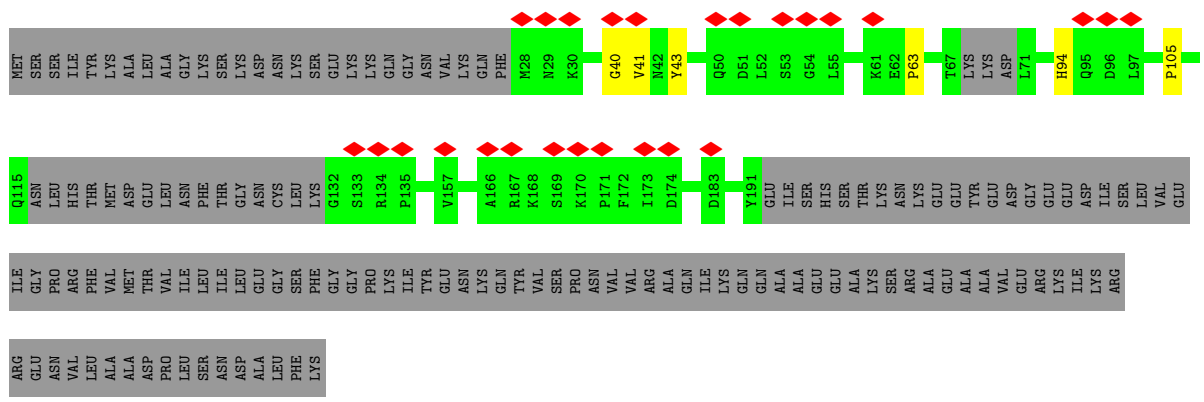
| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| | | | Total | C | O | | | P |
| 36 | 6 | 65 | 780 | 325 | 390 | 65 | 0 | 0 |

- Molecule 37 is a protein called Ribosome biogenesis protein ERB1.

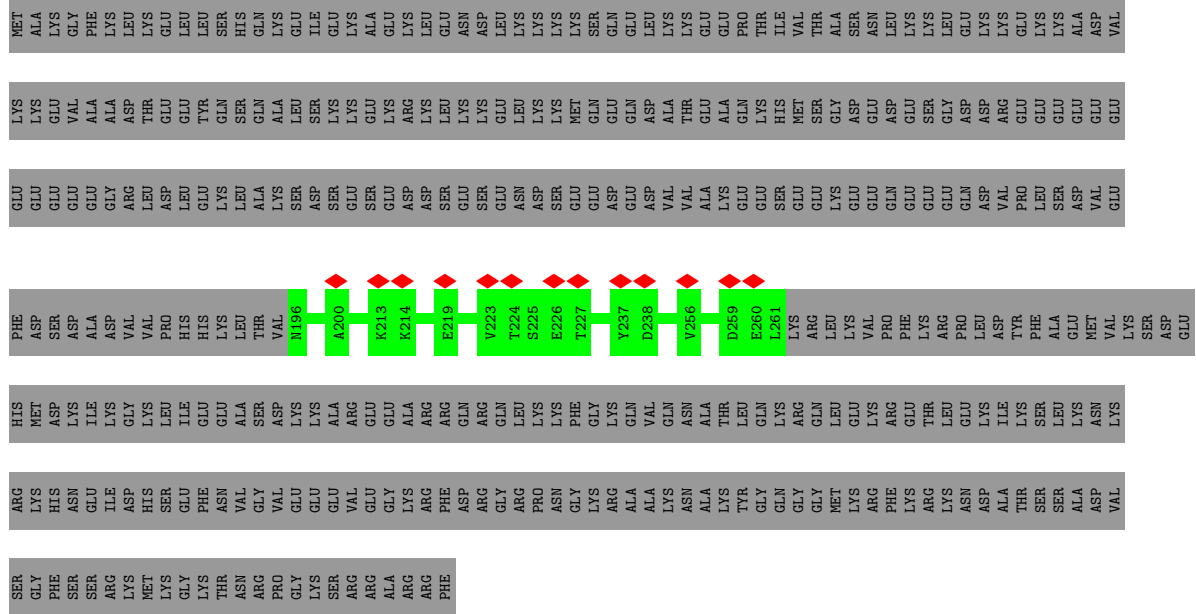
| Mol | Chain | Residues | Atoms | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---------|-------|---|
| | | | Total | C | N | | | O |
| 37 | H | 143 | 572 | 286 | 143 | 143 | 0 | 0 |



● Molecule 6: Ribosome biogenesis protein BRX1

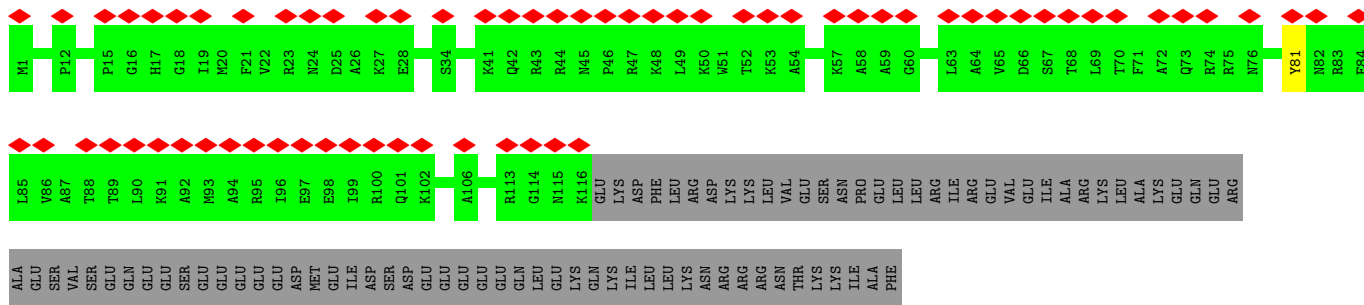


● Molecule 7: rRNA-processing protein EBP2

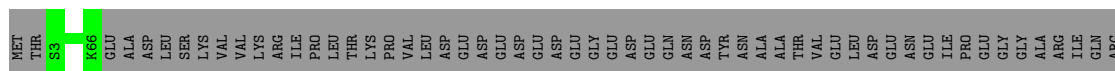


● Molecule 8: Ribosome biogenesis protein RLP24

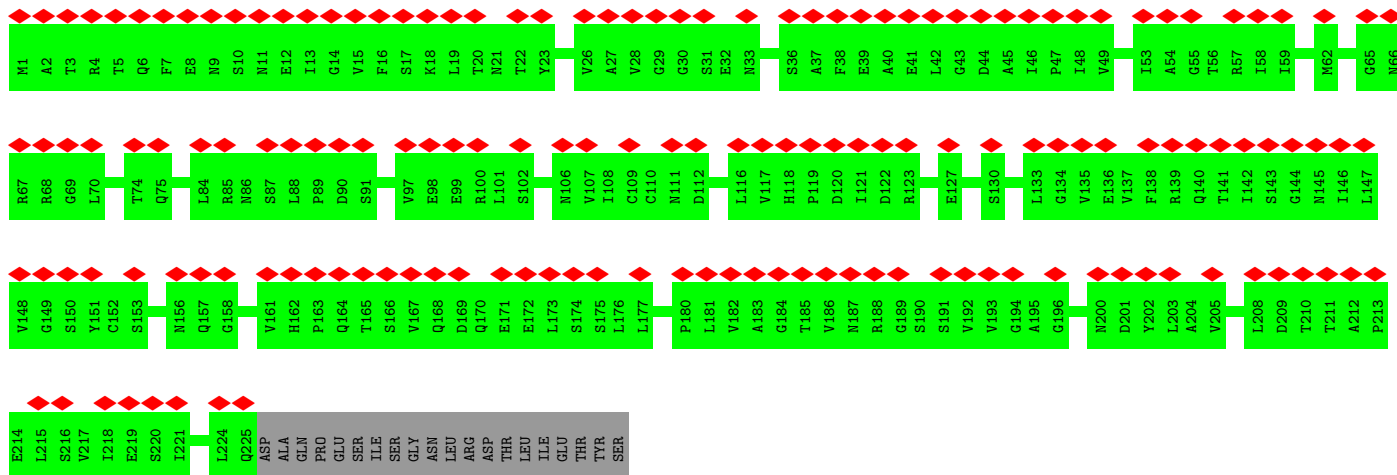
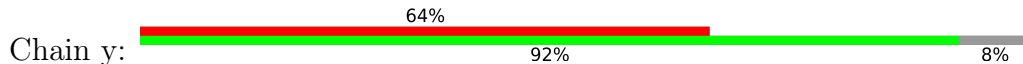




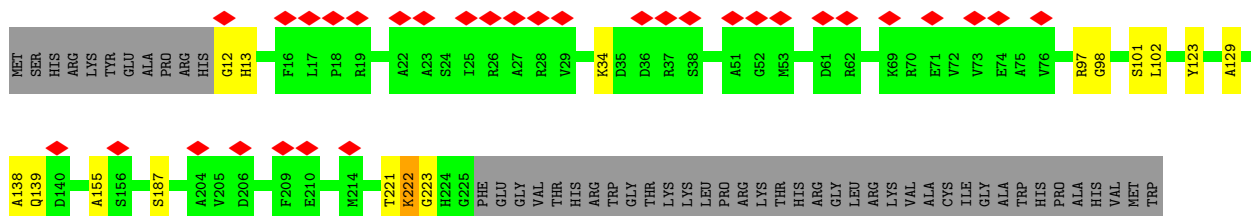
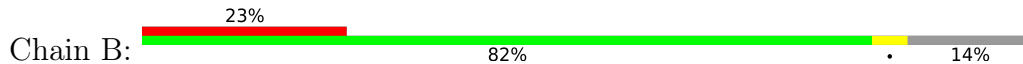
• Molecule 9: Nucleolar protein 16

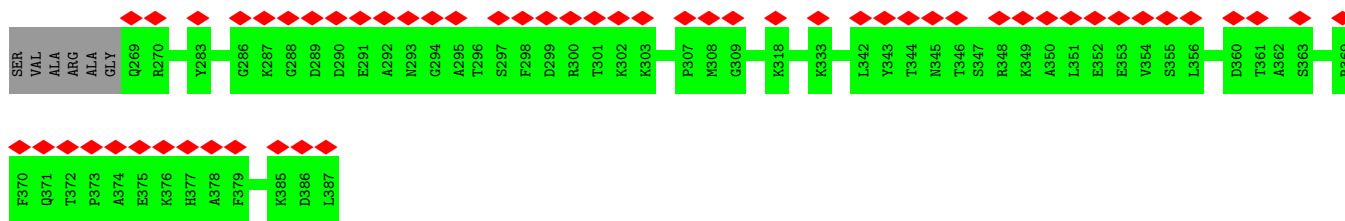


• Molecule 10: Eukaryotic translation initiation factor 6



• Molecule 11: 60S ribosomal protein L3





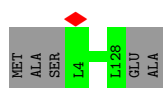
- Molecule 12: 60S ribosomal protein L4-A

Chain C: 93% 5%



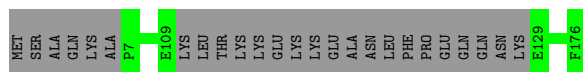
- Molecule 13: 60S ribosomal protein L32

Chain e: 96%



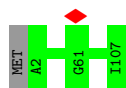
- Molecule 14: 60S ribosomal protein L6-A

Chain E: 86% 14%



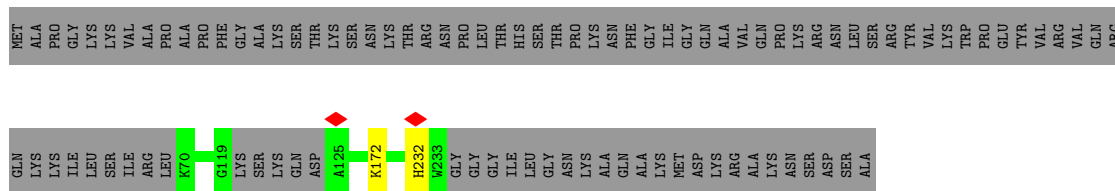
- Molecule 15: 60S ribosomal protein L33-A

Chain f: 99%



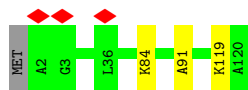
- Molecule 16: 60S ribosomal protein L8-A

Chain G: 61% 38%

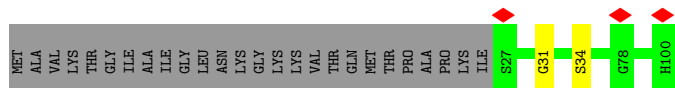


- Molecule 17: 60S ribosomal protein L35-A

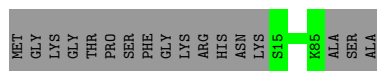
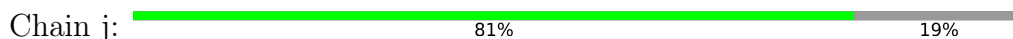
Chain h: 97%



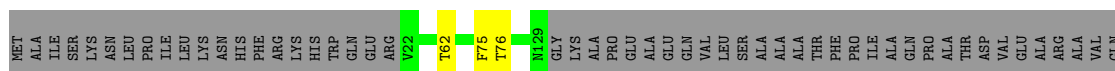
• Molecule 18: 60S ribosomal protein L36-B



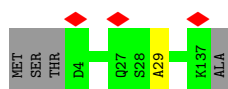
• Molecule 19: 60S ribosomal protein L37-A



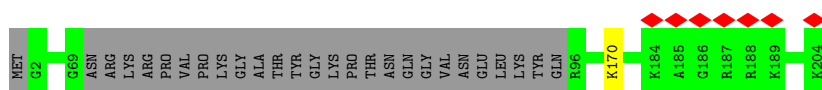
• Molecule 20: 60S ribosomal protein L13-A



• Molecule 21: 60S ribosomal protein L14-A



• Molecule 22: 60S ribosomal protein L15-A

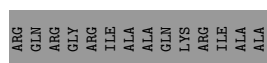
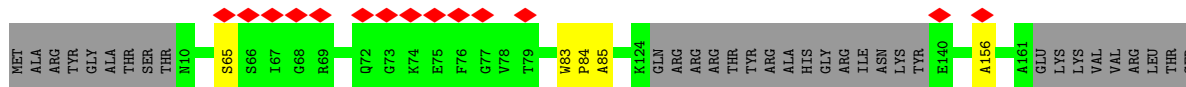


• Molecule 23: 60S ribosomal protein L16-A

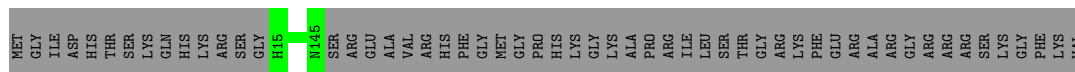




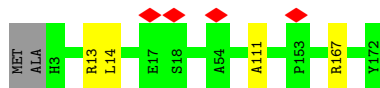
• Molecule 24: 60S ribosomal protein L17-A



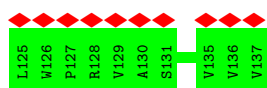
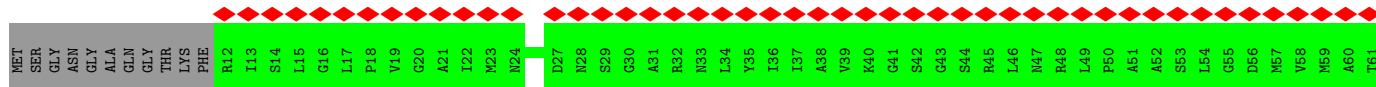
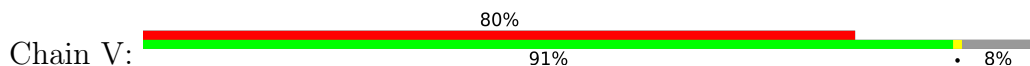
• Molecule 25: 60S ribosomal protein L18-A



• Molecule 26: 60S ribosomal protein L20-A



• Molecule 27: 60S ribosomal protein L23-A

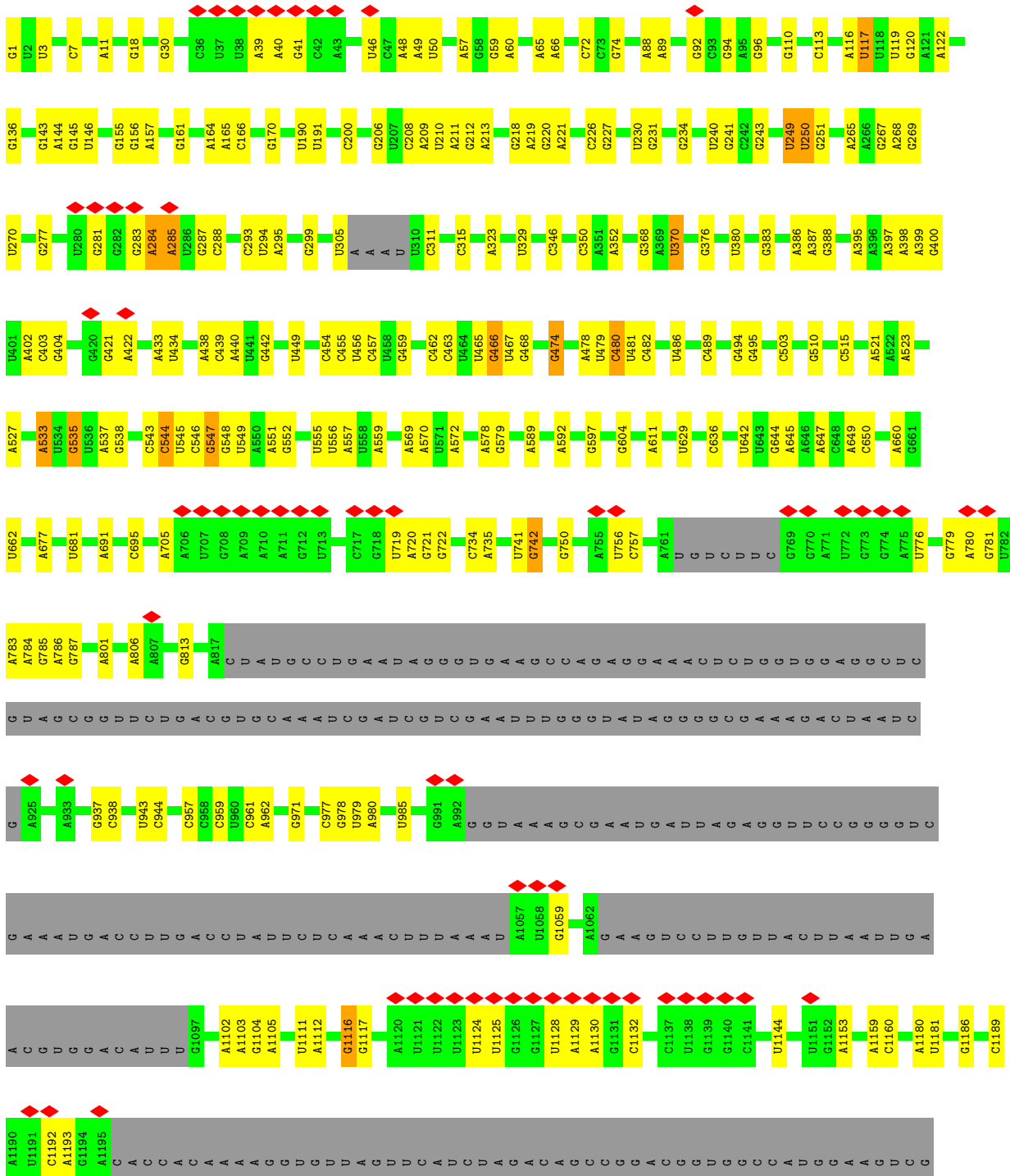
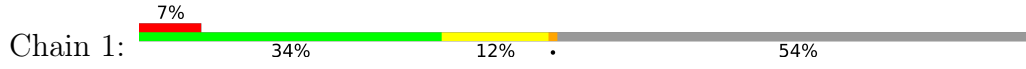


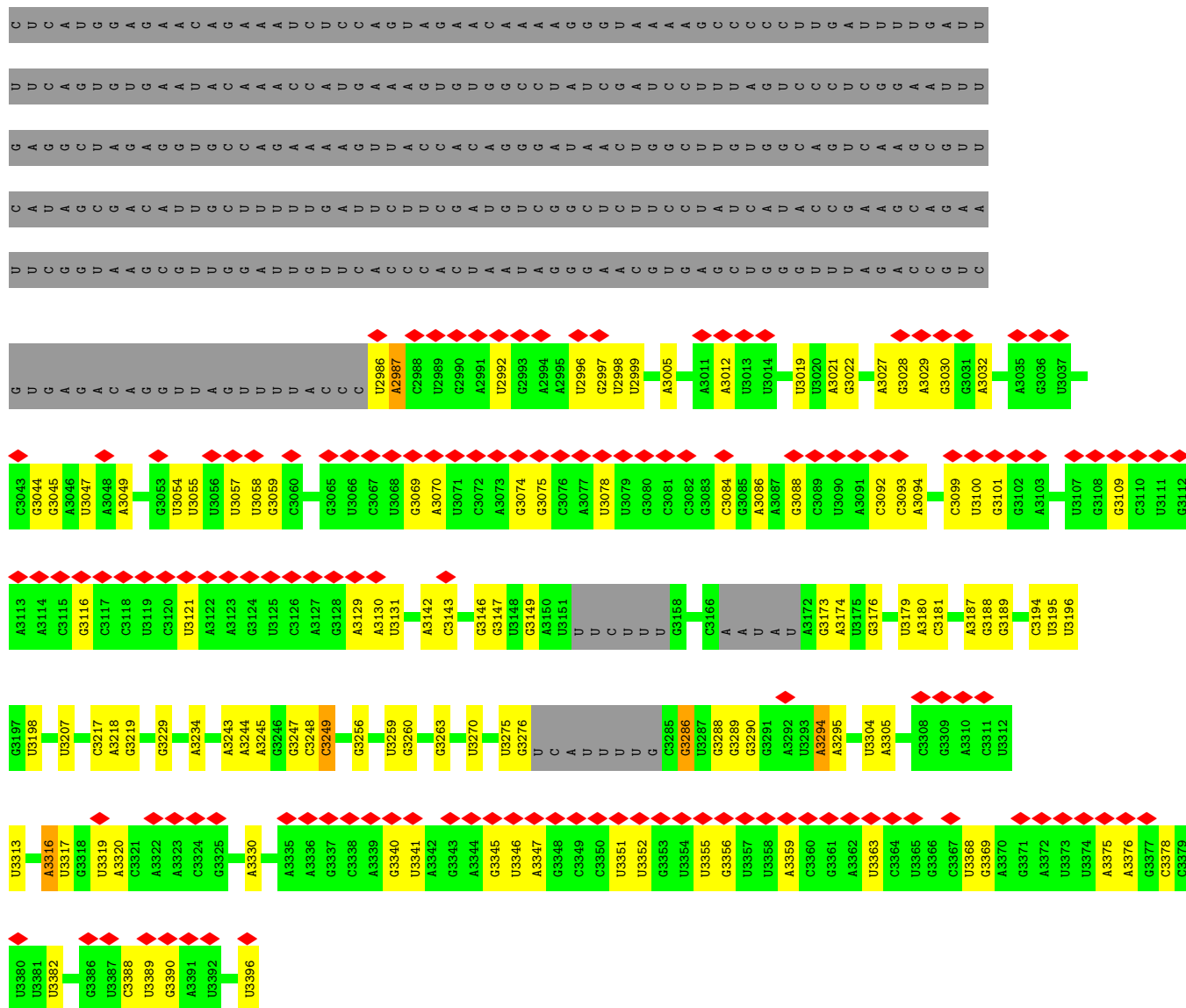
• Molecule 28: 60S ribosomal protein L26-A



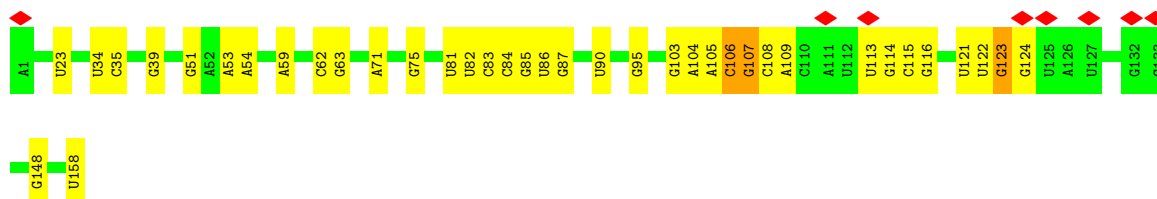
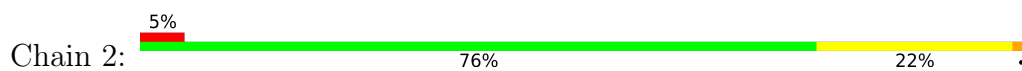


• Molecule 29: 25S ribosomal RNA



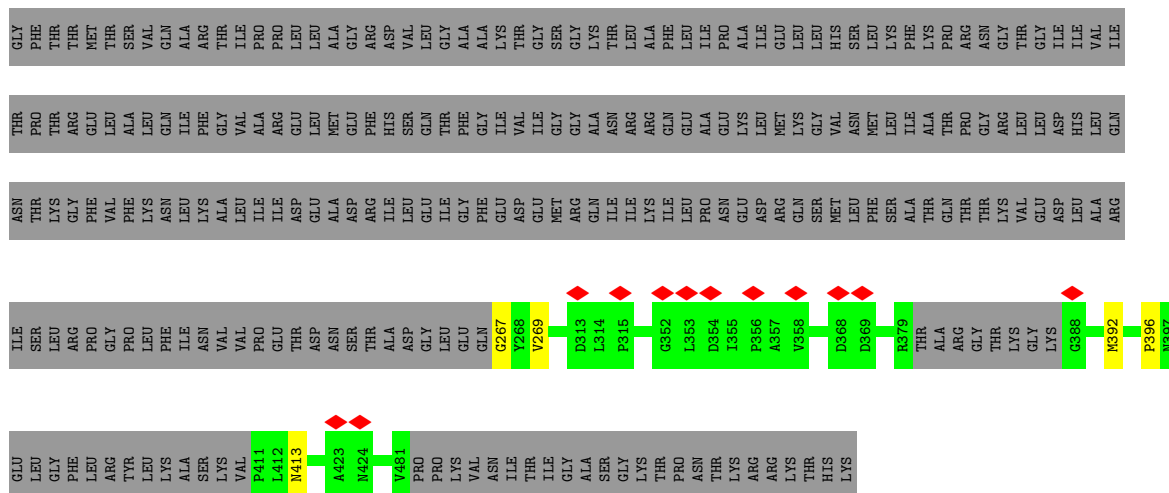


● Molecule 30: 5.8S ribosomal RNA



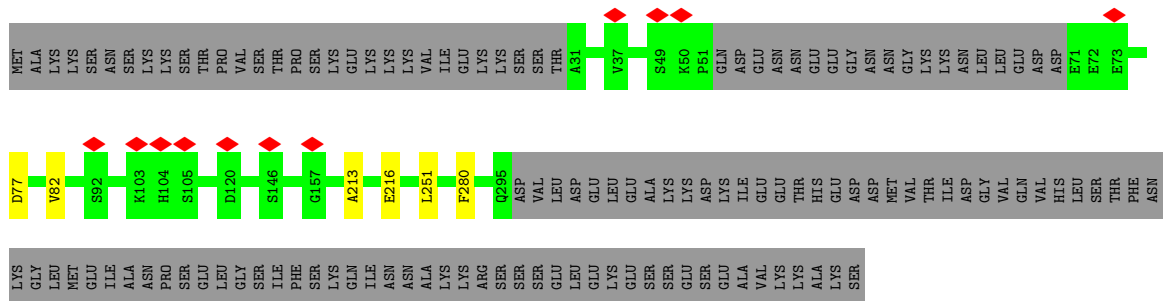
● Molecule 31: ATP-dependent RNA helicase HAS1





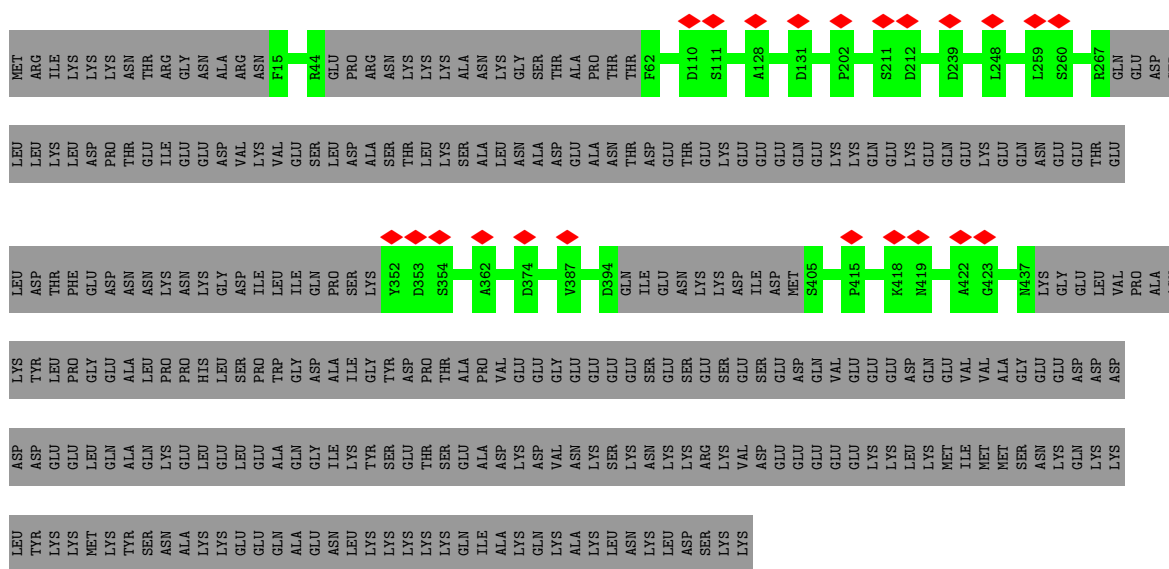
• Molecule 32: Proteasome-interacting protein CIC1

Chain K:



• Molecule 33: Pescadillo homolog

Chain n:



• Molecule 34: Ribosome biogenesis protein 15

4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 65539 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 27 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 0.131 | Depositor |
| Minimum map value | -0.036 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.006 | Depositor |
| Recommended contour level | 0.03 | Depositor |
| Map size (\AA) | 455.28, 455.28, 455.28 | wwPDB |
| Map dimensions | 420, 420, 420 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.084, 1.084, 1.084 | 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 >5 | RMSZ | # Z >5 |
| 1 | x | 0.40 | 0/1064 | 0.67 | 0/1323 |
| 2 | F | 0.35 | 0/963 | 0.57 | 0/1202 |
| 3 | 3 | 0.36 | 0/691 | 0.63 | 0/862 |
| 4 | 4 | 0.29 | 0/878 | 0.75 | 2/1094 (0.2%) |
| 5 | 5 | 0.36 | 0/1536 | 0.57 | 0/1913 |
| 6 | A | 0.43 | 0/577 | 0.60 | 0/716 |
| 7 | J | 0.41 | 0/263 | 0.58 | 0/327 |
| 8 | u | 0.38 | 0/463 | 0.58 | 0/577 |
| 9 | v | 0.34 | 0/517 | 0.53 | 0/641 |
| 10 | y | 0.41 | 0/899 | 0.58 | 0/1122 |
| 11 | B | 0.38 | 0/1330 | 0.60 | 0/1659 |
| 12 | C | 0.37 | 0/1371 | 0.60 | 0/1712 |
| 13 | e | 0.35 | 0/499 | 0.58 | 0/622 |
| 14 | E | 0.35 | 0/602 | 0.59 | 0/749 |
| 15 | f | 0.32 | 0/423 | 0.57 | 0/527 |
| 16 | G | 0.37 | 0/634 | 0.61 | 0/789 |
| 17 | h | 0.36 | 0/475 | 0.55 | 0/592 |
| 18 | i | 0.38 | 0/295 | 0.56 | 0/367 |
| 19 | j | 0.36 | 0/283 | 0.59 | 0/352 |
| 20 | L | 0.35 | 0/431 | 0.61 | 0/537 |
| 21 | M | 0.34 | 0/535 | 0.55 | 0/667 |
| 22 | N | 0.35 | 0/706 | 0.55 | 0/879 |
| 23 | O | 0.25 | 0/787 | 0.41 | 0/982 |
| 24 | P | 0.34 | 0/546 | 0.56 | 0/679 |
| 25 | Q | 0.35 | 0/523 | 0.55 | 0/652 |
| 26 | S | 0.38 | 0/679 | 0.61 | 0/847 |
| 27 | V | 0.41 | 0/503 | 0.58 | 0/627 |
| 28 | Y | 0.33 | 0/499 | 0.55 | 0/622 |
| 29 | 1 | 0.24 | 0/20215 | 0.84 | 5/31068 (0.0%) |
| 30 | 2 | 0.23 | 0/2047 | 0.85 | 1/3132 (0.0%) |
| 31 | D | 0.63 | 0/773 | 0.66 | 0/961 |
| 32 | K | 0.58 | 0/982 | 0.63 | 0/1224 |
| 33 | n | 0.59 | 0/1244 | 0.57 | 0/1548 |
| 34 | o | 0.71 | 0/462 | 0.65 | 0/574 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 35 | t | 0.65 | 0/990 | 0.65 | 0/1234 |
| 36 | 6 | 0.70 | 0/843 | 0.99 | 1/1292 (0.1%) |
| 37 | H | 0.61 | 0/570 | 0.69 | 0/709 |
| All | All | 0.36 | 0/47098 | 0.74 | 9/65380 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 4 | 4 | 0 | 2 |
| 31 | D | 0 | 1 |
| 35 | t | 0 | 2 |
| 37 | H | 0 | 2 |
| All | All | 0 | 7 |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 4 | 4 | 132 | GLN | N-CA-C | -12.69 | 76.73 | 111.00 |
| 29 | 1 | 1102 | A | C2'-C3'-O3' | 7.45 | 125.88 | 109.50 |
| 29 | 1 | 649 | A | C2'-C3'-O3' | 6.42 | 123.97 | 113.70 |
| 4 | 4 | 133 | LEU | N-CA-C | -6.28 | 94.06 | 111.00 |
| 30 | 2 | 114 | G | C2'-C3'-O3' | 6.17 | 123.58 | 113.70 |
| 29 | 1 | 1347 | U | C4'-C3'-O3' | 5.95 | 124.90 | 113.00 |
| 29 | 1 | 480 | C | C2'-C3'-O3' | 5.92 | 123.18 | 113.70 |
| 36 | 6 | 16 | U | P-O3'-C3' | 5.31 | 126.07 | 119.70 |
| 29 | 1 | 456 | U | C2'-C3'-O3' | 5.28 | 122.14 | 113.70 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 4 | 4 | 135 | TYR | Peptide |
| 4 | 4 | 136 | LEU | Peptide |
| 31 | D | 396 | PRO | Peptide |
| 37 | H | 268 | PRO | Peptide |
| 37 | H | 335 | GLU | Peptide |
| 35 | t | 226 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 35 | t | 270 | PRO | Peptide |

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 | x | 1068 | 0 | 271 | 0 | 0 |
| 2 | F | 964 | 0 | 259 | 0 | 0 |
| 3 | 3 | 692 | 0 | 177 | 1 | 0 |
| 4 | 4 | 880 | 0 | 222 | 7 | 0 |
| 5 | 5 | 1540 | 0 | 421 | 1 | 0 |
| 6 | A | 580 | 0 | 142 | 5 | 0 |
| 7 | J | 264 | 0 | 64 | 0 | 0 |
| 8 | u | 464 | 0 | 122 | 0 | 0 |
| 9 | v | 520 | 0 | 139 | 0 | 0 |
| 10 | y | 900 | 0 | 258 | 0 | 0 |
| 11 | B | 1332 | 0 | 372 | 34 | 0 |
| 12 | C | 1372 | 0 | 380 | 0 | 0 |
| 13 | e | 500 | 0 | 133 | 0 | 0 |
| 14 | E | 604 | 0 | 156 | 0 | 0 |
| 15 | f | 424 | 0 | 117 | 0 | 0 |
| 16 | G | 636 | 0 | 159 | 1 | 0 |
| 17 | h | 476 | 0 | 118 | 0 | 0 |
| 18 | i | 296 | 0 | 80 | 0 | 0 |
| 19 | j | 284 | 0 | 83 | 0 | 0 |
| 20 | L | 432 | 0 | 112 | 0 | 0 |
| 21 | M | 536 | 0 | 143 | 0 | 0 |
| 22 | N | 708 | 0 | 191 | 1 | 0 |
| 23 | O | 788 | 0 | 213 | 129 | 0 |
| 24 | P | 548 | 0 | 144 | 6 | 0 |
| 25 | Q | 524 | 0 | 137 | 0 | 0 |
| 26 | S | 680 | 0 | 170 | 1 | 0 |
| 27 | V | 504 | 0 | 146 | 0 | 0 |
| 28 | Y | 500 | 0 | 133 | 1 | 0 |
| 29 | 1 | 18672 | 0 | 9348 | 99 | 0 |
| 30 | 2 | 1896 | 0 | 954 | 8 | 0 |
| 31 | D | 776 | 0 | 199 | 2 | 0 |
| 32 | K | 984 | 0 | 248 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33 | n | 1248 | 0 | 314 | 0 | 0 |
| 34 | o | 464 | 0 | 126 | 0 | 0 |
| 35 | t | 992 | 0 | 263 | 0 | 0 |
| 36 | 6 | 780 | 0 | 392 | 24 | 0 |
| 37 | H | 572 | 0 | 134 | 4 | 0 |
| All | All | 45400 | 0 | 17040 | 251 | 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 4.

All (251) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 29:1:1:G:P | 36:6:232:A:H3' | 1.39 | 1.61 |
| 11:B:12:GLY:C | 29:1:3044:G:H5'' | 1.15 | 1.50 |
| 29:1:1:G:OP2 | 36:6:232:A:H5'' | 1.29 | 1.30 |
| 23:O:98:ALA:O | 23:O:100:GLU:N | 1.60 | 1.29 |
| 23:O:189:ASP:O | 23:O:191:ALA:N | 1.64 | 1.28 |
| 29:1:1:G:OP2 | 36:6:232:A:H3' | 1.27 | 1.27 |
| 11:B:13:HIS:N | 29:1:3044:G:O3' | 1.67 | 1.26 |
| 23:O:52:LEU:O | 23:O:54:TYR:N | 1.72 | 1.22 |
| 30:2:158:U:O2' | 36:6:1:C:OP1 | 1.57 | 1.22 |
| 23:O:88:VAL:O | 23:O:90:HIS:N | 1.74 | 1.21 |
| 11:B:12:GLY:C | 29:1:3044:G:C5' | 2.10 | 1.20 |
| 23:O:187:GLU:O | 23:O:188:SER:O | 1.60 | 1.19 |
| 29:1:1:G:OP2 | 36:6:232:A:C5' | 1.88 | 1.19 |
| 29:1:1:G:OP2 | 36:6:232:A:C3' | 1.92 | 1.16 |
| 11:B:13:HIS:CA | 29:1:3044:G:O3' | 1.92 | 1.16 |
| 29:1:1:G:P | 36:6:232:A:C3' | 2.34 | 1.14 |
| 11:B:13:HIS:CA | 29:1:3044:G:H4' | 1.78 | 1.14 |
| 4:4:84:THR:O | 4:4:86:ASP:N | 1.83 | 1.10 |
| 30:2:158:U:C2' | 36:6:1:C:OP1 | 2.02 | 1.07 |
| 11:B:98:GLY:HA3 | 29:1:3005:A:H5'' | 1.30 | 1.05 |
| 11:B:13:HIS:H | 29:1:3045:G:P | 1.81 | 1.03 |
| 29:1:1:G:O4' | 36:6:232:A:O2' | 1.75 | 1.03 |
| 29:1:1:G:H5' | 36:6:232:A:O2' | 1.59 | 1.02 |
| 23:O:162:VAL:O | 23:O:164:SER:N | 1.93 | 1.01 |
| 11:B:221:THR:C | 29:1:3047:U:OP1 | 2.00 | 1.00 |
| 11:B:12:GLY:O | 29:1:3044:G:H5'' | 1.60 | 1.00 |
| 11:B:98:GLY:HA3 | 29:1:3005:A:C5' | 1.93 | 0.99 |
| 11:B:222:LYS:N | 29:1:3047:U:OP1 | 1.96 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:O:95:GLY:O | 23:O:98:ALA:N | 1.94 | 0.99 |
| 23:O:164:SER:O | 23:O:167:TYR:N | 1.94 | 0.99 |
| 23:O:52:LEU:C | 23:O:54:TYR:H | 1.64 | 0.98 |
| 11:B:12:GLY:CA | 29:1:3044:G:H5'' | 1.95 | 0.97 |
| 29:1:1:G:C4' | 36:6:232:A:O2' | 2.14 | 0.95 |
| 11:B:13:HIS:N | 29:1:3044:G:H5'' | 1.81 | 0.94 |
| 11:B:13:HIS:CA | 29:1:3044:G:C4' | 2.46 | 0.94 |
| 29:1:1:G:H5' | 36:6:232:A:C2' | 1.98 | 0.93 |
| 29:1:1:G:C5' | 36:6:232:A:O2' | 2.18 | 0.91 |
| 23:O:88:VAL:C | 23:O:90:HIS:H | 1.71 | 0.90 |
| 29:1:1:G:H5' | 36:6:232:A:C3' | 2.02 | 0.90 |
| 23:O:54:TYR:O | 23:O:57:PHE:N | 2.06 | 0.89 |
| 23:O:98:ALA:O | 23:O:101:ARG:N | 2.06 | 0.89 |
| 29:1:1:G:OP2 | 36:6:232:A:C4' | 2.19 | 0.88 |
| 11:B:223:GLY:HA3 | 29:1:3305:A:OP1 | 1.74 | 0.88 |
| 23:O:155:LYS:O | 23:O:157:GLU:N | 2.07 | 0.86 |
| 23:O:45:GLY:O | 23:O:46:GLU:O | 1.92 | 0.86 |
| 23:O:89:SER:O | 23:O:91:LYS:N | 2.08 | 0.86 |
| 30:2:158:U:H2' | 36:6:1:C:OP1 | 1.75 | 0.86 |
| 23:O:137:THR:O | 23:O:139:GLY:N | 2.09 | 0.85 |
| 29:1:1:G:O4' | 36:6:232:A:C2' | 2.23 | 0.85 |
| 4:4:129:LEU:O | 4:4:132:GLN:O | 1.94 | 0.85 |
| 4:4:60:ARG:CA | 29:1:466:G:O5' | 2.12 | 0.85 |
| 11:B:13:HIS:N | 29:1:3044:G:C3' | 2.39 | 0.84 |
| 23:O:164:SER:O | 23:O:166:GLU:N | 2.11 | 0.84 |
| 23:O:59:ARG:O | 23:O:60:LYS:O | 1.97 | 0.83 |
| 23:O:130:LYS:O | 23:O:131:PRO:O | 1.96 | 0.83 |
| 11:B:13:HIS:N | 29:1:3044:G:C4' | 2.42 | 0.82 |
| 29:1:1:G:O4' | 36:6:232:A:H2' | 1.80 | 0.82 |
| 11:B:123:TYR:CA | 29:1:3316:A:OP2 | 2.26 | 0.82 |
| 23:O:55:HIS:O | 23:O:58:LEU:N | 2.13 | 0.81 |
| 23:O:95:GLY:O | 23:O:97:ALA:N | 2.14 | 0.80 |
| 29:1:1:G:C5' | 36:6:232:A:C2' | 2.61 | 0.79 |
| 11:B:221:THR:CA | 29:1:3047:U:OP1 | 2.30 | 0.79 |
| 23:O:157:GLU:O | 23:O:159:LYS:N | 2.17 | 0.78 |
| 11:B:13:HIS:CA | 29:1:3044:G:C3' | 2.63 | 0.76 |
| 23:O:157:GLU:O | 23:O:160:ARG:N | 2.19 | 0.76 |
| 23:O:189:ASP:O | 23:O:190:VAL:C | 2.24 | 0.75 |
| 23:O:98:ALA:O | 23:O:99:LEU:C | 2.24 | 0.75 |
| 23:O:82:LYS:O | 23:O:84:LEU:N | 2.20 | 0.74 |
| 23:O:98:ALA:C | 23:O:100:GLU:N | 2.35 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 11:B:12:GLY:O | 29:1:3044:G:C5' | 2.30 | 0.74 |
| 6:A:40:GLY:HA2 | 29:1:285:A:OP2 | 1.87 | 0.74 |
| 23:O:164:SER:O | 23:O:165:ALA:C | 2.26 | 0.74 |
| 11:B:12:GLY:HA2 | 29:1:3044:G:OP1 | 1.90 | 0.72 |
| 23:O:98:ALA:O | 23:O:100:GLU:CA | 2.38 | 0.72 |
| 23:O:189:ASP:C | 23:O:191:ALA:N | 2.42 | 0.71 |
| 23:O:191:ALA:O | 23:O:192:LYS:C | 2.29 | 0.71 |
| 23:O:95:GLY:O | 23:O:96:LYS:C | 2.28 | 0.70 |
| 23:O:171:LYS:O | 23:O:174:PHE:N | 2.26 | 0.69 |
| 23:O:76:PRO:O | 23:O:77:SER:C | 2.30 | 0.69 |
| 29:1:1:G:C5' | 36:6:232:A:C3' | 2.70 | 0.69 |
| 29:1:1:G:O5' | 36:6:232:A:H3' | 1.93 | 0.69 |
| 11:B:13:HIS:N | 29:1:3044:G:C5' | 2.46 | 0.68 |
| 23:O:15:LEU:O | 23:O:16:VAL:C | 2.30 | 0.68 |
| 23:O:18:ARG:O | 23:O:19:LEU:C | 2.33 | 0.68 |
| 11:B:97:ARG:O | 29:1:3005:A:H4' | 1.94 | 0.67 |
| 24:P:83:TRP:O | 29:1:2352:A:H4' | 1.94 | 0.67 |
| 23:O:155:LYS:C | 23:O:157:GLU:H | 1.97 | 0.67 |
| 23:O:112:TYR:O | 23:O:115:LYS:N | 2.23 | 0.67 |
| 23:O:146:GLY:O | 23:O:147:TRP:C | 2.32 | 0.66 |
| 4:4:84:THR:O | 4:4:85:ALA:C | 2.33 | 0.66 |
| 23:O:189:ASP:O | 23:O:191:ALA:CA | 2.42 | 0.66 |
| 4:4:84:THR:C | 4:4:86:ASP:N | 2.48 | 0.66 |
| 23:O:167:TYR:O | 23:O:168:TYR:C | 2.34 | 0.65 |
| 23:O:19:LEU:O | 23:O:20:ALA:C | 2.35 | 0.64 |
| 23:O:20:ALA:O | 23:O:23:VAL:N | 2.30 | 0.64 |
| 23:O:112:TYR:O | 23:O:113:ASP:C | 2.35 | 0.64 |
| 23:O:17:GLY:HA3 | 29:1:1313:G:O3' | 1.97 | 0.64 |
| 23:O:162:VAL:O | 23:O:163:SER:C | 2.36 | 0.64 |
| 23:O:82:LYS:C | 23:O:84:LEU:H | 2.01 | 0.63 |
| 23:O:184:THR:C | 23:O:186:ALA:H | 2.02 | 0.63 |
| 23:O:155:LYS:C | 23:O:157:GLU:N | 2.49 | 0.63 |
| 23:O:20:ALA:O | 23:O:21:SER:C | 2.37 | 0.62 |
| 23:O:138:LEU:O | 23:O:139:GLY:C | 2.38 | 0.62 |
| 23:O:84:LEU:C | 23:O:86:GLY:H | 2.03 | 0.62 |
| 4:4:84:THR:C | 4:4:86:ASP:H | 2.01 | 0.61 |
| 23:O:120:VAL:O | 23:O:122:GLN:N | 2.34 | 0.61 |
| 23:O:76:PRO:O | 23:O:79:ILE:N | 2.33 | 0.61 |
| 23:O:184:THR:O | 23:O:186:ALA:N | 2.35 | 0.60 |
| 29:1:644:G:OP2 | 29:1:1116:G:O2' | 2.19 | 0.59 |
| 23:O:184:THR:C | 23:O:186:ALA:N | 2.56 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 23:O:146:GLY:O | 23:O:147:TRP:O | 2.20 | 0.58 |
| 23:O:187:GLU:C | 23:O:188:SER:O | 2.38 | 0.58 |
| 23:O:131:PRO:O | 23:O:132:GLY:C | 2.42 | 0.58 |
| 23:O:153:VAL:O | 23:O:154:ALA:C | 2.42 | 0.58 |
| 23:O:149:TYR:O | 23:O:151:ASP:N | 2.38 | 0.57 |
| 23:O:7:VAL:O | 23:O:8:VAL:C | 2.43 | 0.57 |
| 23:O:153:VAL:O | 23:O:157:GLU:N | 2.37 | 0.57 |
| 23:O:82:LYS:C | 23:O:84:LEU:N | 2.53 | 0.57 |
| 23:O:37:ARG:N | 23:O:107:GLY:O | 2.27 | 0.57 |
| 29:1:1:G:H5' | 36:6:232:A:O3' | 2.05 | 0.57 |
| 11:B:12:GLY:HA2 | 29:1:3044:G:P | 2.44 | 0.56 |
| 23:O:162:VAL:C | 23:O:164:SER:N | 2.58 | 0.56 |
| 11:B:98:GLY:HA3 | 29:1:3005:A:H5' | 1.84 | 0.56 |
| 23:O:182:ASN:O | 23:O:186:ALA:N | 2.38 | 0.56 |
| 29:1:3248:C:H2' | 29:1:3249:C:O4' | 2.06 | 0.56 |
| 6:A:40:GLY:HA2 | 29:1:285:A:P | 2.46 | 0.56 |
| 29:1:3286:G:H5' | 29:1:3396:U:O3' | 2.06 | 0.56 |
| 23:O:157:GLU:O | 23:O:158:ALA:C | 2.43 | 0.55 |
| 23:O:84:LEU:C | 23:O:86:GLY:N | 2.60 | 0.55 |
| 24:P:84:PRO:C | 29:1:2353:G:OP1 | 2.44 | 0.55 |
| 23:O:11:GLY:O | 23:O:12:LYS:C | 2.45 | 0.55 |
| 29:1:3294:A:H2' | 29:1:3295:A:O4' | 2.06 | 0.55 |
| 23:O:18:ARG:O | 23:O:19:LEU:O | 2.25 | 0.55 |
| 23:O:177:LYS:O | 23:O:180:SER:N | 2.39 | 0.55 |
| 23:O:36:VAL:O | 23:O:38:ALA:N | 2.40 | 0.55 |
| 23:O:89:SER:O | 23:O:90:HIS:C | 2.45 | 0.55 |
| 23:O:191:ALA:O | 23:O:193:GLN:N | 2.40 | 0.55 |
| 24:P:85:ALA:N | 29:1:2353:G:OP1 | 2.38 | 0.55 |
| 23:O:49:ARG:O | 23:O:52:LEU:N | 2.39 | 0.54 |
| 29:1:230:U:H2' | 29:1:231:G:O4' | 2.07 | 0.54 |
| 23:O:149:TYR:O | 23:O:150:GLU:C | 2.46 | 0.54 |
| 23:O:37:ARG:O | 23:O:38:ALA:C | 2.45 | 0.54 |
| 29:1:3388:C:H5'' | 29:1:3389:U:H5' | 1.90 | 0.54 |
| 23:O:95:GLY:C | 23:O:97:ALA:N | 2.62 | 0.54 |
| 24:P:84:PRO:CA | 29:1:2353:G:OP1 | 2.56 | 0.53 |
| 29:1:544:C:H2' | 29:1:545:U:H2' | 1.90 | 0.53 |
| 11:B:98:GLY:CA | 29:1:3005:A:H5'' | 2.20 | 0.53 |
| 26:S:111:ALA:O | 29:1:1321:G:O2' | 2.26 | 0.53 |
| 23:O:168:TYR:O | 23:O:169:ALA:C | 2.46 | 0.53 |
| 23:O:54:TYR:O | 23:O:55:HIS:C | 2.47 | 0.53 |
| 30:2:122:U:H2' | 30:2:123:G:O4' | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 23:O:130:LYS:O | 23:O:131:PRO:C | 2.47 | 0.52 |
| 23:O:76:PRO:O | 23:O:78:ARG:N | 2.42 | 0.52 |
| 23:O:52:LEU:C | 23:O:54:TYR:N | 2.34 | 0.52 |
| 30:2:106:C:H4' | 30:2:107:G:H5'' | 1.92 | 0.52 |
| 23:O:36:VAL:C | 23:O:38:ALA:N | 2.63 | 0.52 |
| 31:D:267:GLY:N | 31:D:413:ASN:O | 2.43 | 0.52 |
| 23:O:63:ALA:O | 23:O:65:ASN:N | 2.43 | 0.52 |
| 23:O:157:GLU:C | 23:O:159:LYS:N | 2.64 | 0.52 |
| 24:P:84:PRO:CA | 29:1:2353:G:P | 2.99 | 0.50 |
| 23:O:63:ALA:O | 23:O:64:PHE:C | 2.49 | 0.50 |
| 23:O:84:LEU:O | 23:O:86:GLY:N | 2.44 | 0.50 |
| 23:O:168:TYR:O | 23:O:171:LYS:N | 2.44 | 0.50 |
| 23:O:59:ARG:O | 23:O:60:LYS:C | 2.49 | 0.50 |
| 23:O:153:VAL:O | 23:O:154:ALA:O | 2.28 | 0.50 |
| 23:O:133:ARG:O | 23:O:134:LYS:O | 2.29 | 0.50 |
| 23:O:164:SER:C | 23:O:166:GLU:N | 2.65 | 0.50 |
| 11:B:129:ALA:O | 29:1:3149:G:O2' | 2.25 | 0.50 |
| 23:O:55:HIS:C | 23:O:58:LEU:H | 2.11 | 0.50 |
| 23:O:138:LEU:O | 23:O:141:LEU:N | 2.45 | 0.50 |
| 6:A:41:VAL:O | 29:1:285:A:H5'' | 2.12 | 0.50 |
| 23:O:194:LEU:O | 23:O:195:ALA:C | 2.50 | 0.50 |
| 23:O:133:ARG:O | 23:O:134:LYS:C | 2.51 | 0.50 |
| 23:O:31:GLN:O | 23:O:32:LYS:C | 2.50 | 0.49 |
| 11:B:12:GLY:CA | 29:1:3044:G:OP1 | 2.61 | 0.49 |
| 31:D:269:VAL:N | 31:D:392:MET:O | 2.44 | 0.49 |
| 23:O:149:TYR:C | 23:O:151:ASP:N | 2.66 | 0.48 |
| 23:O:27:LEU:O | 23:O:29:ASN:N | 2.46 | 0.48 |
| 23:O:27:LEU:C | 23:O:29:ASN:N | 2.67 | 0.48 |
| 11:B:12:GLY:CA | 29:1:3044:G:C5' | 2.78 | 0.48 |
| 23:O:167:TYR:O | 23:O:170:LYS:N | 2.46 | 0.48 |
| 30:2:53:A:H2' | 30:2:54:A:O4' | 2.13 | 0.48 |
| 32:K:77:ASP:O | 32:K:251:LEU:N | 2.42 | 0.48 |
| 16:G:172:LYS:O | 37:H:252:GLU:N | 2.46 | 0.48 |
| 37:H:282:ALA:O | 37:H:286:GLY:N | 2.46 | 0.48 |
| 23:O:36:VAL:C | 23:O:38:ALA:H | 2.17 | 0.48 |
| 29:1:144:A:H2' | 29:1:145:G:O4' | 2.14 | 0.48 |
| 29:1:741:U:H2' | 29:1:742:G:O4' | 2.14 | 0.48 |
| 23:O:19:LEU:O | 23:O:20:ALA:O | 2.32 | 0.47 |
| 23:O:112:TYR:O | 23:O:114:LYS:N | 2.47 | 0.47 |
| 5:5:288:ARG:H | 29:1:474:G:P | 2.37 | 0.47 |
| 29:1:88:A:H2' | 29:1:89:A:O4' | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 23:O:55:HIS:O | 23:O:58:LEU:CA | 2.61 | 0.47 |
| 11:B:101:SER:O | 29:1:3146:G:O2' | 2.33 | 0.47 |
| 23:O:45:GLY:O | 23:O:46:GLU:C | 2.52 | 0.47 |
| 37:H:295:LYS:O | 37:H:299:GLU:N | 2.47 | 0.47 |
| 23:O:74:ARG:O | 23:O:75:ALA:C | 2.53 | 0.47 |
| 29:1:1:G:C5' | 36:6:232:A:H3' | 2.40 | 0.46 |
| 29:1:293:C:H2' | 29:1:294:U:O4' | 2.16 | 0.46 |
| 29:1:2361:A:H2' | 29:1:2362:C:O4' | 2.16 | 0.46 |
| 6:A:40:GLY:CA | 29:1:284:A:O3' | 2.64 | 0.45 |
| 23:O:27:LEU:C | 23:O:29:ASN:H | 2.18 | 0.45 |
| 23:O:189:ASP:C | 23:O:191:ALA:H | 2.10 | 0.45 |
| 22:N:170:LYS:O | 29:1:288:C:H5'' | 2.17 | 0.45 |
| 29:1:734:C:H2' | 29:1:735:A:O4' | 2.15 | 0.45 |
| 37:H:270:LYS:O | 37:H:274:LYS:N | 2.42 | 0.45 |
| 3:3:118:VAL:C | 3:3:120:ILE:H | 2.18 | 0.45 |
| 29:1:433:A:H2' | 29:1:434:U:O4' | 2.17 | 0.45 |
| 23:O:130:LYS:C | 23:O:131:PRO:O | 2.56 | 0.45 |
| 23:O:191:ALA:O | 23:O:194:LEU:N | 2.50 | 0.44 |
| 23:O:45:GLY:C | 23:O:46:GLU:O | 2.51 | 0.44 |
| 23:O:47:PHE:O | 23:O:49:ARG:N | 2.50 | 0.44 |
| 23:O:54:TYR:O | 23:O:57:PHE:CA | 2.65 | 0.44 |
| 29:1:537:A:H2' | 29:1:538:G:O4' | 2.17 | 0.44 |
| 23:O:98:ALA:O | 23:O:100:GLU:C | 2.55 | 0.44 |
| 23:O:47:PHE:C | 23:O:49:ARG:N | 2.71 | 0.44 |
| 23:O:31:GLN:O | 23:O:32:LYS:O | 2.36 | 0.43 |
| 23:O:78:ARG:O | 23:O:79:ILE:C | 2.57 | 0.43 |
| 29:1:533:A:O2' | 29:1:535:G:H5' | 2.18 | 0.43 |
| 29:1:249:U:H3' | 29:1:250:U:H5'' | 1.99 | 0.43 |
| 29:1:208:C:H2' | 29:1:209:A:O4' | 2.18 | 0.43 |
| 11:B:102:LEU:O | 29:1:3147:G:H4' | 2.18 | 0.43 |
| 23:O:82:LYS:O | 23:O:83:ALA:C | 2.56 | 0.43 |
| 23:O:178:VAL:O | 23:O:180:SER:N | 2.52 | 0.43 |
| 11:B:12:GLY:HA2 | 29:1:3044:G:C5' | 2.46 | 0.42 |
| 29:1:1317:A:O2' | 29:1:1318:A:H3' | 2.19 | 0.42 |
| 23:O:178:VAL:C | 23:O:180:SER:N | 2.73 | 0.42 |
| 29:1:786:A:H4' | 29:1:787:G:H5' | 2.01 | 0.42 |
| 23:O:115:LYS:O | 23:O:116:LYS:O | 2.38 | 0.42 |
| 29:1:117:U:O2' | 29:1:119:U:OP2 | 2.33 | 0.42 |
| 30:2:108:C:H2' | 30:2:109:A:O4' | 2.20 | 0.42 |
| 29:1:370:U:H4' | 29:1:404:G:H5' | 2.02 | 0.42 |
| 6:A:40:GLY:HA2 | 29:1:284:A:O3' | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 29:1:2986:U:H4' | 29:1:2987:A:OP1 | 2.19 | 0.42 |
| 4:4:59:PRO:N | 29:1:466:G:OP1 | 2.52 | 0.42 |
| 36:6:14:U:H2' | 36:6:15:C:H3' | 2.00 | 0.42 |
| 28:Y:2:ALA:N | 29:1:212:G:OP2 | 2.53 | 0.41 |
| 30:2:103:G:OP2 | 30:2:105:A:O2' | 2.31 | 0.41 |
| 23:O:142:SER:O | 23:O:143:THR:C | 2.59 | 0.41 |
| 23:O:178:VAL:O | 23:O:179:ALA:C | 2.58 | 0.41 |
| 29:1:226:C:H2' | 29:1:227:G:O4' | 2.20 | 0.41 |
| 23:O:120:VAL:C | 23:O:122:GLN:N | 2.74 | 0.41 |
| 29:1:2998:U:H2' | 29:1:2999:U:O4' | 2.21 | 0.41 |
| 29:1:3286:G:C5' | 29:1:3396:U:O3' | 2.68 | 0.41 |
| 32:K:82:VAL:N | 32:K:280:PHE:O | 2.46 | 0.41 |
| 23:O:24:ALA:O | 23:O:25:LYS:C | 2.59 | 0.41 |
| 32:K:213:ALA:N | 32:K:216:GLU:O | 2.52 | 0.40 |
| 24:P:65:SER:H | 29:1:1447:G:H5' | 1.87 | 0.40 |
| 11:B:223:GLY:CA | 29:1:3305:A:OP1 | 2.57 | 0.40 |
| 29:1:547:G:O2' | 29:1:548:G:H5'' | 2.21 | 0.40 |
| 23:O:168:TYR:O | 23:O:172:ARG:N | 2.49 | 0.40 |

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | x | 259/295 (88%) | 220 (85%) | 28 (11%) | 11 (4%) | 3 | 24 |
| 2 | F | 239/244 (98%) | 227 (95%) | 8 (3%) | 4 (2%) | 9 | 42 |
| 3 | 3 | 171/306 (56%) | 148 (86%) | 19 (11%) | 4 (2%) | 6 | 36 |
| 4 | 4 | 216/278 (78%) | 197 (91%) | 17 (8%) | 2 (1%) | 17 | 54 |
| 5 | 5 | 377/463 (81%) | 356 (94%) | 19 (5%) | 2 (0%) | 29 | 67 |
| 6 | A | 139/291 (48%) | 123 (88%) | 12 (9%) | 4 (3%) | 4 | 32 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 7 | J | 64/427 (15%) | 61 (95%) | 3 (5%) | 0 | 100 | 100 |
| 8 | u | 114/199 (57%) | 108 (95%) | 5 (4%) | 1 (1%) | 17 | 54 |
| 9 | v | 124/231 (54%) | 117 (94%) | 7 (6%) | 0 | 100 | 100 |
| 10 | y | 223/245 (91%) | 215 (96%) | 8 (4%) | 0 | 100 | 100 |
| 11 | B | 329/387 (85%) | 298 (91%) | 25 (8%) | 6 (2%) | 8 | 40 |
| 12 | C | 341/362 (94%) | 304 (89%) | 29 (8%) | 8 (2%) | 6 | 36 |
| 13 | e | 123/130 (95%) | 116 (94%) | 7 (6%) | 0 | 100 | 100 |
| 14 | E | 147/176 (84%) | 134 (91%) | 13 (9%) | 0 | 100 | 100 |
| 15 | f | 104/107 (97%) | 98 (94%) | 6 (6%) | 0 | 100 | 100 |
| 16 | G | 155/256 (60%) | 142 (92%) | 12 (8%) | 1 (1%) | 25 | 63 |
| 17 | h | 117/120 (98%) | 109 (93%) | 5 (4%) | 3 (3%) | 5 | 34 |
| 18 | i | 72/100 (72%) | 67 (93%) | 3 (4%) | 2 (3%) | 5 | 32 |
| 19 | j | 69/88 (78%) | 68 (99%) | 1 (1%) | 0 | 100 | 100 |
| 20 | L | 106/199 (53%) | 94 (89%) | 9 (8%) | 3 (3%) | 5 | 32 |
| 21 | M | 132/138 (96%) | 125 (95%) | 6 (4%) | 1 (1%) | 19 | 58 |
| 22 | N | 173/204 (85%) | 160 (92%) | 13 (8%) | 0 | 100 | 100 |
| 23 | O | 195/199 (98%) | 81 (42%) | 49 (25%) | 65 (33%) | 0 | 0 |
| 24 | P | 133/184 (72%) | 127 (96%) | 5 (4%) | 1 (1%) | 19 | 58 |
| 25 | Q | 129/186 (69%) | 122 (95%) | 7 (5%) | 0 | 100 | 100 |
| 26 | S | 168/172 (98%) | 155 (92%) | 10 (6%) | 3 (2%) | 8 | 40 |
| 27 | V | 124/137 (90%) | 117 (94%) | 5 (4%) | 2 (2%) | 9 | 43 |
| 28 | Y | 123/127 (97%) | 116 (94%) | 7 (6%) | 0 | 100 | 100 |
| 31 | D | 188/505 (37%) | 174 (93%) | 14 (7%) | 0 | 100 | 100 |
| 32 | K | 242/376 (64%) | 227 (94%) | 15 (6%) | 0 | 100 | 100 |
| 33 | n | 304/605 (50%) | 280 (92%) | 24 (8%) | 0 | 100 | 100 |
| 34 | o | 112/220 (51%) | 104 (93%) | 8 (7%) | 0 | 100 | 100 |
| 35 | t | 244/322 (76%) | 214 (88%) | 27 (11%) | 3 (1%) | 13 | 48 |
| 37 | H | 139/807 (17%) | 125 (90%) | 14 (10%) | 0 | 100 | 100 |
| All | All | 5895/9086 (65%) | 5329 (90%) | 440 (8%) | 126 (2%) | 10 | 38 |

All (126) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | x | 128 | PHE |
| 1 | x | 222 | PRO |
| 1 | x | 277 | GLU |
| 3 | 3 | 133 | HIS |
| 4 | 4 | 85 | ALA |
| 4 | 4 | 133 | LEU |
| 6 | A | 43 | TYR |
| 11 | B | 34 | LYS |
| 11 | B | 138 | ALA |
| 12 | C | 5 | GLN |
| 12 | C | 140 | HIS |
| 23 | O | 4 | GLU |
| 23 | O | 16 | VAL |
| 23 | O | 20 | ALA |
| 23 | O | 46 | GLU |
| 23 | O | 53 | LYS |
| 23 | O | 60 | LYS |
| 23 | O | 63 | ALA |
| 23 | O | 83 | ALA |
| 23 | O | 88 | VAL |
| 23 | O | 89 | SER |
| 23 | O | 90 | HIS |
| 23 | O | 96 | LYS |
| 23 | O | 98 | ALA |
| 23 | O | 99 | LEU |
| 23 | O | 116 | LYS |
| 23 | O | 118 | VAL |
| 23 | O | 127 | LEU |
| 23 | O | 131 | PRO |
| 23 | O | 134 | LYS |
| 23 | O | 136 | THR |
| 23 | O | 138 | LEU |
| 23 | O | 154 | ALA |
| 23 | O | 156 | LEU |
| 23 | O | 158 | ALA |
| 23 | O | 162 | VAL |
| 23 | O | 163 | SER |
| 23 | O | 165 | ALA |
| 23 | O | 167 | TYR |
| 23 | O | 188 | SER |
| 23 | O | 190 | VAL |
| 23 | O | 192 | LYS |
| 27 | V | 90 | GLY |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | x | 281 | GLU |
| 1 | x | 287 | ASP |
| 2 | F | 159 | GLN |
| 2 | F | 164 | SER |
| 5 | 5 | 340 | LYS |
| 6 | A | 94 | HIS |
| 11 | B | 155 | ALA |
| 12 | C | 268 | ALA |
| 17 | h | 91 | ALA |
| 18 | i | 31 | GLY |
| 20 | L | 76 | THR |
| 21 | M | 29 | ALA |
| 23 | O | 8 | VAL |
| 23 | O | 19 | LEU |
| 23 | O | 21 | SER |
| 23 | O | 32 | LYS |
| 23 | O | 64 | PHE |
| 23 | O | 103 | LYS |
| 23 | O | 132 | GLY |
| 23 | O | 139 | GLY |
| 23 | O | 147 | TRP |
| 23 | O | 155 | LYS |
| 23 | O | 168 | TYR |
| 23 | O | 185 | ALA |
| 23 | O | 191 | ALA |
| 35 | t | 227 | ILE |
| 1 | x | 65 | VAL |
| 1 | x | 292 | LYS |
| 2 | F | 157 | ASN |
| 6 | A | 63 | PRO |
| 11 | B | 187 | SER |
| 11 | B | 222 | LYS |
| 12 | C | 311 | HIS |
| 17 | h | 119 | LYS |
| 18 | i | 34 | SER |
| 20 | L | 62 | THR |
| 20 | L | 75 | PHE |
| 23 | O | 12 | LYS |
| 23 | O | 37 | ARG |
| 23 | O | 48 | PHE |
| 23 | O | 77 | SER |
| 23 | O | 85 | ARG |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | O | 113 | ASP |
| 23 | O | 123 | ALA |
| 23 | O | 149 | TYR |
| 23 | O | 150 | GLU |
| 24 | P | 156 | ALA |
| 26 | S | 13 | ARG |
| 27 | V | 84 | SER |
| 1 | x | 293 | PHE |
| 2 | F | 163 | LEU |
| 8 | u | 81 | TYR |
| 12 | C | 233 | LEU |
| 16 | G | 232 | HIS |
| 17 | h | 84 | LYS |
| 23 | O | 49 | ARG |
| 23 | O | 121 | PRO |
| 23 | O | 179 | ALA |
| 26 | S | 14 | LEU |
| 1 | x | 132 | LEU |
| 1 | x | 224 | ILE |
| 3 | 3 | 14 | PHE |
| 3 | 3 | 128 | ARG |
| 12 | C | 269 | SER |
| 12 | C | 320 | ASN |
| 23 | O | 28 | LEU |
| 1 | x | 119 | PRO |
| 3 | 3 | 84 | LYS |
| 6 | A | 105 | PRO |
| 11 | B | 139 | GLN |
| 12 | C | 182 | LEU |
| 23 | O | 38 | ALA |
| 23 | O | 61 | ALA |
| 23 | O | 169 | ALA |
| 26 | S | 167 | ARG |
| 23 | O | 76 | PRO |
| 23 | O | 152 | VAL |
| 35 | t | 240 | GLY |
| 23 | O | 34 | VAL |
| 23 | O | 120 | VAL |
| 5 | 5 | 131 | VAL |
| 23 | O | 30 | GLY |
| 35 | t | 270 | PRO |

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 |
|-----|-------|-----------------|-------------------|-----------------|
| 29 | 1 | 1543/3396 (45%) | 354 (22%) | 0 |
| 30 | 2 | 151/158 (95%) | 29 (19%) | 0 |
| 36 | 6 | 63/232 (27%) | 31 (49%) | 0 |
| All | All | 1757/3786 (46%) | 414 (23%) | 0 |

All (414) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29 | 1 | 3 | U |
| 29 | 1 | 7 | C |
| 29 | 1 | 11 | A |
| 29 | 1 | 18 | G |
| 29 | 1 | 30 | G |
| 29 | 1 | 39 | A |
| 29 | 1 | 40 | A |
| 29 | 1 | 41 | G |
| 29 | 1 | 46 | U |
| 29 | 1 | 48 | A |
| 29 | 1 | 49 | A |
| 29 | 1 | 50 | U |
| 29 | 1 | 57 | A |
| 29 | 1 | 59 | G |
| 29 | 1 | 60 | A |
| 29 | 1 | 65 | A |
| 29 | 1 | 66 | A |
| 29 | 1 | 72 | C |
| 29 | 1 | 74 | G |
| 29 | 1 | 92 | G |
| 29 | 1 | 94 | G |
| 29 | 1 | 96 | G |
| 29 | 1 | 110 | G |
| 29 | 1 | 113 | C |
| 29 | 1 | 116 | A |
| 29 | 1 | 117 | U |
| 29 | 1 | 120 | G |
| 29 | 1 | 122 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 136 | G |
| 29 | 1 | 143 | G |
| 29 | 1 | 146 | U |
| 29 | 1 | 155 | G |
| 29 | 1 | 156 | G |
| 29 | 1 | 157 | A |
| 29 | 1 | 161 | G |
| 29 | 1 | 164 | A |
| 29 | 1 | 165 | A |
| 29 | 1 | 166 | C |
| 29 | 1 | 170 | G |
| 29 | 1 | 190 | U |
| 29 | 1 | 191 | U |
| 29 | 1 | 200 | C |
| 29 | 1 | 206 | G |
| 29 | 1 | 210 | U |
| 29 | 1 | 211 | A |
| 29 | 1 | 213 | A |
| 29 | 1 | 218 | G |
| 29 | 1 | 219 | A |
| 29 | 1 | 220 | G |
| 29 | 1 | 221 | A |
| 29 | 1 | 234 | G |
| 29 | 1 | 240 | U |
| 29 | 1 | 241 | G |
| 29 | 1 | 243 | G |
| 29 | 1 | 249 | U |
| 29 | 1 | 250 | U |
| 29 | 1 | 251 | G |
| 29 | 1 | 265 | A |
| 29 | 1 | 267 | G |
| 29 | 1 | 268 | A |
| 29 | 1 | 269 | G |
| 29 | 1 | 270 | U |
| 29 | 1 | 277 | G |
| 29 | 1 | 281 | G |
| 29 | 1 | 283 | G |
| 29 | 1 | 284 | A |
| 29 | 1 | 285 | A |
| 29 | 1 | 287 | G |
| 29 | 1 | 295 | A |
| 29 | 1 | 299 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 305 | U |
| 29 | 1 | 311 | C |
| 29 | 1 | 315 | C |
| 29 | 1 | 323 | A |
| 29 | 1 | 329 | U |
| 29 | 1 | 346 | C |
| 29 | 1 | 350 | C |
| 29 | 1 | 352 | A |
| 29 | 1 | 368 | G |
| 29 | 1 | 370 | U |
| 29 | 1 | 376 | G |
| 29 | 1 | 380 | U |
| 29 | 1 | 383 | G |
| 29 | 1 | 386 | A |
| 29 | 1 | 387 | A |
| 29 | 1 | 388 | G |
| 29 | 1 | 395 | A |
| 29 | 1 | 397 | A |
| 29 | 1 | 398 | A |
| 29 | 1 | 399 | A |
| 29 | 1 | 400 | G |
| 29 | 1 | 402 | A |
| 29 | 1 | 403 | C |
| 29 | 1 | 421 | G |
| 29 | 1 | 422 | A |
| 29 | 1 | 438 | A |
| 29 | 1 | 439 | C |
| 29 | 1 | 440 | A |
| 29 | 1 | 442 | G |
| 29 | 1 | 449 | U |
| 29 | 1 | 454 | C |
| 29 | 1 | 455 | C |
| 29 | 1 | 457 | C |
| 29 | 1 | 459 | G |
| 29 | 1 | 462 | C |
| 29 | 1 | 463 | C |
| 29 | 1 | 465 | U |
| 29 | 1 | 466 | G |
| 29 | 1 | 467 | U |
| 29 | 1 | 468 | G |
| 29 | 1 | 474 | G |
| 29 | 1 | 478 | A |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 479 | U |
| 29 | 1 | 480 | C |
| 29 | 1 | 481 | U |
| 29 | 1 | 482 | C |
| 29 | 1 | 486 | U |
| 29 | 1 | 489 | C |
| 29 | 1 | 494 | G |
| 29 | 1 | 495 | G |
| 29 | 1 | 503 | C |
| 29 | 1 | 510 | G |
| 29 | 1 | 515 | C |
| 29 | 1 | 521 | A |
| 29 | 1 | 523 | A |
| 29 | 1 | 527 | A |
| 29 | 1 | 533 | A |
| 29 | 1 | 535 | G |
| 29 | 1 | 543 | C |
| 29 | 1 | 544 | C |
| 29 | 1 | 546 | C |
| 29 | 1 | 547 | G |
| 29 | 1 | 549 | U |
| 29 | 1 | 551 | A |
| 29 | 1 | 552 | G |
| 29 | 1 | 555 | U |
| 29 | 1 | 556 | U |
| 29 | 1 | 557 | A |
| 29 | 1 | 559 | A |
| 29 | 1 | 569 | A |
| 29 | 1 | 570 | A |
| 29 | 1 | 572 | A |
| 29 | 1 | 578 | A |
| 29 | 1 | 579 | G |
| 29 | 1 | 589 | A |
| 29 | 1 | 592 | A |
| 29 | 1 | 597 | G |
| 29 | 1 | 604 | G |
| 29 | 1 | 611 | A |
| 29 | 1 | 629 | U |
| 29 | 1 | 636 | C |
| 29 | 1 | 642 | U |
| 29 | 1 | 645 | A |
| 29 | 1 | 647 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 650 | C |
| 29 | 1 | 660 | A |
| 29 | 1 | 662 | U |
| 29 | 1 | 677 | A |
| 29 | 1 | 681 | U |
| 29 | 1 | 691 | A |
| 29 | 1 | 695 | C |
| 29 | 1 | 705 | A |
| 29 | 1 | 719 | U |
| 29 | 1 | 720 | A |
| 29 | 1 | 721 | G |
| 29 | 1 | 722 | G |
| 29 | 1 | 742 | G |
| 29 | 1 | 750 | G |
| 29 | 1 | 756 | U |
| 29 | 1 | 757 | C |
| 29 | 1 | 776 | U |
| 29 | 1 | 779 | G |
| 29 | 1 | 780 | A |
| 29 | 1 | 781 | G |
| 29 | 1 | 783 | A |
| 29 | 1 | 784 | A |
| 29 | 1 | 785 | G |
| 29 | 1 | 801 | A |
| 29 | 1 | 806 | A |
| 29 | 1 | 813 | G |
| 29 | 1 | 937 | G |
| 29 | 1 | 938 | C |
| 29 | 1 | 943 | U |
| 29 | 1 | 944 | C |
| 29 | 1 | 957 | C |
| 29 | 1 | 959 | C |
| 29 | 1 | 961 | C |
| 29 | 1 | 962 | A |
| 29 | 1 | 971 | G |
| 29 | 1 | 977 | C |
| 29 | 1 | 978 | G |
| 29 | 1 | 979 | U |
| 29 | 1 | 980 | A |
| 29 | 1 | 985 | U |
| 29 | 1 | 1059 | G |
| 29 | 1 | 1103 | A |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 1104 | G |
| 29 | 1 | 1105 | A |
| 29 | 1 | 1111 | U |
| 29 | 1 | 1112 | A |
| 29 | 1 | 1116 | G |
| 29 | 1 | 1117 | G |
| 29 | 1 | 1124 | U |
| 29 | 1 | 1125 | U |
| 29 | 1 | 1128 | U |
| 29 | 1 | 1129 | A |
| 29 | 1 | 1130 | A |
| 29 | 1 | 1132 | C |
| 29 | 1 | 1144 | U |
| 29 | 1 | 1153 | A |
| 29 | 1 | 1159 | A |
| 29 | 1 | 1160 | C |
| 29 | 1 | 1180 | A |
| 29 | 1 | 1181 | U |
| 29 | 1 | 1186 | G |
| 29 | 1 | 1189 | C |
| 29 | 1 | 1192 | C |
| 29 | 1 | 1193 | A |
| 29 | 1 | 1315 | U |
| 29 | 1 | 1325 | U |
| 29 | 1 | 1330 | A |
| 29 | 1 | 1332 | A |
| 29 | 1 | 1348 | U |
| 29 | 1 | 1349 | G |
| 29 | 1 | 1350 | A |
| 29 | 1 | 1351 | U |
| 29 | 1 | 1352 | A |
| 29 | 1 | 1353 | U |
| 29 | 1 | 1354 | G |
| 29 | 1 | 1355 | A |
| 29 | 1 | 1357 | G |
| 29 | 1 | 1359 | C |
| 29 | 1 | 1380 | G |
| 29 | 1 | 1386 | A |
| 29 | 1 | 1390 | A |
| 29 | 1 | 1392 | G |
| 29 | 1 | 1397 | C |
| 29 | 1 | 1399 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 1400 | G |
| 29 | 1 | 1417 | G |
| 29 | 1 | 1419 | A |
| 29 | 1 | 1434 | G |
| 29 | 1 | 1437 | C |
| 29 | 1 | 1450 | G |
| 29 | 1 | 1452 | A |
| 29 | 1 | 2366 | C |
| 29 | 1 | 2370 | G |
| 29 | 1 | 2371 | G |
| 29 | 1 | 2372 | A |
| 29 | 1 | 2374 | C |
| 29 | 1 | 2375 | G |
| 29 | 1 | 2377 | G |
| 29 | 1 | 2987 | A |
| 29 | 1 | 2992 | U |
| 29 | 1 | 2996 | U |
| 29 | 1 | 2997 | G |
| 29 | 1 | 3012 | A |
| 29 | 1 | 3019 | U |
| 29 | 1 | 3021 | A |
| 29 | 1 | 3022 | G |
| 29 | 1 | 3027 | A |
| 29 | 1 | 3028 | G |
| 29 | 1 | 3029 | A |
| 29 | 1 | 3030 | G |
| 29 | 1 | 3032 | A |
| 29 | 1 | 3049 | A |
| 29 | 1 | 3054 | U |
| 29 | 1 | 3055 | U |
| 29 | 1 | 3057 | U |
| 29 | 1 | 3058 | U |
| 29 | 1 | 3059 | G |
| 29 | 1 | 3069 | G |
| 29 | 1 | 3070 | A |
| 29 | 1 | 3074 | G |
| 29 | 1 | 3075 | G |
| 29 | 1 | 3078 | U |
| 29 | 1 | 3084 | C |
| 29 | 1 | 3086 | A |
| 29 | 1 | 3088 | G |
| 29 | 1 | 3092 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 3093 | C |
| 29 | 1 | 3094 | A |
| 29 | 1 | 3099 | C |
| 29 | 1 | 3100 | U |
| 29 | 1 | 3101 | G |
| 29 | 1 | 3109 | G |
| 29 | 1 | 3116 | G |
| 29 | 1 | 3121 | U |
| 29 | 1 | 3129 | A |
| 29 | 1 | 3130 | A |
| 29 | 1 | 3131 | U |
| 29 | 1 | 3142 | A |
| 29 | 1 | 3143 | C |
| 29 | 1 | 3173 | G |
| 29 | 1 | 3174 | A |
| 29 | 1 | 3176 | G |
| 29 | 1 | 3179 | U |
| 29 | 1 | 3180 | A |
| 29 | 1 | 3181 | C |
| 29 | 1 | 3187 | A |
| 29 | 1 | 3188 | G |
| 29 | 1 | 3189 | G |
| 29 | 1 | 3194 | C |
| 29 | 1 | 3195 | U |
| 29 | 1 | 3196 | U |
| 29 | 1 | 3198 | U |
| 29 | 1 | 3207 | U |
| 29 | 1 | 3217 | C |
| 29 | 1 | 3218 | A |
| 29 | 1 | 3219 | G |
| 29 | 1 | 3229 | G |
| 29 | 1 | 3234 | A |
| 29 | 1 | 3243 | A |
| 29 | 1 | 3244 | A |
| 29 | 1 | 3245 | A |
| 29 | 1 | 3247 | G |
| 29 | 1 | 3249 | C |
| 29 | 1 | 3256 | G |
| 29 | 1 | 3259 | U |
| 29 | 1 | 3260 | G |
| 29 | 1 | 3263 | G |
| 29 | 1 | 3270 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 29 | 1 | 3275 | U |
| 29 | 1 | 3276 | G |
| 29 | 1 | 3286 | G |
| 29 | 1 | 3288 | G |
| 29 | 1 | 3289 | G |
| 29 | 1 | 3290 | G |
| 29 | 1 | 3294 | A |
| 29 | 1 | 3304 | U |
| 29 | 1 | 3313 | U |
| 29 | 1 | 3316 | A |
| 29 | 1 | 3317 | U |
| 29 | 1 | 3319 | U |
| 29 | 1 | 3320 | A |
| 29 | 1 | 3330 | A |
| 29 | 1 | 3340 | G |
| 29 | 1 | 3341 | U |
| 29 | 1 | 3345 | G |
| 29 | 1 | 3346 | U |
| 29 | 1 | 3347 | A |
| 29 | 1 | 3351 | U |
| 29 | 1 | 3352 | U |
| 29 | 1 | 3355 | U |
| 29 | 1 | 3356 | G |
| 29 | 1 | 3359 | A |
| 29 | 1 | 3363 | U |
| 29 | 1 | 3368 | U |
| 29 | 1 | 3369 | G |
| 29 | 1 | 3375 | A |
| 29 | 1 | 3376 | A |
| 29 | 1 | 3378 | C |
| 29 | 1 | 3382 | U |
| 29 | 1 | 3390 | G |
| 30 | 2 | 23 | U |
| 30 | 2 | 34 | U |
| 30 | 2 | 35 | C |
| 30 | 2 | 39 | G |
| 30 | 2 | 51 | G |
| 30 | 2 | 59 | A |
| 30 | 2 | 62 | C |
| 30 | 2 | 63 | G |
| 30 | 2 | 71 | A |
| 30 | 2 | 75 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 30 | 2 | 81 | U |
| 30 | 2 | 82 | U |
| 30 | 2 | 83 | C |
| 30 | 2 | 84 | C |
| 30 | 2 | 85 | G |
| 30 | 2 | 86 | U |
| 30 | 2 | 87 | G |
| 30 | 2 | 90 | U |
| 30 | 2 | 95 | G |
| 30 | 2 | 104 | A |
| 30 | 2 | 106 | C |
| 30 | 2 | 107 | G |
| 30 | 2 | 113 | U |
| 30 | 2 | 115 | C |
| 30 | 2 | 116 | G |
| 30 | 2 | 121 | U |
| 30 | 2 | 123 | G |
| 30 | 2 | 124 | G |
| 30 | 2 | 148 | G |
| 36 | 6 | 2 | C |
| 36 | 6 | 4 | U |
| 36 | 6 | 5 | C |
| 36 | 6 | 6 | U |
| 36 | 6 | 7 | C |
| 36 | 6 | 8 | A |
| 36 | 6 | 13 | U |
| 36 | 6 | 14 | U |
| 36 | 6 | 15 | C |
| 36 | 6 | 16 | U |
| 36 | 6 | 17 | G |
| 36 | 6 | 33 | U |
| 36 | 6 | 36 | U |
| 36 | 6 | 39 | U |
| 36 | 6 | 41 | G |
| 36 | 6 | 42 | G |
| 36 | 6 | 43 | A |
| 36 | 6 | 45 | U |
| 36 | 6 | 47 | A |
| 36 | 6 | 52 | G |
| 36 | 6 | 53 | A |
| 36 | 6 | 54 | A |
| 36 | 6 | 55 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | 6 | 56 | U |
| 36 | 6 | 57 | U |
| 36 | 6 | 58 | G |
| 36 | 6 | 59 | C |
| 36 | 6 | 228 | U |
| 36 | 6 | 229 | U |
| 36 | 6 | 230 | A |
| 36 | 6 | 232 | A |

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 |
|-----|-------|------------------|
| 30 | 2 | 6 |
| 29 | 1 | 1 |
| 1 | x | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 2 | 125:U | O3' | 126:A | P | 7.31 |
| 1 | 2 | 124:G | O3' | 125:U | P | 7.17 |
| 1 | 2 | 110:C | O3' | 111:A | P | 6.69 |
| 1 | 2 | 113:U | O3' | 114:G | P | 4.18 |
| 1 | 2 | 128:U | O3' | 129:C | P | 3.61 |
| 1 | 1 | 3395:G | O3' | 3396:U | P | 3.49 |
| 1 | 2 | 126:A | O3' | 127:U | P | 3.41 |
| 1 | x | 285:GLU | C | 286:MET | N | 3.36 |

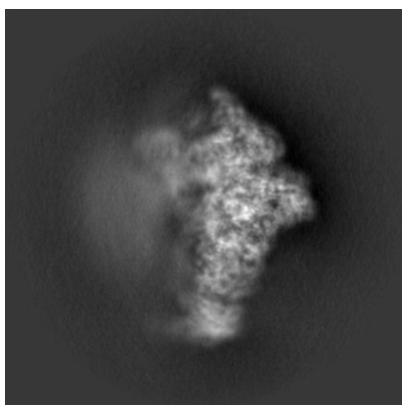
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3889. These allow visual inspection of the internal detail of the map and identification of artifacts.

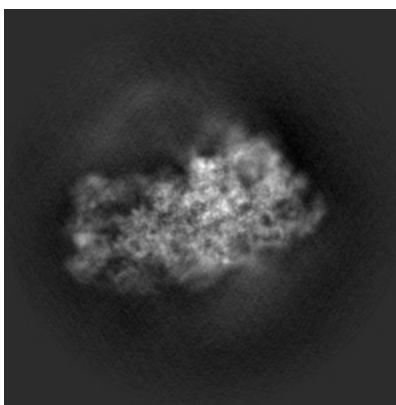
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

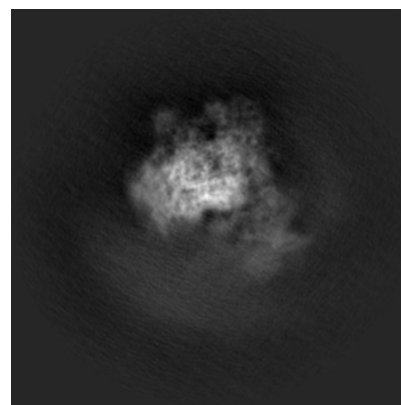
6.1.1 Primary map



X



Y

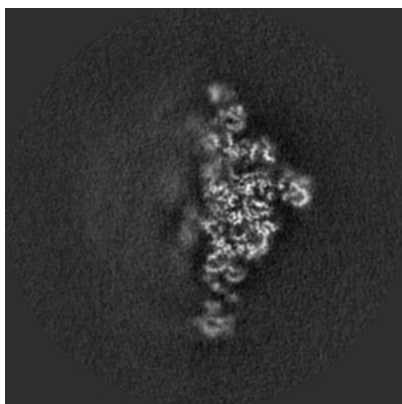


Z

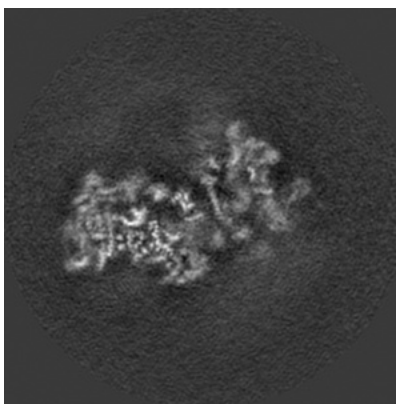
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

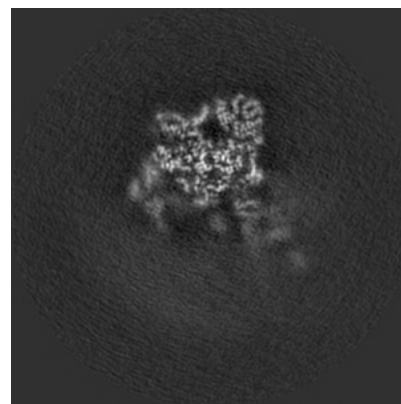
6.2.1 Primary map



X Index: 210



Y Index: 210

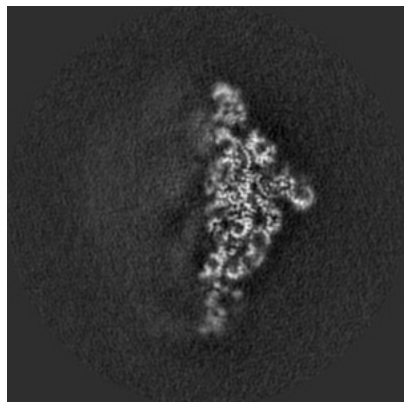


Z Index: 210

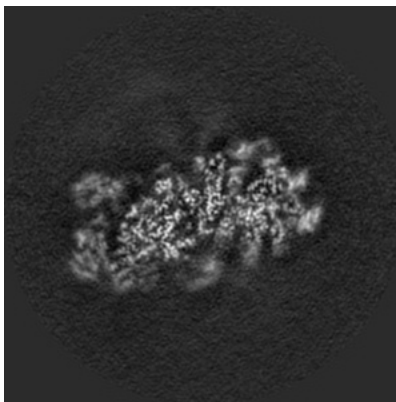
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

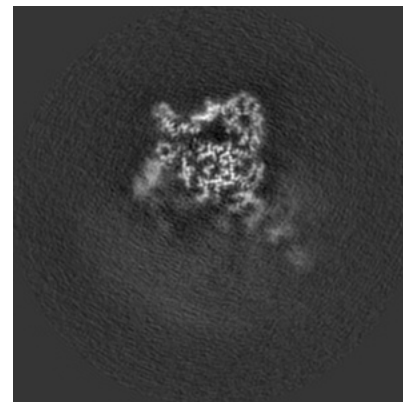
6.3.1 Primary map



X Index: 204



Y Index: 235



Z Index: 215

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

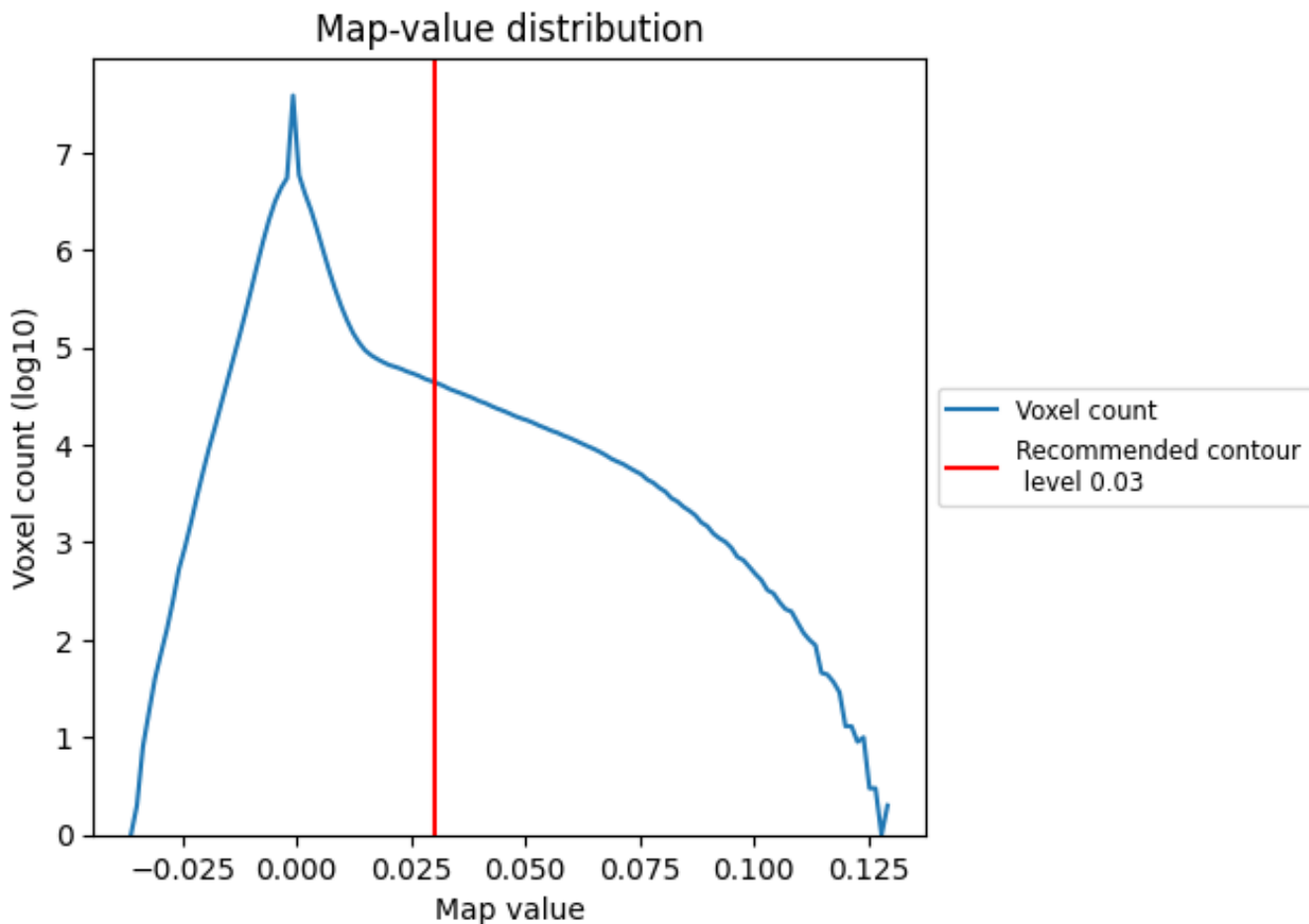
6.5 Mask visualisation

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

7 Map analysis [i](#)

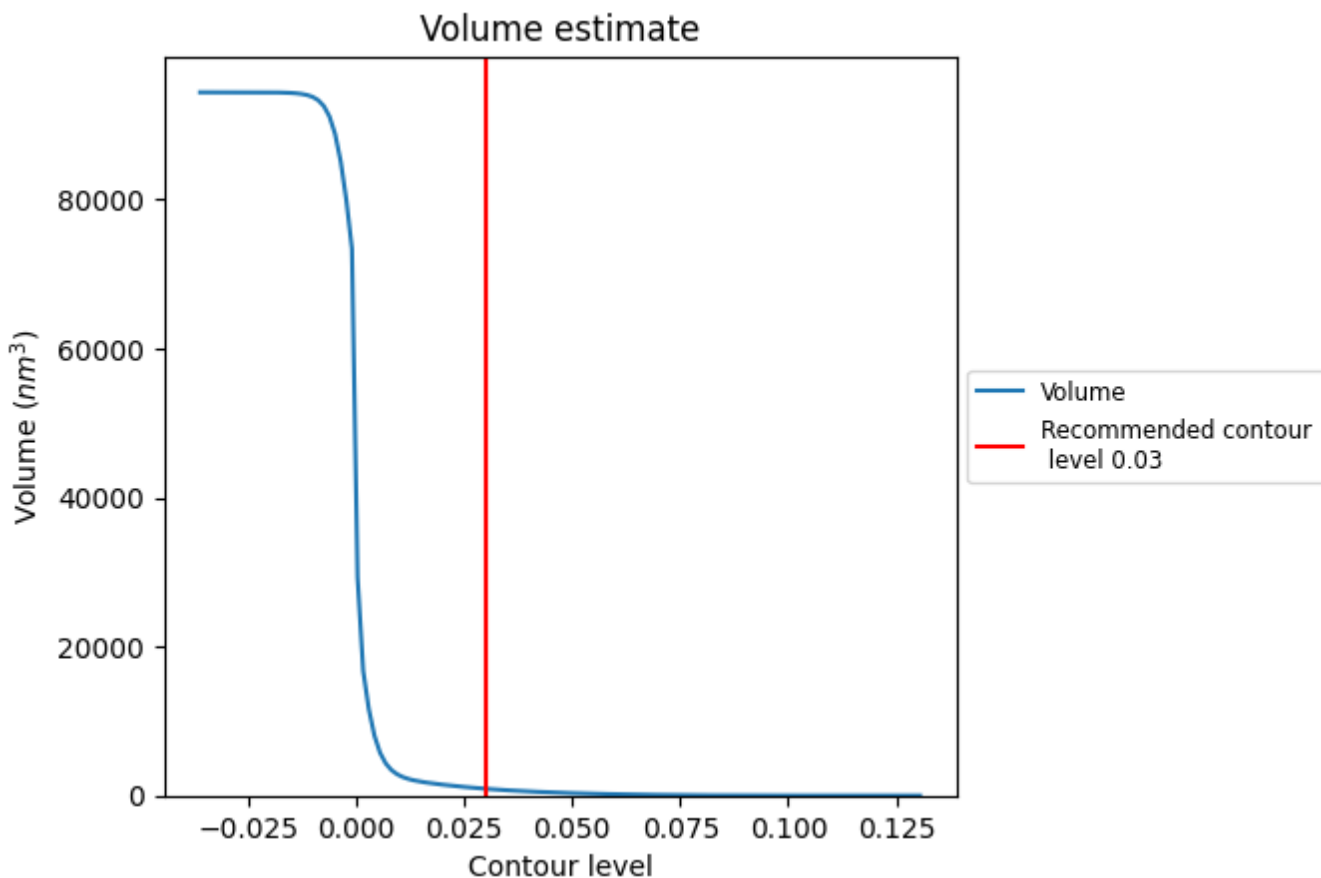
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

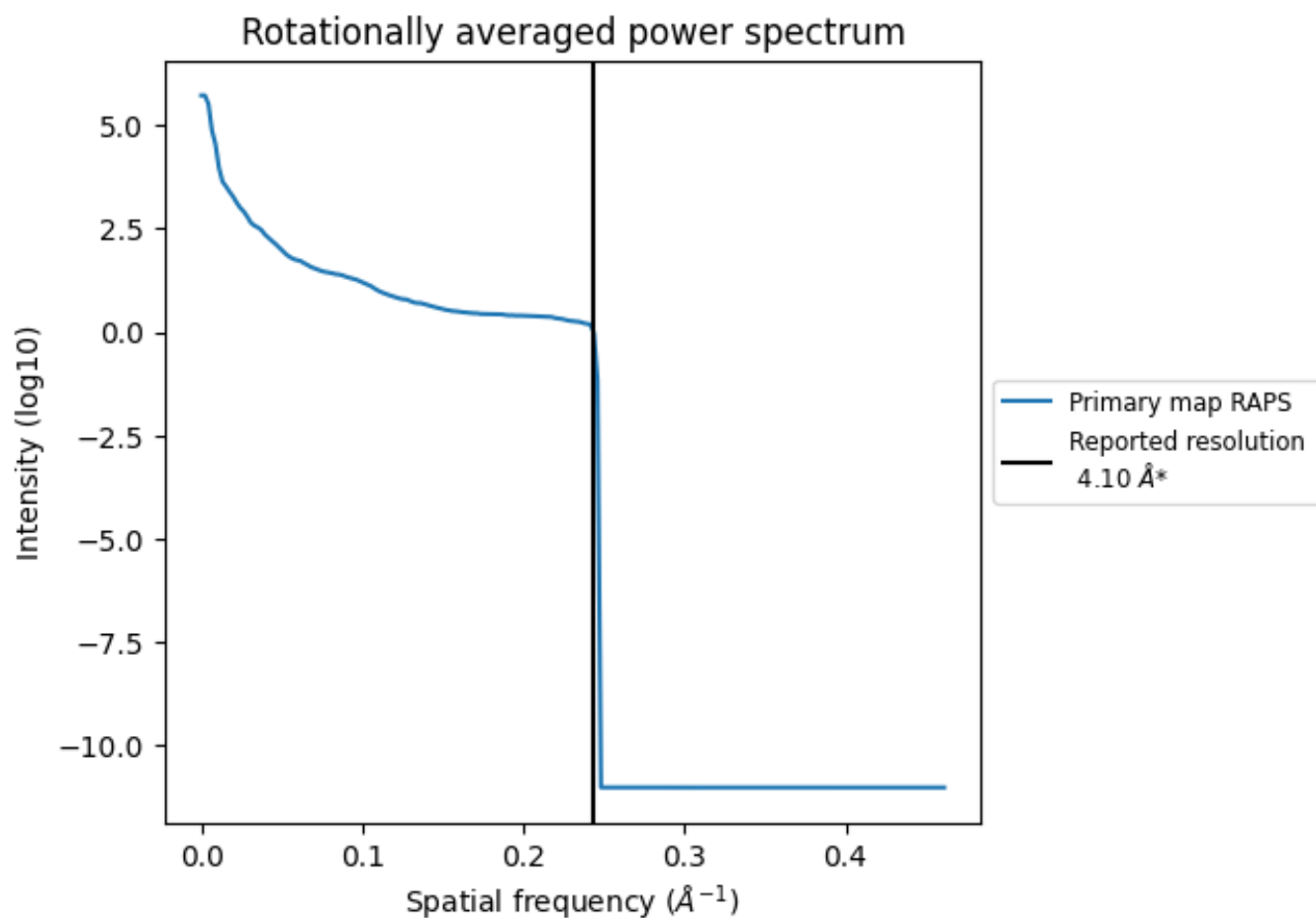
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 908 nm^3 ; this corresponds to an approximate mass of 821 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

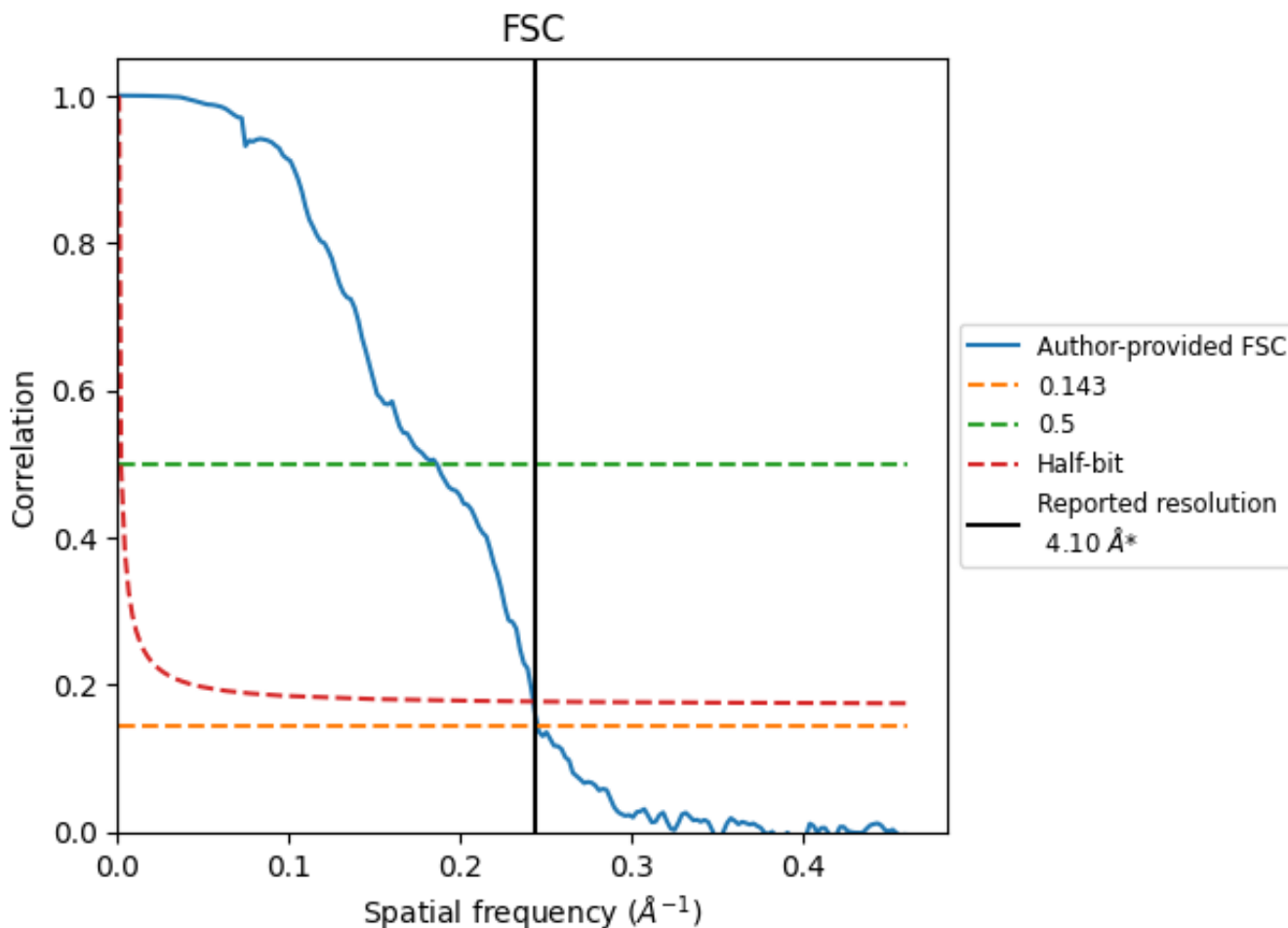


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

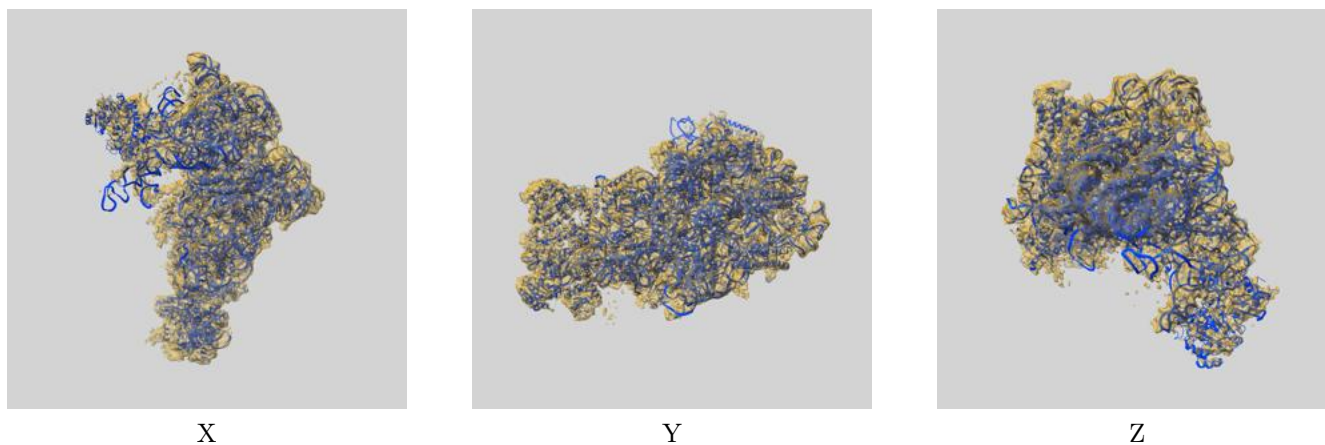
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.10 | - | - |
| Author-provided FSC curve | 4.08 | 5.37 | 4.12 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

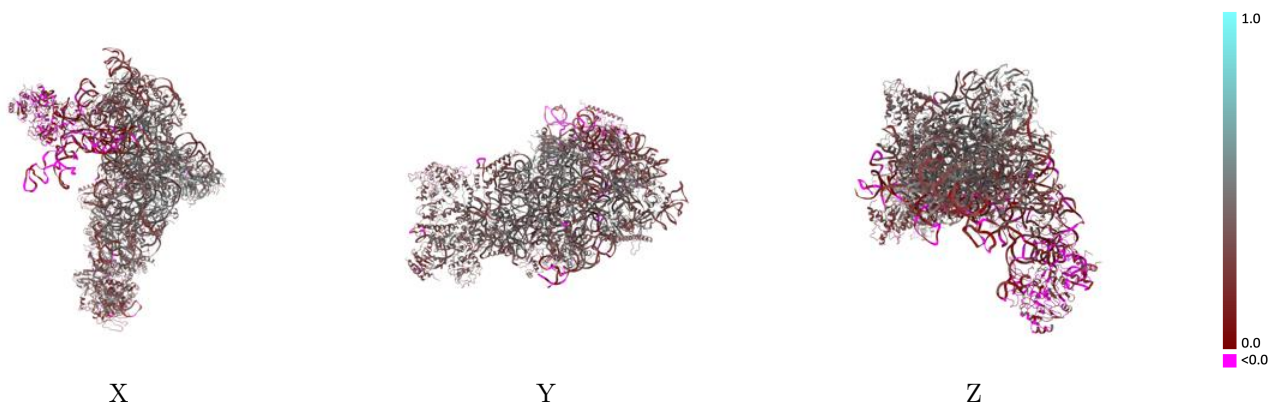
This section contains information regarding the fit between EMDB map EMD-3889 and PDB model 6EM4. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



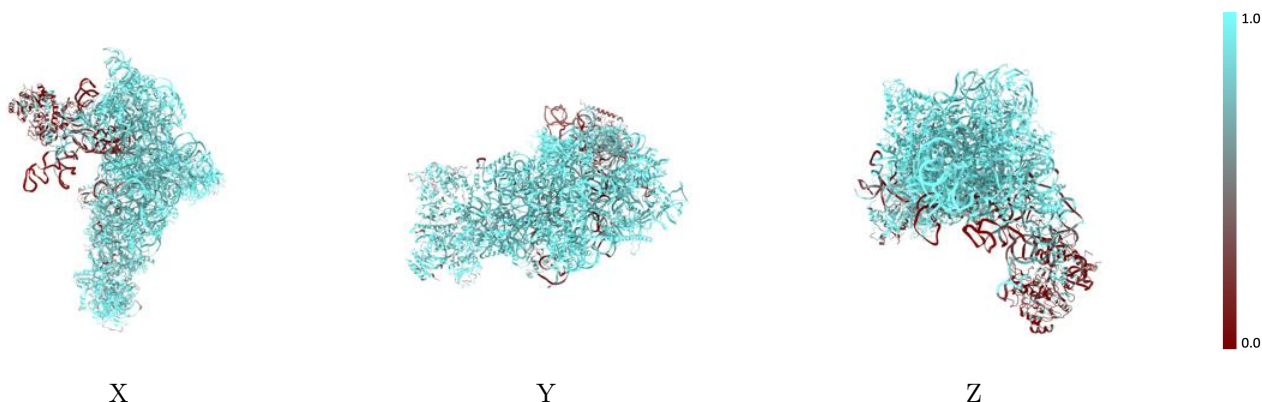
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



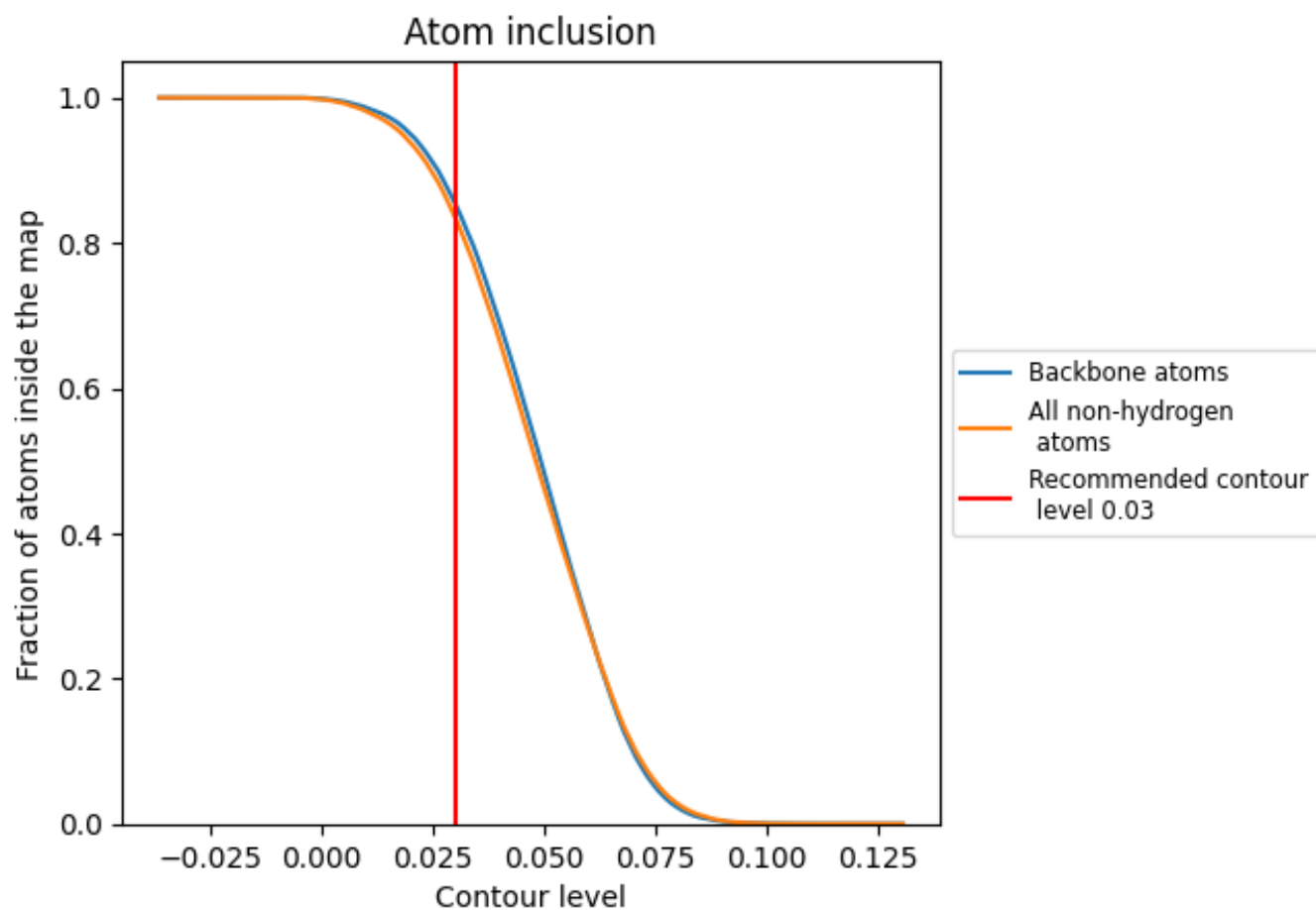
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary







The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8362 |  0.3200 |
| 1 |  0.7927 |  0.2790 |
| 2 |  0.8692 |  0.3380 |
| 3 |  0.9769 |  0.4250 |
| 4 |  0.9875 |  0.3720 |
| 5 |  0.9682 |  0.4360 |
| 6 |  0.9064 |  0.2690 |
| A |  0.7552 |  0.2640 |
| B |  0.6802 |  0.2060 |
| C |  0.9235 |  0.4400 |
| D |  0.8750 |  0.3460 |
| E |  0.9768 |  0.4250 |
| F |  0.9855 |  0.4060 |
| G |  0.9544 |  0.3940 |
| H |  0.8479 |  0.3110 |
| J |  0.7121 |  0.2300 |
| K |  0.9004 |  0.3210 |
| L |  0.9907 |  0.4260 |
| M |  0.9515 |  0.3710 |
| N |  0.9209 |  0.4060 |
| O |  0.9175 |  0.4050 |
| P |  0.8631 |  0.3990 |
| Q |  0.9847 |  0.4340 |
| S |  0.9471 |  0.3880 |
| V |  0.1250 |  0.0620 |
| Y |  0.9800 |  0.4600 |
| e |  0.9420 |  0.4570 |
| f |  0.9693 |  0.4590 |
| h |  0.9517 |  0.3760 |
| i |  0.9155 |  0.3040 |
| j |  0.9648 |  0.4230 |
| n |  0.8734 |  0.3070 |
| o |  0.9612 |  0.3670 |
| t |  0.9042 |  0.3110 |
| u |  0.3772 |  0.0680 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| v |  0.9808 |  0.4040 |
| x |  0.9775 |  0.4170 |
| y |  0.2611 |  0.1040 |