

wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 05:34 pm GMT

| PDB ID | : | 7ASE |
|--------------|---|---|
| EMDB ID | : | EMD-11893 |
| Title | : | 43S preinitiation complex from Trypanosoma cruzi with the kDDX60 helicase |
| Authors | : | Bochler, A.; Brito Querido, J.; Prilepskaja, T.; Soufari, H.; Del Cistia, M.L.; |
| | | Kuhn, L.; Rimoldi Ribeiro, A.; Valasek, L.S.; Hashem, Y. |
| Deposited on | : | 2020-10-27 |
| Resolution | : | 3.33 Å(reported) |
| | | |

This is a wwPDB EM Validation Summary 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

| EMDB validation analysis | : | 0.0.1. dev 43 |
|--------------------------------|---|--|
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7(2018) |
| 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) | : | 2.31.3 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.33 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 | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f EM\ structures}\ (\#{ m Entries})$ |
|-----------------------|--|--|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| 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 $\geq=3, 2, 1$ 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 | Qual | Quality of chain | | | | | | |
|-----|-------|--------|--------------|------------------|----------|--|--|--|--|--|
| 1 | f | 2174 | 54% | 10% • | • 30% | | | | | |
| 2 | 1 | 75 | 13% | | 15% | | | | | |
| 3 | 0 | 2319 | 18% • 74% | | 17% • 7% | | | | | |
| 4 | У | 137 | 9% | 6 | • 10% | | | | | |
| 5 | s | 418 | 58% | 9% | • 29% | | | | | |
| 6 | j | 150 | 35% | 7% | 47% | | | | | |
| 7 | n | 343 | 43% | 7% • | 34% | | | | | |
| 8 | р | 318 | 38% | 3% | ••• | | | | | |

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| Mol | Chain | Length | Quality of chain | |
|-----|-------|--------|--------------------|----------|
| 9 | r | 149 | 86% | 7% • 6% |
| - | _ | | 31% | |
| 10 | u | 153 | 75% 1 | 2% • 11% |
| 11 | m | 143 | 94% | |
| | | | 7% | |
| 12 | Ζ | 221 | 76% · | 21% |
| 13 | 0 | 190 | 94% | 6% |
| 14 | q | 211 | 93% | • 5% |
| 15 | R | 151 | 91% | • 7% |
| 16 | S | 86 | 92% | • 5% |
| 17 | t | 112 | 91% | • 7% |
| 18 | U | 91 | 26% 66% 8% • | 25% |
| 19 | V | 144 | 9% | •• 6% |
| 20 | Х | 173 | 8% | • •• 14% |
| 21 | В | 190 | 9% | 5% 6% |
| 22 | F | 245 | 9% | • 16% |
| 23 | d | 263 | 9% | •• 15% |
| 24 | g | 247 | 3 2% • 66% | |
| 25 | a | 110 | 64% | 36% |
| 26 | J | 257 | 55% 52% 11% • • | 33% |
| 27 | h | 141 | 69% 83% | 14% |
| | | 477 | 77% | |
| 28 | G | 477 | 76% 31% | • 12% |
| 29 | Р | 250 | 96% | • |
| 30 | i | 141 | 74% 9% | • 14% |
| 31 | L | 117 | 78% | 5% • 15% |
| 32 | М | 214 | 87% | 5% • 7% |
| 33 | Ν | 161 | 20% 54% ··· 42% |) |

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| Mol | Chain | Length | Quality of chain | | |
|-----|-------|--------|--------------------|----------|---|
| 34 | О | 167 | 75% 8% | • 16% | - |
| 35 | b | 145 | 88% | • 11% | |
| 36 | с | 66 | 82% | 9% 9% | - |
| 37 | V | 109 | 23% | • 11% | |
| 38 | W | 166 | 41% | 5% • 11% | - |
| 39 | Е | 407 | 96% 68% 20% | 8% • | - |
| 40 | Y | 379 | 45% 41% • • 54% | | - |
| 41 | Q | 57 | 79% | 18% | • |
| 42 | D | 34 | 91% | ••• | |
| 43 | G | 345 | 74% 13 | 3% • 11% | - |
| 44 | K | 203 | 99% | 6% • | |
| 45 | Т | 152 | 79% | 7% • 13% | - |
| 46 | С | 716 | 64% 25% | 7% • • | |
| 47 | 8 | 762 | 59% 14% • | 24% | - |
| 48 | W | 254 | 79% | 6% • 15% | |
| 49 | Ι | 489 | 64% 6% • | 30% | |
| 50 | Н | 334 | 73% 14 | % • 11% | - |
| 51 | А | 502 | 76% | 18% • • | - |
| 52 | 1 | 273 | 6% 88% | 6% • 5% | 6 |

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2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 136847 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 kDDX60.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|----------------|-----------|-----------|-----------|---------|---------|-------|
| 1 | f | 1523 | Total 12257 | С 7734 | N 2165 | O 2292 | S 66 | 0 | 0 |

• Molecule 2 is a RNA chain called initiator tRNA-Met.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|---------|-------|
| 2 | 1 | 75 | Total 1606 | C 718 | N 300 | 0 514 | Р 74 | 0 | 0 |

• Molecule 3 is a RNA chain called 18S.

| Mol | Chain | Residues | | 1 | AltConf | Trace | | | |
|-----|-------|----------|----------------|------------|-----------|------------|-----------|---|---|
| 3 | 0 | 2150 | Total 45795 | C 20471 | N 8144 | O 15037 | Р 2143 | 0 | 0 |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|--------------|
| 0 | 143 | C | А | conflict | GB 320364483 |
| 0 | 805 | С | U | conflict | GB 320364483 |
| 0 | 2321 | U | - | insertion | GB 320364483 |
| 0 | 2322 | U | - | insertion | GB 320364483 |
| 0 | 2323 | U | - | insertion | GB 320364483 |

• Molecule 4 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace | |
|-----|-------|----------|--------------|----------|----------|----------|---|-------|---|
| 4 | У | 123 | Total 989 | C 628 | N 194 | 0 165 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 5 is a protein called Elongation initiation factor 2 alpha subunit, putative.



| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 5 | s | 295 | Total 2365 | C 1489 | N 436 | O 427 | S 13 | 0 | 0 |

• Molecule 6 is a protein called 60S ribosomal protein L40.

| Mol | Chain | Residues | | At | oms | Atoms | | | | | |
|-----|-------|----------|--------------|----------|----------|----------|--------|---|---|--|--|
| 6 | j | 79 | Total 644 | C 409 | N 123 | O 106 | S 6 | 0 | 0 | | |

• Molecule 7 is a protein called Translation initiation factor, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 7 | n | 225 | Total 1796 | C 1111 | N 335 | O 339 | S 11 | 0 | 0 |

• Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | | At | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---|---|
| 8 | р | 310 | Total 2405 | C 1505 | N 424 | 0 463 | S 13 | 0 | 0 |

• Molecule 9 is a protein called 40S ribosomal protein S16, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---------|-------|
| 9 | r | 140 | Total 1113 | C 706 | N 212 | 0 192 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 10 is a protein called 40S ribosomal protein S18, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------------|---------|-------|
| 10 | u | 136 | Total 1108 | C 689 | N 224 | O 190 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 11 is a protein called 40S ribosomal protein S23, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---|---------|-------|
| 11 | m | 142 | Total 1116 | C 706 | N 220 | 0 188 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 12 is a protein called 40S ribosomal protein S8.



| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---------|-------|
| 12 | Z | 175 | Total 1404 | C 885 | N 283 | O 233 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 13 is a protein called 40S ribosomal protein S5, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 13 | О | 190 | Total 1493 | C 932 | N 286 | O 269 | S 6 | 0 | 0 |

• Molecule 14 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | | Ate | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---|---|
| 14 | q | 200 | Total 1670 | C 1063 | N 324 | 0 277 | S 6 | 0 | 0 |

• Molecule 15 is a protein called 40S ribosomal protein S13, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 15 | R | 141 | Total 1143 | С 724 | N 221 | O 190 | S 8 | 0 | 0 |

• Molecule 16 is a protein called 40S ribosomal protein S27, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 16 | S | 82 | Total 630 | C 384 | N 121 | O 116 | S 9 | 0 | 0 |

• Molecule 17 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | | \mathbf{A}^{\dagger} | toms | | AltConf | Trace | |
|-----|-------|----------|--------------|------------------------|----------|----------|---------|-------|---|
| 17 | t | 104 | Total 829 | C 510 | N 177 | 0 132 | S 10 | 0 | 0 |

• Molecule 18 is a protein called 40S ribosomal protein S33.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---------|-------|
| 18 | U | 68 | Total 526 | C 315 | N 107 | O 100 | ${S \atop 4}$ | 0 | 0 |

• Molecule 19 is a protein called 40S ribosomal protein S14, putative.



| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 19 | v | 135 | Total 1011 | C 620 | N 195 | O 187 | S 9 | 0 | 0 |

• Molecule 20 is a protein called 40S ribosomal protein S11, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 20 | Х | 148 | Total 1212 | C 760 | N 239 | O 207 | S 6 | 0 | 0 |

• Molecule 21 is a protein called Putative 40S ribosomal protein S9.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|---------------|----------|----------|----------|--------|---|---|
| 21 | В | 179 | Total 1483 | C 935 | N 297 | 0 243 | S 8 | 0 | 0 |

• Molecule 22 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 22 | F | 207 | Total 1658 | C 1060 | N 299 | 0 288 | S 11 | 0 | 0 |

• Molecule 23 is a protein called 40S ribosomal protein S2, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 23 | d | 223 | Total 1726 | C 1098 | N 304 | 0 314 | S 10 | 0 | 0 |

• Molecule 24 is a protein called Putative 40S ribosomal protein S21.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|-------|
| 24 | g | 83 | Total 635 | C 395 | N 116 | 0 122 | ${ m S} { m 2}$ | 0 | 0 |

• Molecule 25 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | | Atc | \mathbf{ms} | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------------|---------|-----------------|---------|-------|
| 25 | a | 70 | Total 553 | C 356 | N 97 | O 97 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 26 is a protein called RNA-binding protein, putative.



| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---------|-------|
| 26 | J | 173 | Total 1358 | C 862 | N 259 | 0 234 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 27 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|--------------|--|----------|----------|----------------|---|---|
| 27 | h | 121 | Total 958 | $\begin{array}{c} \mathrm{C} \\ 594 \end{array}$ | N 174 | 0 185 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 28 is a protein called Eukaryotic translation initiation factor 2 subunit, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 28 | 5 | 421 | Total 3245 | C 2049 | N 581 | O 596 | S 19 | 0 | 0 |

• Molecule 29 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------------|---------|-------|
| 29 | Р | 249 | Total 1983 | C 1244 | N 402 | O 333 | ${S \atop 4}$ | 0 | 0 |

• Molecule 30 is a protein called 40S ribosomal protein S17, putative.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|--------------|----------|----------|----------|---------------|---|---|
| 30 | i | 121 | Total 992 | C 623 | N 190 | 0 174 | ${S \over 5}$ | 0 | 0 |

• Molecule 31 is a protein called Ribosomal protein S20, putative.

| Mol | Chain | Residues | | At | AltConf | Trace | | | |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---|---|
| 31 | L | 99 | Total 784 | C 497 | N 144 | 0 140 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 32 is a protein called 40S ribosomal protein S3, putative.

| Mol | Chain | Residues | | \mathbf{A} | AltConf | Trace | | | |
|-----|-------|----------|---------------|--------------|----------|----------|---------|---|---|
| 32 | М | 200 | Total 1587 | C 995 | N 302 | 0 279 | S 11 | 0 | 0 |

• Molecule 33 is a protein called 40S ribosomal protein S10, putative.



| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|--------------|--|----------|----------|---------------|---|---|
| 33 | Ν | 93 | Total 780 | $\begin{array}{c} \mathrm{C} \\ 508 \end{array}$ | N 136 | 0 132 | $\frac{S}{4}$ | 0 | 0 |

• Molecule 34 is a protein called Ribosomal protein S19, putative.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|---------------|----------|----------|----------|--------|---|---|
| 34 | Ο | 140 | Total 1116 | C 702 | N 221 | 0 185 | S 8 | 0 | 0 |

• Molecule 35 is a protein called 40S ribosomal protein S15a, putative.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|---------------|----------|----------|----------|--------|---|---|
| 35 | b | 129 | Total 1019 | C 647 | N 188 | 0 176 | S 8 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| b | 83 | THR | ALA | conflict | UNP Q4CXX2 |

• Molecule 36 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | | Ato | \mathbf{ms} | AltConf | Trace | | |
|-----|-------|----------|--------------|----------|---------------|---------|--------|---|---|
| 36 | с | 60 | Total 480 | C 303 | N 98 | O 78 | S 1 | 0 | 0 |

• Molecule 37 is a protein called Protein translation factor SUI1 homolog, putative.

| Mol | Chain | Residues | | At | oms | | AltConf | Trace | |
|-----|-------|----------|--------------|----------|----------|----------|---|-------|---|
| 37 | V | 97 | Total 789 | C 490 | N 152 | 0 145 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 38 is a protein called Putative eukaryotic translation initiation factor 1A.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|---------------|----------|----------|----------|--------|---|---|
| 38 | W | 147 | Total 1162 | C 716 | N 209 | O 236 | S 1 | 0 | 0 |

• Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit E.



| Mol | Chain | Residues | | At | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---|---|
| 39 | Е | 391 | Total 3119 | C 1977 | N 536 | O 593 | S 13 | 0 | 0 |

• Molecule 40 is a protein called Eukaryotic translation initiation factor 5, putative.

| Mol | Chain | Residues | | \mathbf{A} | toms | AltConf | Trace | | |
|-----|-------|----------|---------------|--------------|----------|----------|---------|---|---|
| 40 | Y | 174 | Total 1387 | C 872 | N 243 | O 260 | S 12 | 0 | 0 |

• Molecule 41 is a protein called Ribosomal protein S29, putative.

| Mol | Chain | Residues | | Ato | \mathbf{ms} | AltConf | Trace | | |
|-----|-------|----------|--------------|----------|---------------|---------|--------|---|---|
| 41 | Q | 57 | Total 462 | C 283 | N 96 | O 77 | S 6 | 0 | 0 |

• Molecule 42 is a protein called eL41.

| Mol | Chain | Residues | | Ato | \mathbf{ms} | AltConf | Trace | | |
|-----|-------|----------|-------|-----|---------------|---------|-------|---|---|
| 42 | П | 22 | Total | С | N | 0 | S | 0 | 0 |
| 42 | D | | 294 | 178 | 76 | 38 | 2 | 0 | 0 |

• Molecule 43 is a protein called JAB_MPN domain-containing protein.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 43 | G | 308 | Total 2414 | C 1492 | N 442 | O 466 | S 14 | 0 | 0 |

• Molecule 44 is a protein called CSN8_PSD8_EIF3K domain-containing protein.

| Mol | Chain | Residues | | At | | AltConf | Trace | | |
|-----|-------|----------|---------------|-----------|----------|----------|----------------|---|---|
| 44 | K | 201 | Total 1566 | C 1001 | N 256 | 0 304 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 45 is a protein called 40S ribosomal protein S15, putative.

| Mol | Chain | Residues | | At | oms | AltConf | Trace | | |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---|---|
| 45 | Т | 132 | Total 1057 | C 670 | N 204 | 0 179 | ${S \atop 4}$ | 0 | 0 |

• Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit 8, putative.



| Mol | Chain | Residues | | \mathbf{A} | toms | | | AltConf | Trace |
|-----|-------|----------|---------------|--------------|----------|-----------|---------|---------|-------|
| 46 | С | 696 | Total 5630 | C 3542 | N 973 | O 1092 | S 23 | 0 | 0 |

• Molecule 47 is a protein called eIF3A.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 47 | 8 | 576 | Total 4596 | C 2882 | N 845 | O 847 | S 22 | 0 | 0 |

• Molecule 48 is a protein called 40S ribosomal protein S3a-2.

| Mol | Chain | Residues | | Ate | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---|---|
| 48 | W | 217 | Total 1781 | C 1124 | N 337 | 0 313 | S 7 | 0 | 0 |

• Molecule 49 is a protein called Eukaryotic translation initiation factor 3 (EIF-3) interacting protein, putative.

| Mol | Chain | Residues | | At | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---|---|
| 49 | Ι | 344 | Total 2770 | C 1771 | N 479 | O 503 | S 17 | 0 | 0 |

• Molecule 50 is a protein called eIF3H.

| Mol | Chain | Residues | | At | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---|---|
| 50 | Н | 297 | Total 2388 | C 1498 | N 421 | 0 451 | S 18 | 0 | 0 |

• Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit 7-like protein, putative.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 51 | А | 483 | Total 3891 | C 2446 | N 691 | 0 729 | S 25 | 0 | 0 |

• Molecule 52 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | | At | oms | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 52 | 1 | 258 | Total 2038 | C 1290 | N 383 | 0 354 | S 11 | 0 | 0 |

• Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).



| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 53 | n | 1 | Total Zn 1 1 | 0 |

• Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 54 | 5 | 1 | Total Mg 1 1 | 0 |

• Molecule 55 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



| Mol | Chain | Residues | Atoms | | | | AltConf | |
|------|-------|----------|-------|----|---|----|---------|---|
| 55 | F | 1 | Total | С | Ν | Ο | Р | 0 |
| - 55 | 5 | L | 32 | 10 | 6 | 13 | 3 | 0 |



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: kDDX60































| Chain R: | | 91% | • 7% |
|--|--|--|--|
| MET V2 B32 V37 V37 K43 | 644 R73 E83 F113 F116 0134 0134 | E142 SER SER SER SER ALA ALA ALA ALA | |
| • Molecule 16: | 40S ribosomal protein | S27, putative | |
| Chain S: | | 92% | • 5% |
| MET PHE PHE BF S6 P39 C40 | S 53 E 54 E 654 A 61 A 61 C 60 C 60 C 60 C 60 C 60 C 60 C 60 C 60 | | |
| • Molecule 17: | 40S ribosomal protein | S26 | |
| Chain t: | | 91% | • 7% |
| M1 R21 F41 V42 V43 R44 R45 | L47 D48 D54 A64 G65 G65 R86 D94 D94 K103 | PR0 PR0 PR0 PR0 THR GLY ALA LYS | |
| • Molecule 18: | 40S ribosomal protein | S33 | |
| Chain U: | 26% 66% | 8% • 25% | |
| MET THR GLU VAL ALA ALA ALA LYS LYS ASP ASP LYS | LYS ALA ALA ALA ALA GLU GLU CLU GLU GLU GLU GLU GLU GLU GLU GLU GLU G | 410 861 861 861 861 873 878 878 878 881 883 883 883 883 883 883 883 883 88 | M102 E103 E105 R106 E107 A108 R109 R110 C111 L111 |
| • Molecule 19: | 40S ribosomal protein | S14, putative | |
| Chain v: | | 90% | • • 6% |
| MET SER LYS LYS GLU CJU LYS F9 A15 A15 | K16 D17 E18 B39 M40 A57 D73 K79 | A92 A105 A113 S132 S132 S132 K136 K136 K133 LEU | |
| • Molecule 20: | 40S ribosomal protein | S11, putative | |
| Chain X: | 79% | ••• | 14% |
| MET THR ALA PRO GLU GLU ALA ALA ALA ALA H11 | D14 E20 E20 B32 B33 N32 B35 N35 K38 K38 K39 K39 K39 K39 | N42 N43 844 B78 D78 N36 N130 N132 N133 V158 | SER LYS SER ALA ALA ALA GLY GLY CLY ARG LY ARG CLY SER SER |
| LYS ASN | | | |
| • Molecule 21: | Putative 40S ribosom | al protein S9 | |
| Chain B: | | 89% 5 | % 6% |
| | | | |









WORLDWIDE PROTEIN DATA BANK





• Molecule 37: Protein translation factor SUI1 homolog, putative













89% Chain G: 74% 13% 11%





• Molecule 46: Eukaryotic translation initiation factor 3 subunit 8, putative 87% Chain C: 25% 7% • • 64% S10 L14 D15 H19 H20 D21 E22 Q23 E25 V28 E12 V17 R26 K27 M S2 F4 F5 D6 **S**8 V1 00 E81 K82 A83 **q**169 G164 G165 D166 G168 G170 E167 I190 191 **3232** 1233 2234 A2 18 L2 15 0230 (207 A22E L226 L227 D280 G281 L282 A260 [261 E265 V266 F267 3273 r256 42.62 (264 271 /248 5249 (250 (251 (251 (252 (253 I345 V318 D319 3323 <u> 7</u>328 R333 G334 K335 A336 A336 I337 C338 3344 3350 **351** <mark>1352</mark> 1361 **J32**6 q340 I341 E375 **q**382 E383 387 /453 [454 **1455** A450 456 457 **3475** 480 1528 523 D519 524 V51 T51 V51 M587 M588 P589 N590 G591 D592 1582 1584 1585 1586 3570 0571 1573 580 2558 1559 1560 .<mark>567</mark> (568 556 1557 r561 A562 A563 Y564 Y565 K638 C639 I641 I641 N642 D643 I644 I645 R615 C616 N617 F<mark>618</mark> A619 T620 1621 S622 L<mark>652</mark> I 653 A654 V623 1633 E634 3636 1637 646 3647 R696 ASP SER ASP PHE ARC GLY CLY CLY ARC GLY ARC GLY PHE PHE

• Molecule 47: eIF3A

Chain 8: 59% 14% • 24%







• Molecule 51: Eukaryotic translation initiation factor 3 subunit 7-like protein, putative



 \bullet Molecule 52: 40S ribosomal protein S4

Chain l:

6%

88%







4 Experimental information (i)

| Property | Value | Source |
|------------------------------------|---------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 33775 | 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 $(e^-/\text{\AA}^2)$ | 30 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.118 | Depositor |
| Minimum map value | -0.081 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.005 | Depositor |
| Recommended contour level | 0.0193 | Depositor |
| Map size (Å) | 440.0, 440.0, 440.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles $(^{\circ})$ | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.1, 1.1, 1.1 | Depositor |



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GNP, ZN

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 | | |
|-----------|--------------|--------------|---------------------|-------------|---------------------|--|
| WIOI | Unam | RMSZ | # Z > 5 | RMSZ | # Z > 5 | |
| 1 | f | 1.28 | 79/12510~(0.6%) | 1.48 | 202/16884~(1.2%) | |
| 2 | 1 | 1.61 | 1/1798~(0.1%) | 2.50 | 213/2803~(7.6%) | |
| 3 | 0 | 1.59 | 38/51207~(0.1%) | 2.44 | 5849/79792~(7.3%) | |
| 4 | У | 1.02 | 0/1004 | 1.01 | 0/1335 | |
| 5 | \mathbf{S} | 0.94 | 0/2405 | 1.09 | 8/3247~(0.2%) | |
| 6 | j | 0.94 | 0/658 | 1.04 | 2/871~(0.2%) | |
| 7 | n | 0.92 | 0/1818 | 0.93 | 1/2433~(0.0%) | |
| 8 | р | 0.94 | 0/2461 | 1.10 | 2/3347~(0.1%) | |
| 9 | r | 1.01 | 0/1131 | 1.06 | 1/1520~(0.1%) | |
| 10 | u | 1.06 | 0/1126 | 1.20 | 5/1508~(0.3%) | |
| 11 | m | 0.97 | 0/1137 | 1.02 | 2/1520~(0.1%) | |
| 12 | Ζ | 1.06 | 0/1424 | 1.04 | 0/1904 | |
| 13 | 0 | 0.96 | 0/1515 | 0.97 | 0/2034 | |
| 14 | q | 1.06 | 0/1703 | 1.05 | 2/2290~(0.1%) | |
| 15 | R | 1.01 | 0/1164 | 1.00 | 0/1559 | |
| 16 | S | 0.97 | 0/641 | 0.95 | 0/858 | |
| 17 | \mathbf{t} | 1.14 | 0/845 | 1.05 | 0/1129 | |
| 18 | U | 1.05 | 0/527 | 1.04 | 0/702 | |
| 19 | V | 1.04 | 0/1026 | 1.04 | 1/1376~(0.1%) | |
| 20 | Х | 1.04 | 1/1238~(0.1%) | 1.04 | 1/1662~(0.1%) | |
| 21 | В | 1.06 | 0/1513 | 1.00 | 0/2030 | |
| 22 | F | 0.98 | 0/1693 | 1.05 | 4/2290~(0.2%) | |
| 23 | d | 0.95 | 0/1760 | 1.08 | 5/2376~(0.2%) | |
| 24 | g | 0.93 | 0/644 | 1.01 | 0/875 | |
| 25 | a | 0.93 | 0/559 | 0.98 | 0/748 | |
| 26 | J | 1.07 | 0/1381 | 1.23 | 7/1857~(0.4%) | |
| 27 | h | 0.97 | 0/966 | 0.99 | 0/1295 | |
| 28 | 5 | 1.02 | 2/3302~(0.1%) | 1.27 | 12/4483~(0.3%) | |
| 29 | Р | 1.09 | 0/2008 | 1.04 | 0/2678 | |
| 30 | i | 1.00 | 0/1005 | 1.11 | 3/1341~(0.2%) | |
| 31 | L | 0.99 | 0/794 | 1.09 | 0/1076 | |
| 32 | М | 1.04 | $0/1\overline{606}$ | 1.05 | $0/2\overline{141}$ | |



| Mol Chain | | E | Bond lengths | Bond angles | | |
|-----------|---------|------|-------------------|-------------|--------------------|--|
| | Ullalli | RMSZ | # Z > 5 | RMSZ | # Z > 5 | |
| 33 | N | 0.98 | 0/804 | 1.07 | 2/1082~(0.2%) | |
| 34 | 0 | 1.01 | 0/1140 | 1.05 | 0/1524 | |
| 35 | b | 1.00 | 0/1037 | 1.04 | 0/1391 | |
| 36 | с | 0.92 | 0/488 | 1.02 | 0/644 | |
| 37 | V | 0.75 | 0/799 | 0.84 | 0/1072 | |
| 38 | W | 0.92 | 0/1177 | 0.94 | 1/1588~(0.1%) | |
| 39 | Е | 1.49 | 6/3174~(0.2%) | 1.15 | 13/4304~(0.3%) | |
| 40 | Y | 0.91 | 0/1406 | 1.00 | 2/1890~(0.1%) | |
| 41 | Q | 1.07 | 0/468 | 1.10 | 1/618~(0.2%) | |
| 42 | D | 1.30 | 0/298 | 1.04 | 0/385 | |
| 43 | G | 1.00 | 0/2455 | 1.09 | 4/3323~(0.1%) | |
| 44 | Κ | 0.89 | 0/1597 | 1.06 | 12/2170~(0.6%) | |
| 45 | Т | 1.00 | 0/1079 | 0.98 | 1/1447~(0.1%) | |
| 46 | С | 1.68 | 3/5724~(0.1%) | 1.11 | 20/7724~(0.3%) | |
| 47 | 8 | 0.96 | 0/4685 | 1.04 | 6/6327~(0.1%) | |
| 48 | W | 1.05 | 4/1809~(0.2%) | 1.21 | 7/2437~(0.3%) | |
| 49 | Ι | 0.98 | 0/2826 | 1.01 | 8/3809~(0.2%) | |
| 50 | Н | 1.01 | 0/2431 | 1.11 | 9/3285~(0.3%) | |
| 51 | А | 0.95 | 3/3971~(0.1%) | 1.04 | 4/5366~(0.1%) | |
| 52 | 1 | 1.01 | 0/2073 | 1.05 | 0/2787 | |
| All | All | 1.31 | 137/144010~(0.1%) | 1.78 | 6410/205137~(3.1%) | |

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 |
|-----|-------|---------------------|---------------------|
| 1 | f | 3 | 200 |
| 3 | 0 | 2 | 52 |
| 4 | у | 0 | 1 |
| 5 | s | 0 | 17 |
| 6 | j | 0 | 2 |
| 7 | n | 0 | 1 |
| 8 | р | 0 | 2 |
| 9 | r | 0 | 4 |
| 10 | u | 0 | 2 |
| 11 | m | 0 | 2 |
| 12 | Ζ | 0 | 2 |
| 13 | 0 | 0 | 1 |
| 17 | t | 0 | 1 |
| 19 | V | 0 | 2 |

Continued on next page...



| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 20 | Х | 0 | 10 |
| 21 | В | 0 | 4 |
| 22 | F | 0 | 3 |
| 23 | d | 0 | 3 |
| 24 | g | 0 | 1 |
| 26 | J | 0 | 21 |
| 28 | 5 | 0 | 12 |
| 29 | Р | 0 | 4 |
| 31 | L | 0 | 7 |
| 32 | М | 0 | 2 |
| 33 | N | 0 | 1 |
| 34 | 0 | 0 | 6 |
| 35 | b | 0 | 1 |
| 36 | с | 0 | 3 |
| 38 | W | 0 | 6 |
| 39 | Е | 1 | 73 |
| 40 | Y | 0 | 4 |
| 41 | Q | 0 | 3 |
| 42 | D | 0 | 1 |
| 43 | G | 0 | 36 |
| 44 | Κ | 0 | 2 |
| 45 | Т | 0 | 1 |
| 46 | С | 1 | 137 |
| 47 | 8 | 0 | 69 |
| 48 | W | 0 | 2 |
| 49 | Ι | 2 | 6 |
| 50 | Н | 0 | 26 |
| 51 | А | 0 | 16 |
| 52 | 1 | 0 | 10 |
| All | All | 9 | 759 |

Continued from previous page...

The worst 5 of 137 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 46 | С | 411 | ARG | CD-NE | 105.86 | 3.26 | 1.46 |
| 39 | Е | 279 | TYR | CE1-CZ | 28.41 | 1.75 | 1.38 |
| 39 | Е | 279 | TYR | CE2-CZ | 28.18 | 1.75 | 1.38 |
| 39 | Е | 279 | TYR | CG-CD1 | 28.05 | 1.75 | 1.39 |
| 39 | Е | 279 | TYR | CG-CD2 | 27.28 | 1.74 | 1.39 |

The worst 5 of 6410 bond angle outliers are listed below:



| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $\operatorname{Ideal}(^{o})$ |
|-----|-------|------|------|---------|--------|------------------|------------------------------|
| 28 | 5 | 412 | GLN | O-C-N | -35.37 | 66.11 | 122.70 |
| 1 | f | 234 | GLY | O-C-N | -34.90 | 66.87 | 122.70 |
| 1 | f | 307 | LEU | O-C-N | -26.57 | 80.19 | 122.70 |
| 1 | f | 1147 | ILE | O-C-N | 23.84 | 160.84 | 122.70 |
| 1 | f | 305 | TYR | N-CA-CB | 19.79 | 146.23 | 110.60 |

5 of 9 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | f | 296 | TYR | CA |
| 1 | f | 305 | TYR | CA |
| 1 | f | 772 | TYR | CA |
| 3 | 0 | 974 | А | C1' |
| 3 | 0 | 1833 | G | C1' |

5 of 759 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | f | 26 | SER | Peptide |
| 1 | f | 38 | SER | Peptide |
| 1 | f | 46 | SER | Peptide |
| 1 | f | 55 | VAL | Peptide |
| 1 | f | 56 | THR | Peptide |

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 | f | 1519/2174~(70%) | 1094 (72%) | 295~(19%) | 130 (9%) | 1 5 |

Continued on next page...



| Continued fro | om previous | page |
|---------------|-------------|-------|
| contraca ji | | pagom |

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Perce | entiles |
|-----|--------------|--------------------|-----------|----------|----------|-------|---------|
| 4 | У | 121/137~(88%) | 109 (90%) | 10 (8%) | 2(2%) | 9 | 37 |
| 5 | \mathbf{S} | 293/418~(70%) | 207 (71%) | 51~(17%) | 35~(12%) | 0 | 2 |
| 6 | j | 77/150~(51%) | 68 (88%) | 6 (8%) | 3 (4%) | 3 | 21 |
| 7 | n | 223/343~(65%) | 179 (80%) | 33~(15%) | 11 (5%) | 2 | 16 |
| 8 | р | 308/318~(97%) | 268 (87%) | 31 (10%) | 9 (3%) | 4 | 27 |
| 9 | r | 138/149~(93%) | 101 (73%) | 29 (21%) | 8 (6%) | 1 | 12 |
| 10 | u | 134/153~(88%) | 87 (65%) | 33~(25%) | 14 (10%) | 0 | 3 |
| 11 | m | 140/143~(98%) | 120 (86%) | 18 (13%) | 2 (1%) | 11 | 41 |
| 12 | Z | $171/221 \ (77\%)$ | 145 (85%) | 20 (12%) | 6 (4%) | 3 | 24 |
| 13 | О | 188/190~(99%) | 147 (78%) | 33 (18%) | 8 (4%) | 2 | 19 |
| 14 | q | 198/211~(94%) | 168 (85%) | 28 (14%) | 2 (1%) | 15 | 49 |
| 15 | R | 139/151~(92%) | 121 (87%) | 15 (11%) | 3 (2%) | 6 | 33 |
| 16 | S | 80/86~(93%) | 69 (86%) | 9 (11%) | 2 (2%) | 5 | 30 |
| 17 | t | 102/112~(91%) | 82 (80%) | 19 (19%) | 1 (1%) | 15 | 49 |
| 18 | U | 66/91~(72%) | 54 (82%) | 10 (15%) | 2(3%) | 4 | 27 |
| 19 | V | 133/144~(92%) | 121 (91%) | 10 (8%) | 2 (2%) | 10 | 40 |
| 20 | Х | 146/173~(84%) | 121 (83%) | 20 (14%) | 5 (3%) | 3 | 24 |
| 21 | В | 177/190~(93%) | 149 (84%) | 23~(13%) | 5(3%) | 5 | 27 |
| 22 | F | 205/245~(84%) | 180 (88%) | 23~(11%) | 2(1%) | 15 | 49 |
| 23 | d | 221/263~(84%) | 191 (86%) | 28~(13%) | 2(1%) | 17 | 51 |
| 24 | g | 81/247~(33%) | 68 (84%) | 12~(15%) | 1 (1%) | 13 | 45 |
| 25 | a | 68/110~(62%) | 56 (82%) | 12~(18%) | 0 | 100 | 100 |
| 26 | J | 171/257~(66%) | 132 (77%) | 24~(14%) | 15~(9%) | 1 | 5 |
| 27 | h | 119/141~(84%) | 96 (81%) | 19~(16%) | 4 (3%) | 3 | 24 |
| 28 | 5 | 417/477~(87%) | 325 (78%) | 62~(15%) | 30~(7%) | 1 | 8 |
| 29 | Р | 247/250~(99%) | 219 (89%) | 25~(10%) | 3(1%) | 13 | 45 |
| 30 | i | 119/141~(84%) | 91 (76%) | 16~(13%) | 12 (10%) | 0 | 3 |
| 31 | L | 97/117~(83%) | 75 (77%) | 20 (21%) | 2 (2%) | 7 | 34 |
| 32 | М | 198/214~(92%) | 160 (81%) | 31~(16%) | 7~(4%) | 3 | 24 |
| 33 | Ν | 91/161~(56%) | 78 (86%) | 10 (11%) | 3(3%) | 4 | 24 |
| 34 | Ο | 138/167~(83%) | 103 (75%) | 27~(20%) | 8 (6%) | 1 | 12 |

Continued on next page...



| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-------------------|------------|------------|-----------|-------------|
| 35 | b | 127/145~(88%) | 108 (85%) | 18 (14%) | 1 (1%) | 19 53 |
| 36 | с | 58/66~(88%) | 47 (81%) | 10~(17%) | 1 (2%) | 9 37 |
| 37 | V | 95/109~(87%) | 70 (74%) | 15~(16%) | 10 (10%) | 0 3 |
| 38 | W | 145/166~(87%) | 105~(72%) | 30~(21%) | 10 (7%) | 1 9 |
| 39 | Ε | 389/407~(96%) | 288 (74%) | 46 (12%) | 55~(14%) | 0 1 |
| 40 | Y | 172/379~(45%) | 139 (81%) | 27~(16%) | 6 (4%) | 3 24 |
| 41 | Q | 55/57~(96%) | 40 (73%) | 8 (14%) | 7~(13%) | 0 2 |
| 42 | D | 31/34~(91%) | 25 (81%) | 5~(16%) | 1 (3%) | 4 25 |
| 43 | G | 306/345~(89%) | 254 (83%) | 33~(11%) | 19~(6%) | 1 11 |
| 44 | K | 199/203~(98%) | 185~(93%) | 10~(5%) | 4 (2%) | 7 34 |
| 45 | Т | 130/152~(86%) | 100 (77%) | 21~(16%) | 9~(7%) | 1 9 |
| 46 | С | 694/716~(97%) | 490 (71%) | 82~(12%) | 122 (18%) | 0 1 |
| 47 | 8 | 574/762~(75%) | 462 (80%) | 57~(10%) | 55~(10%) | 0 4 |
| 48 | W | 215/254~(85%) | 181 (84%) | 27~(13%) | 7~(3%) | 4 24 |
| 49 | Ι | 342/489~(70%) | 302 (88%) | 21~(6%) | 19~(6%) | 2 13 |
| 50 | Н | 295/334~(88%) | 231 (78%) | 41 (14%) | 23~(8%) | 1 7 |
| 51 | А | 481/502~(96%) | 341 (71%) | 89~(18%) | 51 (11%) | 0 3 |
| 52 | 1 | 256/273~(94%) | 216 (84%) | 30 (12%) | 10 (4%) | 3 21 |
| All | All | 11089/13737~(81%) | 8768 (79%) | 1572 (14%) | 749 (7%) | 2 9 |

Continued from previous page...

 $5~{\rm of}~749$ Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | f | 56 | THR |
| 1 | f | 91 | ASP |
| 1 | f | 190 | ARG |
| 1 | f | 203 | LEU |
| 1 | f | 235 | LEU |

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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



| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 1 | f | 1318/1862~(71%) | 1270~(96%) | 48 (4%) | 35 65 |
| 4 | У | 104/116~(90%) | 104 (100%) | 0 | 100 100 |
| 5 | s | 252/362~(70%) | 239~(95%) | 13 (5%) | 23 56 |
| 6 | j | 69/123~(56%) | 65~(94%) | 4 (6%) | 20 53 |
| 7 | n | 196/289~(68%) | 181 (92%) | 15 (8%) | 13 41 |
| 8 | р | 262/268~(98%) | 259~(99%) | 3 (1%) | 73 86 |
| 9 | r | 113/121 (93%) | 113 (100%) | 0 | 100 100 |
| 10 | u | 117/132~(89%) | 111 (95%) | 6 (5%) | 24 57 |
| 11 | m | 116/117~(99%) | 112 (97%) | 4 (3%) | 37 67 |
| 12 | Z | 143/184 (78%) | 143 (100%) | 0 | 100 100 |
| 13 | О | 160/160~(100%) | 157 (98%) | 3 (2%) | 57 79 |
| 14 | q | 188/195~(96%) | 187 (100%) | 1 (0%) | 88 93 |
| 15 | R | 125/132~(95%) | 125 (100%) | 0 | 100 100 |
| 16 | S | 70/73~(96%) | 69~(99%) | 1 (1%) | 67 83 |
| 17 | t | 87/93~(94%) | 87 (100%) | 0 | 100 100 |
| 18 | U | 57/74~(77%) | 50 (88%) | 7 (12%) | 4 20 |
| 19 | V | 103/112~(92%) | 102 (99%) | 1 (1%) | 76 87 |
| 20 | Х | 137/157~(87%) | 135~(98%) | 2 (2%) | 65 82 |
| 21 | В | 159/165~(96%) | 159 (100%) | 0 | 100 100 |
| 22 | F | 182/212~(86%) | 182 (100%) | 0 | 100 100 |
| 23 | d | 187/208~(90%) | 186 (100%) | 1 (0%) | 88 93 |
| 24 | g | 68/197~(34%) | 67~(98%) | 1 (2%) | 65 82 |
| 25 | a | 64/96~(67%) | 64 (100%) | 0 | 100 100 |
| 26 | J | 138/191~(72%) | 125~(91%) | 13 (9%) | 8 32 |
| 27 | h | 103/120~(86%) | 102 (99%) | 1 (1%) | 76 87 |
| 28 | 5 | 358/408~(88%) | 337~(94%) | 21 (6%) | 19 52 |
| 29 | Р | 204/205~(100%) | 202~(99%) | 2(1%) | 76 87 |
| 30 | i | 110/124~(89%) | 106 (96%) | 4 (4%) | 35 65 |
| 31 | L | 89/104~(86%) | 89 (100%) | 0 | 100 100 |
| 32 | М | 167/179~(93%) | 161 (96%) | 6 (4%) | 35 65 |
| 33 | Ν | 84/125~(67%) | 82 (98%) | 2 (2%) | 49 75 |

analysed, and the total number of residues.

Continued on next page...



| Mol | Chain | Analysed | Rotameric | Outliers | Perce | entiles |
|-----|-------|------------------|------------|----------|-------|---------|
| 34 | Ο | 118/139~(85%) | 117 (99%) | 1 (1%) | 81 | 90 |
| 35 | b | 110/123~(89%) | 110 (100%) | 0 | 100 | 100 |
| 36 | с | 49/53~(92%) | 47 (96%) | 2 (4%) | 30 | 62 |
| 37 | V | 86/97~(89%) | 71 (83%) | 15 (17%) | 2 | 8 |
| 38 | W | 125/137~(91%) | 115 (92%) | 10 (8%) | 12 | 40 |
| 39 | Ε | 334/350~(95%) | 322~(96%) | 12 (4%) | 35 | 65 |
| 40 | Y | 152/327~(46%) | 145~(95%) | 7 (5%) | 27 | 60 |
| 41 | Q | 49/49~(100%) | 46 (94%) | 3 (6%) | 18 | 51 |
| 42 | D | 30/31~(97%) | 29~(97%) | 1 (3%) | 38 | 68 |
| 43 | G | 260/289~(90%) | 256~(98%) | 4 (2%) | 65 | 82 |
| 44 | Κ | 176/178~(99%) | 174 (99%) | 2 (1%) | 73 | 86 |
| 45 | Т | 111/131~(85%) | 108~(97%) | 3 (3%) | 44 | 72 |
| 46 | С | 616/628~(98%) | 585~(95%) | 31 (5%) | 24 | 57 |
| 47 | 8 | 485/648~(75%) | 465~(96%) | 20 (4%) | 30 | 62 |
| 48 | W | 194/217~(89%) | 186~(96%) | 8 (4%) | 30 | 62 |
| 49 | Ι | 300/430~(70%) | 295~(98%) | 5 (2%) | 60 | 80 |
| 50 | Н | 266/299~(89%) | 261~(98%) | 5 (2%) | 57 | 79 |
| 51 | А | 425/441 (96%) | 380 (89%) | 45 (11%) | 6 | 27 |
| 52 | 1 | 217/230~(94%) | 214 (99%) | 3 (1%) | 67 | 83 |
| All | All | 9633/11701 (82%) | 9297 (96%) | 336 (4%) | 39 | 66 |

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5 of 336 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | С | 190 | ILE |
| 50 | Н | 304 | LEU |
| 46 | С | 274 | LYS |
| 47 | 8 | 82 | GLN |
| 51 | А | 48 | MET |

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such side chains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | W | 34 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | С | 359 | HIS |
| 38 | W | 130 | HIS |
| 43 | G | 231 | ASN |
| 46 | С | 635 | ASN |

5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2 | 1 | 74/75~(98%) | 11 (14%) | 1 (1%) |
| 3 | 0 | 2144/2319~(92%) | 389~(18%) | 28 (1%) |
| All | All | 2218/2394~(92%) | 400 (18%) | 29 (1%) |

5 of 400 RNA backbone outliers are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 2 | 1 | 16 | U |
| 2 | 1 | 17 | G |
| 2 | 1 | 20 | А |
| 2 | 1 | 25 | G |
| 2 | 1 | 32 | U |

5 of 29 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | 0 | 1196 | G |
| 3 | 0 | 2073 | С |
| 3 | 0 | 1450 | G |
| 3 | 0 | 1979 | С |
| 3 | 0 | 1393 | U |

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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mal | Type | Chain | Dog | Bos Link Bond lengths | | Bond angles | | | | |
|-----|-------------------|-------|-----|-----------------------|----------|-------------|---------|----------|------|----------|
| | for Type Cham Res | | nes | | Counts | RMSZ | # Z >2 | Counts | RMSZ | # Z > 2 |
| 55 | GNP | 5 | 502 | 54 | 29,34,34 | 2.06 | 8 (27%) | 33,54,54 | 2.39 | 9 (27%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 55 | GNP | 5 | 502 | 54 | - | 6/14/38/38 | 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) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 55 | 5 | 502 | GNP | PB-O3A | -7.46 | 1.49 | 1.59 |
| 55 | 5 | 502 | GNP | C6-N1 | 3.87 | 1.39 | 1.33 |
| 55 | 5 | 502 | GNP | PB-O2B | -3.60 | 1.47 | 1.56 |
| 55 | 5 | 502 | GNP | PG-O3G | -2.43 | 1.50 | 1.56 |
| 55 | 5 | 502 | GNP | C8-N7 | -2.33 | 1.30 | 1.34 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|-------------|-------|------------------|---------------|
| 55 | 5 | 502 | GNP | C5-C6-N1 | -8.57 | 111.71 | 123.43 |
| 55 | 5 | 502 | GNP | C2-N1-C6 | 5.52 | 124.69 | 115.93 |
| 55 | 5 | 502 | GNP | O3G-PG-O1G | -3.59 | 104.44 | 113.45 |
| 55 | 5 | 502 | GNP | PB-O3A-PA | -3.42 | 120.56 | 132.62 |
| 55 | 5 | 502 | GNP | C3'-C2'-C1' | 3.38 | 106.07 | 100.98 |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:



| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 55 | 5 | 502 | GNP | PG-N3B-PB-O1B |
| 55 | 5 | 502 | GNP | PG-N3B-PB-O3A |
| 55 | 5 | 502 | GNP | C5'-O5'-PA-O3A |
| 55 | 5 | 502 | GNP | O4'-C4'-C5'-O5' |
| 55 | 5 | 502 | GNP | C3'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

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





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 | f | 20 |
| 28 | 5 | 2 |
| 46 | С | 1 |
| 48 | W | 1 |

The worst 5 of 24 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | 5 | 282:ARG | С | 283:GLY | Ν | 2.09 |
| 1 | f | 1149:TYR | С | 1150:VAL | Ν | 1.72 |
| 1 | f | 1221:LEU | С | 1222:PRO | Ν | 1.71 |
| 1 | f | 1254:ALA | С | 1255:GLN | Ν | 1.68 |
| 1 | С | 53:ARG | С | 54:ASN | Ν | 1.67 |



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11893. 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



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

Y Index: 200



Z Index: 200 $\,$

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: 188

Y Index: 200

Z Index: 199

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



The images above show the 3D surface view of the map at the recommended contour level 0.0193. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

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 566 $\rm nm^3;$ this corresponds to an approximate mass of 511 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 0.300 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11893 and PDB model 7ASE. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0193 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 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 (0.0193).



9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0193) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | $\mathbf{Q}	extsf{-score}$ |
|-------|----------------|----------------------------|
| All | 0.4651 | 0.3140 |
| 0 | 0.6863 | 0.4100 |
| 1 | 0.6239 | 0.3900 |
| 5 | 0.1771 | 0.1970 |
| 8 | 0.1055 | 0.1110 |
| А | 0.1799 | 0.2290 |
| В | 0.6629 | 0.4450 |
| C | 0.1366 | 0.1530 |
| D | 0.6494 | 0.4030 |
| E | 0.0184 | 0.0580 |
| F | 0.6586 | 0.4440 |
| G | 0.0085 | 0.0310 |
| Н | 0.0060 | 0.0140 |
| I | 0.0000 | 0.0270 |
| J | 0.2144 | 0.1620 |
| K | 0.0000 | 0.0090 |
| L | 0.5216 | 0.3740 |
| М | 0.5824 | 0.4010 |
| N | 0.5152 | 0.3200 |
| 0 | 0.5157 | 0.2710 |
| P | 0.5254 | 0.3680 |
| Q | 0.6166 | 0.3660 |
| R | 0.6715 | 0.4560 |
| S | 0.6558 | 0.4530 |
| T | 0.5678 | 0.3920 |
| U | 0.4506 | 0.3740 |
| V | 0.5590 | 0.4390 |
| W | 0.6412 | 0.4440 |
| X | 0.7030 | 0.4570 |
| Y | 0.0510 | 0.1140 |
| Z | 0.6632 | 0.4390 |
| a | 0.4438 | 0.3150 |
| b | 0.7233 | 0.4770 |
| С | 0.5107 | 0.3610 |
| d | 0.6771 | 0.4640 |

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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| f | 0.2537 | 0.2210 |
| g | 0.6677 | 0.4600 |
| h | 0.2366 | 0.1980 |
| i | 0.5446 | 0.3570 |
| j | 0.3185 | 0.2750 |
| 1 | 0.6776 | 0.4450 |
| m | 0.7000 | 0.4630 |
| n | 0.2780 | 0.2490 |
| 0 | 0.5774 | 0.3930 |
| р | 0.4877 | 0.3530 |
| q | 0.6075 | 0.4110 |
| r | 0.6475 | 0.4160 |
| s | 0.2066 | 0.1950 |
| t | 0.6915 | 0.4720 |
| u | 0.5258 | 0.3220 |
| V | 0.6547 | 0.4420 |
| W | 0.3930 | 0.3050 |
| У | 0.6420 | 0.4190 |

