



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 03:57 AM GMT

PDB ID : 2HGU
Title : 70S T.Th. ribosome functional complex with mRNA and E- and P-site tRNAs at 4.5Å. This entry 2HGU contains 50S ribosomal subunit. The 30S ribosomal subunit can be found in PDB entry 2HGR.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 4.51 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

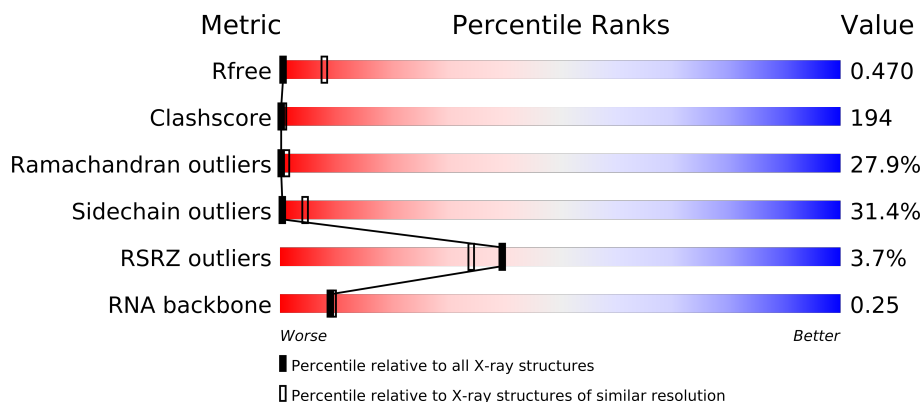
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.51 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R_{free} | 66092 | 1029 (5.50-3.50) |
| Clashscore | 79885 | 1300 (5.50-3.50) |
| Ramachandran outliers | 78287 | 1222 (5.50-3.50) |
| Sidechain outliers | 78261 | 1203 (5.50-3.50) |
| RSRZ outliers | 66119 | 1028 (5.50-3.50) |
| RNA backbone | 1838 | 1031 (6.22-2.80) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 2916 | |
| 2 | B | 123 | |
| 3 | C | 229 | |
| 4 | D | 276 | |
| 5 | E | 206 | |
| 6 | F | 210 | |
| 7 | G | 182 | |
| 8 | H | 180 | |
| 9 | K | 148 | |
| 10 | L | 147 | |
| 11 | M | 140 | |
| 12 | N | 122 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 13 | O | 150 | |
| 14 | P | 141 | |
| 15 | Q | 118 | |
| 16 | R | 112 | |
| 17 | S | 146 | |
| 18 | T | 118 | |
| 19 | U | 101 | |
| 20 | V | 113 | |
| 21 | W | 96 | |
| 22 | X | 110 | |
| 23 | Y | 206 | |
| 24 | Z | 85 | |
| 25 | 1 | 67 | |
| 26 | 2 | 60 | |
| 27 | 3 | 71 | |
| 28 | 4 | 60 | |
| 29 | 5 | 54 | |
| 30 | 6 | 49 | |
| 31 | 7 | 65 | |
| 32 | 8 | 37 | |

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 94012 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | A | 2889 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62218 | 27691 | 11629 | 20009 | 2889 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-----------|
| A | 493 | G | - | INSERTION | GB 48268 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | B | 123 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2641 | 1175 | 488 | 855 | 123 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|-----------|
| B | -1 | A | - | INSERTION | GB 48271 |
| B | 120 | U | - | INSERTION | GB 48271 |

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 228 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1742 | 1102 | 318 | 319 | 3 | | | |

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 272 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2124 | 1339 | 424 | 358 | 3 | | | |

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | E | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1578 | 997 | 302 | 273 | 6 | | | |

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | F | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1034 | 303 | 286 | 2 | | | |

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | G | 182 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1482 | 947 | 269 | 261 | 5 | | | |

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1328 | 844 | 248 | 235 | 1 | | | |

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | K | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 737 | 205 | 212 | 1 | | | |

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | L | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1025 | 654 | 181 | 185 | 5 | | | |

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | M | 139 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1113 | 717 | 207 | 186 | 3 | | | |

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | N | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 587 | 171 | 170 | 4 | | | |

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | O | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1106 | 688 | 226 | 190 | 2 | | | |

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | P | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1080 | 688 | 204 | 183 | 5 | | | |

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | Q | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | | |

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | R | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | | |

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | S | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 976 | 614 | 197 | 164 | 1 | | | |

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | T | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | U | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | V | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 552 | 171 | 151 | 2 | | | |

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | W | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 483 | 133 | 126 | | | | |

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | X | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 844 | 539 | 158 | 141 | 6 | | | |

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | Y | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1435 | 916 | 256 | 260 | 3 | | | |

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | Z | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 670 | 415 | 141 | 112 | 2 | | | |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 25 | 1 | 67 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 567 | 350 | 116 | 99 | 2 | | | |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 26 | 2 | 59 | Total | C | N | O | | | |
| | | | 469 | 298 | 90 | 81 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | 3 | 71 | Total | C | N | O | S | | | |
| | | | 581 | 364 | 108 | 104 | 5 | 0 | 0 | 0 |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 4 | 57 | Total | C | N | O | S | | | |
| | | | 445 | 279 | 87 | 74 | 5 | 0 | 0 | 0 |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | 5 | 49 | Total | C | N | O | S | | | |
| | | | 426 | 265 | 87 | 70 | 4 | 0 | 0 | 0 |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30 | 6 | 49 | Total | C | N | O | S | | | |
| | | | 430 | 263 | 108 | 57 | 2 | 0 | 0 | 0 |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 31 | 7 | 64 | Total | C | N | O | S | | | |
| | | | 515 | 331 | 102 | 79 | 3 | 0 | 0 | 0 |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L36.

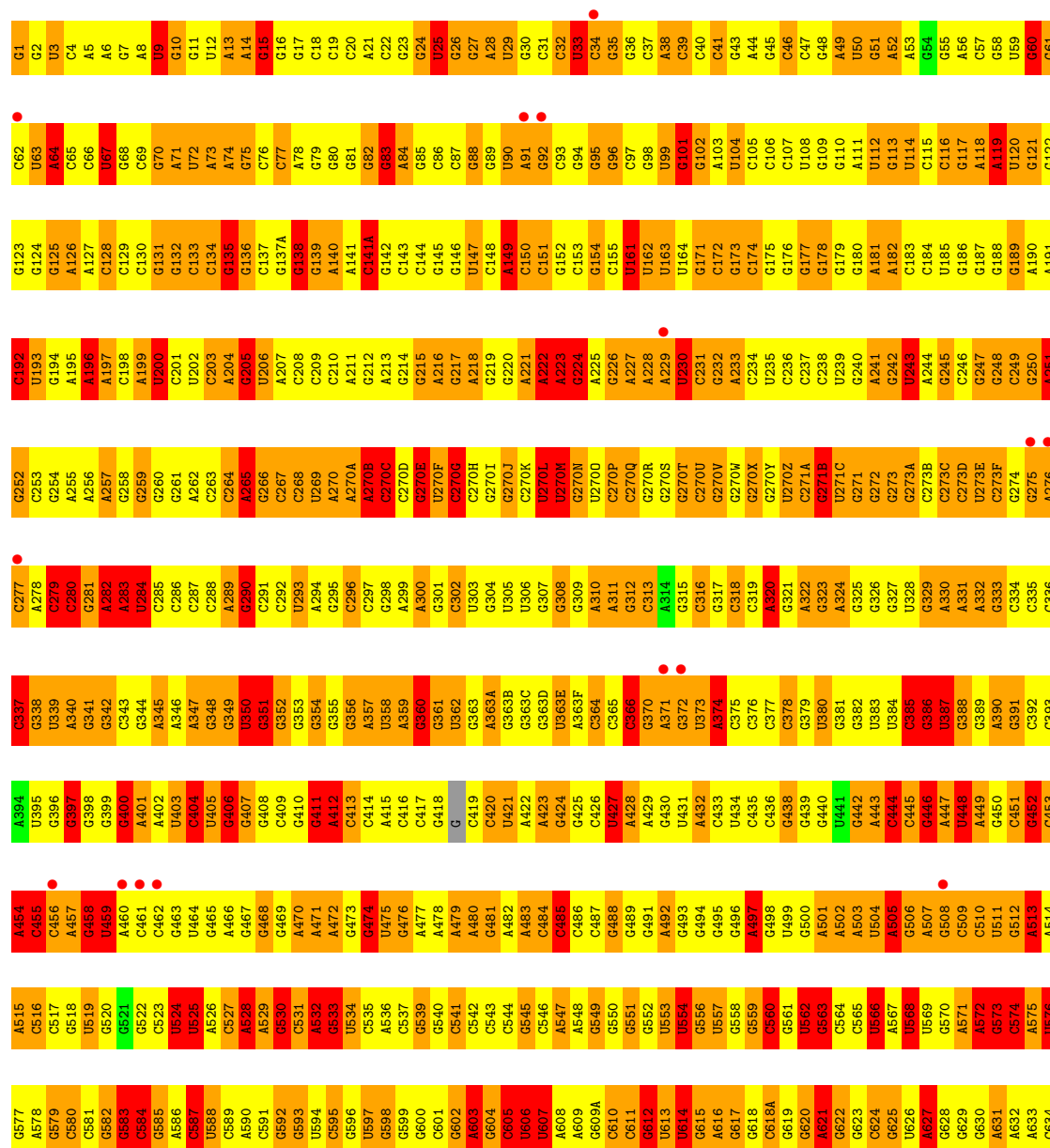
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32 | 8 | 37 | Total | C | N | O | S | | | |
| | | | 307 | 188 | 68 | 47 | 4 | 0 | 0 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

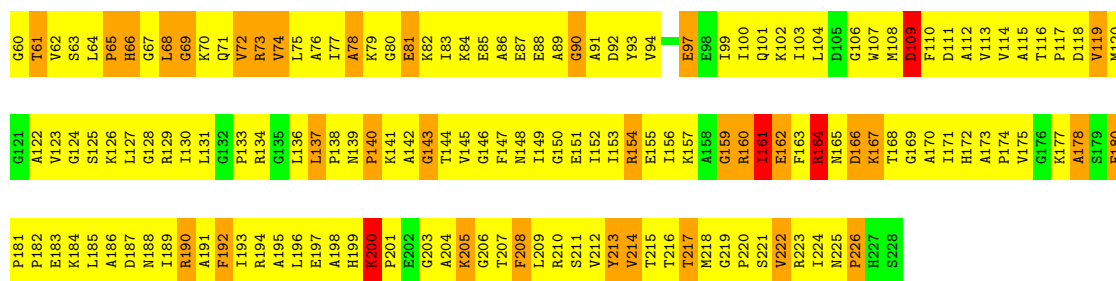
• Molecule 1: 23S rRNA

Chain A: 



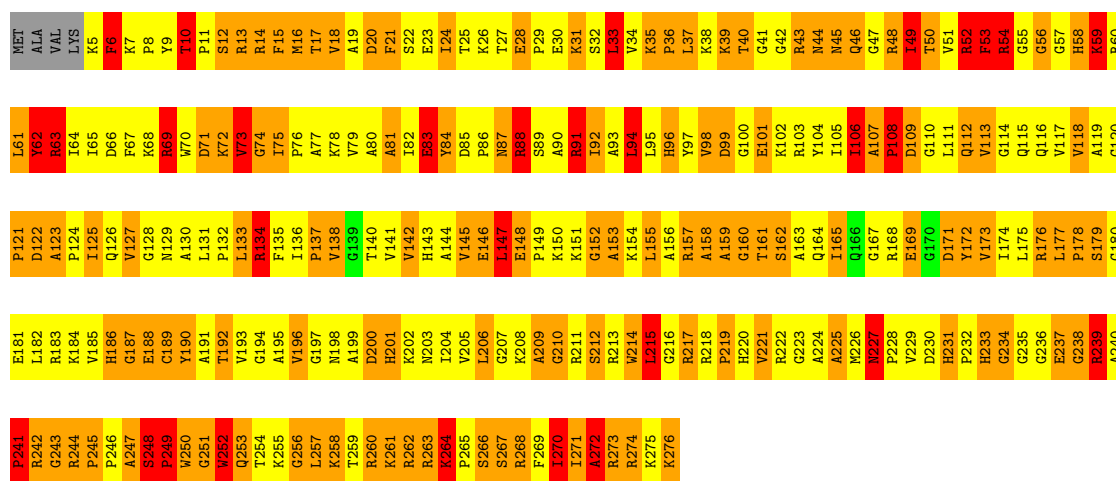
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|-------|-------|------|-------|
| G1455 | G1456 | G1457 | C1398 | G1399 | G1400 | G1401 | G1402 | G1403 | G1404 | G1405 | G1406 | G1407 | G1408 | G1409 | G1410 | G1411 | G1412 | G1413 | G1414 | G1415 | G1416 | G1417 | G1418 | G1419 | G1420 | G1421 | G1422 | G1423 | G1424 | G1425 | G1426 | G1427 | G1428 | G1429 | A1490 | G1491 | G1492 | G1493 | A1494 | A1495 | A1496 | U1497 | G1498 | G1499 | G1500 | C1501 | C1502 | U1503 | C1504 | C1505 | C1506 | A1507 | A1508 | C1509 | A1510 | A1511 | G1512 | C1513 | U1514 | C1515 | | | | | |
| A1336 | G1337 | G1338 | G1339 | U1340 | U1341 | U1342 | G1343 | G1344 | G1345 | G1346 | G1347 | G1348 | A1349 | C1350 | C1351 | U1352 | A1353 | A1354 | G1355 | G1356 | U1357 | G1358 | A1359 | A1360 | G1361 | C1362 | C1363 | G1364 | G1365 | A1366 | A1367 | G1368 | G1369 | C1370 | G1371 | G1372 | U1373 | G1374 | G1375 | G1376 | G1377 | A1378 | G1379 | G1380 | G1381 | G1382 | C1383 | A1384 | G1385 | C1386 | C1387 | G1388 | G1389 | U1390 | U1391 | A1392 | C1393 | U1394 | A1395 | | | | | | |
| G1216 | C1217 | G1218 | G1219 | A1220 | G1221 | C1222 | C1223 | A1224 | G1225 | C1226 | A1227 | G1228 | C1229 | C1230 | G1231 | C1232 | G1233 | U1234 | G1235 | G1236 | A1237 | C1238 | G1239 | U1240 | A1241 | A1242 | C1243 | G1244 | G1245 | A1246 | A1247 | G1248 | U1249 | G1250 | C1251 | G1252 | A1253 | A1254 | U1255 | G1256 | C1257 | G1258 | G1259 | G1260 | C1261 | A1262 | U1263 | G1264 | A1265 | G1266 | U1267 | A1268 | U1269 | A1270 | G1271 | A1272 | U1273 | A1274 | A1275 | | | | | | |
| A1155 | A1156 | G1157 | G1158 | U1159 | G1160 | C1161 | G1162 | G1163 | G1164 | U1165 | G1166 | U1167 | G1168 | G1169 | G1170 | G1171 | G1172 | U1173 | G1174 | U1175 | G1176 | A1177 | C1178 | G1179 | C1180 | C1181 | A1182 | G1183 | G1184 | C1185 | G1186 | G1187 | U1188 | A1189 | G1190 | G1191 | G1192 | G1193 | A1194 | G1195 | C1196 | G1197 | U1198 | U1199 | C1200 | C1201 | C1202 | G1203 | A1204 | U1205 | G1206 | C1207 | C1208 | G1209 | A1210 | C1211 | G1212 | A1213 | A1214 | G1215 | | | | | |
| A1096 | U1097 | A1098 | G1099 | U1100 | U1101 | C1102 | C1103 | C1104 | A1105 | G1106 | G1107 | U1108 | C1109 | G1110 | A1111 | G1112 | U1113 | G1114 | G1115 | G1116 | G1117 | C1118 | G1119 | G1120 | C1121 | G1122 | C1123 | G1124 | G1125 | A1126 | A1127 | A1128 | U1129 | U1130 | G1131 | A1132 | U1133 | G1134 | C1135 | G1136 | G1137 | G1138 | G1139 | C1140 | U1141 | U1142 | A1142A | A1143 | G1144 | C1145 | G1146 | C1147 | A1148 | G1149 | C1150 | G1151 | C1152 | C1153 | G1154 | | | | | | |
| G1036 | G1037 | C1038 | G1039 | C1040 | G1041 | G1042 | C1043 | C1044 | A1045 | A1046 | G1047 | A1048 | C1049 | C1050 | U1051 | G1052 | C1053 | A1054 | G1055 | G1056 | A1057 | G1058 | G1059 | U1060 | U1061 | G1062 | G1063 | A1064 | U1065 | G1066 | A1067 | G1068 | U1069 | A1070 | G1071 | C1072 | A1073 | G1074 | C1075 | C1076 | A1077 | U1078 | C1079 | C1080 | U1081 | G1082 | U1083 | A1084 | A1085 | A1086 | C1087 | A1088 | G1089 | U1090 | U1091 | C1092 | G1093 | U1094 | A1095 | | | | | | |
| C974A | G975 | C976 | G977 | G978 | G979 | A980 | A981 | C982 | A983 | C984 | C985 | C986 | C987 | A988 | G989 | A990 | C991 | C992 | G993 | C994 | C995 | A996 | G997 | C998 | C999 | U999 | A1000 | A1001 | G1002 | U943 | G1003 | C1004 | G1005 | C1006 | G947 | C948 | A1009 | A1010 | G952 | A953 | G954 | C955 | G956 | A957 | U958 | A959 | A960 | G1022 | U1023 | G962 | U963 | C964 | C965 | G966 | A1027 | A1028 | G968 | U969 | G1030 | U1031 | C971 | A1032 | U1033 | A973 | U1035 |
| C914 | C915 | G916 | C917 | A918 | U919 | G920 | G921 | U922 | A923 | C924 | C925 | A926 | G928 | U929 | U930 | G931 | G932 | A933 | G934 | C935 | C936 | U937 | G938 | G939 | G940 | A941 | G942 | U943 | G944 | A945 | C946 | G947 | C948 | A949 | G950 | C951 | G952 | A953 | G954 | C955 | G956 | A957 | U958 | A959 | A960 | G961 | G962 | U963 | C964 | C965 | G966 | A967 | G968 | U969 | C970 | C971 | A972 | A973 | G974 | | | | | | |
| G853 | G854 | C855 | C856 | C857 | U858 | C859 | U860 | A861 | A862 | C863 | G864 | C865 | A866 | C867 | U868 | G869 | A870 | U871 | A872 | C873 | G874 | C875 | C876 | U877 | A878 | G879 | A880 | G881 | C882 | G883 | C884 | C885 | C886 | A887 | C888 | C889 | A890 | C892 | C893 | C894 | U895 | A896 | C897 | C898 | A899 | A900 | U901 | G902 | C903 | C904 | U905 | G906 | U907 | U908 | A909 | A910 | A911 | C912 | U913 | | | | | | |
| A793 | G794 | C795 | C796 | C797 | G798 | G799 | A800 | A801 | A802 | U803 | A804 | C805 | A806 | C807 | U807 | G808 | G809 | U810 | U811 | C812 | U813 | C814 | C815 | C816 | C817 | G818 | A819 | G820 | A821 | U822 | G823 | A824 | C825 | C826 | U827 | C828 | A829 | G830 | G831 | C832 | U833 | C834 | A835 | G836 | C837 | C838 | U839 | C840 | A841 | G842 | C843 | U844 | G845 | C846 | U847 | U848 | A849 | C850 | U851 | G852 | | | | | |
| C673 | G674 | A675 | A676 | C677 | C678 | C679 | G680 | G681 | G682 | C683 | A684 | G685 | A686 | C687 | U688 | A689 | G690 | U691 | C692 | C693 | U694 | C695 | G696 | C697 | C698 | A699 | G700 | G701 | G702 | U703 | G704 | A705 | A706 | C707 | G708 | U709 | G710 | G711 | G712 | G713 | U714 | A715 | A716 | C717 | A718 | C719 | G720 | C721 | A722 | G723 | U724 | G725 | C726 | U727 | G728 | G729 | C730 | C731 | C732 | | | | | | |
| G733 | A734 | C735 | C736 | A737 | G738 | G739 | U740 | G741 | G742 | G743 | A744 | G745 | A746 | U747 | G748 | A749 | A750 | A751 | A752 | C753 | C754 | C755 | C756 | U757 | C758 | A759 | G760 | G761 | U762 | G763 | A764 | G765 | C766 | U767 | G768 | C769 | G770 | G771 | C772 | U773 | A774 | G775 | G776 | A777 | G778 | U779 | G780 | A781 | A782 | U783 | A784 | G785 | C786 | U787 | A788 | A789 | C790 | C791 | G792 | C793 | C794 | | | | |





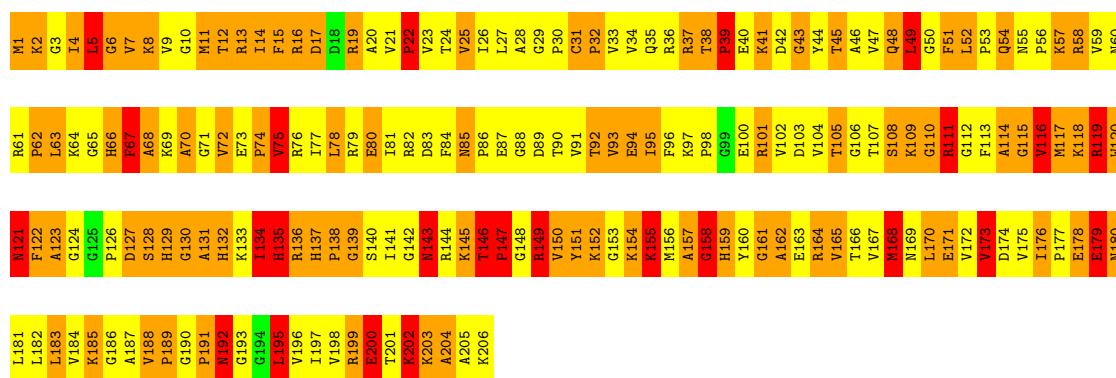
• Molecule 4: 50S RIBOSOMAL PROTEIN L2

Chain D:



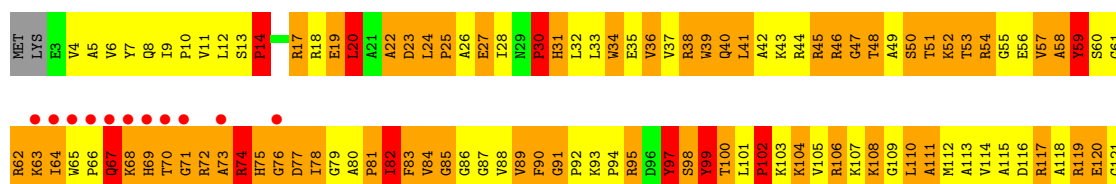
• Molecule 5: 50S RIBOSOMAL PROTEIN L3

Chain E:



• Molecule 6: 50S RIBOSOMAL PROTEIN L4

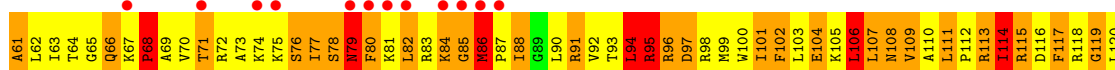
Chain F:





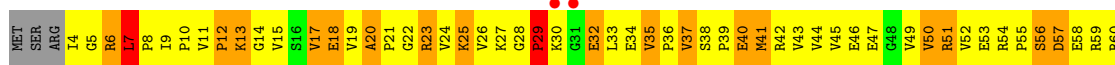
• Molecule 7: 50S RIBOSOMAL PROTEIN L5

Chain G:



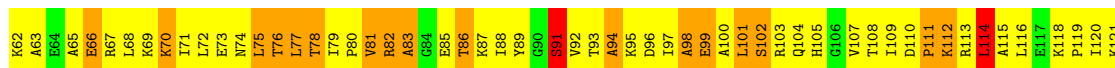
• Molecule 8: 50S RIBOSOMAL PROTEIN L6

Chain H:



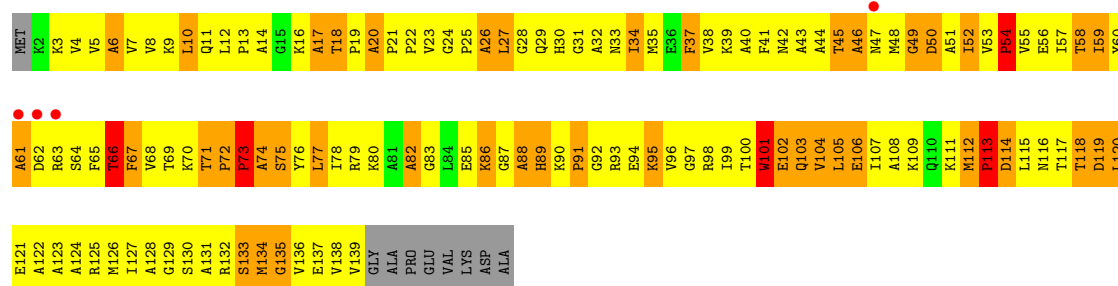
• Molecule 9: 50S RIBOSOMAL PROTEIN L9

Chain K:



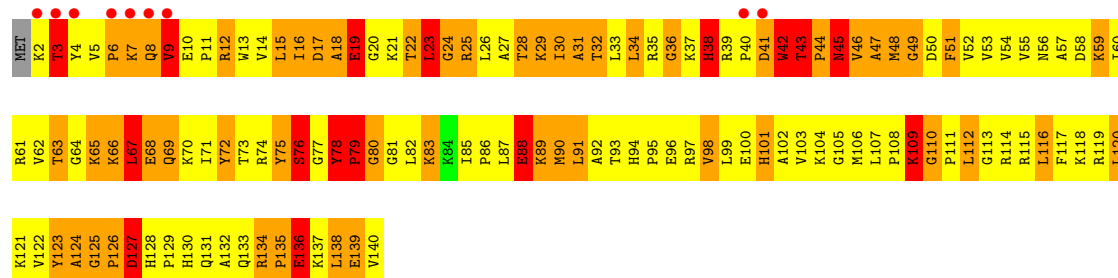
• Molecule 10: 50S RIBOSOMAL PROTEIN L11

Chain L:



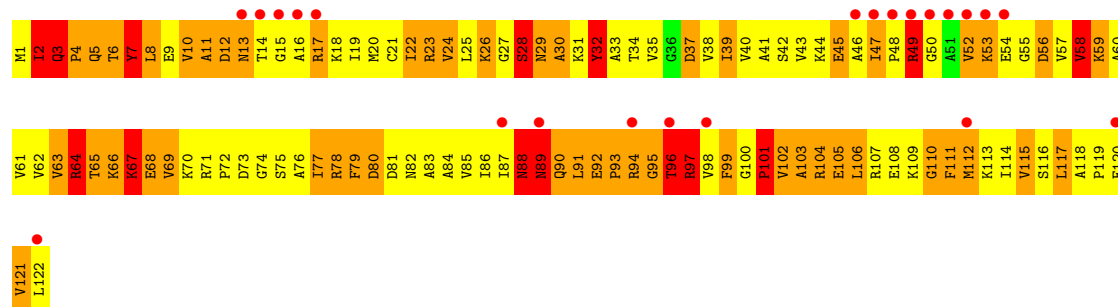
• Molecule 11: 50S RIBOSOMAL PROTEIN L13

Chain M:



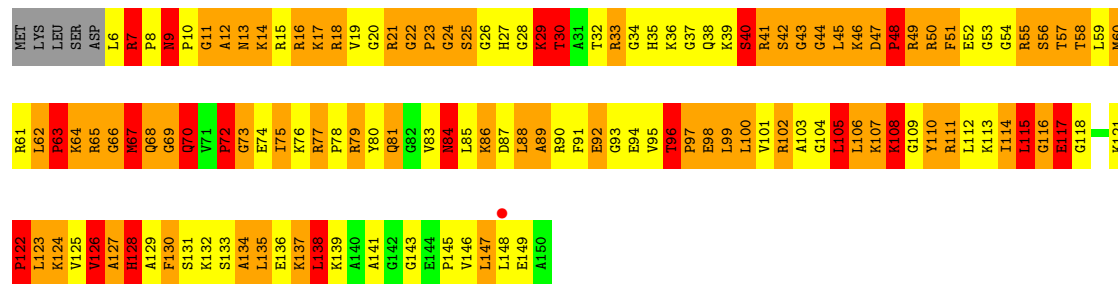
• Molecule 12: 50S RIBOSOMAL PROTEIN L14

Chain N:



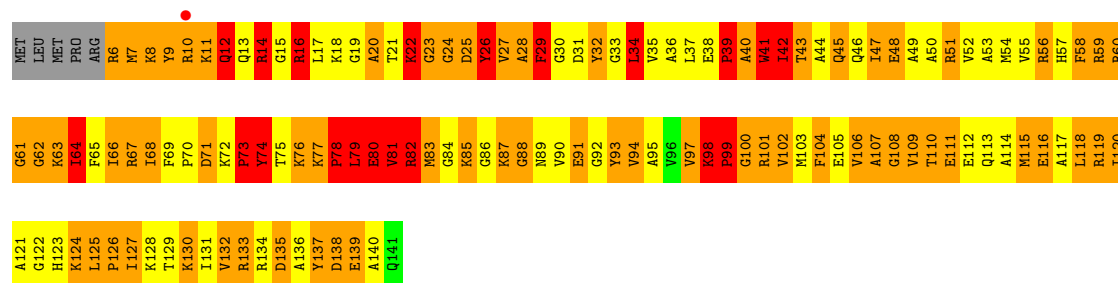
• Molecule 13: 50S RIBOSOMAL PROTEIN L15

Chain O:



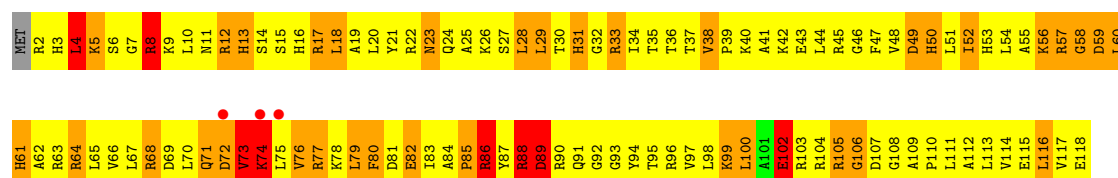
• Molecule 14: 50S RIBOSOMAL PROTEIN L16

Chain P:



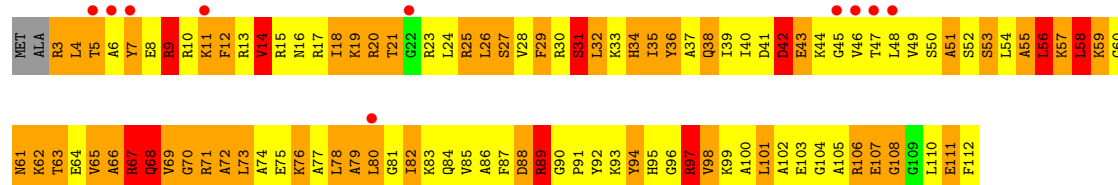
• Molecule 15: 50S RIBOSOMAL PROTEIN L17

Chain Q:



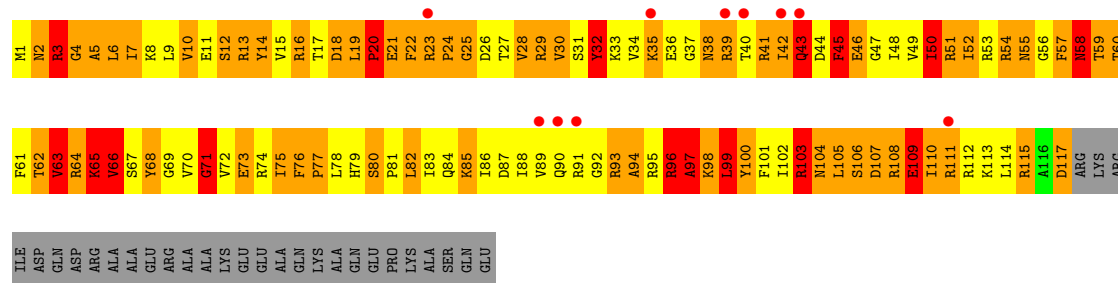
• Molecule 16: 50S RIBOSOMAL PROTEIN L18

Chain R:



• Molecule 17: 50S RIBOSOMAL PROTEIN L19

Chain S:

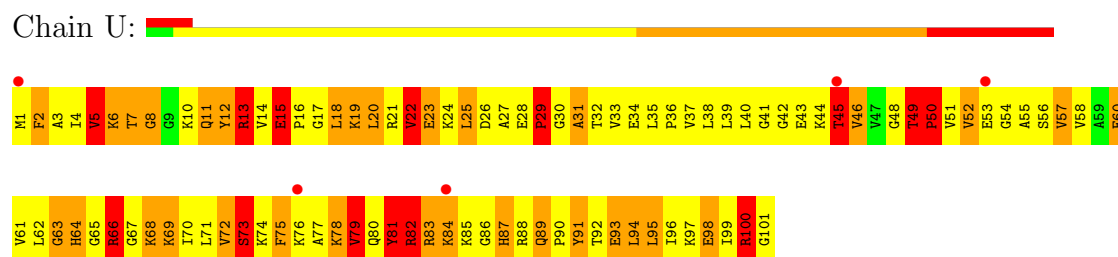


• Molecule 18: 50S RIBOSOMAL PROTEIN L20

Chain T:

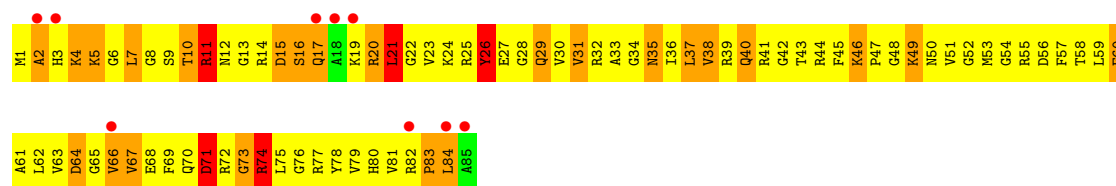


• Molecule 19: 50S RIBOSOMAL PROTEIN L21



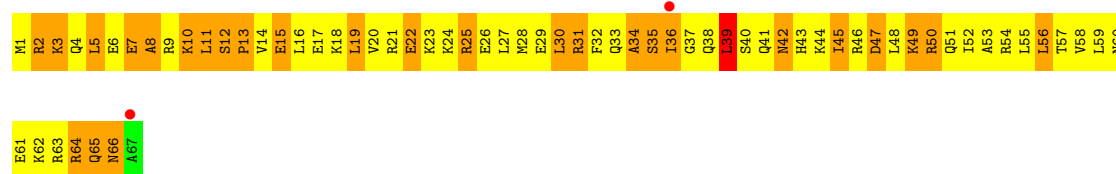
- Molecule 24: 50S RIBOSOMAL PROTEIN L27

Chain Z:



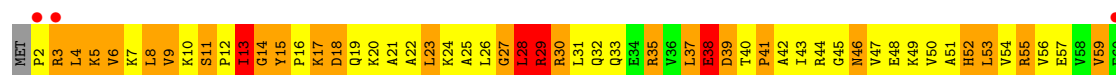
- Molecule 25: 50S RIBOSOMAL PROTEIN L29

Chain 1:



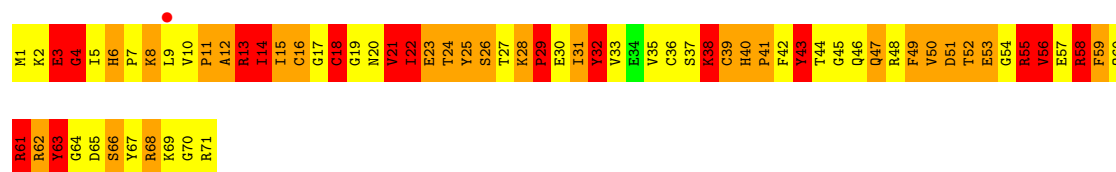
- Molecule 26: 50S RIBOSOMAL PROTEIN L30

Chain 2:



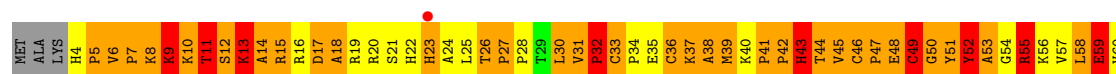
- Molecule 27: 50S RIBOSOMAL PROTEIN L31

Chain 3:



- Molecule 28: 50S RIBOSOMAL PROTEIN L32

Chain 4:



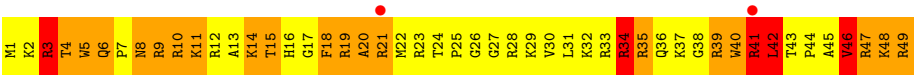
- Molecule 29: 50S RIBOSOMAL PROTEIN L33

Chain 5:



- Molecule 30: 50S RIBOSOMAL PROTEIN L34

Chain 6:



● Molecule 31: 50S RIBOSOMAL PROTEIN L35

Chain 7:



● Molecule 32: 50S RIBOSOMAL PROTEIN L36

Chain 8:



4 Data and refinement statistics

| Property | Value | Source |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group | I 4 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 300.00 – 4.51 429.82 – 3.98 | Depositor EDS |
| % Data completeness (in resolution range) | 90.3 (300.00-4.51) 94.9 (429.82-3.98) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.00 (at 4.02Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.298 , 0.345 0.442 , 0.470 | Depositor DCC |
| R_{free} test set | 14214 reflections (5.13%) | DCC |
| Wilson B-factor (Å ²) | 198.7 | Xtriage |
| Anisotropy | 0.113 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.09 , 112.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$ | Xtriage |
| Outliers | 0 of 441813 reflections | Xtriage |
| F_o, F_c correlation | 0.79 | EDS |
| Total number of atoms | 94012 | wwPDB-VP |
| Average B, all atoms (Å ²) | 249.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 | A | 1.06 | 139/69685 (0.2%) | 1.19 | 514/108786 (0.5%) |
| 2 | B | 0.80 | 2/2954 (0.1%) | 1.00 | 4/4606 (0.1%) |
| 3 | C | 0.50 | 0/1775 | 0.89 | 2/2393 (0.1%) |
| 4 | D | 0.88 | 2/2174 (0.1%) | 1.35 | 22/2927 (0.8%) |
| 5 | E | 0.87 | 0/1611 | 1.36 | 19/2171 (0.9%) |
| 6 | F | 0.74 | 0/1660 | 1.26 | 11/2247 (0.5%) |
| 7 | G | 0.60 | 0/1507 | 1.07 | 5/2027 (0.2%) |
| 8 | H | 0.64 | 0/1354 | 1.08 | 5/1831 (0.3%) |
| 9 | K | 0.68 | 0/1170 | 1.10 | 8/1581 (0.5%) |
| 10 | L | 0.50 | 0/1044 | 0.92 | 1/1415 (0.1%) |
| 11 | M | 0.85 | 1/1140 (0.1%) | 1.19 | 7/1537 (0.5%) |
| 12 | N | 1.07 | 4/942 (0.4%) | 1.42 | 7/1268 (0.6%) |
| 13 | O | 0.75 | 0/1123 | 1.24 | 9/1493 (0.6%) |
| 14 | P | 0.86 | 1/1100 (0.1%) | 1.23 | 9/1470 (0.6%) |
| 15 | Q | 0.70 | 0/974 | 1.07 | 2/1302 (0.2%) |
| 16 | R | 0.73 | 0/887 | 1.14 | 5/1180 (0.4%) |
| 17 | S | 0.98 | 0/990 | 1.52 | 16/1325 (1.2%) |
| 18 | T | 0.81 | 0/982 | 1.19 | 7/1306 (0.5%) |
| 19 | U | 0.94 | 1/790 (0.1%) | 1.40 | 10/1057 (0.9%) |
| 20 | V | 0.73 | 0/886 | 1.21 | 7/1189 (0.6%) |
| 21 | W | 0.60 | 0/756 | 0.97 | 5/1015 (0.5%) |
| 22 | X | 0.61 | 0/857 | 1.10 | 3/1142 (0.3%) |
| 23 | Y | 0.66 | 0/1467 | 1.11 | 5/1992 (0.3%) |
| 24 | Z | 0.67 | 0/679 | 1.02 | 1/902 (0.1%) |
| 25 | 1 | 0.60 | 0/569 | 0.89 | 1/751 (0.1%) |
| 26 | 2 | 0.71 | 1/474 (0.2%) | 1.10 | 4/635 (0.6%) |
| 27 | 3 | 1.05 | 0/594 | 1.44 | 10/795 (1.3%) |
| 28 | 4 | 0.79 | 0/459 | 1.22 | 2/621 (0.3%) |
| 29 | 5 | 0.98 | 1/433 (0.2%) | 1.49 | 6/576 (1.0%) |
| 30 | 6 | 0.84 | 1/438 (0.2%) | 1.08 | 1/575 (0.2%) |
| 31 | 7 | 0.69 | 0/523 | 1.22 | 5/690 (0.7%) |
| 32 | 8 | 0.73 | 0/310 | 1.13 | 1/407 (0.2%) |
| All | All | 0.98 | 153/102307 (0.1%) | 1.18 | 714/153212 (0.5%) |

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 | A | 0 | 610 |
| 2 | B | 0 | 20 |
| 4 | D | 0 | 1 |
| 6 | F | 0 | 1 |
| 8 | H | 0 | 3 |
| 12 | N | 0 | 2 |
| 14 | P | 0 | 3 |
| 17 | S | 0 | 2 |
| 18 | T | 0 | 1 |
| 19 | U | 0 | 2 |
| 20 | V | 0 | 1 |
| 27 | 3 | 0 | 2 |
| 28 | 4 | 0 | 1 |
| 29 | 5 | 0 | 1 |
| 32 | 8 | 0 | 1 |
| All | All | 0 | 651 |

The worst 5 of 153 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | A | 1203 | G | O3'-P | -34.71 | 1.19 | 1.61 |
| 1 | A | 1202 | C | O3'-P | 29.90 | 1.97 | 1.61 |
| 1 | A | 2447 | G | O3'-P | -21.30 | 1.35 | 1.61 |
| 1 | A | 2601 | C | O3'-P | 19.66 | 1.84 | 1.61 |
| 1 | A | 2756 | U | O3'-P | 19.18 | 1.84 | 1.61 |

The worst 5 of 714 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1 | A | 412 | A | O5'-P-OP2 | -28.87 | 76.06 | 110.70 |
| 1 | A | 1203 | G | P-O3'-C3' | 27.73 | 152.97 | 119.70 |
| 1 | A | 2448 | A | C5'-C4'-O4' | -27.33 | 76.31 | 109.10 |
| 6 | F | 20 | LEU | O-C-N | -25.54 | 81.83 | 122.70 |
| 1 | A | 412 | A | O5'-P-OP1 | -19.34 | 87.50 | 110.70 |

There are no chirality outliers.

5 of 651 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 10 | G | Sidechain |
| 1 | A | 14 | A | Sidechain |
| 1 | A | 15 | G | Sidechain |
| 1 | A | 3 | U | Sidechain |
| 1 | A | 9 | U | Sidechain |

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 62218 | 0 | 31354 | 15612 | 0 |
| 2 | B | 2641 | 0 | 1337 | 598 | 0 |
| 3 | C | 1742 | 0 | 1796 | 753 | 0 |
| 4 | D | 2124 | 0 | 2207 | 1429 | 0 |
| 5 | E | 1578 | 0 | 1647 | 1120 | 0 |
| 6 | F | 1625 | 0 | 1666 | 862 | 0 |
| 7 | G | 1482 | 0 | 1546 | 788 | 0 |
| 8 | H | 1328 | 0 | 1408 | 664 | 0 |
| 9 | K | 1155 | 0 | 1244 | 574 | 0 |
| 10 | L | 1025 | 0 | 1074 | 414 | 0 |
| 11 | M | 1113 | 0 | 1183 | 722 | 0 |
| 12 | N | 932 | 0 | 994 | 702 | 0 |
| 13 | O | 1106 | 0 | 1183 | 801 | 0 |
| 14 | P | 1080 | 0 | 1127 | 691 | 0 |
| 15 | Q | 960 | 0 | 1021 | 505 | 0 |
| 16 | R | 877 | 0 | 938 | 472 | 0 |
| 17 | S | 976 | 0 | 1033 | 690 | 0 |
| 18 | T | 964 | 0 | 1022 | 709 | 0 |
| 19 | U | 779 | 0 | 852 | 626 | 0 |
| 20 | V | 876 | 0 | 941 | 423 | 0 |
| 21 | W | 742 | 0 | 800 | 336 | 0 |
| 22 | X | 844 | 0 | 930 | 493 | 0 |
| 23 | Y | 1435 | 0 | 1463 | 683 | 0 |
| 24 | Z | 670 | 0 | 700 | 361 | 0 |
| 25 | 1 | 567 | 0 | 621 | 303 | 0 |
| 26 | 2 | 469 | 0 | 518 | 302 | 0 |
| 27 | 3 | 581 | 0 | 577 | 371 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28 | 4 | 445 | 0 | 459 | 271 | 0 |
| 29 | 5 | 426 | 0 | 452 | 307 | 0 |
| 30 | 6 | 430 | 0 | 480 | 275 | 0 |
| 31 | 7 | 515 | 0 | 587 | 413 | 0 |
| 32 | 8 | 307 | 0 | 335 | 126 | 0 |
| All | All | 94012 | 0 | 63495 | 30488 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 194.

The worst 5 of 30488 close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---------------|----------------|-------------|----------|
| 1:A:1204:A:C2 | 6:F:188:ARG:HA | 1.17 | 1.61 |
| 1:A:2459:A:N3 | 1:A:2460:U:H1' | 1.22 | 1.46 |
| 1:A:1204:A:C2 | 6:F:188:ARG:CA | 1.98 | 1.45 |
| 1:A:2745:C:N4 | 1:A:2756:U:C5 | 1.85 | 1.45 |
| 1:A:1475:G:H1 | 1:A:1477:A:N6 | 1.11 | 1.44 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 3 | C | 226/229 (99%) | 137 (61%) | 52 (23%) | 37 (16%) | 0 | 7 |
| 4 | D | 270/276 (98%) | 129 (48%) | 49 (18%) | 92 (34%) | 0 | 0 |
| 5 | E | 204/206 (99%) | 106 (52%) | 39 (19%) | 59 (29%) | 0 | 1 |
| 6 | F | 206/210 (98%) | 100 (48%) | 47 (23%) | 59 (29%) | 0 | 1 |
| 7 | G | 180/182 (99%) | 79 (44%) | 42 (23%) | 59 (33%) | 0 | 0 |
| 8 | H | 172/180 (96%) | 89 (52%) | 41 (24%) | 42 (24%) | 0 | 2 |
| 9 | K | 146/148 (99%) | 88 (60%) | 32 (22%) | 26 (18%) | 0 | 6 |
| 10 | L | 136/147 (92%) | 66 (48%) | 32 (24%) | 38 (28%) | 0 | 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|------------|-------------|---|
| 11 | M | 137/140 (98%) | 66 (48%) | 31 (23%) | 40 (29%) | 0 | 1 |
| 12 | N | 120/122 (98%) | 63 (52%) | 21 (18%) | 36 (30%) | 0 | 1 |
| 13 | O | 143/150 (95%) | 60 (42%) | 31 (22%) | 52 (36%) | 0 | 0 |
| 14 | P | 134/141 (95%) | 51 (38%) | 35 (26%) | 48 (36%) | 0 | 0 |
| 15 | Q | 115/118 (98%) | 64 (56%) | 33 (29%) | 18 (16%) | 0 | 8 |
| 16 | R | 108/112 (96%) | 45 (42%) | 30 (28%) | 33 (31%) | 0 | 1 |
| 17 | S | 115/146 (79%) | 53 (46%) | 26 (23%) | 36 (31%) | 0 | 0 |
| 18 | T | 115/118 (98%) | 49 (43%) | 39 (34%) | 27 (24%) | 0 | 3 |
| 19 | U | 99/101 (98%) | 51 (52%) | 22 (22%) | 26 (26%) | 0 | 2 |
| 20 | V | 108/113 (96%) | 69 (64%) | 15 (14%) | 24 (22%) | 0 | 3 |
| 21 | W | 92/96 (96%) | 59 (64%) | 14 (15%) | 19 (21%) | 0 | 4 |
| 22 | X | 108/110 (98%) | 41 (38%) | 27 (25%) | 40 (37%) | 0 | 0 |
| 23 | Y | 178/206 (86%) | 93 (52%) | 48 (27%) | 37 (21%) | 0 | 4 |
| 24 | Z | 83/85 (98%) | 50 (60%) | 14 (17%) | 19 (23%) | 0 | 3 |
| 25 | 1 | 65/67 (97%) | 27 (42%) | 26 (40%) | 12 (18%) | 0 | 5 |
| 26 | 2 | 57/60 (95%) | 32 (56%) | 16 (28%) | 9 (16%) | 0 | 8 |
| 27 | 3 | 69/71 (97%) | 26 (38%) | 19 (28%) | 24 (35%) | 0 | 0 |
| 28 | 4 | 55/60 (92%) | 16 (29%) | 12 (22%) | 27 (49%) | 0 | 0 |
| 29 | 5 | 47/54 (87%) | 13 (28%) | 7 (15%) | 27 (57%) | 0 | 0 |
| 30 | 6 | 47/49 (96%) | 16 (34%) | 16 (34%) | 15 (32%) | 0 | 0 |
| 31 | 7 | 62/65 (95%) | 29 (47%) | 11 (18%) | 22 (36%) | 0 | 0 |
| 32 | 8 | 35/37 (95%) | 20 (57%) | 4 (11%) | 11 (31%) | 0 | 0 |
| All | All | 3632/3799 (96%) | 1787 (49%) | 831 (23%) | 1014 (28%) | 0 | 1 |

5 of 1014 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 20 | TYR |
| 3 | C | 22 | ILE |
| 3 | C | 35 | ALA |
| 3 | C | 37 | PHE |
| 3 | C | 50 | ASP |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | C | 180/181 (99%) | 151 (84%) | 29 (16%) | 3 | 26 |
| 4 | D | 215/218 (99%) | 151 (70%) | 64 (30%) | 0 | 5 |
| 5 | E | 166/166 (100%) | 102 (61%) | 64 (39%) | 0 | 1 |
| 6 | F | 164/166 (99%) | 104 (63%) | 60 (37%) | 0 | 2 |
| 7 | G | 156/156 (100%) | 112 (72%) | 44 (28%) | 0 | 5 |
| 8 | H | 143/148 (97%) | 97 (68%) | 46 (32%) | 0 | 4 |
| 9 | K | 124/124 (100%) | 87 (70%) | 37 (30%) | 0 | 5 |
| 10 | L | 105/111 (95%) | 85 (81%) | 20 (19%) | 2 | 17 |
| 11 | M | 118/119 (99%) | 80 (68%) | 38 (32%) | 0 | 4 |
| 12 | N | 100/100 (100%) | 65 (65%) | 35 (35%) | 0 | 2 |
| 13 | O | 111/116 (96%) | 64 (58%) | 47 (42%) | 0 | 1 |
| 14 | P | 106/111 (96%) | 55 (52%) | 51 (48%) | 0 | 0 |
| 15 | Q | 100/101 (99%) | 69 (69%) | 31 (31%) | 0 | 5 |
| 16 | R | 87/88 (99%) | 55 (63%) | 32 (37%) | 0 | 1 |
| 17 | S | 105/127 (83%) | 69 (66%) | 36 (34%) | 0 | 3 |
| 18 | T | 93/94 (99%) | 64 (69%) | 29 (31%) | 0 | 4 |
| 19 | U | 82/82 (100%) | 59 (72%) | 23 (28%) | 0 | 6 |
| 20 | V | 90/92 (98%) | 56 (62%) | 34 (38%) | 0 | 1 |
| 21 | W | 76/78 (97%) | 55 (72%) | 21 (28%) | 0 | 6 |
| 22 | X | 91/91 (100%) | 66 (72%) | 25 (28%) | 0 | 6 |
| 23 | Y | 159/179 (89%) | 110 (69%) | 49 (31%) | 0 | 5 |
| 24 | Z | 67/67 (100%) | 52 (78%) | 15 (22%) | 1 | 11 |
| 25 | 1 | 62/62 (100%) | 46 (74%) | 16 (26%) | 1 | 8 |
| 26 | 2 | 51/52 (98%) | 34 (67%) | 17 (33%) | 0 | 3 |
| 27 | 3 | 63/63 (100%) | 42 (67%) | 21 (33%) | 0 | 3 |
| 28 | 4 | 50/52 (96%) | 30 (60%) | 20 (40%) | 0 | 1 |
| 29 | 5 | 48/52 (92%) | 32 (67%) | 16 (33%) | 0 | 3 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 30 | 6 | 42/42 (100%) | 30 (71%) | 12 (29%) | 0 | 5 |
| 31 | 7 | 54/55 (98%) | 40 (74%) | 14 (26%) | 1 | 7 |
| 32 | 8 | 34/34 (100%) | 25 (74%) | 9 (26%) | 1 | 7 |
| All | All | 3042/3127 (97%) | 2087 (69%) | 955 (31%) | 0 | 4 |

5 of 955 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | N | 97 | ARG |
| 14 | P | 139 | GLU |
| 27 | 3 | 66 | SER |
| 13 | O | 33 | ARG |
| 14 | P | 6 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 68 | GLN |
| 16 | R | 84 | GLN |
| 29 | 5 | 26 | ASN |
| 14 | P | 12 | GLN |
| 15 | Q | 23 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2888/2916 (99%) | 1241 (42%) | 313 (10%) |
| 2 | B | 122/123 (99%) | 46 (37%) | 5 (4%) |
| All | All | 3010/3039 (99%) | 1287 (42%) | 318 (10%) |

5 of 1287 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | U |
| 1 | A | 13 | A |
| 1 | A | 25 | U |
| 1 | A | 26 | G |
| 1 | A | 29 | U |

5 of 318 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1302 | A |
| 1 | A | 1626 | G |
| 1 | A | 2712 | U |
| 1 | A | 1349 | A |
| 1 | A | 1528 | A |

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 2889/2916 (99%) | -0.52 | 75 (2%) 53 43 | 168, 241, 340, 398 | 0 |
| 2 | B | 123/123 (100%) | -0.48 | 2 (1%) 68 56 | 236, 293, 329, 343 | 0 |
| 3 | C | 228/229 (99%) | -0.43 | 0 100 100 | 299, 326, 342, 347 | 0 |
| 4 | D | 272/276 (98%) | -0.53 | 0 100 100 | 184, 216, 235, 256 | 0 |
| 5 | E | 206/206 (100%) | -0.68 | 0 100 100 | 155, 205, 250, 276 | 0 |
| 6 | F | 208/210 (99%) | -0.28 | 11 (5%) 25 25 | 186, 255, 283, 288 | 0 |
| 7 | G | 182/182 (100%) | -0.05 | 14 (7%) 13 17 | 247, 283, 306, 311 | 0 |
| 8 | H | 174/180 (96%) | -0.33 | 5 (2%) 49 40 | 230, 260, 278, 284 | 0 |
| 9 | K | 148/148 (100%) | -0.64 | 1 (0%) 84 73 | 212, 241, 261, 265 | 0 |
| 10 | L | 138/147 (93%) | -0.31 | 4 (2%) 49 40 | 305, 358, 399, 403 | 0 |
| 11 | M | 139/140 (99%) | -0.06 | 9 (6%) 18 21 | 187, 217, 245, 270 | 0 |
| 12 | N | 122/122 (100%) | 0.80 | 22 (18%) 2 4 | 172, 201, 228, 240 | 0 |
| 13 | O | 145/150 (96%) | -0.50 | 1 (0%) 84 73 | 189, 271, 304, 346 | 0 |
| 14 | P | 136/141 (96%) | -0.54 | 1 (0%) 84 73 | 199, 234, 257, 266 | 0 |
| 15 | Q | 117/118 (99%) | -0.22 | 3 (2%) 53 43 | 195, 214, 246, 256 | 0 |
| 16 | R | 110/112 (98%) | 0.37 | 10 (9%) 9 14 | 232, 266, 293, 300 | 0 |
| 17 | S | 117/146 (80%) | 0.36 | 10 (8%) 11 15 | 182, 205, 238, 244 | 0 |
| 18 | T | 117/118 (99%) | -0.10 | 0 100 100 | 191, 221, 241, 250 | 0 |
| 19 | U | 101/101 (100%) | 0.16 | 5 (4%) 28 26 | 190, 244, 272, 277 | 0 |
| 20 | V | 110/113 (97%) | 1.45 | 28 (25%) 1 3 | 203, 226, 250, 260 | 0 |
| 21 | W | 94/96 (97%) | 0.95 | 22 (23%) 1 3 | 237, 253, 304, 309 | 0 |
| 22 | X | 110/110 (100%) | -0.13 | 7 (6%) 19 21 | 244, 282, 303, 312 | 0 |
| 23 | Y | 180/206 (87%) | -0.28 | 0 100 100 | 235, 267, 281, 287 | 0 |
| 24 | Z | 85/85 (100%) | 0.42 | 9 (10%) 7 11 | 236, 259, 272, 289 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 25 | 1 | 67/67 (100%) | -0.32 | 2 (2%) 48 39 | 251, 264, 276, 281 | 0 |
| 26 | 2 | 59/60 (98%) | -0.04 | 3 (5%) 27 26 | 208, 244, 261, 268 | 0 |
| 27 | 3 | 71/71 (100%) | -0.02 | 1 (1%) 72 58 | 212, 239, 259, 276 | 0 |
| 28 | 4 | 57/60 (95%) | -0.06 | 1 (1%) 65 53 | 200, 227, 276, 299 | 0 |
| 29 | 5 | 49/54 (90%) | -0.15 | 1 (2%) 62 49 | 211, 247, 269, 277 | 0 |
| 30 | 6 | 49/49 (100%) | 0.21 | 2 (4%) 35 31 | 189, 228, 244, 250 | 0 |
| 31 | 7 | 64/65 (98%) | 0.04 | 0 100 100 | 201, 220, 235, 247 | 0 |
| 32 | 8 | 37/37 (100%) | -0.45 | 0 100 100 | 212, 230, 240, 244 | 0 |
| All | All | 6704/6838 (98%) | -0.30 | 249 (3%) 39 34 | 155, 244, 337, 403 | 0 |

The worst 5 of 249 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | W | 96 | ILE | 11.7 |
| 20 | V | 83 | LYS | 9.6 |
| 7 | G | 71 | THR | 9.3 |
| 12 | N | 49 | ARG | 8.8 |
| 1 | A | 1537 | C | 8.8 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.