



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:10 PM BST

PDB ID : 3J3W  
EMDB ID: : EMD-5643  
Title : Atomic model of the immature 50S subunit from *Bacillus subtilis* (state II-a)  
Authors : Li, N.; Guo, Q.; Zhang, Y.; Yuan, Y.; Ma, C.; Lei, J.; Gao, N.  
Deposited on : 2013-04-28  
Resolution : 10.70 Å (reported)  
Based on PDB ID : 2J01, 2AW4

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

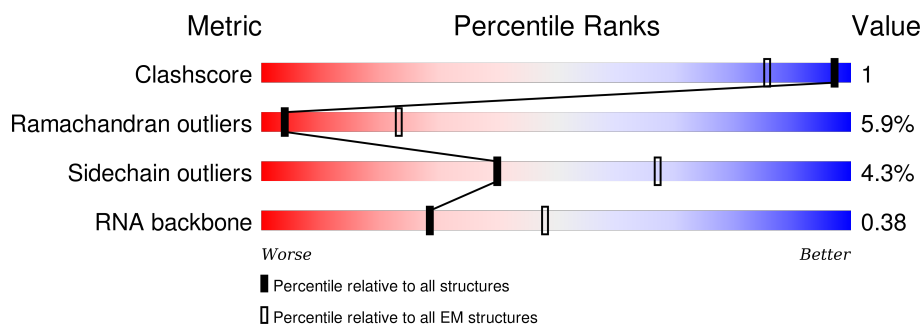
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.70 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<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |
| RNA backbone          | 3027                        | 244                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 2927   | 53% 32% 7% 8%    |
| 2   | O     | 59     | 83% 10% 7%       |
| 3   | C     | 277    | 88% 12%          |
| 4   | N     | 120    | 96% .            |
| 5   | G     | 179    | 84% 7% 9%        |
| 6   | J     | 145    | 87% 10% ..       |
| 7   | K     | 122    | 93% 7%           |
| 8   | L     | 146    | 88% 10% .        |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 9   | P     | 115    |  72%23% . . |
| 10  | Q     | 119    |  91%8% .    |
| 11  | D     | 209    |  91%6% ..   |
| 12  | R     | 102    |  88%11% .   |
| 13  | S     | 113    |  92%6% ..   |
| 14  | T     | 95     |  86%13% .   |
| 15  | U     | 103    |  83%17% .   |
| 16  | X     | 66     |  82%11%8%   |
| 17  | 2     | 44     |  91%9%      |
| 18  | 5     | 232    |  48% .48%   |
| 19  | 6     | 141    |  94%5% .    |
| 20  | E     | 207    |  86%13%    |

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 76573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | A     | 2685     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 57639 | 25720 | 10638 | 18600 | 2681 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 0     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 433   | 267 | 87 | 72 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2129  | 1323 | 419 | 380 | 7 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | N     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 962   | 588 | 187 | 182 | 5 |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | G     | 163      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1246  | 776 | 226 | 242 | 2 |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | J     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 717 | 207 | 204 | 6 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | K     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 921   | 571 | 173 | 173 | 4 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | L     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1082  | 671 | 207 | 202 | 2 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | P     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 916   | 584 | 178 | 154 |   |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | Q     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 940   | 591 | 189 | 156 | 4 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | D     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1568  | 984 | 289 | 290 | 5 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | R     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 795   | 506 | 140 | 148 | 1 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | S     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 541 | 168 | 155 | 4 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | T     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 767   | 480 | 139 | 144 | 4 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | U     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 780   | 488 | 145 | 143 | 4 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | X     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 504   | 312 | 97 | 93 | 2 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | 2     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 368   | 222 | 89 | 55 | 2 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | 5     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 910   | 576 | 156 | 176 | 2 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | 6     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1044  | 657 | 184 | 196 | 7 |         |       |

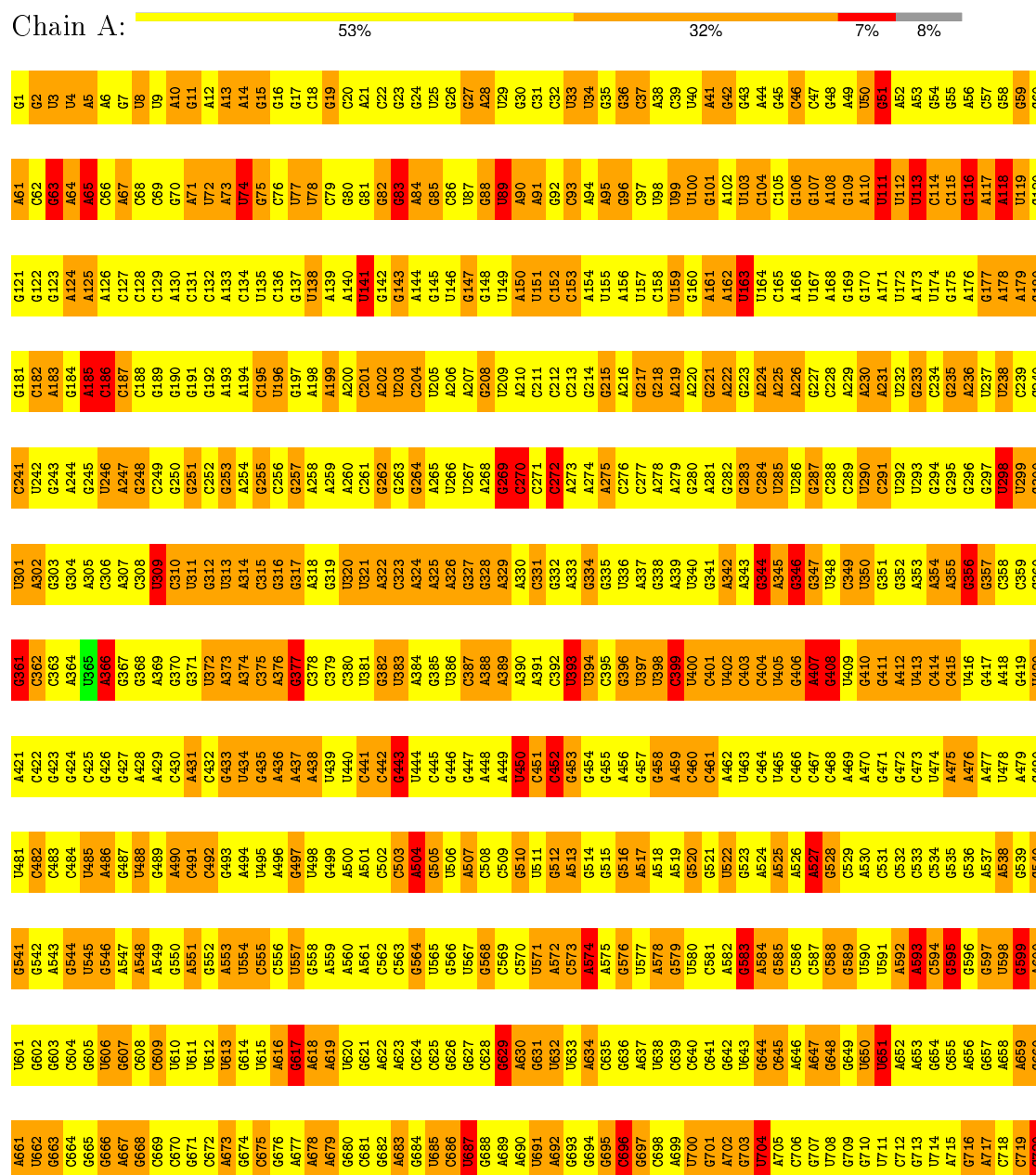
- Molecule 20 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | E     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1567  | 983 | 290 | 292 | 2 |         |       |

### 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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

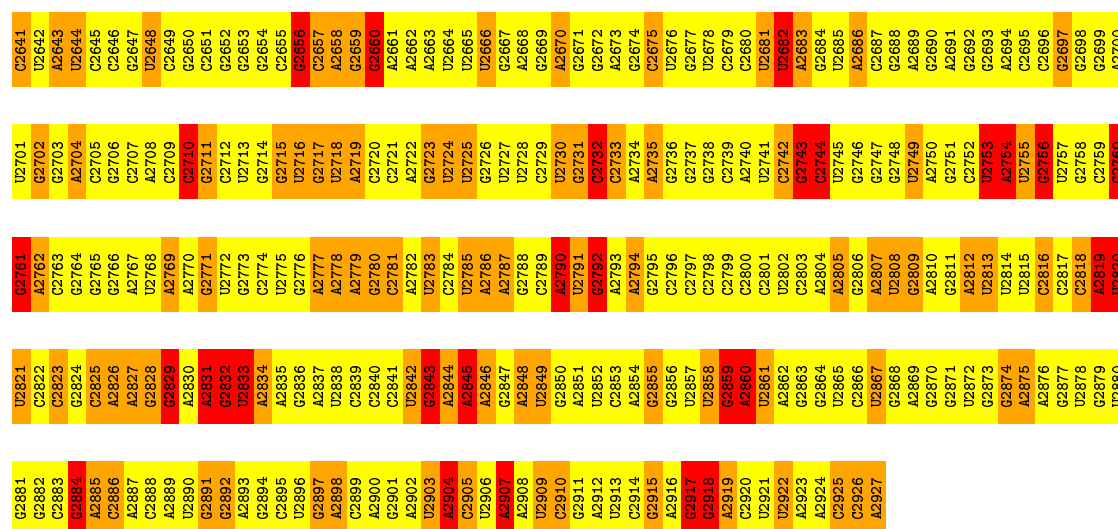
- Molecule 1: ribosome RNA 23S



|       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|
| G1621 | A1381 | U1501 | U1441 | G1381 | U1321 | G1261 | A1201 | A1141 | U1081 | A1021 | C961  | U901 | A841 | A781 | G721 |
| C1622 | A1382 | G1502 | A1442 | G1382 | G1322 | C1262 | A1202 | A1142 | G1082 | G1022 | C962  | G902 | C842 | A782 | A722 |
| C1623 | G1383 | G1503 | C1443 | G1383 | A1323 | C1263 | G1203 | A1143 | G1083 | G1023 | G963  | G903 | C843 | C783 | A723 |
| U1624 | C1384 | A1504 | C1444 | G1384 | G1324 | G1264 | C1204 | A1144 | A1084 | G1024 | A964  | A904 | U844 | C784 | A724 |
| C1625 | A1445 | A1505 | A1445 | G1385 | A1325 | A1265 | U1205 | G1145 | G1085 | A1025 | U965  | G905 | G845 | C785 | C725 |
| U1626 | G1386 | A1506 | C1446 | G1386 | A1326 | A1266 | G1206 | U1146 | U1086 | A1026 | U966  | G906 | G846 | C786 | C726 |
| A1627 | U1387 | U1507 | C1447 | G1387 | U1327 | G1267 | C1207 | U1147 | U1087 | A1027 | G967  | U907 | A847 | C787 | A727 |
| G1628 | C1388 | G1508 | U1448 | G1388 | C1328 | G1268 | G1208 | C1148 | G1088 | C1028 | C968  | A908 | G848 | C788 | G728 |
| A1629 | G1389 | C1509 | C1449 | G1389 | C1329 | A1269 | G1209 | A1149 | U1089 | A1029 | C969  | G909 | A849 | C789 | G729 |
| G1630 | U1390 | C1510 | C1450 | C1390 | C1330 | C1270 | A1210 | C1150 | U1090 | G1030 | A970  | A910 | U850 | U730 |      |
| A1631 | U1451 | U1511 | U1451 | C1391 | C1331 | C1271 | C1211 | U1151 | U1091 | G1031 | A971  | G911 | A851 | C731 | G731 |
| G1632 | G1512 | G1512 | A1452 | A1392 | U1332 | G1272 | U1212 | G1152 | A1092 | C1032 | U972  | G912 | G852 | G792 |      |
| G1633 | U1513 | U1513 | A1453 | A1393 | C1333 | G1273 | G1213 | G1153 | G1093 | C1033 | U973  | A913 | C853 | U793 |      |
| U1634 | C1514 | C1514 | C1454 | G1394 | C1334 | U1274 | U1214 | U1154 | A1094 | A1034 | A974  | C914 | U854 | U794 | C734 |
| A1635 | A1515 | A1515 | C1455 | C1395 | A1335 | G1275 | U1215 | C1155 | G1095 | G1035 | U975  | U915 | G855 | G795 | U735 |
| G1636 | G1516 | A1516 | A1456 | C1396 | C1336 | G1276 | A1216 | G1156 | A1096 | A1036 | U976  | G916 | G856 | A796 | A736 |
| A1637 | C1517 | U1517 | U1457 | G1397 | C1337 | A1277 | U1217 | A1157 | A1097 | C1037 | U977  | A917 | U857 | A797 | C737 |
| G1638 | G1518 | A1518 | U1458 | A1398 | G1338 | G1278 | U1218 | G1158 | C1098 | C1038 | A978  | U918 | U858 | A798 | C738 |
| A1639 | U1519 | G1519 | U1459 | G1399 | A1339 | C1279 | C1219 | U1159 | C1099 | G1039 | U979  | U919 | C859 | A799 | C739 |
| G1640 | A1520 | A1520 | G1460 | C1400 | A1340 | G1280 | G1220 | G1160 | A1100 | C1040 | C980  | G920 | U860 | G800 | A740 |
| U1641 | U1521 | A1521 | A1461 | C1401 | U1341 | C1281 | A1221 | A1161 | G1101 | C1041 | C981  | G921 | C861 | U801 | U741 |
| G1642 | U1522 | G1522 | G1462 | C1402 | G1342 | U1282 | A1222 | C1162 | G1102 | A1042 | U982  | A922 | U862 | G802 | G742 |
| A1643 | U1523 | C1463 | C1463 | G1403 | C1343 | U1283 | C1223 | U1163 | A1103 | G1043 | U983  | C923 | C863 | C743 | U743 |
| C1644 | U1524 | A1464 | A1464 | A1404 | C1344 | A1284 | A1224 | C1164 | U1104 | C1044 | G984  | U924 | C864 | G804 | C744 |
| A1645 | G1525 | A1465 | A1465 | A1405 | U1345 | G1285 | G1225 | U1165 | G1105 | U1045 | G985  | A925 | G865 | G805 | C745 |
| G1646 | G1526 | U1466 | U1466 | A1406 | A1346 | A1286 | U1226 | G1166 | U1106 | A1046 | G986  | G926 | A866 | G806 | A746 |
| U1647 | U1527 | G1467 | G1467 | G1407 | A1347 | A1287 | G1227 | C1167 | U1107 | A1047 | A987  | G927 | A867 | G807 | G747 |
| A1648 | U1528 | G1468 | G1468 | G1408 | G1348 | G1288 | G1228 | C1168 | G1108 | C1048 | A988  | G928 | A868 | A808 | G748 |
| G1649 | G1529 | G1469 | G1469 | C1409 | G1349 | U1289 | U1229 | C1169 | G1109 | C1049 | U989  | G929 | U869 | U809 | G749 |
| C1650 | G1530 | G1470 | G1470 | G1410 | U1350 | G1290 | A1230 | C1170 | A1110 | U1050 | C990  | G930 | A870 | G810 | U750 |
| G1651 | G1531 | G1471 | U1471 | U1411 | U1351 | A1291 | G1231 | G1171 | U1111 | C1051 | A991  | C931 | G871 | A811 | G751 |
| A1652 | A1532 | A1532 | G1472 | G1412 | C1352 | G1292 | G1232 | A1172 | U1112 | C1052 | G992  | C932 | C872 | G812 | A752 |
| G1653 | U1533 | G1413 | C1353 | C1353 | U1353 | A1293 | A1233 | A1173 | A1113 | C1053 | A993  | C933 | C873 | G813 | A753 |
| A1654 | A1534 | C1474 | C1354 | C1354 | C1354 | U1294 | A1234 | A1174 | G1114 | A1054 | U994  | U934 | U874 | U814 | G754 |
| A1655 | U1535 | G1475 | U1355 | G1415 | U1355 | U1295 | A1235 | A1175 | A1115 | A1055 | U995  | A935 | U875 | U815 | U755 |
| U1656 | A1536 | C1476 | G1356 | G1416 | G1356 | G1296 | G1236 | U1176 | A1116 | A1056 | G996  | C936 | A876 | U816 | U756 |
| C1657 | G1537 | A1477 | A1357 | A1417 | A1357 | G1297 | C1237 | G1177 | G1117 | G1057 | C997  | G937 | G877 | G817 | C757 |
| G1658 | G1538 | U1418 | G1358 | U1418 | G1358 | C1298 | G1238 | U1178 | C1118 | U1058 | G998  | G938 | G878 | G818 | A758 |
| U1659 | C1539 | G1479 | G1359 | G1419 | G1359 | G1299 | U1239 | A1179 | A1119 | C1059 | A999  | G939 | G879 | G819 | G759 |
| G1660 | A1540 | A1480 | A1360 | G1420 | A1360 | G1300 | U1240 | C1180 | G1120 | U1060 | C999  | G940 | C880 | U820 | G760 |
| A1661 | A1541 | G1481 | A1361 | A1421 | A1361 | U1301 | C1241 | C1181 | C1121 | A1061 | U1001 | U941 | U881 | A821 | A761 |
| C1662 | A1542 | G1482 | G1362 | C1422 | G1362 | A1302 | U1242 | G1182 | C1122 | C1062 | G1002 | U942 | A882 | G822 | A762 |
| A1663 | U1543 | A1483 | G1363 | A1423 | G1363 | U1303 | A1243 | G1183 | A1123 | G1063 | A1003 | A943 | G883 | G823 | A763 |
| G1664 | G1544 | A1484 | C1364 | A1424 | C1364 | G1304 | A1244 | G1184 | C1124 | U1064 | C944  | C944 | C884 | G824 | C764 |
| C1665 | C1545 | A1485 | U1365 | C1425 | U1365 | A1305 | G1245 | G1185 | C1125 | U1065 | A1005 | C945 | C885 | G825 | A765 |
| A1666 | G1546 | G1486 | C1366 | A1426 | C1366 | G1306 | G1246 | C1186 | A1126 | A1066 | U886  | G946 | U886 | U826 | C766 |
| U1667 | U1547 | G1487 | G1367 | G1427 | G1367 | U1307 | G1247 | U1187 | U1127 | A1067 | C947  | A947 | C887 | U767 |      |
| G1668 | U1548 | G1488 | U1368 | G1428 | U1368 | A1308 | C1248 | A1188 | U1128 | G1068 | A1008 | A948 | A888 | A828 | G768 |
| C1669 | U1549 | U1489 | C1369 | U1429 | C1369 | G1309 | U1249 | A1189 | U1129 | U1069 | U1009 | U949 | A889 | A829 | A769 |
| U1670 | C1550 | A1490 | C1370 | U1430 | C1370 | C1310 | G1250 | A1190 | A1130 | G1070 | C1010 | U950 | G890 | A830 | A770 |
| G1671 | C1551 | A1491 | G1371 | G1431 | G1371 | G1311 | U1251 | C1191 | A1131 | G1071 | C1011 | C951 | G891 | U831 | U771 |
| A1672 | A1552 | A1492 | C1372 | A1432 | C1372 | A1312 | G1252 | G1192 | A1132 | A1072 | G1012 | A952 | U892 | G832 | G772 |
| G1673 | U1553 | U1433 | U1373 | A1433 | C1373 | A1313 | A1253 | U1193 | G1133 | A1073 | U1013 | G953 | A893 | C833 | G773 |
| C1674 | A1554 | G1494 | C1374 | A1434 | C1374 | A1314 | A1254 | A1194 | A1134 | A1074 | A1014 | U954 | A894 | C834 | A774 |
| A1675 | G1555 | C1495 | U1435 | A1435 | A1375 | G1315 | G1255 | U1195 | G1135 | A1075 | G1015 | C955 | G895 | A835 | G775 |
| G1676 | A1556 | U1436 | G1376 | U1436 | A1376 | A1316 | C1256 | C1196 | U1136 | G1076 | U1016 | A956 | A896 | A836 | G776 |
| A1677 | G1557 | C1437 | G1377 | C1437 | G1377 | G1317 | C1257 | A1197 | G1137 | G1077 | C1017 | A957 | G897 | U837 | C777 |
| G1678 | U1558 | C1438 | U1378 | G1438 | G1378 | G1318 | A1258 | C1198 | C1138 | A1078 | G1018 | A958 | U898 | C838 | C778 |
| A1679 | U1559 | U1439 | G1379 | U1439 | G1379 | G1319 | G1259 | C1199 | C1139 | U1079 | A1019 | C959 | C899 | G779 |      |
| A1680 | U1560 | G1440 | U1380 | G1440 | U1380 | G1320 | A1260 | G1200 | U1140 | G1080 | A1020 | U960 | U900 | A840 | G780 |



|       |       |       |       |   |   |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|---|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U2581 | U2521 | A2461 | G     | U | G | C2221 | G2161 | G2101 | G2041 | A     | C     | C1861 | G1801 | G1741 | U1681 |
| G2582 | U2522 | A2462 | A     | C | G | C2222 | G2162 | C2102 | A2042 | A     | C     | C1862 | A1802 | G1742 | C1682 |
| U2583 | G2523 | A2463 | C     | A | C | U2223 | A2163 | C2103 | A2043 | U     | C     | C1863 | A1803 | A1743 | C1683 |
| U2584 | U2524 | A2464 | G     | U | G | U2224 | A2164 | U2104 | A2044 | G     | C     | G1864 | U1804 | G1744 | U1684 |
| C2585 | G2525 | A2465 | A     | U | U | C2225 | A2165 | U2105 | U2045 | U     | A     | C1865 | G1805 | A1745 | A1685 |
| C2586 | G2526 | A2466 | A     | C | U | U2226 | C2166 | A2106 | U2046 | C     | G     | C     | U1806 | A1746 | A1686 |
| C2587 | G2527 | U2467 | A     | G | G | A2227 | G2167 | C2107 | A2047 | C     | U     | C     | U1807 | G1747 | G1687 |
| C2588 | C2528 | A2468 | G     | C | C | A2228 | G2168 | U2108 | U2048 | G     | A     | G     | U1808 | G1748 | G1688 |
| C2589 | U2529 | A2469 | U     | A | C | C2229 | G2169 | G2109 | A2049 | A     | A     | G     | A1809 | G1749 | U1689 |
| U2590 | C2530 | C2470 | C     | G | A | C2230 | A2170 | C2110 | G2050 | C     | A     | U     | C1810 | G1750 | G1690 |
| U2591 | G2531 | C2471 | G     | A | U | C2231 | G2171 | A2111 | U2051 | C     | C     | U     | C1811 | G1751 | A1691 |
| C2592 | A2532 | C2472 | G     | U | C | G2232 | C2172 | G2112 | A2052 | C     | G     | G     | A1812 | G1752 | U1692 |
| C2593 | G2533 | G2473 | G     | U | C | C2233 | G2173 | C2113 | C2053 | G     | C     | U     | A1813 | C1753 | C1693 |
| A2594 | G2534 | C     | C     | G | U | C2234 | C2174 | C2114 | C2054 | C     | C     | G     | A1814 | U1754 | G1694 |
| A2595 | U2535 | G2475 | U     | A | A | G2235 | C2175 | U2115 | U2055 | A     | A     | G     | A1815 | C1755 | A1695 |
| A2596 | G2536 | G2476 | U     | A | A | G2236 | A2176 | G2116 | G2056 | C     | G1936 | G     | A1816 | U1756 | G1696 |
| C2597 | G2537 | A2477 | A     | A | A | C2237 | G2177 | A2117 | U2057 | G1997 | C1937 | G     | C1817 | G1757 | A1697 |
| C2598 | U2538 | U2478 | A     | A | A | C2238 | C2178 | U2118 | G2058 | A1998 | C1938 | G     | A1818 | U1758 | G1698 |
| C2599 | G2539 | A2479 | G     | G | G | U2239 | U2179 | A2119 | A2059 | A1999 | G1939 | G     | C1819 | U1759 | A1699 |
| U2600 | U2540 | C2480 | U2419 | G | G | U2240 | U2180 | U2120 | A2060 | A2000 | U1940 | U     | A1820 | A1760 | A1700 |
| C2601 | C2481 | A2420 | A2421 | C | U | A2241 | U2181 | U2121 | G2061 | G2001 | A1941 | U     | G1821 | G1761 | C1701 |
| C2602 | A2542 | U2422 | A2422 | A | A | U2242 | G2182 | G2122 | A2062 | G2002 | A1942 | A     | U1822 | G1762 | U1702 |
| G2603 | U2543 | G2483 | C2423 | C | A | C2243 | G2183 | A2123 | U2063 | C2003 | C1943 | A     | U1823 | G1763 | C1703 |
| C2604 | C2544 | G2484 | C2424 | A | C | G2244 | U2184 | A2124 | G2064 | G2004 | U1944 | G     | A1824 | U1764 | U1704 |
| C2605 | G2545 | C2485 | G2425 | A | G | G2245 | G2185 | U2125 | C2065 | C2005 | A1945 | A     | U1825 | G1765 | C1705 |
| A2606 | C2546 | U2486 | G2426 | G | G | G2246 | G2186 | G2126 | A2066 | A2006 | U1946 | G     | C1826 | C1766 | G1706 |
| G2607 | A2547 | U2487 | U2427 | G | A | C2247 | A2187 | U2127 | G2067 | A2007 | A1947 | G     | U1827 | A1767 | U1707 |
| C2608 | U2548 | G2488 | G2428 | G | G | G2248 | G2188 | U2128 | G2068 | C2008 | A1948 | A     | G1828 | A1768 | U1708 |
| U2609 | C2549 | U2489 | G2429 | A | G | U2249 | G2189 | G2129 | U2069 | G2009 | C1949 | G     | C1829 | G1769 | A1709 |
| G2610 | C2550 | C2490 | U2430 | G | C | G2250 | C2190 | G2130 | U2070 | A2010 | G1950 | C     | G1830 | C1770 | A1710 |
| C2611 | U2551 | U2491 | U2431 | C | G | G2251 | A2191 | U2131 | A2071 | U2011 | G1951 | G     | A1831 | C1771 | G1711 |
| G2612 | G2552 | C2492 | C2432 | U | U | A2252 | U2192 | A2132 | C2072 | C2012 | U1952 | C     | A1832 | C1772 | G1712 |
| G2613 | G2553 | C2493 | C2433 | U | C | C2253 | C2193 | C2133 | C2073 | U2013 | C1953 | C     | G1833 | G1773 | A1713 |
| U2614 | G2554 | C2494 | G2434 | G | C | A2254 | G2194 | A2134 | C2074 | G2014 | C1954 | U     | C1834 | A1774 | A1714 |
| C2615 | C2555 | C2495 | C2435 | A | A | C2255 | G2195 | G2135 | G2075 | G2015 | U1955 | A     | C1835 | G1775 | C1715 |
| A2616 | C2556 | A2496 | A2436 | C | A | A2256 | U2196 | C2136 | C2076 | G2016 | A1956 | G     | G1836 | A1776 | U1716 |
| G2617 | U2557 | C2497 | U2437 | U | A | G2257 | G2197 | U2137 | G2077 | C2017 | A1957 | C     | U1837 | G1777 | C1717 |
| A2618 | G2558 | A2498 | G2438 | G | G | U2258 | G2198 | U2138 | A2078 | A2018 | G1958 | G     | A1838 | A1778 | G1718 |
| A2619 | U2559 | G2499 | G2439 | C | G | G2259 | G2199 | G2139 | C2079 | C2019 | G1959 | U     | A1839 | G1779 | G1719 |
| C2620 | A2560 | A2500 | A2440 | G | U | U2260 | A2200 | U2140 | A2080 | U2020 | U1960 | A     | G1840 | C1780 | G1720 |
| G2621 | G2561 | C2501 | A2441 | A | U | C2261 | U2201 | A2141 | G2081 | G2021 | A1961 | A     | G1841 | C1781 | A1721 |
| U2622 | U2562 | U2502 | G2442 | G | C | A2262 | A2202 | C2142 | G2082 | U2022 | G1962 | G     | C1842 | G1782 | A1722 |
| C2623 | C2563 | C2503 | G2443 | C | C | G2263 | C2203 | A2143 | A2083 | C2023 | C1963 | C     | G1843 | C1783 | A1723 |
| G2624 | A2564 | C2504 | G2444 | C | C | G2264 | U2204 | G2144 | G2084 | U2024 | G     | G     | A1844 | A1784 | A1724 |
| U2625 | G2565 | A2505 | C2445 | C | U | U2265 | A2205 | G2145 | G2085 | C2025 | A     | A     | A1845 | G1785 | U1725 |
| G2626 | U2566 | C2506 | C2446 | U | C | G2266 | C2206 | A2146 | G2086 | A2026 | A     | A     | G1846 | U1786 | G1726 |
| A2627 | C2567 | A2507 | U2447 | A | A | G2267 | C2207 | U2147 | A2087 | A2027 | A     | G     | U1847 | G1787 | A1727 |
| G2628 | C2568 | U2508 | U2448 | C | G | G2268 | C2208 | A2148 | A2088 | C2028 | U     | U     | A1848 | A1788 | C1728 |
| A2629 | C2569 | C2509 | C2449 | A | A | C2269 | U2209 | G2149 | A2089 | G2029 | U     | G     | U1849 | A1789 | C1729 |
| C2630 | A2570 | G2510 | G2450 | G | A | A2270 | G2210 | G2150 | G2090 | A2030 | C     | G     | A1850 | U1790 | G1730 |
| A2631 | G2571 | A2511 | C2451 | G | U | G2271 | G2211 | U2151 | A2091 | G2031 | C     | C     | G1851 | A1791 | C1731 |
| G2632 | G2572 | U2512 | U2452 | U | G | U2272 | C2212 | A2152 | C2092 | U2032 | U     | G     | G1852 | G1792 | G1732 |
| C2633 | U2573 | G2513 | C2453 | C | U | U2273 | G2213 | G2153 | C2093 | G2033 | U     | A     | G1853 | G1793 | U1733 |
| U2634 | G2574 | G2514 | A2454 | G | U | U2274 | G2214 | G2154 | C2094 | A2034 | G     | A     | G1854 | A1794 | A1734 |
| C2635 | U2575 | G2515 | A2455 | G | U | G2275 | U2215 | A2155 | C2095 | C2035 | U     | U     | C1855 | C1795 | A1735 |
| C2636 | U2576 | G2516 | C2456 | G | U | A     | A2216 | G2156 | G2096 | U2036 | C     | U     | U1856 | G1796 | C1736 |
| G2637 | G2577 | A2517 | G2457 | C | G | C     | U2217 | C2157 | U2097 | C2037 | G     | G     | G1857 | A1797 | U1737 |
| U2638 | C2578 | G2518 | G2458 | A | A | U     | U2218 | C2158 | G2098 | G2038 | G     | A     | A1858 | G1798 | U1738 |
| C2639 | G2579 | G2519 | A2459 | G | A | G     | G2219 | U2159 | G2099 | G2039 | G     | A     | G1799 | G1799 | C1739 |
| C2640 | C2580 | U2520 | U2460 | G | A | G     | A2220 | U2160 | A2100 | U2040 | U     | G     | G1860 | C1800 | G1740 |



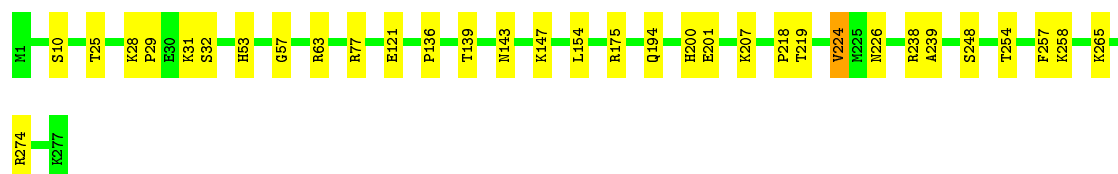
- Molecule 2: 50S ribosomal protein L32

Chain 0: 83% 10% 7%



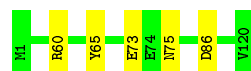
- Molecule 3: 50S ribosomal protein L2

Chain C: 88% 12%



- Molecule 4: 50S ribosomal protein L17

Chain N: 96% 0% 0%



- Molecule 5: 50S ribosomal protein L6

Chain G: 84% 7% 9%



- Molecule 6: 50S ribosomal protein L13

Chain J: 87% 10% 0%



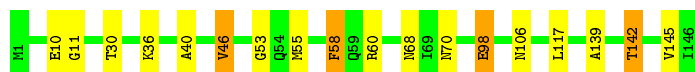
- Molecule 7: 50S ribosomal protein L14

Chain K: 93% 7%



- Molecule 8: 50S ribosomal protein L15

Chain L: 88% 10%



- Molecule 9: 50S ribosomal protein L19

Chain P: 72% 23%



- Molecule 10: 50S ribosomal protein L20

Chain Q: 91% 8%



- Molecule 11: 50S ribosomal protein L3

Chain D: 91% 6%



- Molecule 12: 50S ribosomal protein L21

Chain R: 88% 11%

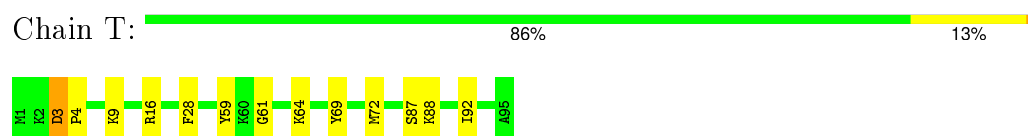


- Molecule 13: 50S ribosomal protein L22

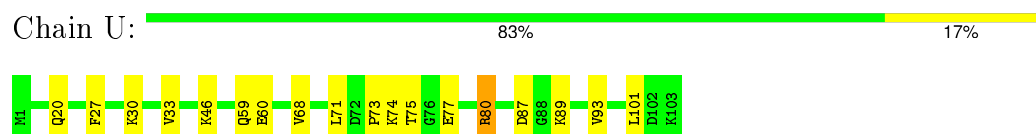
Chain S: 92% 6%



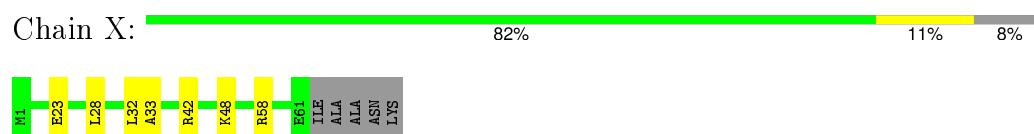
- Molecule 14: 50S ribosomal protein L23



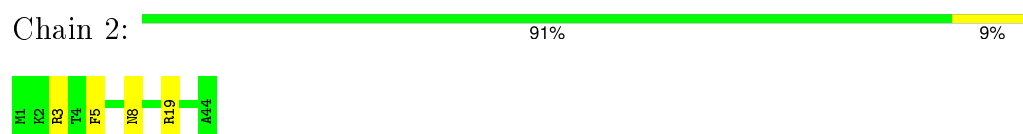
- Molecule 15: 50S ribosomal protein L24



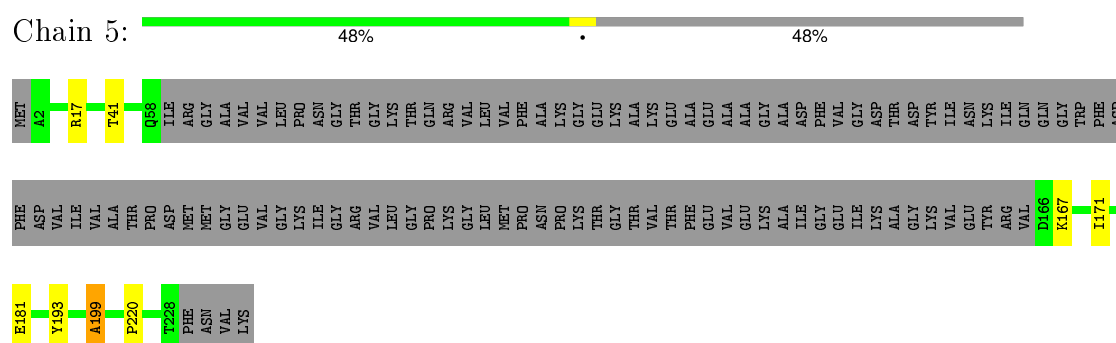
- Molecule 16: 50S ribosomal protein L29



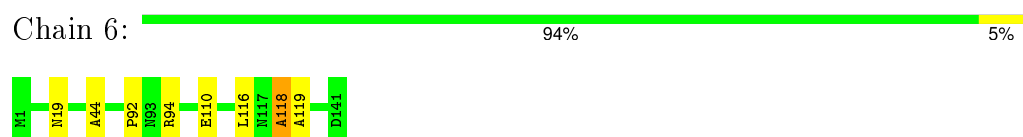
- Molecule 17: 50S ribosomal protein L34



- Molecule 18: 50S ribosomal protein L1



- Molecule 19: 50S ribosomal protein L11



- Molecule 20: 50S ribosomal protein L4





## 4 Experimental information

| Property                             | Value   | Source    |
|--------------------------------------|---|-----------|
| Reconstruction method                | SINGLE PARTICLE   | Depositor |
| Imposed symmetry                     | POINT, Not provided   | Depositor |
| Number of images                     | 27652   | Depositor |
| Resolution determination method      | SSNR-MAP(an optimized approach of Spectral Single-to Noise Ratio) at 1.0 cutoff | Depositor |
| CTF correction method                | Each particle   | Depositor |
| Microscope                           | FEI TITAN KRIOS   | Depositor |
| Voltage (kV)                         | 300   | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20  | Depositor |
| Minimum defocus (nm)                 | 1000  | Depositor |
| Maximum defocus (nm)                 | 4000  | Depositor |
| Magnification                        | 59000   | Depositor |
| Image detector                       | FEI Eagle 4K*4K CCD   | Depositor |

## 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  > 2$     | RMSZ        | # $ Z  > 2$        |
| 1   | A     | 1.68         | 83/64560 (0.1%) | 2.67        | 8132/100715 (8.1%) |
| 10  | Q     | 1.05         | 0/952           | 1.06        | 2/1266 (0.2%)      |
| 11  | D     | 0.96         | 0/1590          | 1.09        | 2/2130 (0.1%)      |
| 12  | R     | 0.92         | 0/806           | 1.13        | 1/1080 (0.1%)      |
| 13  | S     | 1.01         | 0/877           | 1.10        | 0/1179             |
| 14  | T     | 1.01         | 0/774           | 1.15        | 2/1030 (0.2%)      |
| 15  | U     | 0.87         | 0/790           | 1.16        | 3/1054 (0.3%)      |
| 16  | X     | 1.04         | 0/505           | 1.01        | 0/671              |
| 17  | 2     | 1.26         | 0/371           | 1.04        | 0/483              |
| 18  | 5     | 0.87         | 0/921           | 1.05        | 2/1239 (0.2%)      |
| 19  | 6     | 0.92         | 0/1058          | 1.06        | 1/1427 (0.1%)      |
| 2   | 0     | 1.04         | 0/440           | 1.20        | 2/584 (0.3%)       |
| 20  | E     | 0.97         | 0/1586          | 1.10        | 1/2139 (0.0%)      |
| 3   | C     | 1.00         | 0/2166          | 1.09        | 0/2902             |
| 4   | N     | 1.09         | 0/969           | 1.05        | 0/1294             |
| 5   | G     | 0.97         | 0/1264          | 1.04        | 0/1709             |
| 6   | J     | 0.95         | 0/1157          | 1.08        | 2/1557 (0.1%)      |
| 7   | K     | 1.02         | 0/928           | 1.05        | 0/1245             |
| 8   | L     | 0.97         | 0/1094          | 1.10        | 2/1457 (0.1%)      |
| 9   | P     | 1.10         | 0/929           | 1.17        | 2/1243 (0.2%)      |
| All | All   | 1.55         | 83/83737 (0.1%) | 2.43        | 8154/126404 (6.5%) |

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                   | 320                 |
| 14  | T     | 0                   | 2                   |
| 15  | U     | 0                   | 1                   |
| 20  | E     | 0                   | 2                   |
| 4   | N     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 8   | L     | 0                   | 2                   |
| 9   | P     | 0                   | 2                   |
| All | All   | 0                   | 330                 |

The worst 5 of 83 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1339 | A    | O3'-P | -7.12 | 1.52        | 1.61     |
| 1   | A     | 1831 | A    | N7-C5 | -6.74 | 1.35        | 1.39     |
| 1   | A     | 52   | A    | N7-C5 | -6.72 | 1.35        | 1.39     |
| 1   | A     | 653  | A    | N7-C5 | -6.68 | 1.35        | 1.39     |
| 1   | A     | 1839 | A    | N7-C5 | -6.64 | 1.35        | 1.39     |

The worst 5 of 8154 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 1339 | A    | P-O3'-C3' | 34.26 | 160.81      | 119.70   |
| 1   | A     | 313  | U    | P-O3'-C3' | 20.76 | 144.62      | 119.70   |
| 1   | A     | 178  | A    | P-O3'-C3' | 20.05 | 143.75      | 119.70   |
| 1   | A     | 74   | U    | P-O3'-C3' | 19.98 | 143.68      | 119.70   |
| 1   | A     | 375  | C    | P-O3'-C3' | 19.92 | 143.60      | 119.70   |

There are no chirality outliers.

5 of 330 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 15  | G    | Sidechain |
| 1   | A     | 27  | G    | Sidechain |
| 1   | A     | 28  | A    | Sidechain |
| 1   | A     | 33  | U    | Sidechain |
| 1   | A     | 5   | A    | Sidechain |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 57639 | 0        | 29016    | 104     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 0     | 433   | 0        | 454      | 0       | 0            |
| 3   | C     | 2129  | 0        | 2225     | 4       | 0            |
| 4   | N     | 962   | 0        | 995      | 0       | 0            |
| 5   | G     | 1246  | 0        | 1273     | 2       | 0            |
| 6   | J     | 1134  | 0        | 1178     | 0       | 0            |
| 7   | K     | 921   | 0        | 977      | 0       | 0            |
| 8   | L     | 1082  | 0        | 1132     | 0       | 0            |
| 9   | P     | 916   | 0        | 987      | 5       | 0            |
| 10  | Q     | 940   | 0        | 1005     | 0       | 0            |
| 11  | D     | 1568  | 0        | 1635     | 0       | 0            |
| 12  | R     | 795   | 0        | 838      | 0       | 0            |
| 13  | S     | 868   | 0        | 930      | 0       | 0            |
| 14  | T     | 767   | 0        | 813      | 2       | 0            |
| 15  | U     | 780   | 0        | 838      | 0       | 0            |
| 16  | X     | 504   | 0        | 541      | 1       | 0            |
| 17  | 2     | 368   | 0        | 410      | 1       | 0            |
| 18  | 5     | 910   | 0        | 944      | 0       | 0            |
| 19  | 6     | 1044  | 0        | 1098     | 1       | 0            |
| 20  | E     | 1567  | 0        | 1652     | 1       | 0            |
| All | All   | 76573 | 0        | 48941    | 116     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1        | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------|--------------------------|-------------------|
| 1:A:1245:G:H1 | 1:A:1281:C:H41 | 1.25                     | 0.84              |
| 1:A:898:U:H3  | 1:A:973:G:H1   | 1.41                     | 0.68              |
| 1:A:2557:U:H3 | 1:A:2564:A:H61 | 1.41                     | 0.68              |
| 1:A:1799:G:H1 | 1:A:2011:U:H3  | 1.46                     | 0.63              |
| 1:A:2543:U:H3 | 1:A:2599:G:H1  | 1.48                     | 0.62              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2   | 0     | 53/59 (90%)     | 43 (81%)   | 6 (11%)   | 4 (8%)   | 1           | 21 |
| 3   | C     | 275/277 (99%)   | 217 (79%)  | 40 (14%)  | 18 (6%)  | 1           | 25 |
| 4   | N     | 118/120 (98%)   | 101 (86%)  | 14 (12%)  | 3 (2%)   | 7           | 46 |
| 5   | G     | 161/179 (90%)   | 148 (92%)  | 7 (4%)    | 6 (4%)   | 4           | 38 |
| 6   | J     | 141/145 (97%)   | 124 (88%)  | 9 (6%)    | 8 (6%)   | 2           | 28 |
| 7   | K     | 120/122 (98%)   | 106 (88%)  | 9 (8%)    | 5 (4%)   | 3           | 34 |
| 8   | L     | 144/146 (99%)   | 100 (69%)  | 30 (21%)  | 14 (10%) | 1           | 14 |
| 9   | P     | 110/115 (96%)   | 76 (69%)   | 20 (18%)  | 14 (13%) | 0           | 8  |
| 10  | Q     | 115/119 (97%)   | 101 (88%)  | 9 (8%)    | 5 (4%)   | 3           | 34 |
| 11  | D     | 204/209 (98%)   | 175 (86%)  | 21 (10%)  | 8 (4%)   | 4           | 36 |
| 12  | R     | 100/102 (98%)   | 79 (79%)   | 15 (15%)  | 6 (6%)   | 2           | 26 |
| 13  | S     | 110/113 (97%)   | 97 (88%)   | 10 (9%)   | 3 (3%)   | 6           | 45 |
| 14  | T     | 93/95 (98%)     | 77 (83%)   | 11 (12%)  | 5 (5%)   | 2           | 29 |
| 15  | U     | 101/103 (98%)   | 70 (69%)   | 20 (20%)  | 11 (11%) | 0           | 11 |
| 16  | X     | 59/66 (89%)     | 55 (93%)   | 2 (3%)    | 2 (3%)   | 5           | 40 |
| 17  | 2     | 42/44 (96%)     | 37 (88%)   | 4 (10%)   | 1 (2%)   | 7           | 47 |
| 18  | 5     | 116/232 (50%)   | 97 (84%)   | 13 (11%)  | 6 (5%)   | 2           | 30 |
| 19  | 6     | 139/141 (99%)   | 117 (84%)  | 17 (12%)  | 5 (4%)   | 4           | 38 |
| 20  | E     | 204/207 (99%)   | 161 (79%)  | 25 (12%)  | 18 (9%)  | 1           | 17 |
| All | All   | 2405/2594 (93%) | 1981 (82%) | 282 (12%) | 142 (6%) | 4           | 27 |

5 of 142 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 0     | 19  | HIS  |
| 3   | C     | 219 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | K     | 30  | ARG  |
| 7   | K     | 73  | ASP  |
| 8   | L     | 117 | LEU  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | 0     | 49/53 (92%)     | 48 (98%)   | 1 (2%)   | 63          | 85 |
| 3   | C     | 225/225 (100%)  | 215 (96%)  | 10 (4%)  | 35          | 69 |
| 4   | N     | 100/100 (100%)  | 99 (99%)   | 1 (1%)   | 82          | 92 |
| 5   | G     | 138/151 (91%)   | 135 (98%)  | 3 (2%)   | 60          | 83 |
| 6   | J     | 122/123 (99%)   | 111 (91%)  | 11 (9%)  | 12          | 44 |
| 7   | K     | 101/101 (100%)  | 98 (97%)   | 3 (3%)   | 48          | 77 |
| 8   | L     | 110/110 (100%)  | 105 (96%)  | 5 (4%)   | 34          | 69 |
| 9   | P     | 97/100 (97%)    | 90 (93%)   | 7 (7%)   | 18          | 55 |
| 10  | Q     | 96/98 (98%)     | 93 (97%)   | 3 (3%)   | 47          | 77 |
| 11  | D     | 167/170 (98%)   | 159 (95%)  | 8 (5%)   | 31          | 67 |
| 12  | R     | 84/84 (100%)    | 78 (93%)   | 6 (7%)   | 18          | 55 |
| 13  | S     | 93/93 (100%)    | 87 (94%)   | 6 (6%)   | 21          | 58 |
| 14  | T     | 85/85 (100%)    | 82 (96%)   | 3 (4%)   | 43          | 74 |
| 15  | U     | 87/87 (100%)    | 82 (94%)   | 5 (6%)   | 25          | 62 |
| 16  | X     | 54/57 (95%)     | 50 (93%)   | 4 (7%)   | 17          | 54 |
| 17  | 2     | 39/39 (100%)    | 37 (95%)   | 2 (5%)   | 29          | 66 |
| 18  | 5     | 98/185 (53%)    | 97 (99%)   | 1 (1%)   | 82          | 92 |
| 19  | 6     | 110/110 (100%)  | 109 (99%)  | 1 (1%)   | 84          | 93 |
| 20  | E     | 169/170 (99%)   | 162 (96%)  | 7 (4%)   | 37          | 71 |
| All | All   | 2024/2141 (94%) | 1937 (96%) | 87 (4%)  | 40          | 70 |

5 of 87 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | P     | 74  | PHE  |
| 11  | D     | 130 | ARG  |
| 20  | E     | 29  | ASN  |
| 9   | P     | 83  | LYS  |
| 11  | D     | 19  | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | R     | 90  | GLN  |
| 13  | S     | 57  | ASN  |
| 18  | 5     | 172 | HIS  |
| 10  | Q     | 38  | GLN  |
| 19  | 6     | 34  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 2681/2927 (91%) | 823 (30%)         | 200 (7%)        |

5 of 823 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | G    |
| 1   | A     | 3   | U    |
| 1   | A     | 4   | U    |
| 1   | A     | 8   | U    |
| 1   | A     | 10  | A    |

5 of 200 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1313 | A    |
| 1   | A     | 1497 | G    |
| 1   | A     | 2807 | A    |
| 1   | A     | 1340 | A    |
| 1   | A     | 1448 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.