



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:49 PM BST

PDB ID : 3J2H
EMDB ID: : EMD-5510
Title : Dissecting the in vivo assembly of the 30S ribosomal subunit reveals the role of RimM
Authors : Guo, Q.; Goto, S.; Chen, Y.; Muto, A.; Himeno, H.; Deng, H.; Lei, J.; Gao, N.
Deposited on : 2012-09-28
Resolution : 18.80 Å(reported)
Based on PDB ID : 3OFA

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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

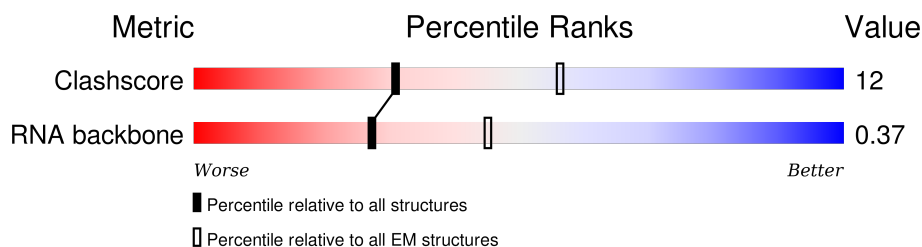
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 18.80 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|--------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| 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 ≥ 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 | N | 1533 |  17% 38% 45% |

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 49446 atoms, of which 16554 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.

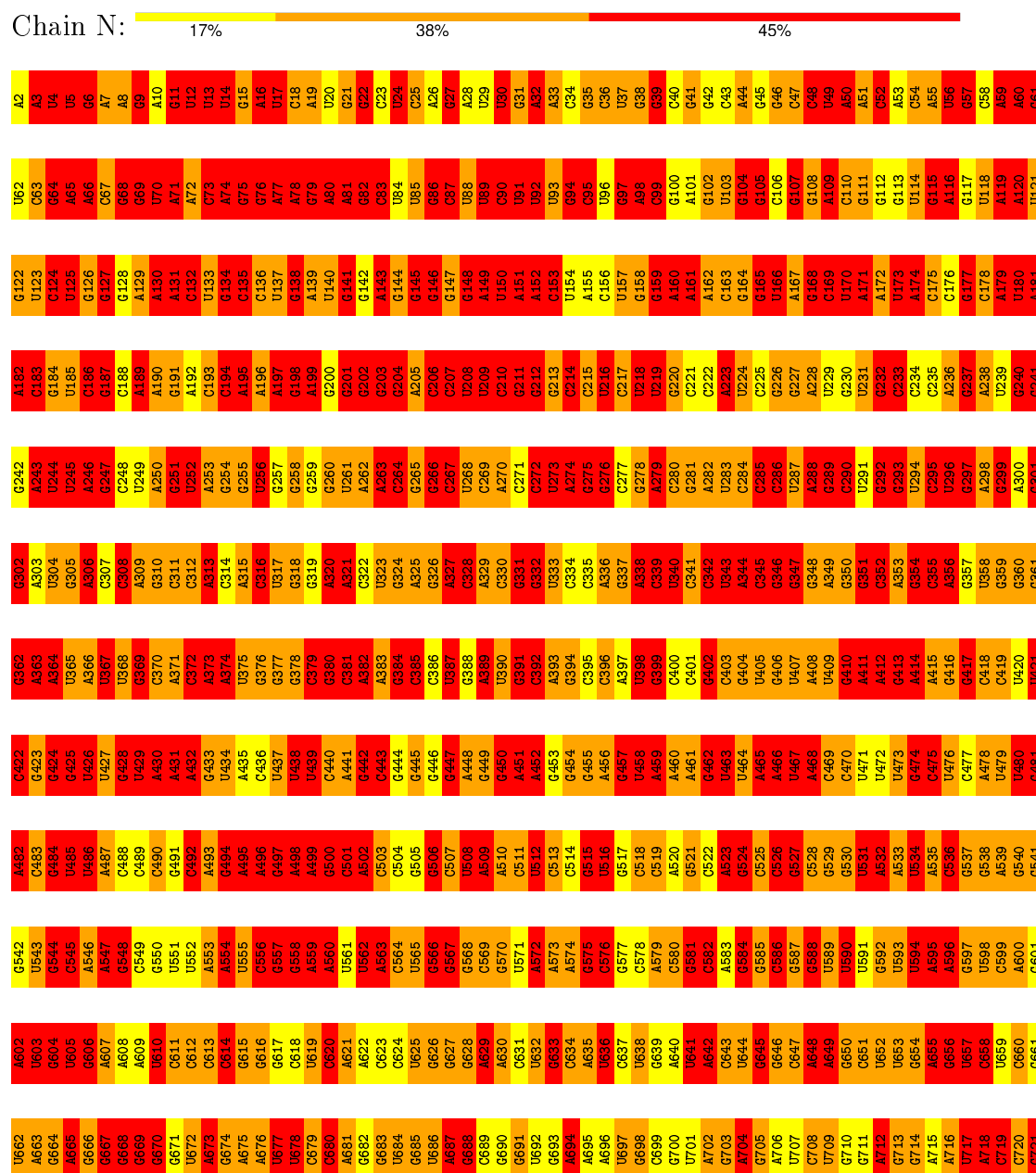
- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|-------|------|---------|-------|
| 1 | N | 1533 | Total | C | H | N | O | P | 0 | 0 |
| | | | 49446 | 14671 | 16554 | 6036 | 10653 | 1532 | | |

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: 16S rRNA



| | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|
| A1502 | G1442 | C1382 | G1322 | C1262 | U1202 | G1142 | A1082 | A1022 | C982 | G902 | U842 | A782 | G722 |
| A1503 | C1443 | C1383 | G1323 | C1263 | C1203 | G1143 | U1083 | U1023 | G963 | G903 | U843 | C782 | U723 |
| G1504 | U1444 | C1384 | A1324 | C1264 | G1204 | G1144 | U1084 | G1024 | A964 | U904 | U844 | A784 | G724 |
| G1505 | U1445 | G1385 | C1325 | C1265 | U1205 | A1145 | U1085 | U1025 | U965 | U905 | A845 | G785 | G725 |
| A1506 | A1446 | G1386 | U1326 | C1266 | G1206 | C1146 | U1086 | G1026 | G966 | A906 | G846 | G786 | G726 |
| A1507 | A1447 | G1387 | C1327 | C1267 | G1207 | C1147 | G1087 | G1027 | G967 | A907 | G847 | A787 | G727 |
| A1508 | C1448 | C1388 | C1328 | C1268 | C1208 | U1148 | G1088 | C1028 | A968 | A908 | C848 | U788 | A728 |
| C1509 | C1449 | C1389 | A1329 | A1269 | C1209 | C1149 | G1089 | U1029 | A969 | A909 | C849 | U789 | A729 |
| U1510 | U1450 | U1390 | U1330 | G1270 | C1210 | A1150 | U1090 | U1030 | C970 | C910 | U850 | A790 | G730 |
| G1511 | U1451 | G1391 | G1331 | A1271 | U1211 | A1151 | U1091 | C1031 | G971 | U911 | G851 | G791 | C731 |
| A1512 | C1452 | G1392 | A1332 | C1272 | U1212 | A1152 | A1092 | G1032 | C972 | C912 | G852 | A792 | C732 |
| A1513 | G1453 | U1393 | A1333 | C1273 | C1213 | G1153 | A1093 | G1033 | G973 | A913 | C853 | U793 | G733 |
| G1514 | G1454 | A1394 | G1334 | A1274 | C1214 | G1154 | G1094 | G1034 | A974 | A914 | U854 | G794 | G734 |
| G1515 | G1455 | C1395 | U1335 | A1275 | G1215 | A1155 | U1095 | A1035 | A975 | A915 | U855 | C795 | C735 |
| G1516 | A1456 | A1396 | G1336 | G1276 | C1216 | G1156 | C1096 | A1036 | A976 | U916 | C856 | C796 | C736 |
| G1517 | G1457 | C1397 | G1337 | C1277 | A1217 | A1157 | C1097 | C1037 | G977 | G917 | C857 | C797 | C737 |
| A1518 | G1458 | A1398 | G1338 | G1278 | C1218 | C1158 | G1098 | C1038 | A978 | A918 | C858 | U798 | C738 |
| A1519 | G1459 | C1399 | A1339 | G1279 | C1219 | U1159 | G1099 | G1039 | G979 | A919 | C859 | G799 | C739 |
| C1520 | C1460 | C1400 | A1340 | A1280 | G1220 | G1160 | C1100 | U1040 | C980 | U920 | A860 | G800 | U740 |
| C1521 | G1461 | G1401 | U1341 | C1281 | G1221 | C1161 | A1101 | G1041 | U981 | U921 | G861 | U801 | G741 |
| U1522 | C1462 | C1402 | G1342 | C1282 | G1222 | C1162 | A1102 | A1042 | U982 | G922 | C862 | A802 | G742 |
| G1523 | U1463 | C1403 | G1343 | U1283 | C1223 | A1163 | C1103 | G1043 | A983 | A923 | U863 | G803 | A743 |
| C1524 | U1464 | C1404 | C1344 | C1284 | U1224 | G1164 | G1104 | A1044 | C984 | C924 | A864 | U804 | C744 |
| G1525 | A1465 | U1405 | U1345 | A1285 | A1225 | U1165 | A1105 | C1045 | C985 | G925 | A865 | C805 | G745 |
| G1526 | U1466 | U1406 | A1346 | U1286 | C1226 | G1166 | U1106 | A1046 | U986 | G926 | C866 | C806 | A746 |
| U1527 | C1467 | C1407 | G1347 | A1287 | A1227 | A1167 | C1107 | G1047 | G987 | G927 | G867 | A807 | A747 |
| U1528 | A1468 | A1408 | U1348 | A1288 | C1228 | U1168 | C1108 | G1048 | G988 | G928 | C868 | C808 | G748 |
| G1529 | C1469 | C1409 | A1349 | A1289 | A1229 | A1169 | C1109 | U1049 | U989 | G929 | C869 | G809 | A749 |
| G1530 | A1470 | A1410 | A1350 | G1290 | C1230 | A1170 | A1110 | G1050 | C990 | C930 | U870 | C810 | C750 |
| A1531 | U1471 | C1411 | U1351 | C1291 | G1231 | A1171 | A1111 | C1051 | U991 | C931 | U871 | C811 | U751 |
| C1532 | U1472 | C1412 | C1352 | G1292 | U1232 | C1172 | C1112 | U1052 | U992 | G932 | A872 | G812 | G752 |
| C1533 | C1473 | A1413 | G1353 | C1293 | G1233 | U1173 | C1113 | G1053 | G993 | C933 | A873 | U813 | A753 |
| A1534 | U1474 | A1414 | U1354 | G1294 | C1234 | G1174 | C1114 | C1054 | A994 | C934 | G874 | A814 | C754 |
| | G1475 | G1415 | G1355 | U1295 | U1235 | G1175 | U1115 | A1055 | C995 | A935 | U875 | A815 | G755 |
| | A1476 | G1416 | G1356 | C1296 | A1236 | A1176 | U1116 | U1056 | A996 | C936 | C876 | A816 | C756 |
| | U1477 | G1417 | A1357 | G1297 | C1237 | G1177 | A1117 | G1057 | U997 | A937 | G877 | C817 | U757 |
| | U1478 | A1418 | U1358 | U1298 | A1238 | G1178 | U1118 | G1058 | G998 | A938 | A878 | G818 | C758 |
| | C1479 | G1419 | C1359 | A1299 | A1239 | A1179 | C1119 | C1059 | C999 | C939 | C879 | A819 | A759 |
| | A1480 | U1420 | A1360 | G1300 | U1240 | A1180 | C1120 | U1060 | A1000 | C940 | C880 | U820 | G760 |
| | U1481 | G1421 | G1361 | U1301 | G1241 | G1181 | U1121 | G1061 | C1001 | G941 | G881 | G821 | G761 |
| | G1482 | C1422 | A1362 | C1302 | G1242 | U1182 | U1122 | U1062 | G1002 | G942 | C882 | U822 | U762 |
| | A1483 | G1423 | A1363 | C1303 | C1243 | U1183 | U1123 | C1063 | G1003 | U943 | C883 | C823 | G763 |
| | C1484 | U1424 | U1364 | G1304 | G1244 | G1184 | G1124 | G1064 | A1004 | G944 | U884 | G824 | C764 |
| | U1485 | U1425 | G1365 | G1305 | C1245 | G1185 | U1125 | U1065 | A1005 | G945 | C885 | A825 | G765 |
| | G1486 | G1426 | C1366 | A1306 | A1246 | G1186 | U1126 | C1066 | G1006 | A946 | G886 | C826 | A766 |
| | G1487 | C1427 | C1367 | U1307 | U1247 | G1187 | G1127 | A1067 | U1007 | G947 | G887 | U827 | A767 |
| | G1488 | A1428 | A1368 | U1308 | A1248 | A1188 | C1128 | G1068 | U1008 | C948 | G888 | U828 | A768 |
| | G1489 | A1429 | C1369 | G1309 | C1249 | U1189 | C1129 | C1069 | U1009 | A949 | A889 | G829 | G769 |
| | U1490 | A1430 | G1370 | G1310 | A1250 | G1190 | A1130 | U1070 | U1010 | U950 | G890 | G830 | C770 |
| | G1491 | A1431 | G1371 | A1311 | A1251 | A1191 | G1131 | C1071 | C1011 | G951 | U891 | A831 | G771 |
| | A1492 | G1432 | U1372 | G1312 | A1252 | C1192 | C1132 | G1072 | A1012 | U952 | A892 | G832 | U772 |
| | A1493 | A1433 | G1373 | C1313 | G1253 | G1193 | G1133 | U1073 | C893 | G953 | C893 | G833 | G773 |
| | G1494 | A1434 | A1374 | C1314 | A1254 | U1194 | G1134 | G1074 | A1014 | G954 | G894 | U834 | G774 |
| | U1495 | G1435 | A1375 | U1315 | G1255 | C1195 | U1135 | U1075 | G895 | U955 | G895 | U835 | G775 |
| | C1496 | U1436 | U1376 | G1316 | A1256 | A1196 | C1136 | U1076 | A1016 | U956 | C896 | G836 | G776 |
| | G1497 | A1437 | G1377 | C1317 | A1257 | A1197 | C1137 | G1077 | U1017 | U957 | C897 | U837 | A777 |
| | U1498 | C1438 | C1378 | A1318 | G1258 | G1198 | G1138 | U1078 | G1018 | A958 | G898 | G838 | G778 |
| | A1499 | G1439 | G1379 | A1319 | C1259 | U1199 | G1139 | G1079 | A1019 | A959 | C899 | C839 | C779 |
| | U1500 | U1440 | U1380 | C1320 | G1260 | U1200 | C1140 | A1080 | U1020 | A960 | A900 | C840 | A780 |
| | C1501 | A1441 | U1381 | U1321 | A1261 | A1201 | C1141 | A1081 | A1021 | U961 | A901 | C841 | A781 |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | 11474 | Depositor |
| Resolution determination method | FSC at 0.5 cut-off | Depositor |
| CTF correction method | Weiner filter | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 20 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3800 | Depositor |
| Magnification | 59000 | Depositor |
| Image detector | FEI Eagle 4k*4k CCD | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------------|-------------|--------------------|
| | | RMSZ | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | N | 3.47 | 5192/36831 (14.1%) | 3.99 | 9508/57458 (16.5%) |

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 | N | 0 | 978 |

The worst 5 of 5192 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | N | 815 | A | N7-C5 | -18.92 | 1.27 | 1.39 |
| 1 | N | 435 | A | N7-C5 | -18.59 | 1.28 | 1.39 |
| 1 | N | 572 | A | N7-C5 | -18.24 | 1.28 | 1.39 |
| 1 | N | 367 | U | C2-N3 | 17.85 | 1.50 | 1.37 |
| 1 | N | 202 | G | N7-C5 | 16.97 | 1.49 | 1.39 |

The worst 5 of 9508 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1 | N | 567 | G | C5-C6-O6 | -27.97 | 111.82 | 128.60 |
| 1 | N | 184 | G | N1-C6-O6 | 26.91 | 136.04 | 119.90 |
| 1 | N | 184 | G | C5-C6-O6 | -26.87 | 112.48 | 128.60 |
| 1 | N | 567 | G | N1-C6-O6 | 25.95 | 135.47 | 119.90 |
| 1 | N | 713 | G | N1-C6-O6 | 24.64 | 134.69 | 119.90 |

There are no chirality outliers.

5 of 978 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | N | 3 | A | Sidechain |
| 1 | N | 4 | U | Sidechain |
| 1 | N | 5 | U | Sidechain |
| 1 | N | 6 | G | Sidechain |
| 1 | N | 9 | G | Sidechain |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | N | 32892 | 16554 | 16521 | 571 | 0 |
| All | All | 32892 | 16554 | 16521 | 571 | 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 12.

The worst 5 of 571 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:N:32:A:H4' | 1:N:48:C:H42 | 1.50 | 0.75 |
| 1:N:594:U:C4 | 1:N:595:A:C6 | 2.74 | 0.75 |
| 1:N:338:A:H61 | 1:N:351:G:H1 | 1.36 | 0.73 |
| 1:N:116:A:H61 | 1:N:313:A:H1' | 1.53 | 0.73 |
| 1:N:197:A:H2 | 1:N:198:G:C4 | 2.08 | 0.70 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | N | 1532/1533 (99%) | 449 (29%) | 152 (9%) |

5 of 449 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 3 | A |
| 1 | N | 4 | U |
| 1 | N | 5 | U |
| 1 | N | 6 | G |
| 1 | N | 7 | A |

5 of 152 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | N | 535 | A |
| 1 | N | 777 | A |
| 1 | N | 1380 | U |
| 1 | N | 559 | A |
| 1 | N | 686 | 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 ⓘ

There are no chain breaks in this entry.