Full wwPDB EM Validation Report ⓘ

May 20, 2024 – 03:05 pm BST

PDB ID	:	8RC0
EMDB ID	:	EMD-19041
Title	:	Structure of the human 20S U5 snRNP
Authors	:	Schneider, S.; Galej, W.P.
Deposited on	:	2023-12-05
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

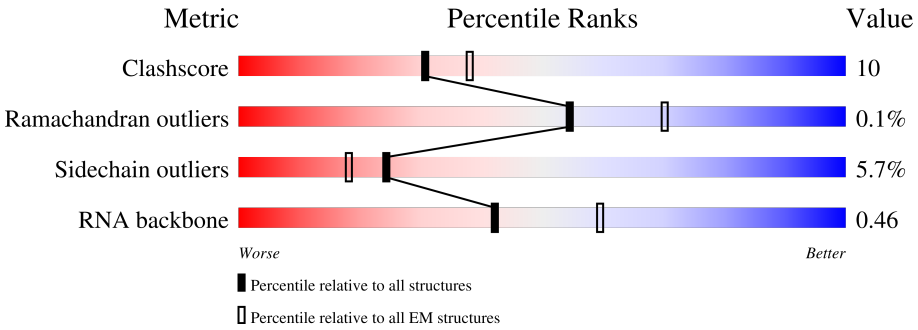
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	F	341	28% 11% 59%
2	A	2335	23% 65% 25% 8%
3	5	117	30% 46% 9% 11%
4	E	941	5% 94%
5	D	820	28% 65% 5% 29%
6	G	357	75% 81% 14%
7	B	2136	81% 81% 18%

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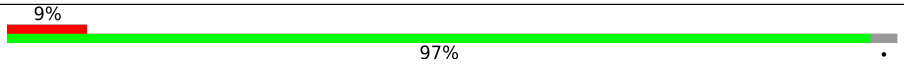
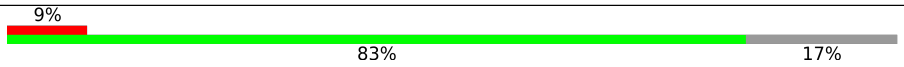
Mol	Chain	Length	Quality of chain
8	i	119	
9	k	126	
10	l	92	
11	m	86	
12	n	76	
13	j	118	
14	h	240	
15	C	972	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 40648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CD2 antigen cytoplasmic tail-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	140	Total	C	N	O	S	0	0
			889	554	165	169	1		

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2153	Total	C	N	O	S	0	0
			16709	10694	2952	2994	69		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 4 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	60	Total	C	N	O	S	0	0
			516	314	93	108	1		

- Molecule 5 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	580	Total	C	N	O	S	7	0
			2941	1609	666	664	2		

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	306	Total	C	N	O	0	0
			1507	894	306	307		

- Molecule 7 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	1748	Total	C	N	O	0	0
			6992	3496	1748	1748		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	i	81	Total	C	N	O	0	0
			324	162	81	81		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	k	84	Total	C	N	O	0	0
			336	168	84	84		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	77	Total	C	N	O	0	0
			308	154	77	77		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	m	73	Total	C	N	O	0	0
			292	146	73	73		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	n	74	Total	C	N	O	0	0
			297	148	74	75		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	j	98	Total	C	N	O	0	0
			392	196	98	98		

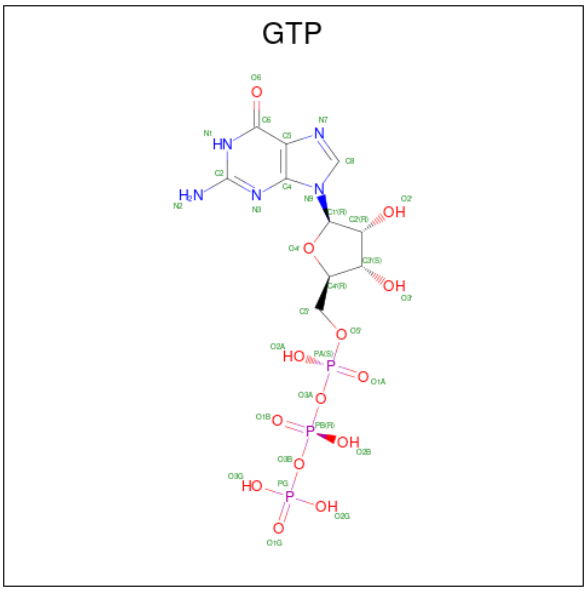
- Molecule 14 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	h	73	Total	C	N	O	0	0
			292	146	73	73		

- Molecule 15 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	847	Total	C	N	O	S	0	0
			6629	4238	1108	1250	33		

- Molecule 16 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

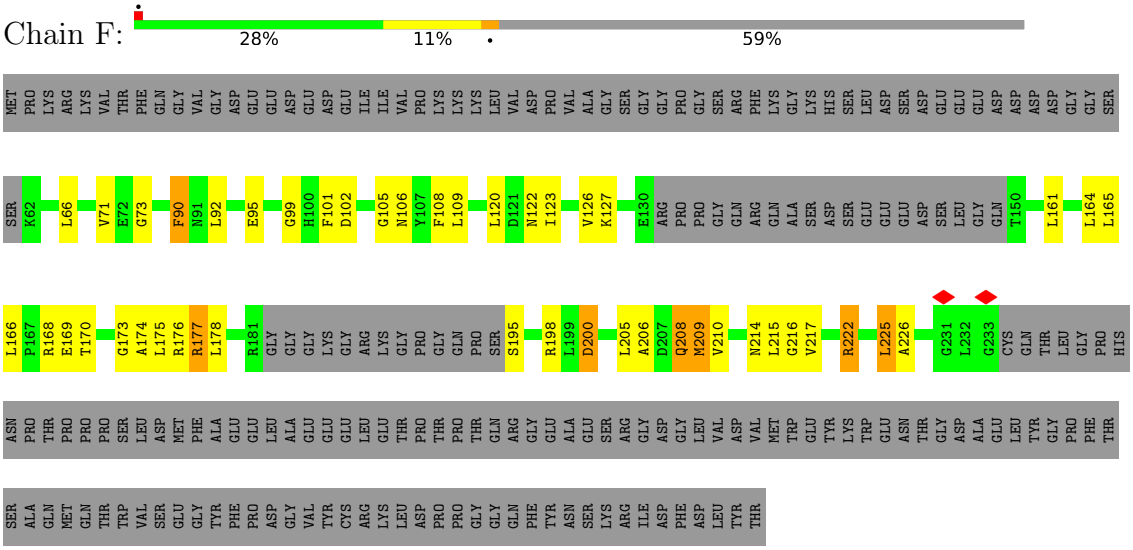


Mol	Chain	Residues	Atoms					AltConf
16	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

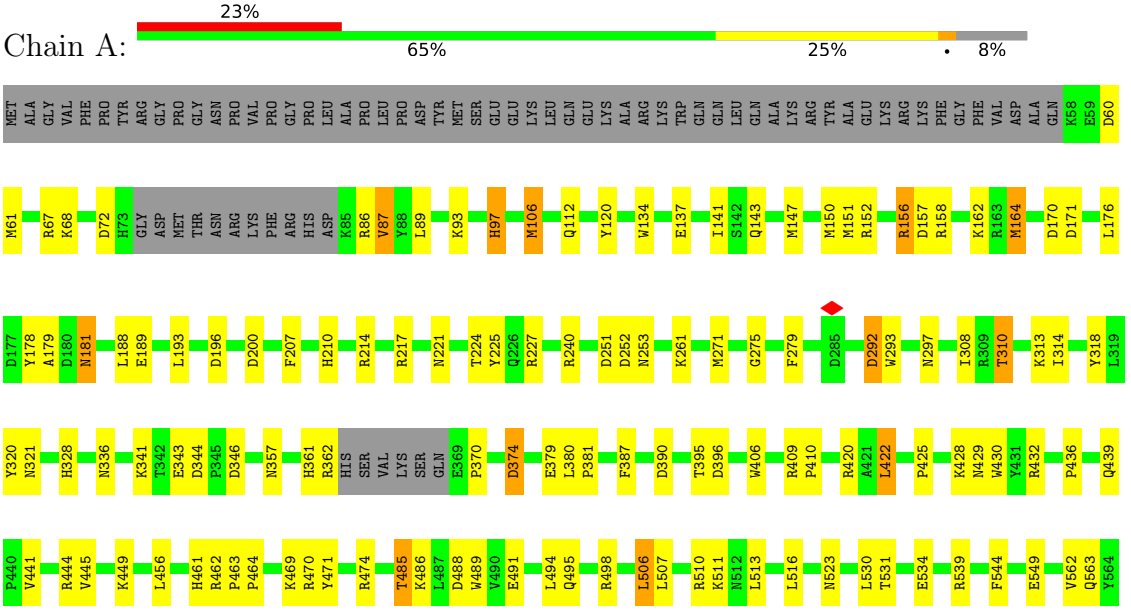
3 Residue-property plots (i)

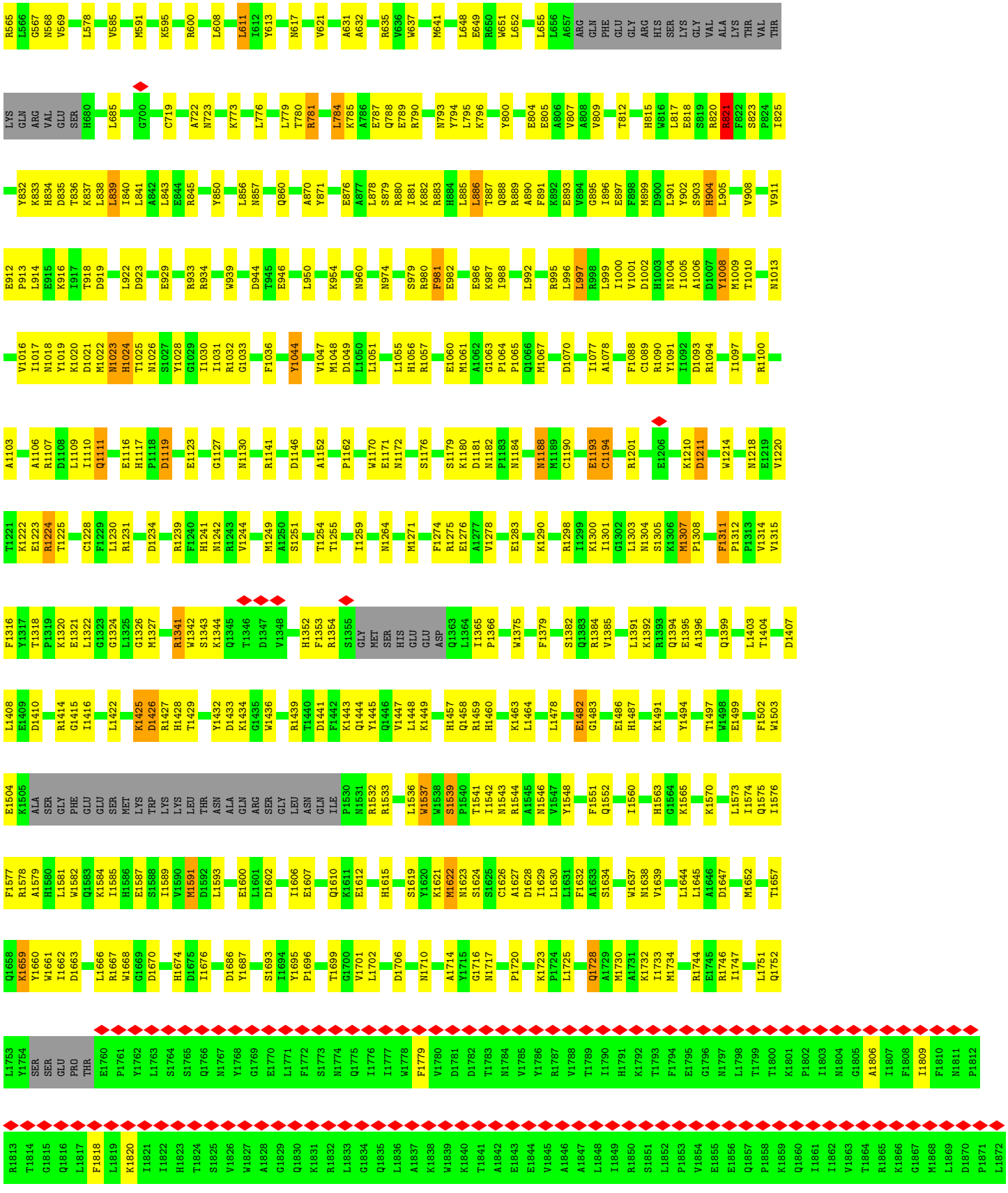
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CD2 antigen cytoplasmic tail-binding protein 2



• Molecule 2: Pre-mRNA-processing-splicing factor 8

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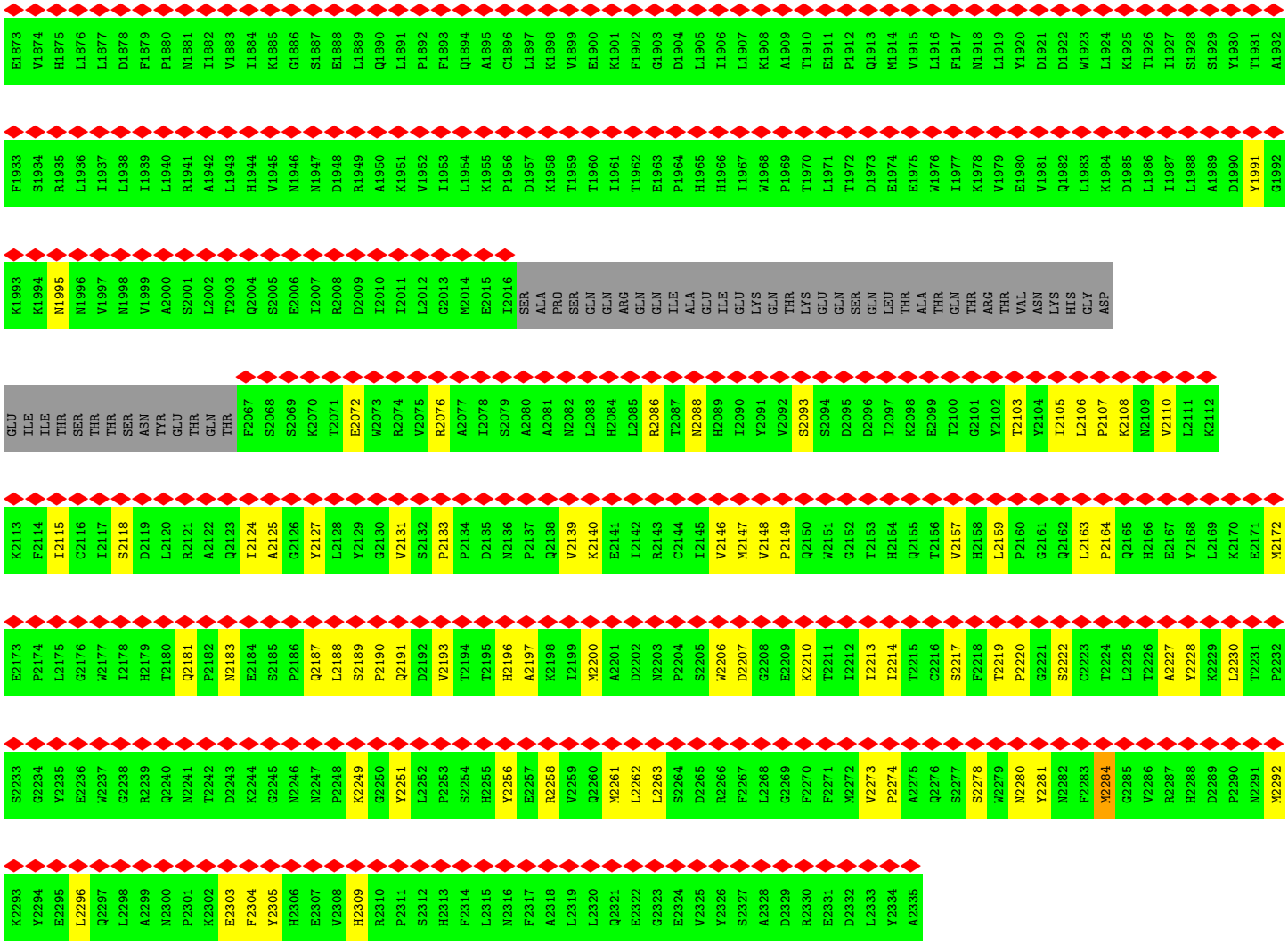
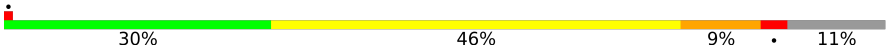
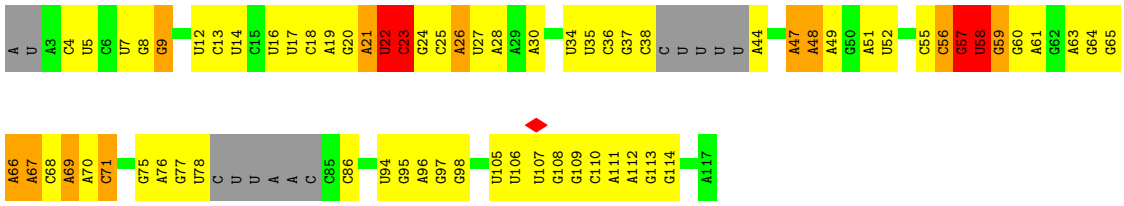
LYS GLN ARG VAL GLU SER H680 L685 G700 C719 A722 N723 K773 L776 L779 T780 R781 L784 K785 A786 E787 Q788 E789 R790 N793 Y794 L795 K796 Y800 E804 E805 A806 V807 A808 V809 T812 H815 W816 L817 E818 S819 R820 R821 F822 S823 P824 I825
Y832 K833 H834 D835 T836 K837 L838 L839 I840 L841 A842 L843 E844 R845 Y850 L856 N857 Q860 A870 Y871 E876 A877 L878 S879 R880 I881 K882 R883 H884 L885 L886 T887 Q888 R889 A890 F891 K892 E893 V894 G895 I896 E897 F898 M899 D900 L901 Y902 S903 H904 L905 V908 V911
E912 P913 L914 E915 K916 I917 T918 D919 L922 D923 E929 R933 R934 W939 D944 T945 E946 L950 K964 N960 N974 S979 R980 F981 E982 E986 K987 I988 L992 R995 L996 L997 R998 L999 I1000 V1001 D1002 H1003 N1004 I1005 A1006 D1007 Y1008 M1009 T1010 N1013
V1016 I1017 N1018 Y1019 K1020 D1021 M1022 N1023 H1024 T1025 N1026 S1027 Y1028 G1029 I1030 I1031 R1032 G1033 F1036 Y1044 V1047 M1048 D1049 L1050 L1051 L1055 H1056 R1057 E1060 M1061 A1062 G1063 P1064 P1065 Q1066 M1067 D1070 I1077 A1078 F1088 C1089 R1090 Y1091 I1092 D1093 R1094 I1097 R1100
A1103 A1106 R1107 D1108 L1109 I1110 Q1111 E1116 H1117 P1118 D1119 E1123 G1127 N1130 R1141 D1146 A1152 P1162 W1170 E1171 N1172 S1176 S1179 K1180 D1181 N1182 P1183 N1184 N1188 M1189 C1190 E1193 C1194 R1201 E1206 K1210 D1211 W1214 N1218 E1219 V1220
T1221 K1222 E1223 R1224 T1225 C1228 F1229 L1230 R1231 D1234 R1239 F1240 H1241 N1242 R1243 V1244 M1249 A1250 S1251 T1254 T1255 I1259 N1264 M1271 F1274 R1275 E1276 A1277 V1278 E1283 K1290 R1298 I1299 K1300 I1301 G1302 L1303 N1304 S1305 K1306 M1307 P1308 F1311 P1312 P1313 V1314 V1315
F1316 Y1317 T1318 P1319 K1320 E1321 L1322 G1323 G1324 L1325 G1326 M1327 R1341 W1342 S1343 K1344 Q1345 T1346 D1347 V1348 H1352 F1353 R1354 S1355 GLY MET SER HIS GLU GLU ASP Q1363 L1364 I1365 P1366 W1375 F1379 S1382 Q1383 R1384 V1385 L1391 K1392 R1393 Q1394 E1395 A1396 Q1399 L1403 T1404 D1407
L1408 E1409 D1410 R1414 G1415 I1416 L1422 K1425 D1426 R1427 H1428 T1429 Y1432 D1433 K1434 G1435 W1436 R1439 T1440 D1441 F1442 K1443 Q1444 Y1445 Q1446 V1447 L1448 K1449 H1457 Q1458 R1459 H1460 K1463 L1464 L1478 E1482 G1483 E1486 H1487 K1491 Y1494 T1497 W1498 E1499 F1502 W1503
E1504 K1505 ALA SER GLY PHE GLU GLU SER MET LYS TRP LYS LYS LEU THR ASN ALA GLN ARG SER GLY LEU ASN GLN ILE P1530 N1531 R1532 R1533 L1536 W1537 W1538 S1539 P1540 T1541 I1542 N1543 R1544 A1545 N1546 V1547 Y1548 F1551 Q1552 I1560 H1563 G1564 K1565 K1570 L1573 I1574 Q1575 I1576
F1577 R1578 A1579 H1580 L1581 W1582 Q1583 K1584 I1585 H1586 E1587 S1588 I1589 V1590 M1591 D1592 L1593 E1600 L1601 D1602 I1606 E1607 Q1610 K1611 E1612 H1615 S1619 Y1620 K1621 M1622 N1623 S1624 S1625 C1626 A1627 D1628 I1629 L1630 L1631 F1632 A1633 S1634 W1637 N1638 V1639 L1644 L1645 A1646 D1647 M1652 T1657
Q1658 K1659 Y1660 W1661 I1662 D1663 L1666 R1667 W1668 G1669 D1670 H1674 D1675 I1676 D1686 Y1687 S1693 I1694 Y1695 P1696 T1699 G1700 V1701 L1702 D1706 N1710 A1714 Y1715 G1716 N1717 P1720 K1723 P1724 L1725 Q1728 A1729 M1730 A1731 K1732 I1733 M1734 R1744 E1745 R1746 I1747 L1751 Q1752
L1753 Y1754 SER SER GLU PRO THR E1760 P1761 Y1762 L1763 S1764 S1765 Q1766 N1767 Y1768 G1769 E1770 L1771 F1772 S1773 N1774 Q1775 I1776 I1777 W1778 F1779 V1780 D1781 D1782 T1783 N1784 V1785 Y1786 R1787 V1788 T1789 I1790 H1791 K1792 T1793 F1794 E1795 G1796 N1797 L1798 T1799 T1800 K1801 P1802 I1803 N1804 G1805 A1806 I1807 F1808 I1809 F1810 N1811 P1812
R1813 T1814 G1815 Q1816 L1817 F1818 L1819 K1820 I1821 I1822 H1823 T1824 S1825 V1826 W1827 A1828 G1829 Q1830 K1831 R1832 L1833 G1834 Q1835 L1836 A1837 K1838 W1839 K1840 T1841 A1842 E1843 E1844 V1845 A1846 A1847 L1848 I1849 R1850 S1851 L1852 P1853 V1854 E1855 E1856 Q1857 P1858 K1859 Q1860 I1861 I1862 V1863 T1864 R1865 K1866 G1867 M1868 L1869 D1870 P1871 L1872



• Molecule 3: U5 snRNA

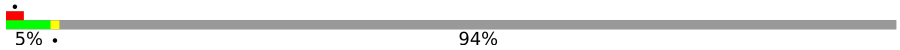
Chain 5:

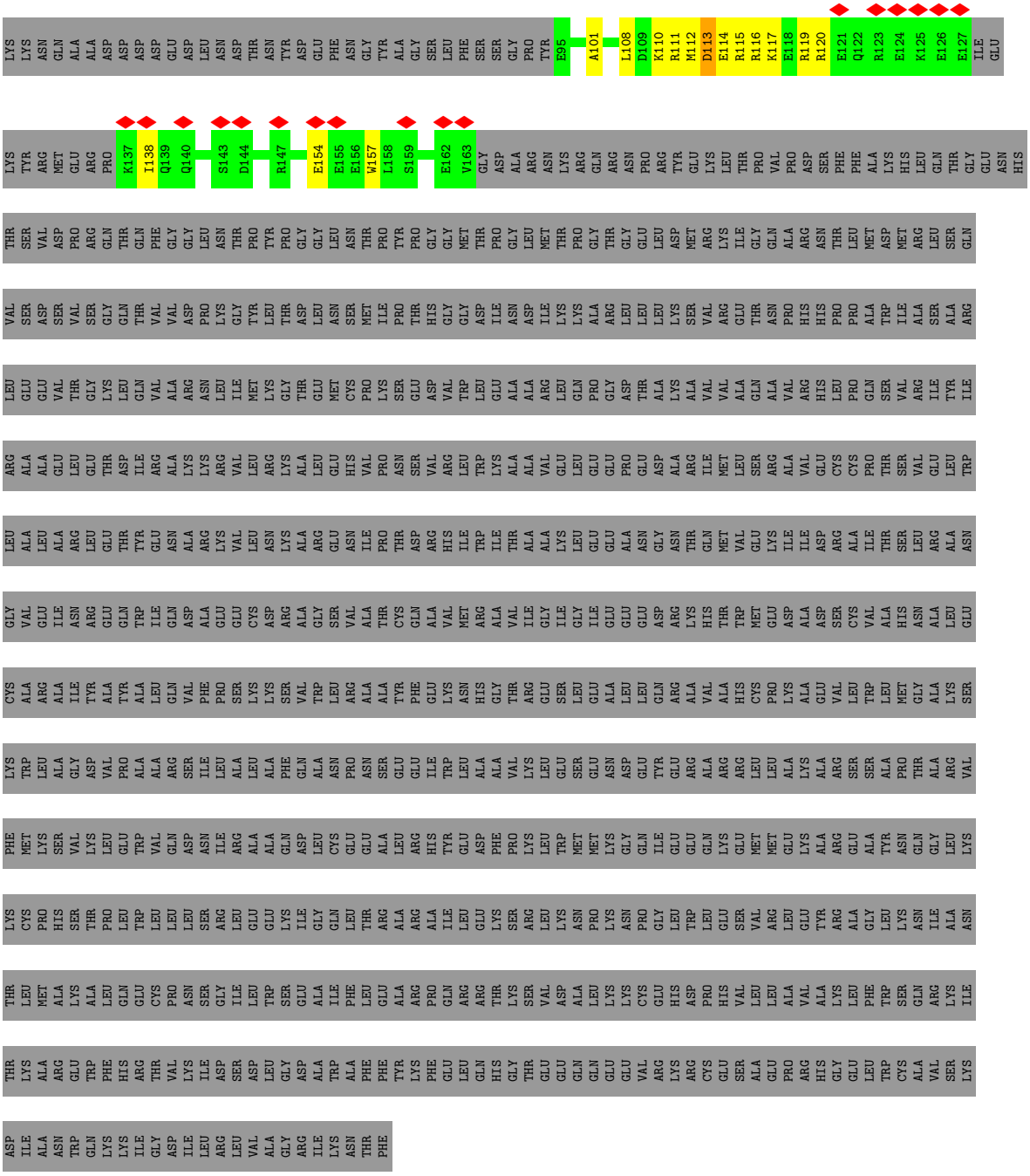




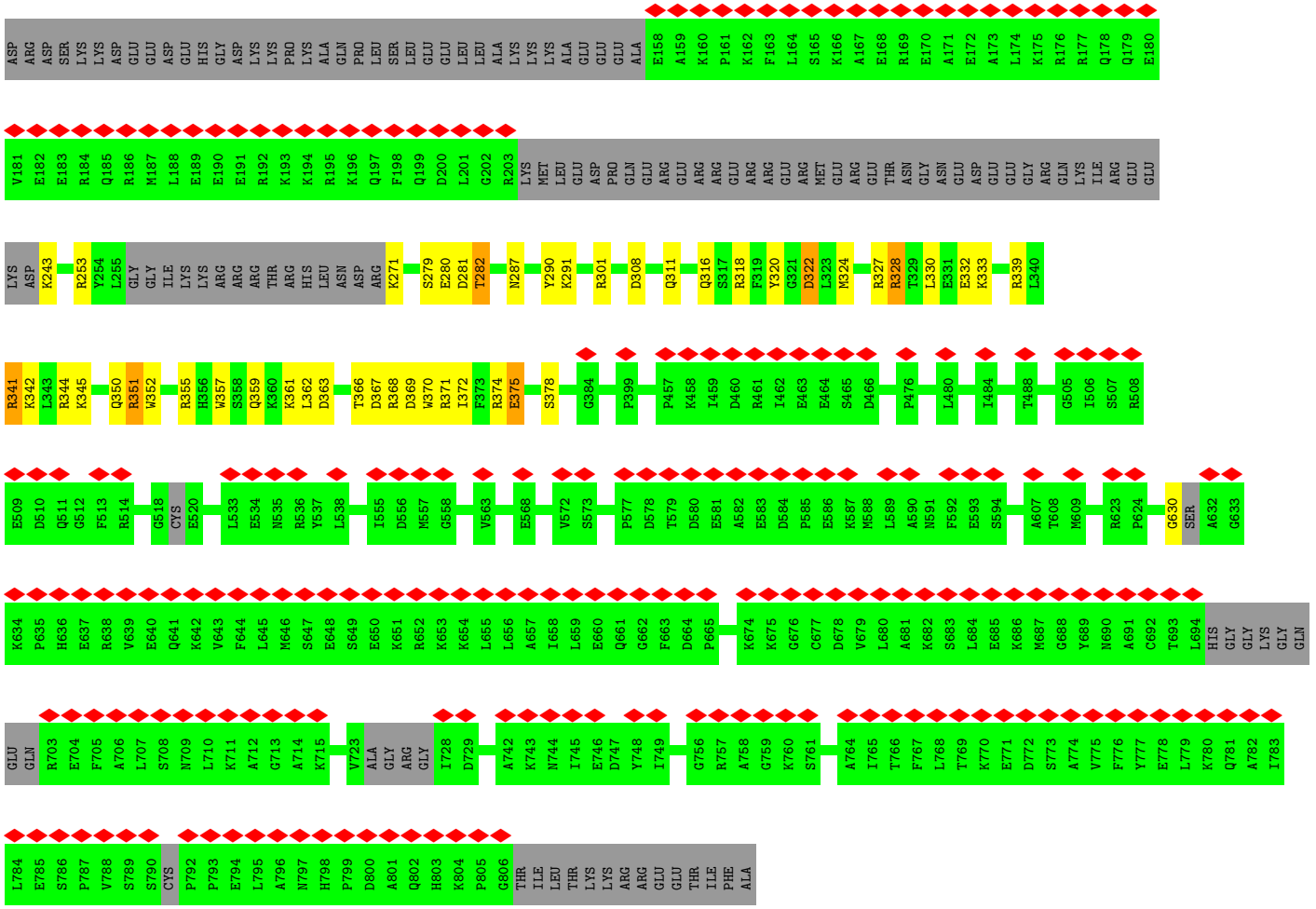
• Molecule 4: Pre-mRNA-processing factor 6

Chain E:



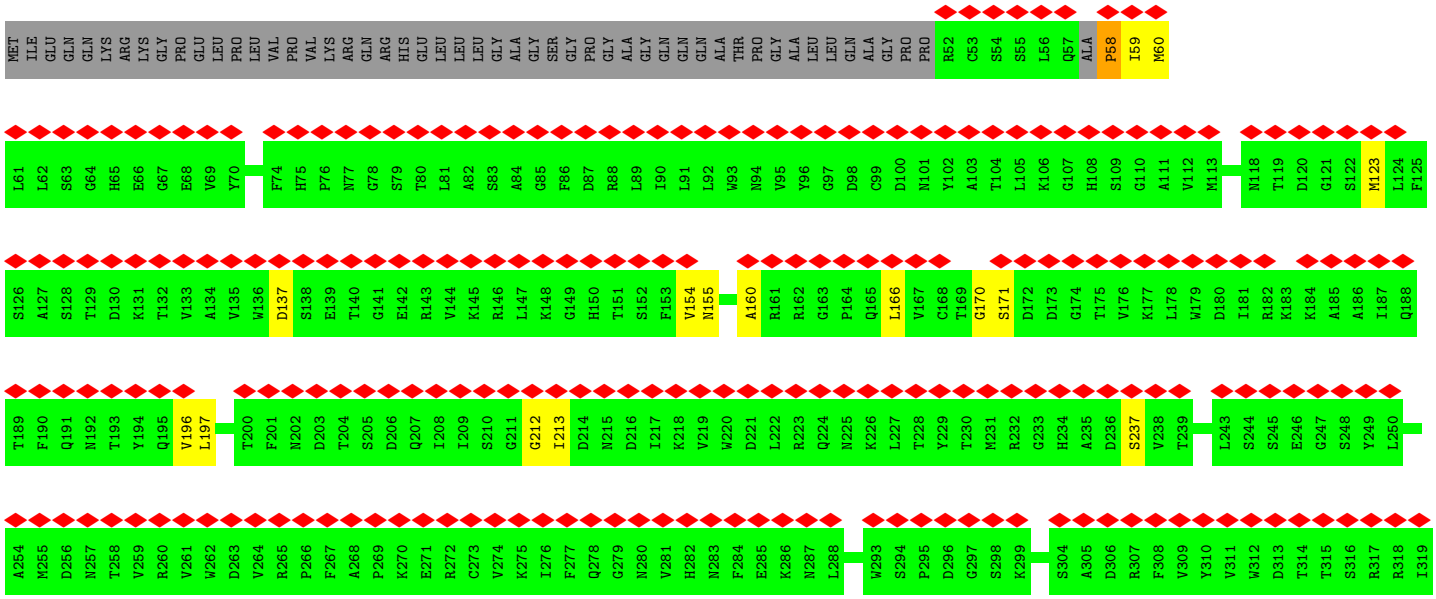


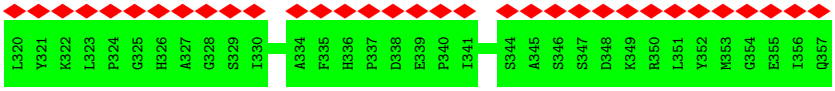
• Molecule 5: Probable ATP-dependent RNA helicase DDX23



• Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein

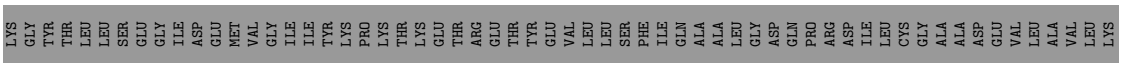
Chain G:

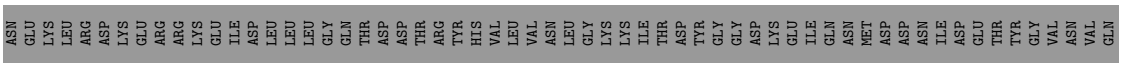


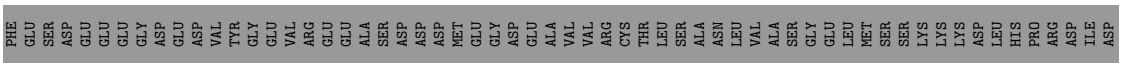


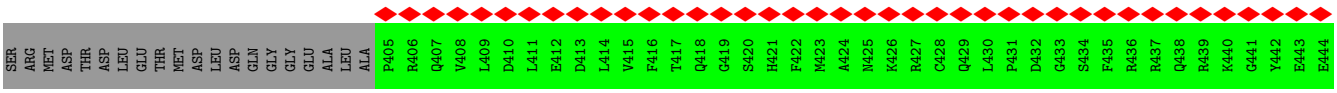
• Molecule 7: U5 small nuclear ribonucleoprotein 200 kDa helicase

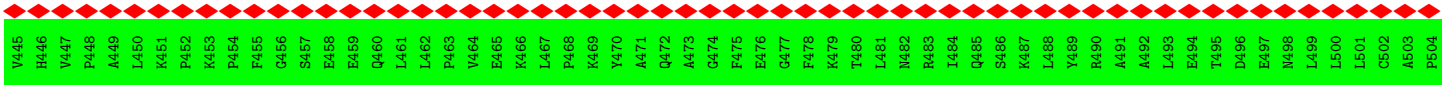
Chain B:

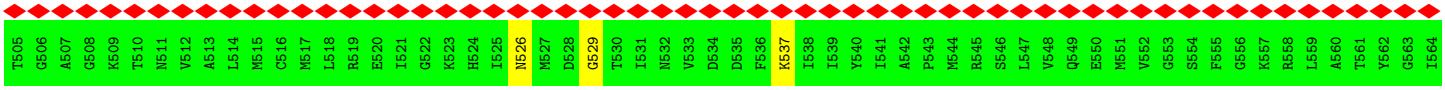


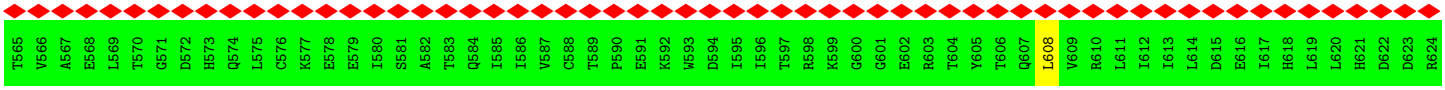


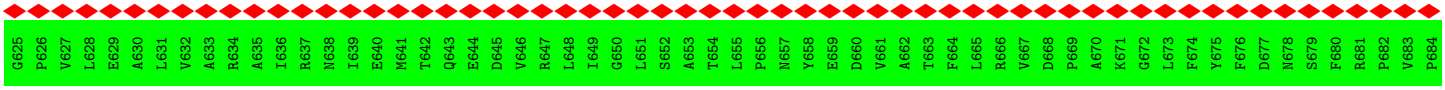


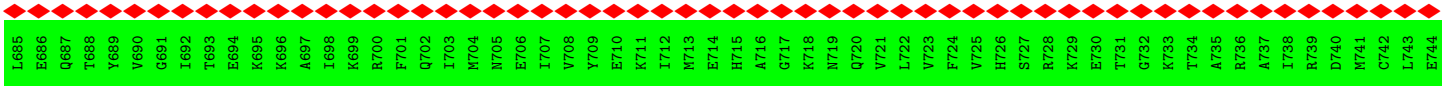


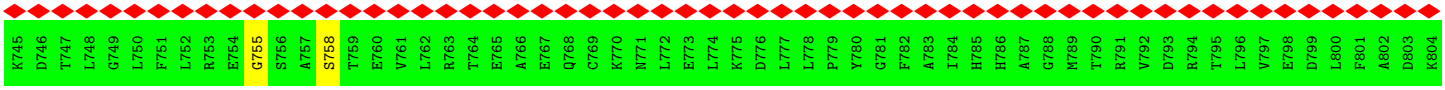


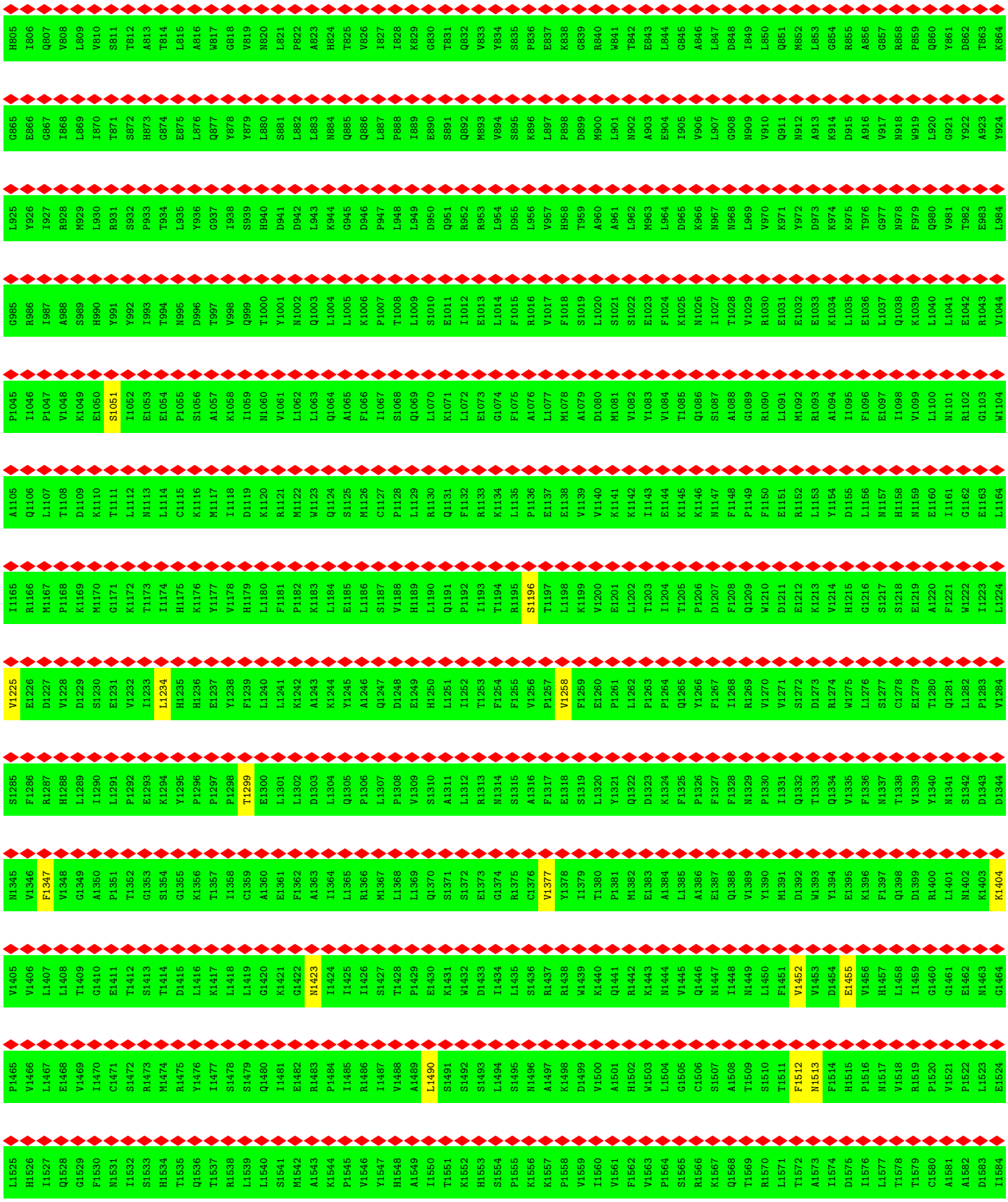








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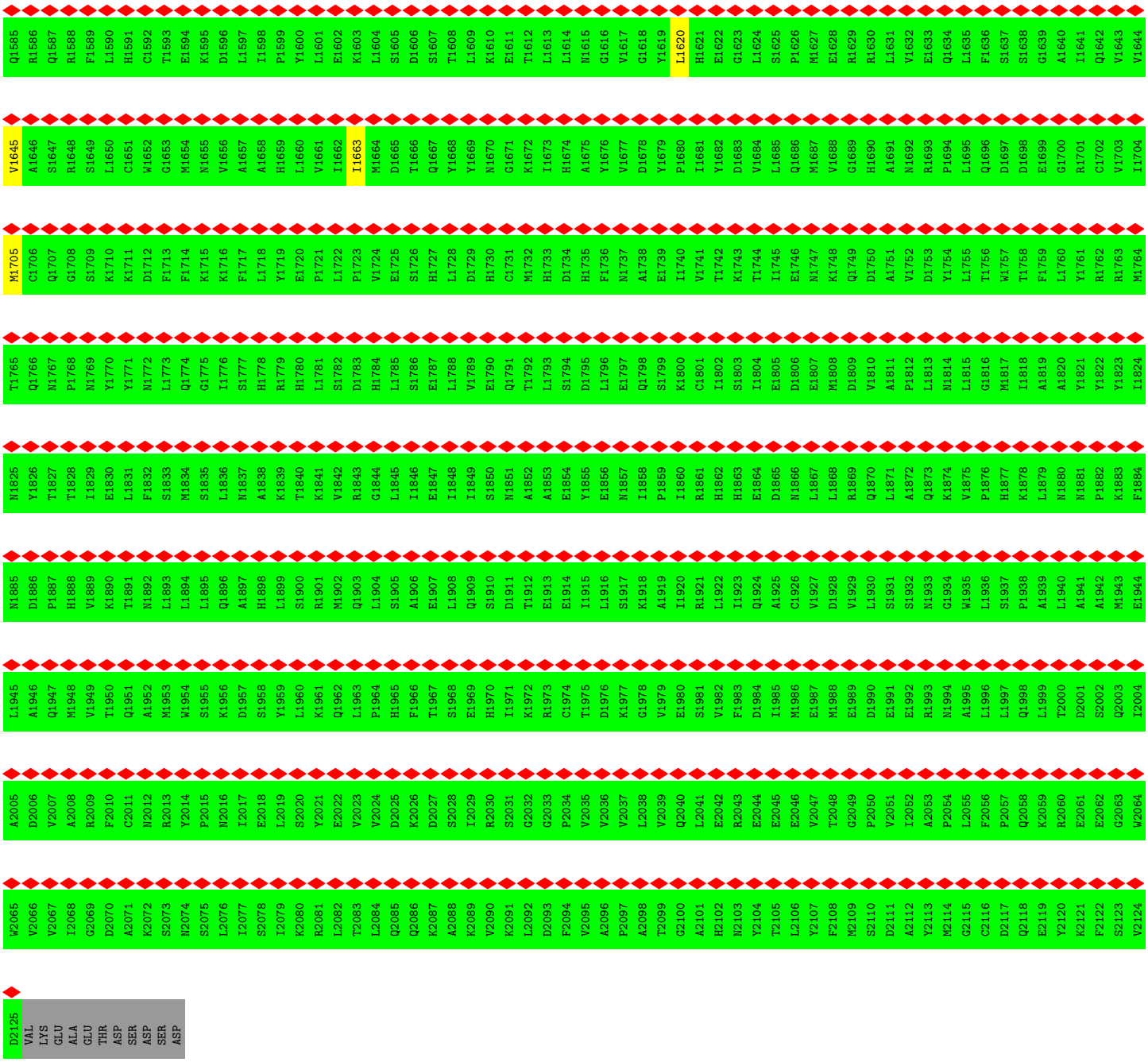
G865 E866 G867 I868 L869 I870 T871 S872 H873 G874 E875 L876 Q877 Y878 Y879 L880 S881 L882 L883 N884 Q885 Q886 L887 P888 I889 E890 S891 Q892 M893 V894 S895 K896 L897 P898 D899 M900 L901 N902 A903 E904 I905 V906 L907 G908 N909 V910 Q911 N912 A913 K914 D915 A916 V917 N918 W919 L920 G921 Y922 A923 Y924
L925 Y926 I927 R928 M929 L930 R931 S932 P933 T934 L935 Y936 G937 I938 S939 H940 D941 D942 L943 K944 G945 D946 P947 L948 L949 D950 Q951 R952 R953 L954 D955 L956 V957 H958 T959 A960 A961 L962 M963 L964 D965 K966 N967 N968 L969 V970 K971 Y972 D973 K974 K975 T976 G977 N978 F979 Q980 V981 T982 E983 L984
G985 R986 I987 A988 S989 H990 Y991 Y992 I993 T994 N995 D996 T997 V998 Q999 T1000 Y1001 N1002 Q1003 L1004 L1005 K1006 P1007 T1008 L1009 S1010 E1011 I1012 E1013 L1014 F1015 R1016 V1017 F1018 S1019 L1020 S1021 S1022 E1023 F1024 K1025 N1026 I1027 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 Q1038 K1039 L1040 L1041 E1042 R1043 V1044
P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 E1053 E1054 P1055 S1056 A1057 K1058 I1059 N1060 V1061 L1062 L1063 Q1064 A1065 F1066 I1067 S1068 Q1069 L1070 K1071 L1072 E1073 G1074 F1075 A1076 L1077 M1078 A1079 D1080 M1081 V1082 Y1083 V1084 T1085 Q1086 S1087 A1088 G1089 R1090 L1091 M1092 R1093 A1094 I1095 F1096 E1097 I1098 V1099 L1100 N1101 R1102 G1103 W1104
A1105 Q1106 L1107 T1108 D1109 K1110 T1111 L1112 N1113 L1114 C1115 K1116 M1117 I1118 D1119 K1120 R1121 M1122 W1123 Q1124 S1125 M1126 C1127 P1128 L1129 R1130 Q1131 F1132 R1133 K1134 L1135 P1136 E1137 E1138 V1139 V1140 K1141 K1142 I1143 E1144 K1145 K1146 N1147 F1148 P1149 F1150 E1151 R1152 L1153 Y1154 D1155 L1156 N1157 H1158 N1159 E1160 I1161 G1162 E1163 L1164
I1165 R1166 M1167 P1168 K1169 M1170 G1171 K1172 T1173 I1174 H1175 K1176 Y1177 V1178 H1179 L1180 F1181 P1182 K1183 L1184 E1185 L1186 S1187 V1188 H1189 L1190 Q1191 P1192 I1193 T1194 R1195 S1196 T1197 L1198 K1199 V1200 E1201 L1202 T1203 I1204 T1205 P1206 D1207 F1208 Q1209 W1210 D1211 E1212 K1213 V1214 H1215 G1216 S1217 S1218 E1219 A1220 F1221 W1222 I1223 L1224
V1225 E1226 D1227 V1228 D1229 S1230 E1231 V1232 I1233 L1234 H1235 H1236 E1237 Y1238 F1239 L1240 L1241 K1242 A1243 K1244 Y1245 A1246 Q1247 D1248 E1249 H1250 L1251 I1252 T1253 F1254 F1255 V1256 P1257 V1258 F1259 E1260 P1261 L1262 P1263 P1264 Q1265 Y1266 F1267 I1268 R1269 V1270 V1271 S1272 D1273 R1274 W1275 L1276 S1277 C1278 E1279 T1280 Q1281 L1282 P1283 V1284
S1285 F1286 R1287 H1288 L1289 I1290 L1291 P1292 E1293 K1294 Y1295 P1296 P1297 P1298 T1299 E1300 L1301 L1302 D1303 L1304 Q1305 P1306 L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 F1317 E1318 S1319 L1320 Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336 N1337 T1338 V1339 Y1340 N1341 S1342 D1343 D1344
N1345 V1346 F1347 V1348 G1349 A1350 P1351 T1352 G1353 S1354 G1355 K1356 T1357 I1358 C1359 A1360 E1361 F1362 A1363 I1364 L1365 R1366 M1367 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 R1375 C1376 V1377 Y1378 I1379 T1380 P1381 M1382 E1383 A1384 L1385 A1386 E1387 Q1388 V1389 Y1390 M1391 D1392 W1393 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404
V1405 V1406 L1407 L1408 T1409 G1410 E1411 T1412 S1413 T1414 D1415 L1416 K1417 L1418 L1419 G1420 K1421 G1422 N1423 I1424 I1425 I1426 S1427 T1428 P1429 E1430 K1431 W1432 D1433 I1434 L1435 S1436 R1437 R1438 W1439 K1440 Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 V1453 D1454 E1455 V1456 H1457 L1458 I1459 G1460 G1461 E1462 N1463 G1464
P1465 V1466 L1467 E1468 V1469 I1470 C1471 S1472 R1473 M1474 R1475 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483 P1484 I1485 R1486 I1487 V1488 A1489 L1490 S1491 S1492 S1493 L1494 S1495 N1496 A1497 K1498 D1499 V1500 A1501 H1502 W1503 L1504 G1505 C1506 S1507 A1508 T1509 S1510 T1511 F1512 N1513 F1514 H1515 P1516 N1517 V1518 R1519 P1520 V1521 P1522 L1523 E1524
L1525 H1526 I1527 Q1528 G1529 F1530 N1531 I1532 S1533 H1534 T1535 Q1536 T1537 R1538 L1539 L1540 S1541 M1542 A1543 K1544 P1545 V1546 Y1547 H1548 A1549 I1550 T1551 K1552 H1553 S1554 P1555 K1556 K1557 P1558 V1559 I1560 V1561 F1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584

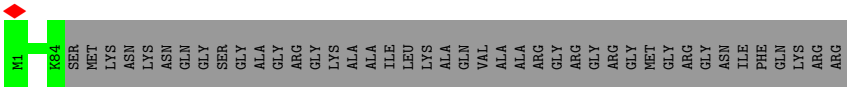


• Molecule 8: Small nuclear ribonucleoprotein Sm D1

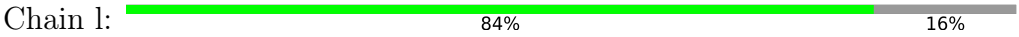
Chain i:

• Molecule 9: Small nuclear ribonucleoprotein Sm D3

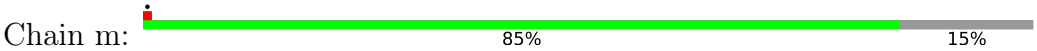
Chain k:

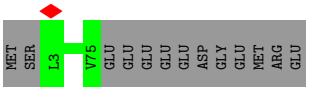


• Molecule 10: Small nuclear ribonucleoprotein E

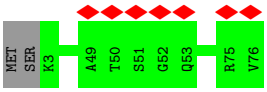


• Molecule 11: Small nuclear ribonucleoprotein F

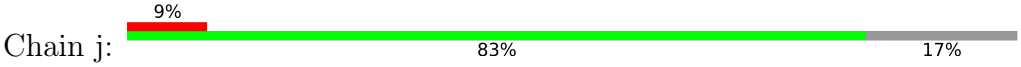


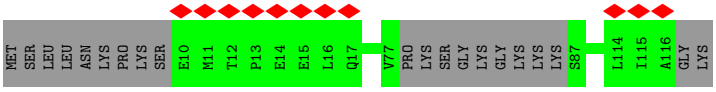


• Molecule 12: Small nuclear ribonucleoprotein G

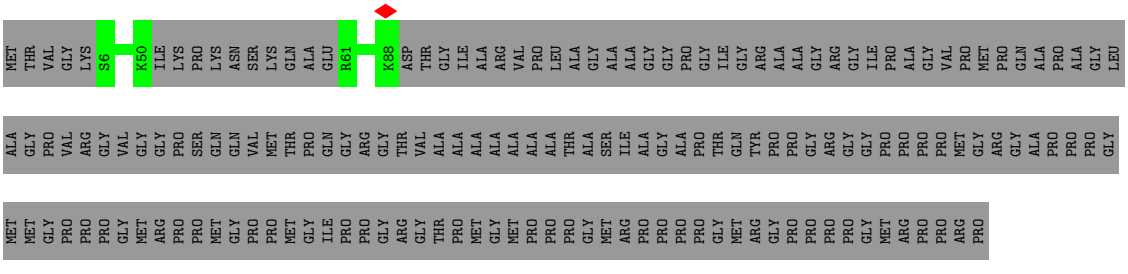


• Molecule 13: Small nuclear ribonucleoprotein Sm D2

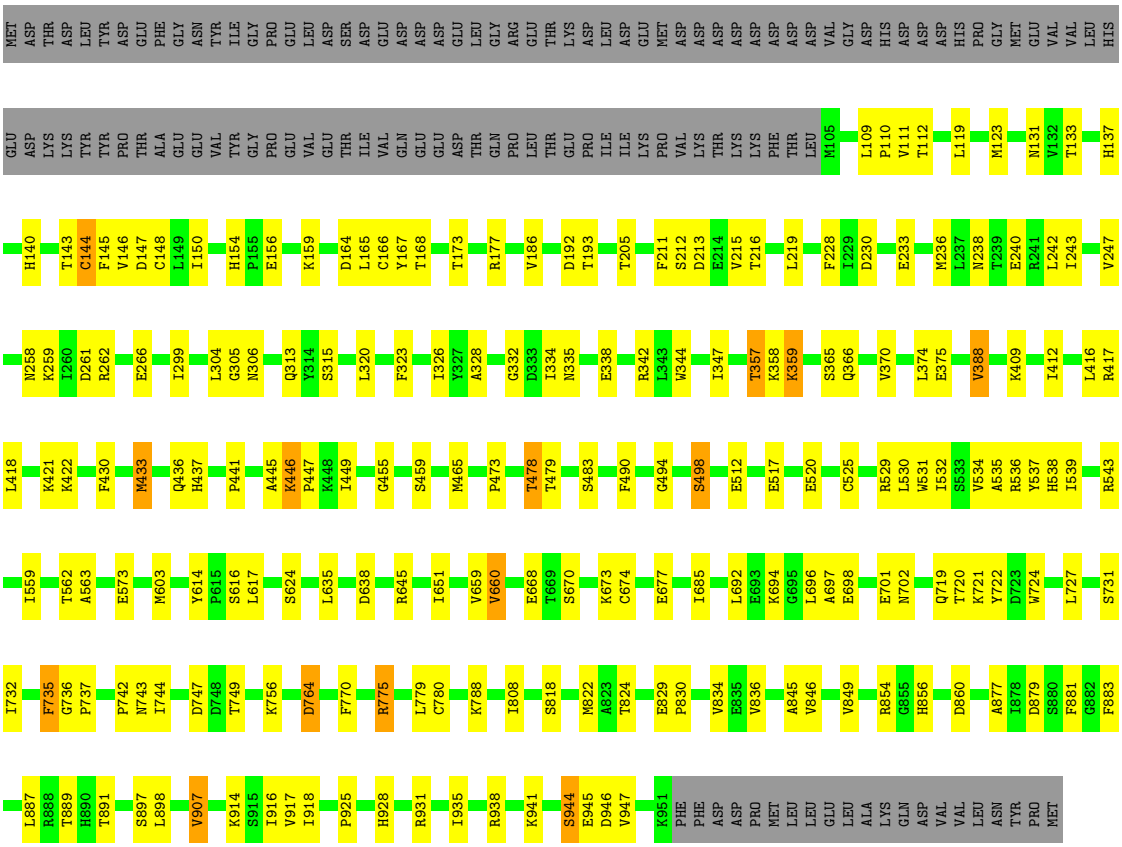




• Molecule 14: Small nuclear ribonucleoprotein-associated proteins B and B'



• Molecule 15: 116 kDa U5 small nuclear ribonucleoprotein component


MET ASP THR ASP LEU TYR ASP GLU PHE GLY ASN TYR ILE GLY PRO GLU LEU ASP SER ASP GLU ASP ASP GLU LEU GLY ARG GLU THR LYS ASP LEU ASP GLU MET ASP ASP ASP ASP ASP ASP ASP VAL GLY ASP HIS ASP ASP ASP HIS PRO GLY MET GLU VAL VAL LEU HIS
GLU ASP LYS LYS TYR TYR PRO THR ALA GLU GLU VAL TYR GLY PRO GLU VAL GLU THR ILE VAL GLN GLU GLU ASP THR GLN PRO LEU THR GLU PRO ILE ILE LYS PRO VAL LYS THR LYS LYS PHE THR LEU M105 L109 P110 V111 T112 L119 M123 N131 V132 T133 H137
H140 T143 C144 F145 V146 D147 C148 L149 I150 K159 H154 P155 E156 D164 L165 C166 Y167 T168 T173 R177 V186 D192 T193 T205 F211 S212 D213 E214 V215 T216 L219 F228 I229 D230 E233 M236 L237 N238 T239 E240 R241 L242 I243 V247
N258 K259 I260 D261 R262 E266 I299 L304 G305 N306 Q313 Y314 S315 L320 F323 I326 Y327 A328 G332 D333 I334 N335 E338 R342 L343 W344 I347 T357 K358 K359 S365 Q366 V370 L374 E375 V388 K409 I412 L416 R417
L418 K421 K422 F430 M433 Q436 H437 P441 A445 K446 P447 K448 I449 G455 S459 M465 P473 T478 T479 S483 F490 G494 S498 E512 E517 E520 C525 R529 L530 W531 I532 S533 V534 A535 R536 Y537 H538 I539 R543
I559 T562 A563 E573 M603 Y614 P615 S616 L617 S624 L635 D638 R645 I651 V659 V660 E668 T669 S670 K673 C674 E677 I685 L692 E693 K694 G695 L696 A697 E698 E701 N702 Q719 T720 K721 Y722 D723 W724 L727 S731
I732 F735 G736 P737 P742 N743 I744 D747 D748 T749 K756 D764 F770 R775 L779 C780 K788 I808 S818 M822 A823 T824 E829 P830 V834 E835 V836 A845 V846 V849 R854 G855 H856 D860 A877 I878 D879 S880 F881 G882 F883
L887 R888 T889 H890 T891 S897 L898 V907 K914 S915 I916 V917 I918 P925 H928 R931 I935 R938 K941 S944 E945 D946 V947 K951 PHE PHE ASP ASP PRO MET LEU LEU GLU LEU ALA LYS GLN ASP VAL VAL LEU ASN TYR PRO MET

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	237698	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.462	Depositor
Minimum map value	-1.224	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	526.68, 526.68, 526.68	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	F	0.28	0/898	0.61	1/1227 (0.1%)
2	A	0.33	0/17137	0.55	8/23327 (0.0%)
3	5	0.34	0/2444	0.93	9/3798 (0.2%)
4	E	0.24	0/519	0.54	0/688
5	D	0.26	0/2955	0.55	0/3773
6	G	0.24	0/1506	0.49	0/2091
7	B	0.23	0/6990	0.45	0/8734
8	i	0.22	0/323	0.49	0/402
9	k	0.23	0/335	0.50	0/417
10	l	0.22	0/307	0.49	0/382
11	m	0.24	0/291	0.49	0/362
12	n	0.23	0/296	0.50	0/367
13	j	0.23	0/390	0.48	0/484
14	h	0.24	0/290	0.50	0/359
15	C	0.40	0/6777	0.57	2/9214 (0.0%)
All	All	0.31	0/41458	0.57	20/55625 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	784	LEU	CA-CB-CG	9.26	136.59	115.30
3	5	23	C	N1-C2-O2	8.27	123.86	118.90
3	5	57	G	O4'-C1'-N9	7.79	114.43	108.20
3	5	58	U	O5'-P-OP2	-7.53	98.92	105.70
3	5	23	C	C2-N1-C1'	7.30	126.84	118.80
3	5	23	C	N3-C2-O2	-7.06	116.96	121.90
2	A	1119	ASP	CB-CG-OD1	6.68	124.31	118.30
1	F	209	MET	CA-CB-CG	5.51	122.66	113.30
3	5	22	U	N1-C2-O2	5.48	126.63	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	71	C	N1-C2-O2	5.40	122.14	118.90
15	C	144	CYS	N-CA-CB	5.29	120.12	110.60
2	A	839	LEU	CA-CB-CG	5.26	127.41	115.30
3	5	23	C	C6-N1-C1'	-5.23	114.53	120.80
2	A	997	LEU	CA-CB-CG	5.23	127.32	115.30
2	A	856	LEU	CA-CB-CG	5.21	127.29	115.30
3	5	71	C	C2-N1-C1'	5.21	124.53	118.80
15	C	860	ASP	CB-CG-OD1	5.07	122.87	118.30
2	A	1426	ASP	CB-CG-OD1	5.05	122.84	118.30
2	A	821	ARG	CA-CB-CG	5.02	124.45	113.40
2	A	1307	MET	CA-CB-CG	5.01	121.82	113.30

There are no chirality outliers.

There are no planarity outliers.

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	F	889	0	721	36	0
2	A	16709	0	15543	439	0
3	5	2192	0	1111	42	0
4	E	516	0	501	10	0
5	D	2941	0	1555	41	0
6	G	1507	0	682	8	0
7	B	6992	0	1835	13	0
8	i	324	0	85	0	0
9	k	336	0	95	0	0
10	l	308	0	83	0	0
11	m	292	0	86	0	0
12	n	297	0	84	0	0
13	j	392	0	98	0	0
14	h	292	0	78	0	0
15	C	6629	0	6607	134	0
16	C	32	0	12	1	0
All	All	40648	0	29176	679	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 10.

All (679) 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)
15:C:173:THR:O	15:C:177:ARG:HB2	1.68	0.94
2:A:200:ASP:OD1	2:A:240:ARG:NH2	2.09	0.86
2:A:370:PRO:HG2	15:C:304:LEU:HD21	1.59	0.82
2:A:1013:ASN:HA	2:A:1031:ILE:HD13	1.62	0.81
2:A:143:GLN:NE2	2:A:207:PHE:O	2.14	0.81
2:A:886:LEU:HD12	2:A:887:THR:HG23	1.64	0.79
5:D:351:ARG:HH22	5:D:355:ARG:HA	1.49	0.77
2:A:821:ARG:HH12	2:A:823:SER:HB3	1.52	0.75
1:F:168:ARG:H	1:F:222:ARG:HD2	1.52	0.74
1:F:166:LEU:O	1:F:222:ARG:NH1	2.21	0.74
2:A:147:MET:O	2:A:151:MET:HG3	1.89	0.73
2:A:469:LYS:NZ	3:5:59:G:N7	2.36	0.73
15:C:829:GLU:HG3	15:C:907:VAL:HG22	1.70	0.73
2:A:585:VAL:HG11	2:A:637:TRP:CZ2	2.24	0.72
2:A:1016:VAL:HA	2:A:1025:THR:HA	1.69	0.72
2:A:1536:LEU:O	2:A:1539:SER:OG	2.08	0.72
2:A:904:HIS:HE1	2:A:1239:ARG:HH12	1.37	0.71
2:A:781:ARG:NH2	2:A:1022:MET:HB3	2.04	0.71
2:A:1628:ASP:H	2:A:1661:TRP:HE1	1.38	0.71
15:C:140:HIS:NE2	15:C:233:GLU:OE1	2.24	0.71
2:A:461:HIS:HD2	3:5:27:U:H3	1.39	0.70
15:C:156:GLU:OE2	15:C:156:GLU:N	2.18	0.70
2:A:817:LEU:HD13	2:A:999:LEU:HD22	1.72	0.70
2:A:885:LEU:HD23	2:A:1008:TYR:HD2	1.56	0.69
2:A:1303:LEU:HD11	2:A:1542:ILE:HD13	1.73	0.69
2:A:1094:ARG:HH22	2:A:1190:CYS:H	1.37	0.69
6:G:160:ALA:HB3	6:G:166:LEU:H	1.58	0.69
2:A:549:GLU:HB3	2:A:591:MET:HG2	1.76	0.68
2:A:1701:VAL:HA	2:A:1716:GLY:HA3	1.75	0.68
5:D:351:ARG:HH12	5:D:355:ARG:HG2	1.57	0.68
15:C:685:ILE:HD11	15:C:808:ILE:HD11	1.74	0.67
2:A:1660:TYR:OH	2:A:1717:ASN:O	2.12	0.67
2:A:1577:PHE:HA	2:A:1581:LEU:HD13	1.75	0.67
15:C:573:GLU:OE1	15:C:573:GLU:N	2.28	0.67
2:A:1425:LYS:HE2	2:A:1425:LYS:H	1.58	0.67
2:A:318:TYR:O	15:C:645:ARG:NH1	2.27	0.67
2:A:1444:GLN:HG3	2:A:1445:TYR:HD1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1626:CYS:SG	2:A:1627:ALA:N	2.67	0.67
2:A:474:ARG:NH2	3:5:14:U:OP2	2.28	0.67
2:A:1005:ILE:O	2:A:1009:MET:HG2	1.95	0.66
2:A:1581:LEU:HD12	2:A:1746:ARG:HH11	1.60	0.66
2:A:1607:GLU:N	2:A:1632:PHE:O	2.27	0.66
2:A:444:ARG:NH2	5:D:281:ASP:OD2	2.28	0.66
2:A:1316:PHE:HB3	2:A:1327:MET:HG3	1.76	0.66
2:A:1622:MET:O	2:A:1687:TYR:OH	2.13	0.66
2:A:1499:GLU:N	2:A:1499:GLU:OE1	2.27	0.66
2:A:150:MET:HE2	2:A:193:LEU:HD12	1.77	0.66
2:A:292:ASP:OD2	2:A:1130:ASN:ND2	2.27	0.66
15:C:887:LEU:O	15:C:891:THR:OG1	2.12	0.66
2:A:1123:GLU:N	2:A:1123:GLU:OE2	2.29	0.66
2:A:170:ASP:OD1	2:A:171:ASP:N	2.29	0.66
2:A:341:LYS:O	5:D:301:ARG:NH1	2.28	0.66
2:A:879:SER:HB2	2:A:883:ARG:HH21	1.61	0.66
15:C:215:VAL:HG11	15:C:242:LEU:HD22	1.78	0.66
2:A:1730:MET:SD	2:A:1730:MET:N	2.69	0.65
2:A:158:ARG:HG2	5:D:372:ILE:HG12	1.77	0.65
1:F:165:LEU:HG	1:F:222:ARG:HH12	1.61	0.65
2:A:1544:ARG:HG2	2:A:1546:ASN:H	1.62	0.65
2:A:820:ARG:NH1	2:A:1063:GLY:O	2.23	0.65
15:C:674:CYS:SG	15:C:818:SER:OG	2.53	0.65
15:C:146:VAL:HG11	15:C:186:VAL:HG21	1.79	0.65
1:F:206:ALA:O	1:F:210:VAL:HG23	1.97	0.64
2:A:530:LEU:HD22	2:A:534:GLU:HB3	1.79	0.64
2:A:950:LEU:HD12	2:A:1379:PHE:CD1	2.33	0.64
2:A:1179:SER:O	2:A:1201:ARG:NH2	2.19	0.64
15:C:335:ASN:ND2	15:C:338:GLU:OE1	2.30	0.64
15:C:517:GLU:N	15:C:517:GLU:OE2	2.31	0.64
2:A:156:ARG:NH1	2:A:157:ASP:OD1	2.31	0.64
2:A:1589:ILE:HA	2:A:1733:ILE:HD11	1.80	0.64
2:A:1425:LYS:HE2	2:A:1425:LYS:N	2.13	0.64
2:A:2103:THR:HB	2:A:2139:VAL:HG23	1.80	0.63
15:C:359:LYS:HE3	15:C:359:LYS:HA	1.80	0.63
15:C:692:LEU:HD12	15:C:788:LYS:HB2	1.80	0.63
2:A:97:HIS:ND1	2:A:649:GLU:OE2	2.22	0.63
15:C:366:GLN:NE2	15:C:375:GLU:OE2	2.31	0.63
2:A:825:ILE:HB	2:A:1001:VAL:HA	1.81	0.63
2:A:974:ASN:OD1	2:A:1100:ARG:NH1	2.32	0.63
2:A:1094:ARG:NH2	2:A:1190:CYS:H	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2196:HIS:HD2	2:A:2230:LEU:HD22	1.63	0.63
2:A:171:ASP:OD2	2:A:523:ASN:ND2	2.31	0.63
2:A:832:TYR:HB3	2:A:835:ASP:HB3	1.81	0.63
2:A:485:THR:OG1	2:A:486:LYS:N	2.31	0.62
2:A:2207:ASP:HB3	2:A:2210:LYS:HG2	1.80	0.62
15:C:603:MET:HB2	15:C:651:ILE:HD11	1.81	0.62
1:F:165:LEU:HG	1:F:222:ARG:NH1	2.13	0.62
2:A:857:ASN:H	2:A:860:GLN:HB2	1.63	0.62
2:A:1579:ALA:O	2:A:1584:LYS:NZ	2.29	0.62
1:F:164:LEU:O	1:F:198:ARG:NH2	2.32	0.62
2:A:2086:ARG:NH1	2:A:2219:THR:O	2.32	0.62
2:A:923:ASP:OD2	2:A:1439:ARG:NH1	2.27	0.62
15:C:512:GLU:OE1	15:C:562:THR:OG1	2.18	0.62
2:A:1687:TYR:O	2:A:1693:SER:OG	2.16	0.62
2:A:608:LEU:HD13	2:A:632:ALA:HB1	1.81	0.62
3:5:17:U:H3	3:5:60:G:H1	1.48	0.62
5:D:361:LYS:HD3	5:D:362:LEU:HD22	1.82	0.62
2:A:1141:ARG:H	2:A:1182:ASN:ND2	1.97	0.62
15:C:473:PRO:O	15:C:498:SER:OG	2.13	0.62
2:A:1002:ASP:OD2	2:A:1004:ASN:ND2	2.33	0.62
2:A:157:ASP:OD2	5:D:368:ARG:NH2	2.22	0.61
15:C:780:CYS:O	15:C:941:LYS:NZ	2.33	0.61
2:A:885:LEU:HD22	2:A:1005:ILE:HD12	1.82	0.61
2:A:2278:SER:OG	2:A:2309:HIS:NE2	2.25	0.61
15:C:133:THR:HG21	15:C:219:LEU:HD23	1.80	0.61
4:E:113:ASP:OD1	4:E:113:ASP:N	2.33	0.61
2:A:784:LEU:HB2	2:A:1024:HIS:NE2	2.16	0.61
2:A:1612:GLU:HG2	2:A:1627:ALA:HB3	1.81	0.61
2:A:946:GLU:HB2	2:A:950:LEU:HD22	1.83	0.61
2:A:1576:ILE:HG23	2:A:1577:PHE:HD1	1.65	0.61
5:D:370:TRP:HB3	5:D:374:ARG:HH12	1.66	0.61
2:A:2105:ILE:HG12	2:A:2262:LEU:HD21	1.82	0.61
2:A:2197:ALA:HA	2:A:2200:MET:HG2	1.83	0.61
2:A:1482:GLU:OE1	2:A:1483:GLY:N	2.35	0.60
2:A:343:GLU:N	2:A:343:GLU:OE1	2.33	0.60
2:A:837:LYS:HA	2:A:840:ILE:HD12	1.83	0.60
5:D:370:TRP:O	5:D:374:ARG:HG2	2.02	0.60
15:C:834:VAL:HG11	15:C:883:PHE:HE2	1.67	0.60
15:C:144:CYS:SG	15:C:147:ASP:HB2	2.41	0.60
2:A:1426:ASP:O	2:A:1429:THR:N	2.34	0.60
3:5:47:A:O2'	3:5:48:A:O5'	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:56:C:H2'	3:5:57:G:H5'	1.84	0.60
2:A:1365:ILE:HG12	2:A:1366:PRO:HD2	1.83	0.59
5:D:361:LYS:HD3	5:D:362:LEU:H	1.66	0.59
2:A:2188:LEU:O	2:A:2251:TYR:OH	2.18	0.59
4:E:154:GLU:HA	4:E:157:TRP:HD1	1.67	0.59
2:A:112:GLN:HE21	2:A:189:GLU:HA	1.67	0.59
5:D:341:ARG:HH22	5:D:342:LYS:HE2	1.68	0.59
2:A:790:ARG:HH22	2:A:1028:TYR:HB3	1.67	0.59
2:A:1384:ARG:HH11	2:A:2220:PRO:HB2	1.68	0.59
2:A:1676:ILE:HD13	2:A:1706:ASP:HB2	1.84	0.59
2:A:470:ARG:HB2	4:E:115:ARG:HG3	1.84	0.58
2:A:2214:ILE:HG12	2:A:2227:ALA:HB2	1.85	0.58
2:A:494:LEU:HD21	2:A:562:VAL:HG21	1.86	0.58
2:A:1576:ILE:HG23	2:A:1577:PHE:CD1	2.38	0.58
5:D:352:TRP:O	5:D:355:ARG:NE	2.33	0.58
2:A:381:PRO:HD2	15:C:334:ILE:HG22	1.85	0.58
2:A:436:PRO:HG2	2:A:439:GLN:HG3	1.84	0.58
2:A:888:GLN:OE1	2:A:889:ARG:N	2.35	0.58
2:A:164:MET:HG2	2:A:569:VAL:HG11	1.85	0.58
2:A:2278:SER:HG	2:A:2309:HIS:CD2	2.18	0.58
3:5:17:U:H2'	3:5:18:C:C6	2.38	0.58
2:A:1300:LYS:HG2	2:A:1311:PHE:CD2	2.38	0.58
2:A:1570:LYS:O	2:A:1574:ILE:HG22	2.03	0.58
2:A:1497:THR:OG1	2:A:1499:GLU:OE1	2.16	0.58
15:C:144:CYS:O	15:C:148:CYS:SG	2.62	0.58
2:A:780:THR:O	2:A:784:LEU:HD23	2.04	0.58
2:A:805:GLU:O	2:A:809:VAL:HG12	2.04	0.58
2:A:835:ASP:O	2:A:839:LEU:HD12	2.03	0.58
15:C:165:LEU:HD12	15:C:167:TYR:HB2	1.86	0.57
2:A:2193:VAL:HG23	2:A:2230:LEU:HD11	1.86	0.57
15:C:166:CYS:O	15:C:168:THR:N	2.37	0.57
2:A:2149:PRO:HB3	2:A:2281:TYR:CE1	2.38	0.57
15:C:145:PHE:HE2	15:C:430:PHE:CD1	2.22	0.57
2:A:1434:LYS:O	2:A:1439:ARG:NH2	2.35	0.57
2:A:1637:TRP:N	2:A:1657:THR:O	2.38	0.57
15:C:436:GLN:OE1	15:C:437:HIS:NE2	2.38	0.57
1:F:169:GLU:OE2	1:F:174:ALA:N	2.38	0.57
2:A:776:LEU:O	2:A:780:THR:HG23	2.03	0.57
2:A:946:GLU:CB	2:A:950:LEU:HD22	2.35	0.57
2:A:1304:ASN:OD1	2:A:1305:SER:N	2.38	0.57
15:C:159:LYS:HA	15:C:165:LEU:HD23	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:488:ASP:OD1	2:A:489:TRP:N	2.38	0.56
15:C:258:ASN:OD1	15:C:259:LYS:N	2.39	0.56
2:A:252:ASP:OD1	2:A:252:ASP:N	2.37	0.56
2:A:511:LYS:HB2	2:A:513:LEU:HG	1.86	0.56
1:F:161:LEU:HD11	1:F:225:LEU:HD22	1.86	0.56
2:A:850:TYR:HE1	2:A:860:GLN:HG2	1.71	0.56
2:A:1403:LEU:HD13	2:A:1408:LEU:HD11	1.87	0.56
15:C:110:PRO:HD2	15:C:537:TYR:CE2	2.41	0.56
15:C:213:ASP:OD2	15:C:616:SER:OG	2.17	0.56
6:G:197:LEU:H	6:G:212:GLY:HA2	1.69	0.56
2:A:1587:GLU:O	2:A:1591:MET:HG3	2.06	0.56
2:A:839:LEU:O	2:A:843:LEU:HD12	2.06	0.55
2:A:903:SER:OG	2:A:904:HIS:ND1	2.40	0.55
2:A:1283:GLU:N	2:A:1283:GLU:OE1	2.36	0.55
2:A:1342:TRP:NE1	2:A:1353:PHE:HB2	2.21	0.55
3:5:66:A:HO2'	3:5:67:A:H8	1.55	0.55
2:A:1193:GLU:HB3	2:A:1231:ARG:HB2	1.89	0.55
2:A:1251:SER:O	2:A:1254:THR:HG23	2.05	0.55
2:A:1264:ASN:ND2	2:A:1326:GLY:O	2.33	0.55
5:D:316:GLN:HE22	5:D:318:ARG:HA	1.70	0.55
15:C:559:ILE:HG21	15:C:563:ALA:HB2	1.87	0.55
15:C:677:GLU:N	15:C:677:GLU:OE1	2.40	0.55
1:F:210:VAL:HG13	1:F:215:LEU:HA	1.87	0.55
2:A:357:ASN:OD1	5:D:327:ARG:NH2	2.39	0.55
2:A:1094:ARG:HH22	2:A:1190:CYS:N	2.03	0.55
2:A:1602:ASP:OD1	2:A:1602:ASP:N	2.35	0.55
2:A:876:GLU:OE1	2:A:880:ARG:NH1	2.31	0.55
3:5:109:G:H2'	3:5:110:C:C6	2.42	0.55
2:A:1047:VAL:HG12	2:A:1048:MET:HE3	1.89	0.55
1:F:123:ILE:O	1:F:127:LYS:N	2.37	0.54
1:F:71:VAL:HG21	2:A:1574:ILE:HG23	1.88	0.54
2:A:1276:GLU:OE1	2:A:1375:TRP:N	2.40	0.54
15:C:737:PRO:O	15:C:775:ARG:NH2	2.40	0.54
15:C:846:VAL:HG22	15:C:887:LEU:HD11	1.88	0.54
15:C:946:ASP:OD1	15:C:947:VAL:N	2.38	0.54
1:F:71:VAL:HG23	2:A:1575:GLN:HB2	1.89	0.54
2:A:1384:ARG:HD2	2:A:1384:ARG:C	2.27	0.54
15:C:186:VAL:HG22	15:C:535:ALA:HB2	1.89	0.54
1:F:66:LEU:HD21	1:F:101:PHE:HD2	1.72	0.54
1:F:95:GLU:N	1:F:95:GLU:OE1	2.40	0.54
2:A:904:HIS:CE1	2:A:1239:ARG:HH12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:19:A:N3	3:5:21:A:N6	2.56	0.54
2:A:1730:MET:HA	2:A:1733:ILE:HG22	1.90	0.54
2:A:1560:ILE:HD11	2:A:1668:TRP:CD1	2.43	0.54
2:A:2146:VAL:HG11	2:A:2164:PRO:HB3	1.89	0.54
2:A:881:ILE:HG12	2:A:918:THR:HA	1.89	0.53
2:A:1573:LEU:HA	2:A:1576:ILE:HG22	1.90	0.53
15:C:357:THR:OG1	15:C:359:LYS:O	2.26	0.53
1:F:165:LEU:O	1:F:222:ARG:NH2	2.39	0.53
1:F:105:GLY:HA3	2:A:1532:ARG:HD2	1.88	0.53
2:A:1404:THR:OG1	2:A:1407:ASP:OD2	2.24	0.53
2:A:2181:GLN:HB2	2:A:2217:SER:HA	1.91	0.53
2:A:939:TRP:NE1	2:A:1049:ASP:OD2	2.39	0.53
4:E:116:ARG:HE	4:E:119:ARG:HD2	1.73	0.53
1:F:168:ARG:N	1:F:222:ARG:HD2	2.22	0.53
2:A:835:ASP:OD1	2:A:836:THR:N	2.42	0.53
2:A:1537:TRP:HB2	2:A:1751:LEU:HD22	1.91	0.53
3:5:111:A:H2'	3:5:112:A:C8	2.43	0.53
1:F:102:ASP:OD1	1:F:106:ASN:N	2.29	0.53
2:A:429:ASN:OD1	2:A:432:ARG:NH1	2.41	0.53
5:D:320:TYR:O	5:D:324:MET:HG2	2.09	0.53
2:A:178:TYR:HB2	2:A:494:LEU:HD12	1.90	0.53
2:A:648:LEU:O	2:A:652:LEU:HD13	2.08	0.53
2:A:881:ILE:HG23	2:A:918:THR:HG23	1.89	0.53
2:A:885:LEU:HD23	2:A:1008:TYR:CD2	2.41	0.53
2:A:1032:ARG:HD3	2:A:1445:TYR:CE2	2.43	0.53
2:A:1342:TRP:HB2	2:A:1486:GLU:HB2	1.91	0.53
15:C:144:CYS:SG	15:C:144:CYS:O	2.67	0.53
15:C:145:PHE:CG	15:C:228:PHE:HZ	2.27	0.53
15:C:614:TYR:HB2	15:C:617:LEU:HB2	1.90	0.53
3:5:7:U:H3'	3:5:8:G:H8	1.74	0.53
15:C:749:THR:O	15:C:756:LYS:NZ	2.36	0.53
3:5:12:U:H3	3:5:65:G:H1	1.58	0.52
3:5:69:A:H2'	3:5:70:A:O4'	2.09	0.52
3:5:67:A:H2'	3:5:68:C:C6	2.44	0.52
15:C:150:ILE:O	15:C:154:HIS:HB2	2.09	0.52
15:C:724:TRP:HZ3	15:C:732:ILE:HD11	1.74	0.52
2:A:651:TRP:CE3	2:A:652:LEU:HD12	2.44	0.52
5:D:370:TRP:HB3	5:D:374:ARG:NH1	2.25	0.52
15:C:243:ILE:O	15:C:247:VAL:HG13	2.08	0.52
2:A:837:LYS:HD2	2:A:1429:THR:HG23	1.90	0.52
15:C:829:GLU:OE2	15:C:854:ARG:NH1	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:63:A:H2'	3:5:64:G:H8	1.73	0.52
2:A:1410:ASP:OD1	2:A:1410:ASP:N	2.41	0.52
3:5:63:A:H2'	3:5:64:G:C8	2.45	0.52
2:A:1031:ILE:HG22	2:A:1033:GLY:H	1.74	0.52
3:5:110:C:H2'	3:5:111:A:H8	1.75	0.52
15:C:836:VAL:HG22	15:C:897:SER:HB3	1.91	0.52
5:D:344:ARG:O	5:D:344:ARG:HD3	2.09	0.51
7:B:526:ASN:O	7:B:529:GLY:N	2.44	0.51
15:C:144:CYS:HA	15:C:147:ASP:CG	2.31	0.51
2:A:992:LEU:O	2:A:996:LEU:HD23	2.10	0.51
2:A:1107:ARG:O	2:A:1111:GLN:NE2	2.36	0.51
2:A:2103:THR:O	2:A:2140:LYS:N	2.33	0.51
2:A:2125:ALA:HB3	2:A:2159:LEU:HD21	1.93	0.51
7:B:1225:VAL:O	7:B:1234:LEU:N	2.41	0.51
2:A:888:GLN:OE1	2:A:890:ALA:N	2.43	0.51
2:A:1447:VAL:HG12	2:A:1449:LYS:H	1.76	0.51
2:A:1582:TRP:CZ2	2:A:1666:LEU:HB2	2.45	0.51
15:C:779:LEU:O	15:C:938:ARG:NH1	2.43	0.51
2:A:1458:GLN:HE22	2:A:1463:LYS:HE2	1.75	0.51
15:C:731:SER:HB3	15:C:747:ASP:OD1	2.11	0.51
15:C:166:CYS:C	15:C:168:THR:H	2.13	0.51
2:A:979:SER:OG	2:A:980:ARG:N	2.43	0.51
2:A:1000:ILE:HD13	2:A:1001:VAL:HG13	1.93	0.51
2:A:1311:PHE:HE1	2:A:1315:VAL:HG21	1.76	0.51
15:C:212:SER:O	15:C:216:THR:HG23	2.11	0.51
2:A:214:ARG:HG3	2:A:225:TYR:CD1	2.45	0.51
2:A:1119:ASP:OD1	2:A:1119:ASP:O	2.29	0.51
2:A:1544:ARG:HD2	2:A:1546:ASN:HB2	1.92	0.51
4:E:114:GLU:HA	4:E:117:LYS:HB2	1.92	0.51
5:D:341:ARG:NH1	5:D:342:LYS:HA	2.25	0.51
15:C:478:THR:HA	15:C:494:GLY:HA3	1.93	0.51
2:A:982:GLU:OE2	2:A:1172:ASN:ND2	2.44	0.51
2:A:880:ARG:O	2:A:883:ARG:HG2	2.12	0.50
1:F:95:GLU:OE2	2:A:1570:LYS:NZ	2.39	0.50
2:A:897:GLU:O	2:A:908:VAL:N	2.41	0.50
15:C:305:GLY:O	15:C:433:MET:HG3	2.11	0.50
2:A:395:THR:HG22	2:A:396:ASP:H	1.75	0.50
2:A:595:LYS:NZ	3:5:30:A:OP1	2.44	0.50
15:C:944:SER:OG	15:C:945:GLU:N	2.44	0.50
2:A:441:VAL:O	2:A:445:VAL:HG23	2.12	0.50
2:A:1056:HIS:O	2:A:1060:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1384:ARG:HE	2:A:1385:VAL:HG23	1.77	0.50
2:A:321:ASN:O	15:C:645:ARG:NH2	2.45	0.50
2:A:1659:LYS:HZ3	2:A:1661:TRP:HB2	1.75	0.50
3:5:57:G:O2'	3:5:58:U:O5'	2.19	0.50
15:C:727:LEU:O	15:C:731:SER:OG	2.17	0.50
15:C:918:ILE:O	15:C:918:ILE:HD12	2.12	0.50
2:A:1006:ALA:O	2:A:1010:THR:OG1	2.21	0.50
3:5:51:A:H2'	3:5:52:U:C6	2.46	0.50
2:A:631:ALA:O	2:A:635:ARG:HG3	2.11	0.50
2:A:1606:ILE:HG12	2:A:1637:TRP:HZ2	1.76	0.50
2:A:1433:ASP:HB3	2:A:1460:HIS:HE1	1.77	0.50
15:C:111:VAL:N	15:C:156:GLU:OE1	2.45	0.50
15:C:483:SER:HB2	15:C:490:PHE:CE2	2.47	0.50
2:A:162:LYS:N	5:D:375:GLU:OE1	2.35	0.49
2:A:224:THR:OG1	3:5:12:U:OP1	2.16	0.49
2:A:534:GLU:N	2:A:534:GLU:OE1	2.46	0.49
2:A:1021:ASP:OD1	2:A:1022:MET:N	2.45	0.49
3:5:60:G:H2'	3:5:61:A:C8	2.46	0.49
2:A:809:VAL:O	2:A:812:THR:HG22	2.12	0.49
2:A:1503:TRP:HE1	2:A:1533:ARG:HD2	1.77	0.49
3:5:12:U:H2'	3:5:13:C:C6	2.48	0.49
5:D:341:ARG:HH12	5:D:342:LYS:HE2	1.77	0.49
15:C:455:GLY:O	15:C:459:SER:OG	2.27	0.49
15:C:701:GLU:HG3	15:C:742:PRO:HG3	1.93	0.49
2:A:825:ILE:HD12	2:A:929:GLU:HB3	1.94	0.49
3:5:34:U:H2'	3:5:35:U:C6	2.47	0.49
15:C:299:ILE:O	15:C:306:ASN:ND2	2.45	0.49
2:A:1093:ASP:N	2:A:1093:ASP:OD1	2.45	0.49
3:5:26:A:H2'	3:5:27:U:O4'	2.12	0.49
2:A:420:ARG:NH1	3:5:57:G:H5"	2.28	0.49
2:A:469:LYS:HB3	2:A:471:TYR:CE1	2.47	0.49
15:C:304:LEU:O	15:C:437:HIS:NE2	2.45	0.49
2:A:469:LYS:HB3	2:A:471:TYR:HE1	1.78	0.49
2:A:981:PHE:HB2	2:A:1093:ASP:O	2.12	0.49
2:A:293:TRP:HB2	2:A:1141:ARG:HB3	1.94	0.49
5:D:328:ARG:HG2	5:D:332:GLU:HB2	1.94	0.49
5:D:359:GLN:OE1	5:D:359:GLN:N	2.46	0.49
15:C:925:PRO:HD2	15:C:928:HIS:NE2	2.27	0.49
2:A:261:LYS:HD2	2:A:328:HIS:HB3	1.93	0.49
2:A:1645:LEU:HB2	2:A:1714:ALA:H	1.78	0.49
2:A:2124:ILE:HD12	2:A:2147:MET:HE1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:893:GLU:OE1	2:A:893:GLU:N	2.45	0.49
2:A:1382:SER:HA	2:A:1415:GLY:HA2	1.94	0.49
15:C:320:LEU:HD21	15:C:344:TRP:HB2	1.95	0.48
2:A:613:TYR:HD2	2:A:617:ASN:HD21	1.61	0.48
2:A:1342:TRP:CD1	2:A:1353:PHE:HB2	2.48	0.48
2:A:1693:SER:HB2	2:A:1695:TYR:CZ	2.48	0.48
5:D:371:ARG:HG2	5:D:374:ARG:HH21	1.77	0.48
1:F:214:ASN:OD1	1:F:216:GLY:N	2.38	0.48
2:A:2227:ALA:HB3	2:A:2261:MET:SD	2.54	0.48
7:B:537:LYS:N	7:B:608:LEU:O	2.45	0.48
7:B:1663:ILE:O	7:B:1705:MET:N	2.45	0.48
2:A:196:ASP:N	2:A:200:ASP:OD2	2.46	0.48
2:A:794:TYR:HA	2:A:800:TYR:CE1	2.48	0.48
2:A:1308:PRO:HB3	2:A:1548:TYR:CE1	2.48	0.48
2:A:1385:VAL:HG21	2:A:1414:ARG:HB3	1.95	0.48
15:C:659:VAL:HG22	15:C:660:VAL:H	1.77	0.48
2:A:530:LEU:HD22	2:A:534:GLU:CB	2.42	0.48
2:A:651:TRP:CZ3	2:A:652:LEU:HD12	2.49	0.48
2:A:1581:LEU:HD12	2:A:1746:ARG:NH1	2.26	0.48
3:5:16:U:H2'	3:5:17:U:C6	2.48	0.48
2:A:336:ASN:O	15:C:262:ARG:NH2	2.46	0.48
2:A:395:THR:HG22	2:A:396:ASP:N	2.28	0.48
15:C:697:ALA:HB1	15:C:742:PRO:HB3	1.95	0.48
2:A:181:ASN:OD1	2:A:181:ASN:N	2.47	0.48
15:C:624:SER:O	15:C:624:SER:OG	2.30	0.48
2:A:815:HIS:HA	2:A:818:GLU:OE1	2.13	0.48
2:A:1030:ILE:HG22	2:A:1032:ARG:H	1.79	0.48
15:C:144:CYS:HA	15:C:147:ASP:HB2	1.95	0.48
2:A:845:ARG:HH12	2:A:1457:HIS:CD2	2.31	0.48
2:A:1127:GLY:O	2:A:1170:TRP:NE1	2.33	0.48
2:A:1659:LYS:HE2	2:A:1696:PRO:HB2	1.96	0.48
4:E:112:MET:HA	4:E:112:MET:HE2	1.96	0.48
15:C:724:TRP:CZ3	15:C:732:ILE:HD11	2.49	0.48
1:F:175:LEU:HD13	2:A:61:MET:HE1	1.96	0.47
2:A:1399:GLN:HA	7:B:1051:SER:N	2.29	0.47
2:A:1581:LEU:O	2:A:1585:ILE:HG12	2.14	0.47
2:A:112:GLN:NE2	2:A:189:GLU:HA	2.28	0.47
2:A:1657:THR:HG21	2:A:1699:THR:HG21	1.97	0.47
2:A:152:ARG:HH22	5:D:308:ASP:HB2	1.79	0.47
2:A:804:GLU:HA	2:A:807:VAL:HG22	1.96	0.47
2:A:1582:TRP:NE1	2:A:1619:SER:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:320:TYR:OH	15:C:881:PHE:HB3	2.12	0.47
5:D:357:TRP:HB3	5:D:369:ASP:OD1	2.14	0.47
2:A:67:ARG:HD3	2:A:179:ALA:HB2	1.97	0.47
2:A:1744:ARG:O	2:A:1747:ILE:HG22	2.15	0.47
2:A:2108:LYS:HD3	2:A:2263:LEU:HD23	1.97	0.47
2:A:2280:ASN:HB3	2:A:2309:HIS:CG	2.50	0.47
7:B:1620:LEU:N	7:B:1645:VAL:O	2.46	0.47
7:B:1196:SER:O	7:B:1258:VAL:N	2.41	0.47
7:B:1347:PHE:O	7:B:1512:PHE:N	2.43	0.47
15:C:144:CYS:HA	15:C:147:ASP:CB	2.45	0.47
2:A:422:LEU:H	2:A:422:LEU:HD23	1.79	0.47
2:A:787:GLU:OE2	2:A:790:ARG:NE	2.42	0.47
2:A:795:LEU:HD12	2:A:796:LYS:HD3	1.98	0.47
2:A:1314:VAL:HG13	2:A:1478:LEU:HD13	1.96	0.47
15:C:736:GLY:N	15:C:743:ASN:O	2.48	0.47
2:A:1644:LEU:N	2:A:1647:ASP:OD2	2.41	0.46
2:A:2131:VAL:HG13	2:A:2172:MET:HG2	1.97	0.46
6:G:154:VAL:HA	6:G:171:SER:HA	1.97	0.46
15:C:720:THR:HG23	15:C:721:LYS:HD3	1.97	0.46
2:A:343:GLU:HG2	2:A:344:ASP:OD1	2.15	0.46
2:A:776:LEU:HA	2:A:779:LEU:HD12	1.98	0.46
2:A:2190:PRO:HA	2:A:2193:VAL:HG12	1.98	0.46
2:A:2281:TYR:HA	2:A:2284:MET:HE3	1.98	0.46
2:A:1991:TYR:O	2:A:1995:ASN:N	2.47	0.46
5:D:322:ASP:OD1	5:D:322:ASP:N	2.49	0.46
15:C:230:ASP:OD2	15:C:262:ARG:NH1	2.49	0.46
15:C:445:ALA:O	15:C:449:ILE:HG12	2.15	0.46
2:A:834:HIS:O	2:A:838:LEU:HD13	2.16	0.46
2:A:1391:LEU:O	2:A:1394:GLN:HG3	2.14	0.46
5:D:351:ARG:HG3	5:D:351:ARG:HH11	1.80	0.46
2:A:843:LEU:HD21	2:A:870:ALA:HB3	1.97	0.46
2:A:980:ARG:NH2	2:A:1094:ARG:HD2	2.30	0.46
3:5:60:G:H2'	3:5:61:A:H8	1.79	0.46
1:F:173:GLY:HA2	1:F:176:ARG:HB2	1.98	0.46
2:A:1487:HIS:HB3	2:A:1541:THR:HB	1.98	0.46
15:C:421:LYS:HE3	15:C:421:LYS:HB2	1.58	0.46
15:C:347:ILE:HG13	15:C:357:THR:O	2.16	0.46
2:A:817:LEU:HD13	2:A:999:LEU:CD2	2.44	0.46
2:A:887:THR:O	2:A:889:ARG:HG2	2.16	0.46
2:A:1271:MET:O	2:A:1271:MET:HG3	2.15	0.46
15:C:696:LEU:HD13	15:C:722:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:GLY:HA3	1:F:109:LEU:HD22	1.97	0.46
2:A:361:HIS:CE1	2:A:362:ARG:HG2	2.50	0.46
4:E:112:MET:HA	4:E:112:MET:CE	2.46	0.46
1:F:200:ASP:O	2:A:68:LYS:HE2	2.15	0.45
2:A:313:LYS:HZ1	5:D:253:ARG:HH22	1.64	0.45
7:B:1455:GLU:N	7:B:1490:LEU:O	2.48	0.45
15:C:520:GLU:OE2	15:C:520:GLU:N	2.45	0.45
15:C:531:TRP:HB3	15:C:538:HIS:HB3	1.98	0.45
2:A:530:LEU:HD23	2:A:530:LEU:HA	1.83	0.45
2:A:1391:LEU:HD23	2:A:1391:LEU:HA	1.85	0.45
3:5:65:G:O6	3:5:66:A:N6	2.49	0.45
5:D:361:LYS:HG3	5:D:363:ASP:OD1	2.16	0.45
2:A:899:MET:O	2:A:905:LEU:HD13	2.16	0.45
2:A:1274:PHE:O	2:A:1278:VAL:HG23	2.16	0.45
2:A:794:TYR:HA	2:A:800:TYR:HE1	1.82	0.45
2:A:899:MET:HE2	2:A:908:VAL:HG21	1.99	0.45
15:C:479:THR:HA	15:C:562:THR:HG22	1.99	0.45
2:A:719:CYS:O	2:A:723:ASN:N	2.50	0.45
2:A:922:LEU:HD12	2:A:1036:PHE:CD2	2.52	0.45
2:A:2107:PRO:HG2	2:A:2110:VAL:HG22	1.98	0.45
2:A:2164:PRO:HB3	2:A:2296:LEU:HD11	1.98	0.45
2:A:2303:GLU:O	2:A:2309:HIS:ND1	2.48	0.45
15:C:668:GLU:OE1	15:C:824:THR:OG1	2.28	0.45
2:A:120:TYR:HE2	2:A:485:THR:HG22	1.82	0.45
15:C:192:ASP:OD1	15:C:193:THR:N	2.47	0.45
2:A:374:ASP:N	2:A:374:ASP:OD1	2.48	0.45
2:A:788:GLN:OE1	2:A:1024:HIS:HB3	2.16	0.45
2:A:823:SER:OG	2:A:933:ARG:NH1	2.48	0.45
2:A:896:ILE:HA	2:A:908:VAL:O	2.17	0.45
2:A:1422:LEU:HD12	2:A:1427:ARG:HH21	1.82	0.45
2:A:1533:ARG:HD3	2:A:1752:GLN:OE1	2.15	0.45
15:C:670:SER:HB2	15:C:822:MET:HB2	1.97	0.45
15:C:674:CYS:SG	15:C:822:MET:HG3	2.57	0.45
15:C:830:PRO:HG2	15:C:877:ALA:HB3	1.99	0.45
2:A:2187:GLN:HB2	2:A:2256:TYR:OH	2.17	0.45
6:G:213:ILE:HA	6:G:237:SER:HA	1.98	0.45
2:A:1659:LYS:HD2	2:A:1660:TYR:N	2.31	0.45
1:F:210:VAL:HA	1:F:214:ASN:O	2.17	0.44
15:C:137:HIS:HA	15:C:238:ASN:HB3	2.00	0.44
2:A:308:ILE:HD12	2:A:320:TYR:HE1	1.81	0.44
2:A:1426:ASP:OD1	2:A:1429:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2106:LEU:HD12	2:A:2107:PRO:HD2	2.00	0.44
2:A:1146:ASP:OD2	2:A:1181:ASP:HB2	2.16	0.44
2:A:1341:ARG:HG2	2:A:1354:ARG:HG3	1.98	0.44
15:C:143:THR:HG22	15:C:147:ASP:OD2	2.18	0.44
1:F:200:ASP:N	1:F:200:ASP:OD1	2.43	0.44
2:A:409:ARG:HG3	2:A:410:PRO:HA	2.00	0.44
3:5:17:U:H2'	3:5:18:C:H6	1.82	0.44
7:B:755:GLY:O	7:B:758:SER:N	2.50	0.44
1:F:90:PHE:O	2:A:1574:ILE:HD12	2.18	0.44
2:A:997:LEU:HG	2:A:1000:ILE:HD11	2.00	0.44
2:A:1051:LEU:HD12	2:A:1162:PRO:HD3	2.00	0.44
2:A:1251:SER:HB2	2:A:1259:ILE:HD11	1.99	0.44
2:A:464:PRO:HG2	3:5:23:C:C6	2.52	0.44
2:A:895:GLY:HA2	2:A:1018:ASN:O	2.16	0.44
2:A:913:PRO:HA	2:A:916:LYS:HB2	1.99	0.44
2:A:988:ILE:HG12	2:A:1044:TYR:CE2	2.52	0.44
2:A:2207:ASP:H	2:A:2210:LYS:HZ2	1.66	0.44
2:A:912:GLU:OE1	2:A:914:LEU:HB2	2.17	0.44
2:A:1577:PHE:HE2	2:A:1582:TRP:CE3	2.36	0.44
2:A:2280:ASN:ND2	2:A:2304:PHE:O	2.49	0.44
3:5:76:A:H2'	3:5:77:G:C8	2.53	0.44
2:A:1018:ASN:HB2	2:A:1023:ASN:HB3	2.00	0.44
3:5:48:A:H2'	3:5:49:A:H8	1.83	0.44
5:D:341:ARG:HH11	5:D:345:LYS:HE3	1.82	0.44
1:F:120:LEU:HD22	2:A:539:ARG:HD2	2.00	0.44
2:A:613:TYR:HD2	2:A:617:ASN:ND2	2.15	0.44
2:A:986:GLU:OE1	2:A:986:GLU:N	2.44	0.44
2:A:1416:ILE:HD13	2:A:1416:ILE:HA	1.87	0.44
2:A:1661:TRP:CD1	2:A:1662:ILE:N	2.86	0.44
15:C:236:MET:O	15:C:240:GLU:HG3	2.18	0.44
15:C:534:VAL:HG12	15:C:535:ALA:H	1.82	0.44
2:A:950:LEU:HD12	2:A:1379:PHE:CE1	2.53	0.43
2:A:1088:PHE:CD1	2:A:1097:ILE:HG12	2.53	0.43
2:A:2149:PRO:HB2	2:A:2292:MET:HE3	2.00	0.43
2:A:491:GLU:O	2:A:495:GLN:HG3	2.18	0.43
2:A:944:ASP:N	2:A:944:ASP:OD1	2.51	0.43
2:A:1116:GLU:HG2	2:A:1117:HIS:CD2	2.53	0.43
2:A:1621:LYS:N	2:A:1622:MET:HE3	2.33	0.43
2:A:1779:PHE:O	2:A:1809:ILE:HA	2.17	0.43
2:A:445:VAL:HG22	5:D:281:ASP:HB2	2.00	0.43
2:A:899:MET:HE1	2:A:1448:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1342:TRP:CH2	2:A:1344:LYS:HB2	2.53	0.43
4:E:113:ASP:HB2	4:E:120:ARG:NH2	2.33	0.43
5:D:366:THR:OG1	5:D:367:ASP:N	2.51	0.43
2:A:188:LEU:HD11	2:A:567:GLY:HA2	2.01	0.43
2:A:960:ASN:OD1	2:A:1225:THR:OG1	2.34	0.43
2:A:1342:TRP:CZ3	2:A:1344:LYS:HB2	2.53	0.43
15:C:446:LYS:HB3	15:C:447:PRO:HD3	2.00	0.43
2:A:839:LEU:HD11	2:A:878:LEU:HG	2.00	0.43
2:A:1396:ALA:HA	2:A:1399:GLN:HB2	2.01	0.43
2:A:1606:ILE:HG12	2:A:1637:TRP:CZ2	2.54	0.43
2:A:2133:PRO:HD2	2:A:2139:VAL:HG13	2.00	0.43
3:5:8:G:C2'	3:5:9:G:H5'	2.49	0.43
15:C:205:THR:HB	15:C:215:VAL:HG22	1.99	0.43
15:C:537:TYR:HD1	15:C:537:TYR:H	1.67	0.43
15:C:698:GLU:O	15:C:702:ASN:HB2	2.19	0.43
2:A:2086:ARG:NH1	2:A:2222:SER:O	2.47	0.43
15:C:370:VAL:HA	15:C:374:LEU:HB2	2.00	0.43
2:A:176:LEU:HD23	2:A:181:ASN:ND2	2.34	0.43
2:A:1318:THR:HB	2:A:1324:GLY:HA3	2.00	0.43
15:C:137:HIS:CE1	15:C:898:LEU:HD12	2.54	0.43
2:A:275:GLY:H	5:D:282:THR:HB	1.84	0.43
2:A:449:LYS:HD3	2:A:449:LYS:HA	1.84	0.43
2:A:919:ASP:N	2:A:919:ASP:OD1	2.52	0.43
2:A:1223:GLU:HA	2:A:1224:ARG:NH2	2.33	0.43
2:A:106:MET:HE2	2:A:578:LEU:HD13	2.01	0.43
2:A:430:TRP:HB3	2:A:611:LEU:HD11	2.00	0.43
2:A:950:LEU:HD21	2:A:954:LYS:HE3	2.01	0.43
2:A:1103:ALA:O	2:A:1107:ARG:HG3	2.19	0.43
2:A:1222:LYS:NZ	2:A:2088:ASN:O	2.39	0.43
2:A:1459:ARG:HG3	2:A:1459:ARG:HH11	1.83	0.43
2:A:2115:ILE:O	2:A:2118:SER:OG	2.36	0.43
5:D:324:MET:O	5:D:328:ARG:HB2	2.19	0.43
7:B:1299:THR:N	7:B:1513:ASN:O	2.46	0.43
2:A:833:LYS:HE3	2:A:834:HIS:HE1	1.84	0.43
2:A:1320:LYS:HA	2:A:1324:GLY:O	2.19	0.43
2:A:1607:GLU:HB2	2:A:1634:SER:N	2.34	0.43
2:A:1728:GLN:O	2:A:1732:LYS:HG2	2.18	0.43
15:C:164:ASP:OD1	15:C:164:ASP:N	2.46	0.43
2:A:318:TYR:HB2	15:C:638:ASP:OD1	2.19	0.42
2:A:722:ALA:HA	2:A:1022:MET:HB2	2.00	0.42
2:A:841:LEU:HD21	2:A:1429:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2188:LEU:HD13	2:A:2228:TYR:CD1	2.54	0.42
3:5:22:U:O2	3:5:22:U:H2'	2.19	0.42
15:C:374:LEU:HA	15:C:374:LEU:HD23	1.82	0.42
1:F:205:LEU:HA	1:F:208:GLN:OE1	2.19	0.42
2:A:513:LEU:HD13	2:A:516:LEU:HD12	2.00	0.42
2:A:1600:GLU:HG2	2:A:1725:LEU:HD13	2.01	0.42
2:A:1623:ASN:OD1	2:A:1624:SER:N	2.52	0.42
5:D:287:ASN:O	5:D:291:LYS:HG3	2.19	0.42
2:A:89:LEU:HD21	2:A:506:LEU:HD11	2.01	0.42
2:A:251:ASP:HB3	2:A:253:ASN:H	1.84	0.42
2:A:279:PHE:HE2	2:A:456:LEU:HG	1.84	0.42
2:A:462:ARG:HG3	2:A:463:PRO:HD2	2.02	0.42
2:A:809:VAL:HG22	2:A:996:LEU:HD11	2.01	0.42
2:A:901:LEU:HD22	2:A:901:LEU:H	1.84	0.42
2:A:1275:ARG:HH22	2:A:1464:LEU:HB3	1.85	0.42
2:A:1311:PHE:CD1	2:A:1312:PRO:HD2	2.54	0.42
2:A:2273:VAL:HG22	2:A:2274:PRO:HD2	2.02	0.42
5:D:328:ARG:HB3	5:D:333:LYS:HG3	2.01	0.42
6:G:196:VAL:HA	6:G:212:GLY:HA3	2.00	0.42
2:A:685:LEU:HA	4:E:138:ILE:HD13	2.01	0.42
2:A:785:LYS:O	2:A:789:GLU:HG2	2.19	0.42
2:A:911:VAL:HG12	2:A:916:LYS:HG3	2.01	0.42
2:A:1188:ASN:C	2:A:1188:ASN:HD22	2.21	0.42
2:A:1384:ARG:NE	2:A:1385:VAL:HG23	2.33	0.42
6:G:123:MET:HA	6:G:137:ASP:HA	2.00	0.42
15:C:133:THR:HG21	15:C:219:LEU:CD2	2.48	0.42
1:F:209:MET:HG3	1:F:217:VAL:CG2	2.50	0.42
2:A:93:LYS:HB3	2:A:93:LYS:HE3	1.86	0.42
2:A:406:TRP:CZ2	15:C:266:GLU:HG2	2.55	0.42
2:A:425:PRO:HB2	2:A:428:LYS:HB2	2.01	0.42
2:A:563:GLN:NE2	2:A:568:ASN:OD1	2.51	0.42
2:A:1426:ASP:HB3	2:A:1459:ARG:NH2	2.34	0.42
2:A:1663:ASP:HB3	2:A:1702:LEU:HA	2.01	0.42
2:A:1806:ALA:HA	2:A:1820:LYS:O	2.19	0.42
3:5:113:G:H2'	3:5:114:G:H8	1.84	0.42
7:B:1377:VAL:O	7:B:1452:VAL:N	2.46	0.42
15:C:328:ALA:O	15:C:332:GLY:HA2	2.19	0.42
15:C:412:ILE:HD13	15:C:412:ILE:HA	1.88	0.42
2:A:1414:ARG:NH1	2:A:1414:ARG:HG3	2.33	0.42
15:C:735:PHE:HD1	15:C:735:PHE:HA	1.69	0.42
15:C:845:ALA:O	15:C:849:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:ASP:OD1	1:F:105:GLY:N	2.52	0.42
1:F:165:LEU:HD11	1:F:170:THR:O	2.20	0.42
2:A:134:TRP:HZ2	3:5:58:U:OP2	2.02	0.42
2:A:380:LEU:HA	2:A:380:LEU:HD12	1.82	0.42
2:A:888:GLN:HG3	2:A:891:PHE:CE1	2.54	0.42
2:A:1077:ILE:HD12	2:A:1078:ALA:N	2.34	0.42
2:A:1109:LEU:HG	2:A:1152:ALA:HB1	2.01	0.42
5:D:366:THR:HG23	5:D:369:ASP:H	1.84	0.42
2:A:544:PHE:HA	2:A:651:TRP:CH2	2.55	0.42
2:A:1504:GLU:N	2:A:1504:GLU:OE1	2.53	0.42
2:A:2196:HIS:CG	2:A:2213:ILE:HD11	2.55	0.42
15:C:211:PHE:HE2	15:C:635:LEU:HD23	1.85	0.42
15:C:719:GLN:HG2	15:C:724:TRP:O	2.20	0.42
2:A:902:TYR:HB2	2:A:1242:ASN:CG	2.40	0.42
2:A:1090:ARG:HG2	2:A:1091:TYR:O	2.19	0.42
2:A:1344:LYS:HA	2:A:1491:LYS:NZ	2.35	0.42
2:A:1565:LYS:HB3	2:A:1565:LYS:HE2	1.73	0.42
7:B:1404:LYS:O	7:B:1423:ASN:N	2.47	0.42
15:C:532:ILE:HD13	15:C:532:ILE:HA	1.88	0.42
2:A:950:LEU:CD2	2:A:954:LYS:HE3	2.50	0.42
2:A:1241:HIS:HE1	2:A:1290:LYS:HE2	1.84	0.42
2:A:1343:SER:OG	2:A:1352:HIS:ND1	2.48	0.42
15:C:313:GLN:HB2	16:C:1001:GTP:C6	2.55	0.42
2:A:152:ARG:NH2	5:D:308:ASP:HB2	2.35	0.41
2:A:944:ASP:HB3	2:A:1436:TRP:NE1	2.35	0.41
2:A:1218:ASN:OD1	2:A:1220:VAL:HG22	2.20	0.41
2:A:1341:ARG:HD3	2:A:1352:HIS:HB3	2.01	0.41
3:5:37:G:N2	3:5:44:A:N3	2.68	0.41
3:5:112:A:H2'	3:5:113:G:C8	2.55	0.41
2:A:2127:TYR:HE2	2:A:2148:VAL:HG21	1.85	0.41
2:A:1612:GLU:HB2	2:A:1630:LEU:HD21	2.02	0.41
15:C:388:VAL:HG11	15:C:412:ILE:HD11	2.01	0.41
2:A:1194:CYS:HB3	2:A:1228:CYS:SG	2.60	0.41
2:A:1458:GLN:NE2	2:A:1463:LYS:HE2	2.35	0.41
5:D:378:SER:OG	5:D:630:GLY:O	2.37	0.41
15:C:537:TYR:CE2	15:C:539:ILE:HD11	2.56	0.41
15:C:692:LEU:HD11	15:C:744:ILE:HG13	2.03	0.41
2:A:902:TYR:HB2	2:A:1242:ASN:ND2	2.36	0.41
2:A:1392:LYS:O	2:A:1395:GLU:HG3	2.20	0.41
2:A:1548:TYR:HB3	2:A:1551:PHE:CE2	2.55	0.41
2:A:1576:ILE:HD11	2:A:1746:ARG:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2093:SER:HB3	2:A:2258:ARG:NH2	2.36	0.41
6:G:58:PRO:O	6:G:60:MET:N	2.53	0.41
2:A:310:THR:O	2:A:314:ILE:HG12	2.20	0.41
2:A:1443:LYS:HA	2:A:1443:LYS:HD3	1.88	0.41
2:A:1482:GLU:H	2:A:1482:GLU:HG3	1.53	0.41
2:A:2149:PRO:HB2	2:A:2292:MET:CE	2.51	0.41
5:D:290:TYR:CE2	15:C:889:THR:HG21	2.54	0.41
15:C:418:LEU:O	15:C:422:LYS:HG2	2.20	0.41
15:C:736:GLY:HA2	15:C:743:ASN:HB2	2.03	0.41
2:A:461:HIS:HD2	3:5:27:U:N3	2.12	0.41
2:A:1384:ARG:NH1	2:A:2220:PRO:HB2	2.34	0.41
2:A:1414:ARG:HG3	2:A:1414:ARG:HH11	1.86	0.41
2:A:2163:LEU:HD21	2:A:2206:TRP:NE1	2.35	0.41
2:A:2183:ASN:OD1	2:A:2183:ASN:N	2.53	0.41
15:C:529:ARG:O	15:C:530:LEU:HD23	2.21	0.41
15:C:916:ILE:HD12	15:C:928:HIS:ND1	2.36	0.41
2:A:344:ASP:OD1	5:D:339:ARG:NE	2.53	0.41
2:A:1321:GLU:HG2	2:A:1322:LEU:HD12	2.02	0.41
2:A:1582:TRP:NE1	2:A:1666:LEU:HD12	2.36	0.41
2:A:1593:LEU:HD12	2:A:1629:ILE:HD12	2.02	0.41
15:C:177:ARG:NH2	15:C:638:ASP:OD2	2.50	0.41
15:C:931:ARG:O	15:C:935:ILE:HG23	2.20	0.41
1:F:73:GLY:HA3	2:A:1578:ARG:HB2	2.02	0.41
2:A:137:GLU:O	2:A:141:ILE:HG13	2.20	0.41
2:A:882:LYS:HA	2:A:885:LEU:HD12	2.03	0.41
2:A:1627:ALA:HA	2:A:1661:TRP:NE1	2.36	0.41
2:A:1638:ASN:O	2:A:1720:PRO:HD3	2.20	0.41
2:A:1670:ASP:O	2:A:1674:HIS:HB3	2.21	0.41
6:G:155:ASN:N	6:G:170:GLY:O	2.44	0.41
15:C:110:PRO:HD2	15:C:537:TYR:CD2	2.55	0.41
15:C:131:ASN:ND2	15:C:441:PRO:HG3	2.35	0.41
15:C:449:ILE:HD12	15:C:465:MET:HE3	2.03	0.41
15:C:854:ARG:NE	15:C:879:ASP:OD2	2.49	0.41
2:A:87:VAL:HG13	4:E:101:ALA:HB2	2.03	0.41
2:A:565:ARG:HD2	2:A:565:ARG:HA	1.95	0.41
2:A:1017:ILE:N	2:A:1024:HIS:O	2.33	0.41
2:A:1057:ARG:HA	2:A:1057:ARG:HD2	1.81	0.41
2:A:1106:ALA:O	2:A:1110:ILE:HG13	2.20	0.41
2:A:1645:LEU:O	2:A:1723:LYS:HE3	2.20	0.41
3:5:37:G:C2	3:5:44:A:C4	3.09	0.41
15:C:119:LEU:O	15:C:123:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:764:ASP:OD1	15:C:764:ASP:C	2.59	0.41
1:F:225:LEU:HD12	1:F:226:ALA:N	2.36	0.40
2:A:387:PHE:CZ	15:C:326:ILE:HG22	2.56	0.40
2:A:507:LEU:HD22	2:A:655:LEU:HD23	2.03	0.40
2:A:531:THR:HB	2:A:534:GLU:OE1	2.21	0.40
2:A:836:THR:O	2:A:840:ILE:HG13	2.20	0.40
2:A:1171:GLU:H	2:A:1171:GLU:HG3	1.63	0.40
2:A:1543:ASN:O	2:A:1563:HIS:ND1	2.51	0.40
2:A:641:MET:HE2	2:A:641:MET:HB3	1.95	0.40
2:A:987:LYS:HA	2:A:1028:TYR:CE2	2.57	0.40
15:C:145:PHE:CE2	15:C:430:PHE:CD1	3.05	0.40
15:C:215:VAL:HG11	15:C:242:LEU:CD2	2.49	0.40
2:A:1214:TRP:CE2	2:A:1230:LEU:HD11	2.56	0.40
2:A:1809:ILE:O	2:A:1818:PHE:N	2.40	0.40
2:A:2076:ARG:HB3	2:A:2305:TYR:OH	2.21	0.40
2:A:2189:SER:OG	2:A:2191:GLN:OE1	2.39	0.40
1:F:108:PHE:CD1	1:F:108:PHE:N	2.89	0.40
2:A:444:ARG:HE	2:A:444:ARG:HB2	1.67	0.40
2:A:1551:PHE:HB3	2:A:1552:GLN:H	1.60	0.40
2:A:2125:ALA:HB3	2:A:2157:VAL:HG11	2.03	0.40
2:A:2284:MET:SD	2:A:2284:MET:O	2.80	0.40
1:F:177:ARG:HD3	1:F:178:LEU:N	2.36	0.40
2:A:72:ASP:N	2:A:72:ASP:OD1	2.55	0.40
2:A:1064:PRO:HA	2:A:1065:PRO:HD3	1.97	0.40
2:A:1211:ASP:OD1	2:A:1211:ASP:N	2.53	0.40
2:A:1639:VAL:HG21	2:A:1699:THR:HG21	2.04	0.40
2:A:2072:GLU:HG3	2:A:2076:ARG:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	134/341 (39%)	121 (90%)	12 (9%)	1 (1%)	22 61
2	A	2137/2335 (92%)	2045 (96%)	91 (4%)	1 (0%)	100 100
4	E	56/941 (6%)	55 (98%)	1 (2%)	0	100 100
5	D	571/820 (70%)	566 (99%)	5 (1%)	0	100 100
6	G	304/357 (85%)	284 (93%)	18 (6%)	2 (1%)	22 61
7	B	1744/2136 (82%)	1716 (98%)	28 (2%)	0	100 100
8	i	79/119 (66%)	76 (96%)	3 (4%)	0	100 100
9	k	82/126 (65%)	79 (96%)	3 (4%)	0	100 100
10	l	75/92 (82%)	75 (100%)	0	0	100 100
11	m	71/86 (83%)	70 (99%)	1 (1%)	0	100 100
12	n	72/76 (95%)	72 (100%)	0	0	100 100
13	j	94/118 (80%)	92 (98%)	2 (2%)	0	100 100
14	h	69/240 (29%)	68 (99%)	1 (1%)	0	100 100
15	C	845/972 (87%)	802 (95%)	43 (5%)	0	100 100
All	All	6333/8759 (72%)	6121 (97%)	208 (3%)	4 (0%)	54 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1020	LYS
1	F	126	VAL
6	G	59	ILE
6	G	58	PRO

5.3.2 Protein sidechains (i)

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
1	F	59/281 (21%)	50 (85%)	9 (15%)	2 13
2	A	1626/2108 (77%)	1536 (94%)	90 (6%)	21 57
4	E	55/792 (7%)	51 (93%)	4 (7%)	14 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	D	115/721 (16%)	102 (89%)	13 (11%)	6 25
15	C	737/866 (85%)	704 (96%)	33 (4%)	27 63
All	All	2592/4768 (54%)	2443 (94%)	149 (6%)	24 56

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	90	PHE
1	F	92	LEU
1	F	122	ASN
1	F	177	ARG
1	F	195	SER
1	F	200	ASP
1	F	208	GLN
1	F	222	ARG
1	F	225	LEU
2	A	60	ASP
2	A	86	ARG
2	A	87	VAL
2	A	97	HIS
2	A	106	MET
2	A	156	ARG
2	A	164	MET
2	A	181	ASN
2	A	210	HIS
2	A	217	ARG
2	A	221	ASN
2	A	227	ARG
2	A	271	MET
2	A	292	ASP
2	A	297	ASN
2	A	310	THR
2	A	346	ASP
2	A	374	ASP
2	A	379	GLU
2	A	390	ASP
2	A	422	LEU
2	A	485	THR
2	A	498	ARG
2	A	506	LEU
2	A	510	ARG

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Mol	Chain	Res	Type
2	A	600	ARG
2	A	611	LEU
2	A	621	VAL
2	A	773	LYS
2	A	781	ARG
2	A	793	ASN
2	A	821	ARG
2	A	871	TYR
2	A	886	LEU
2	A	904	HIS
2	A	934	ARG
2	A	981	PHE
2	A	995	ARG
2	A	1008	TYR
2	A	1019	TYR
2	A	1023	ASN
2	A	1024	HIS
2	A	1026	ASN
2	A	1044	TYR
2	A	1055	LEU
2	A	1061	MET
2	A	1067	MET
2	A	1070	ASP
2	A	1089	CYS
2	A	1111	GLN
2	A	1176	SER
2	A	1180	LYS
2	A	1184	ASN
2	A	1188	ASN
2	A	1193	GLU
2	A	1194	CYS
2	A	1210	LYS
2	A	1211	ASP
2	A	1224	ARG
2	A	1234	ASP
2	A	1244	VAL
2	A	1249	MET
2	A	1255	THR
2	A	1298	ARG
2	A	1301	ILE
2	A	1307	MET
2	A	1311	PHE

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Mol	Chain	Res	Type
2	A	1341	ARG
2	A	1425	LYS
2	A	1428	HIS
2	A	1432	TYR
2	A	1441	ASP
2	A	1482	GLU
2	A	1494	TYR
2	A	1502	PHE
2	A	1537	TRP
2	A	1539	SER
2	A	1591	MET
2	A	1610	GLN
2	A	1615	HIS
2	A	1622	MET
2	A	1652	MET
2	A	1659	LYS
2	A	1667	ARG
2	A	1686	ASP
2	A	1710	ASN
2	A	1728	GLN
2	A	1734	MET
2	A	2249	LYS
2	A	2284	MET
4	E	108	LEU
4	E	110	LYS
4	E	111	ARG
4	E	113	ASP
5	D	243	LYS
5	D	271	LYS
5	D	279	SER
5	D	280	GLU
5	D	282	THR
5	D	311	GLN
5	D	322	ASP
5	D	328	ARG
5	D	330	LEU
5	D	341	ARG
5	D	350	GLN
5	D	351	ARG
5	D	375	GLU
15	C	109	LEU
15	C	112	THR

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Mol	Chain	Res	Type
15	C	261	ASP
15	C	315	SER
15	C	323	PHE
15	C	342	ARG
15	C	357	THR
15	C	358	LYS
15	C	359	LYS
15	C	365	SER
15	C	388	VAL
15	C	409	LYS
15	C	416	LEU
15	C	417	ARG
15	C	433	MET
15	C	446	LYS
15	C	478	THR
15	C	498	SER
15	C	525	CYS
15	C	536	ARG
15	C	543	ARG
15	C	660	VAL
15	C	673	LYS
15	C	694	LYS
15	C	735	PHE
15	C	764	ASP
15	C	770	PHE
15	C	775	ARG
15	C	856	HIS
15	C	907	VAL
15	C	914	LYS
15	C	917	VAL
15	C	944	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	994	ASN
2	A	1026	ASN
2	A	1182	ASN
2	A	1188	ASN
2	A	1460	HIS
2	A	1615	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	5	101/117 (86%)	35 (34%)	4 (3%)

All (35) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	5	4	C
3	5	5	U
3	5	9	G
3	5	20	G
3	5	21	A
3	5	22	U
3	5	23	C
3	5	24	G
3	5	25	C
3	5	26	A
3	5	28	A
3	5	36	C
3	5	38	C
3	5	47	A
3	5	48	A
3	5	55	C
3	5	56	C
3	5	57	G
3	5	58	U
3	5	59	G
3	5	66	A
3	5	67	A
3	5	69	A
3	5	71	C
3	5	75	G
3	5	78	U
3	5	86	C
3	5	94	U
3	5	95	G
3	5	97	G
3	5	98	G
3	5	105	U
3	5	106	U
3	5	107	U
3	5	108	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	57	G
3	5	58	U
3	5	96	A
3	5	105	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	GTP	C	1001	-	26,34,34	1.06	3 (11%)	32,54,54	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	GTP	C	1001	-	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	1001	GTP	C5-C6	-2.71	1.41	1.47
16	C	1001	GTP	C8-N7	-2.18	1.31	1.35
16	C	1001	GTP	C5-C4	-2.01	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	C	1001	GTP	O4'-C4'-C5'-O5'
16	C	1001	GTP	C3'-C4'-C5'-O5'

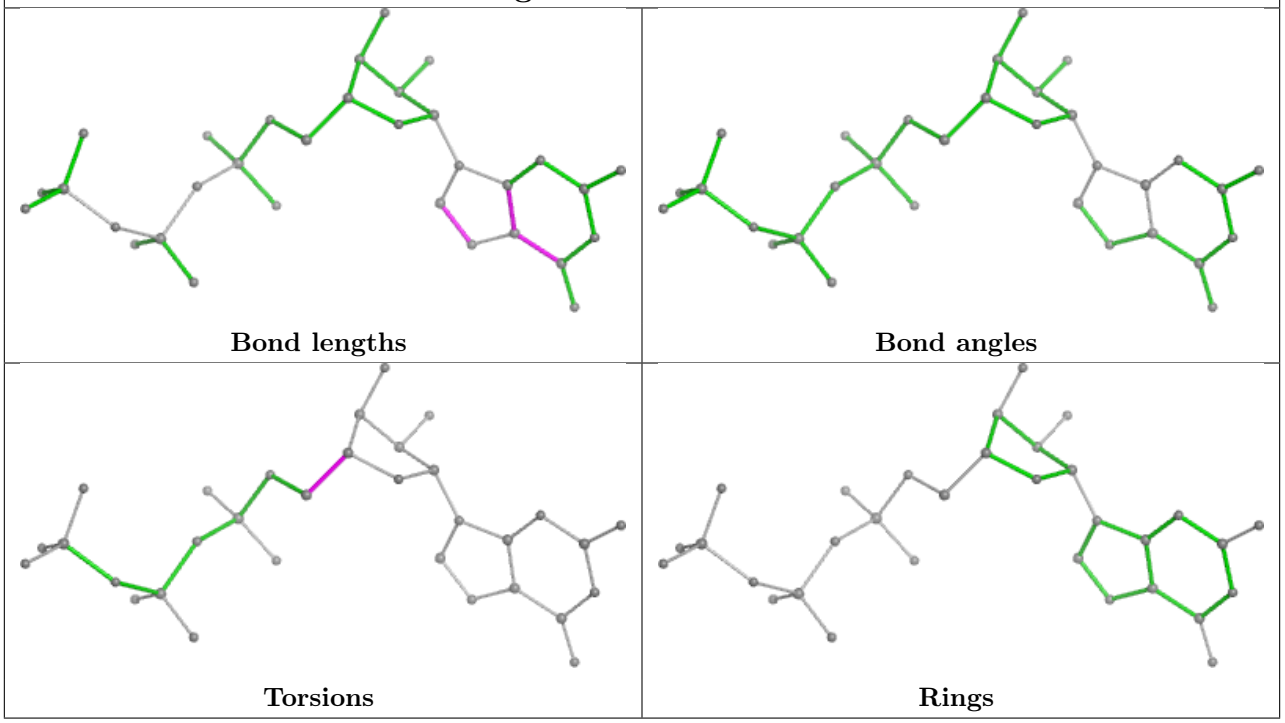
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	1001	GTP	1	0

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

Ligand GTP C 1001



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.

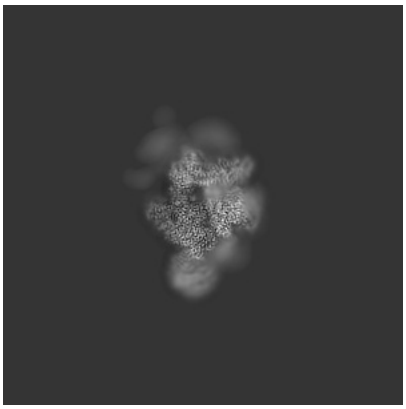
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19041. These allow visual inspection of the internal detail of the map and identification of artifacts.

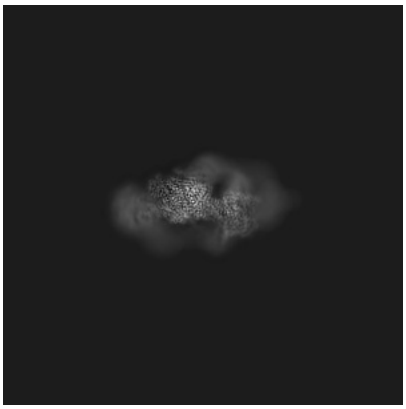
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

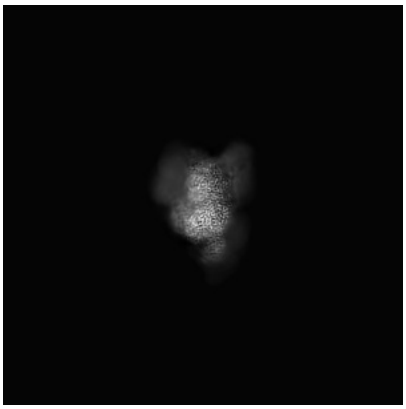
6.1.1 Primary map



X

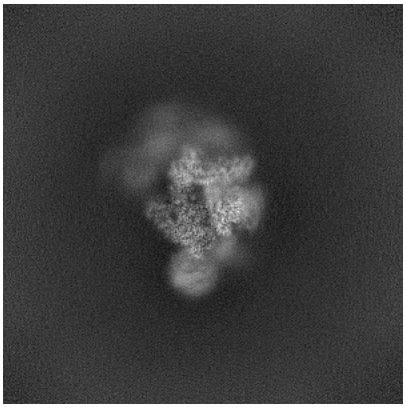


Y

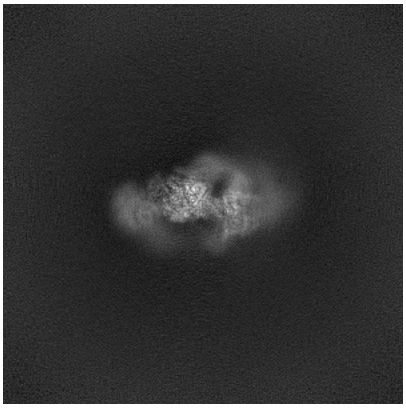


Z

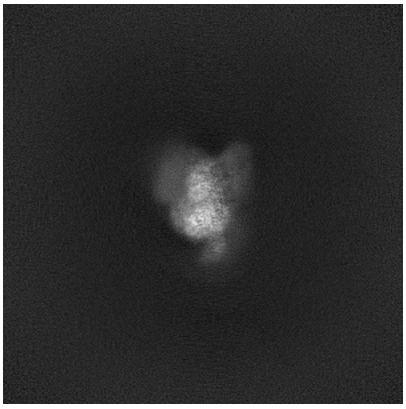
6.1.2 Raw map



X



Y

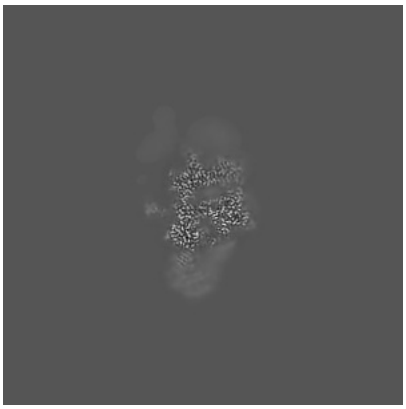


Z

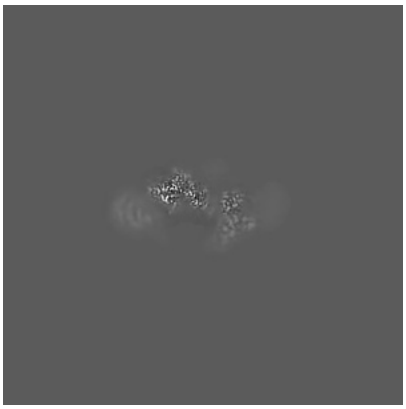
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

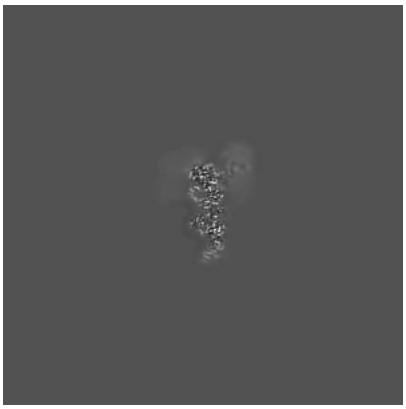
6.2.1 Primary map



X Index: 252

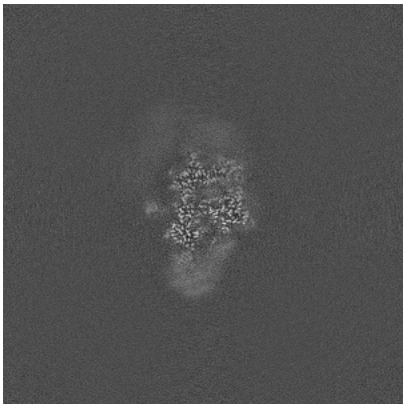


Y Index: 252

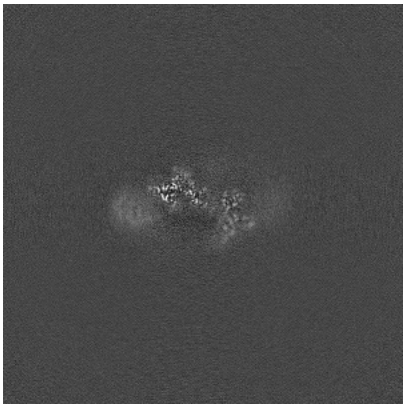


Z Index: 252

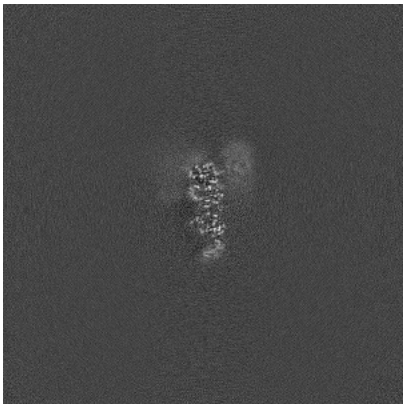
6.2.2 Raw map



X Index: 252



Y Index: 252

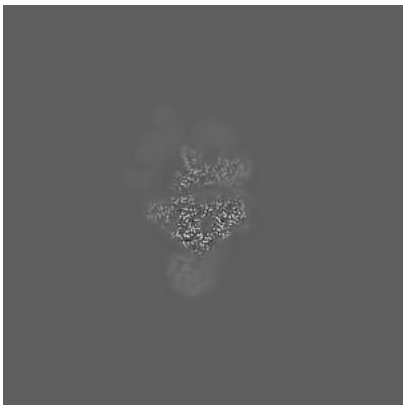


Z Index: 252

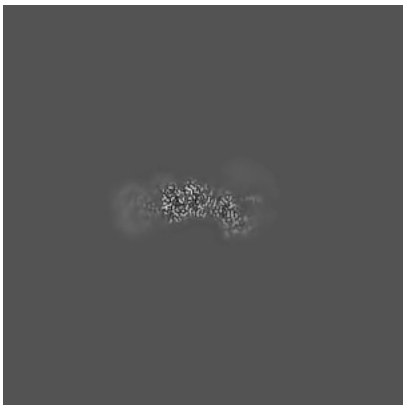
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

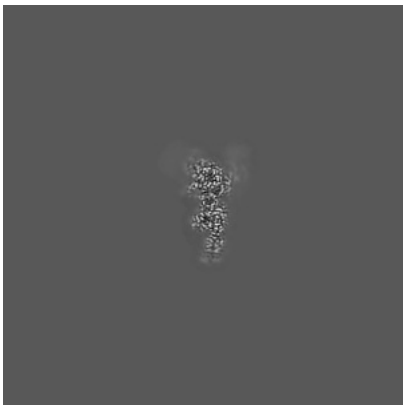
6.3.1 Primary map



X Index: 260

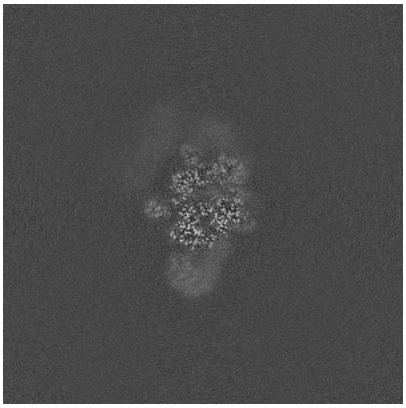


Y Index: 228

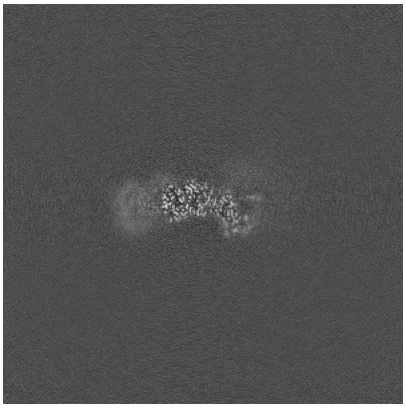


Z Index: 241

6.3.2 Raw map



X Index: 256



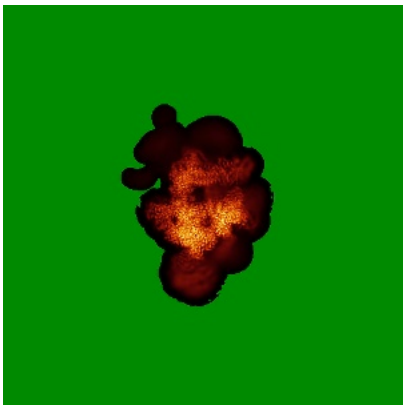
Y Index: 228

Z Index: 241

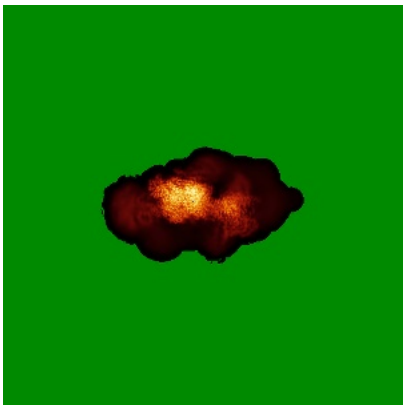
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

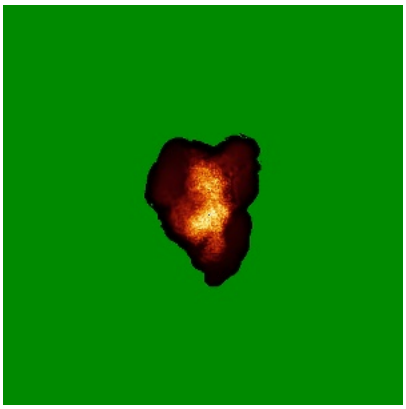
6.4.1 Primary map



X

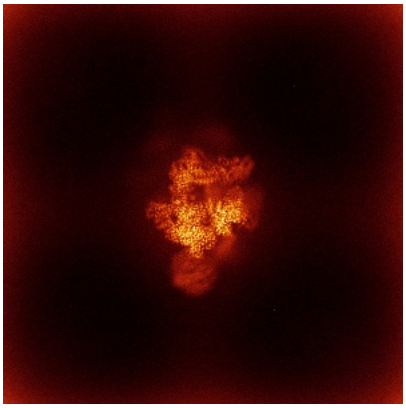


Y

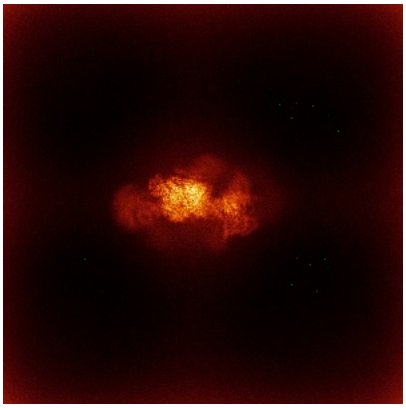


Z

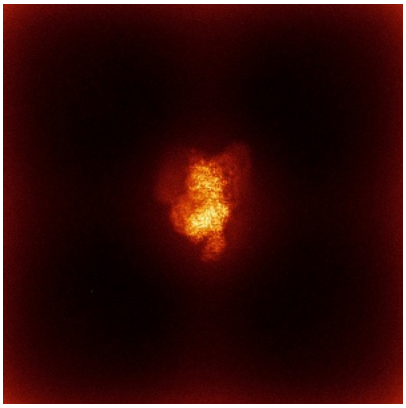
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

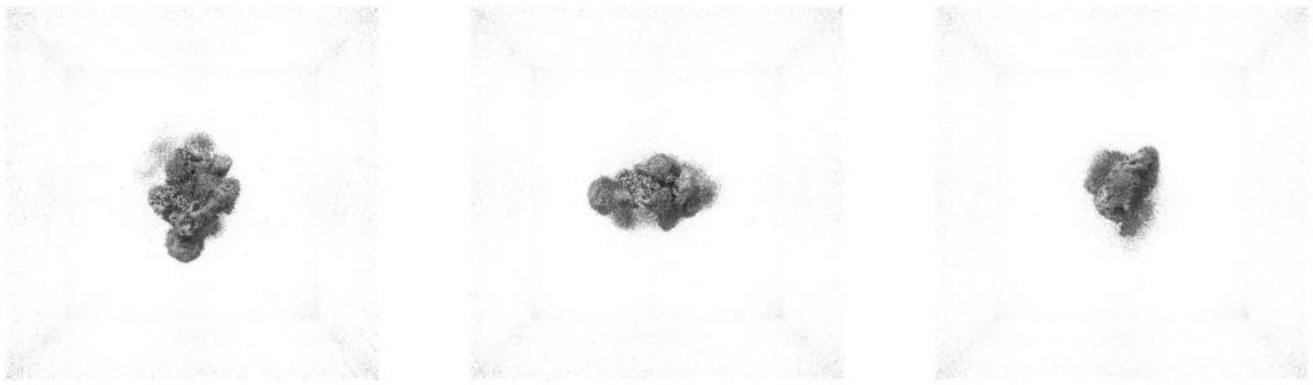
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

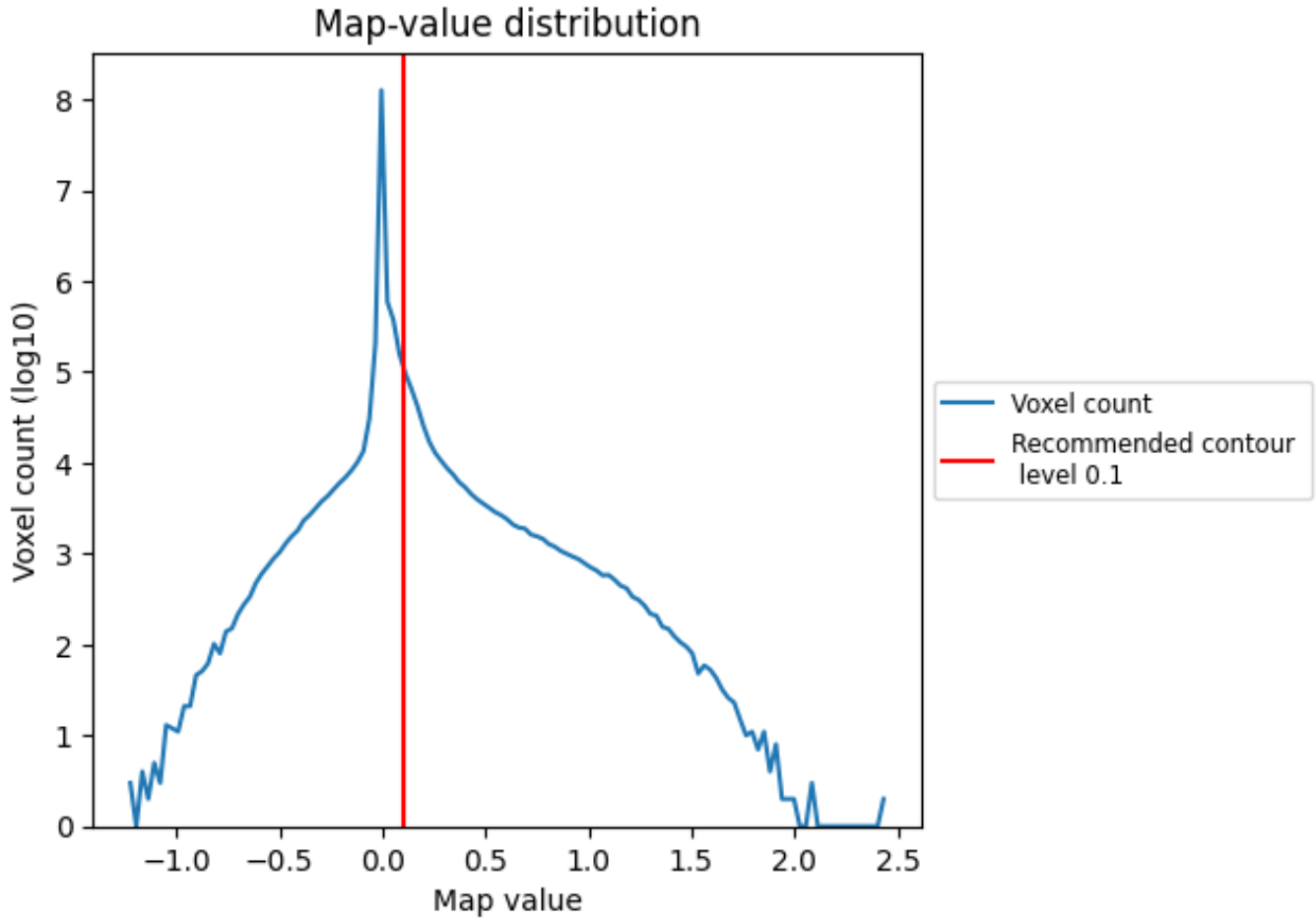
6.6 Mask visualisation (i)

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

7 Map analysis

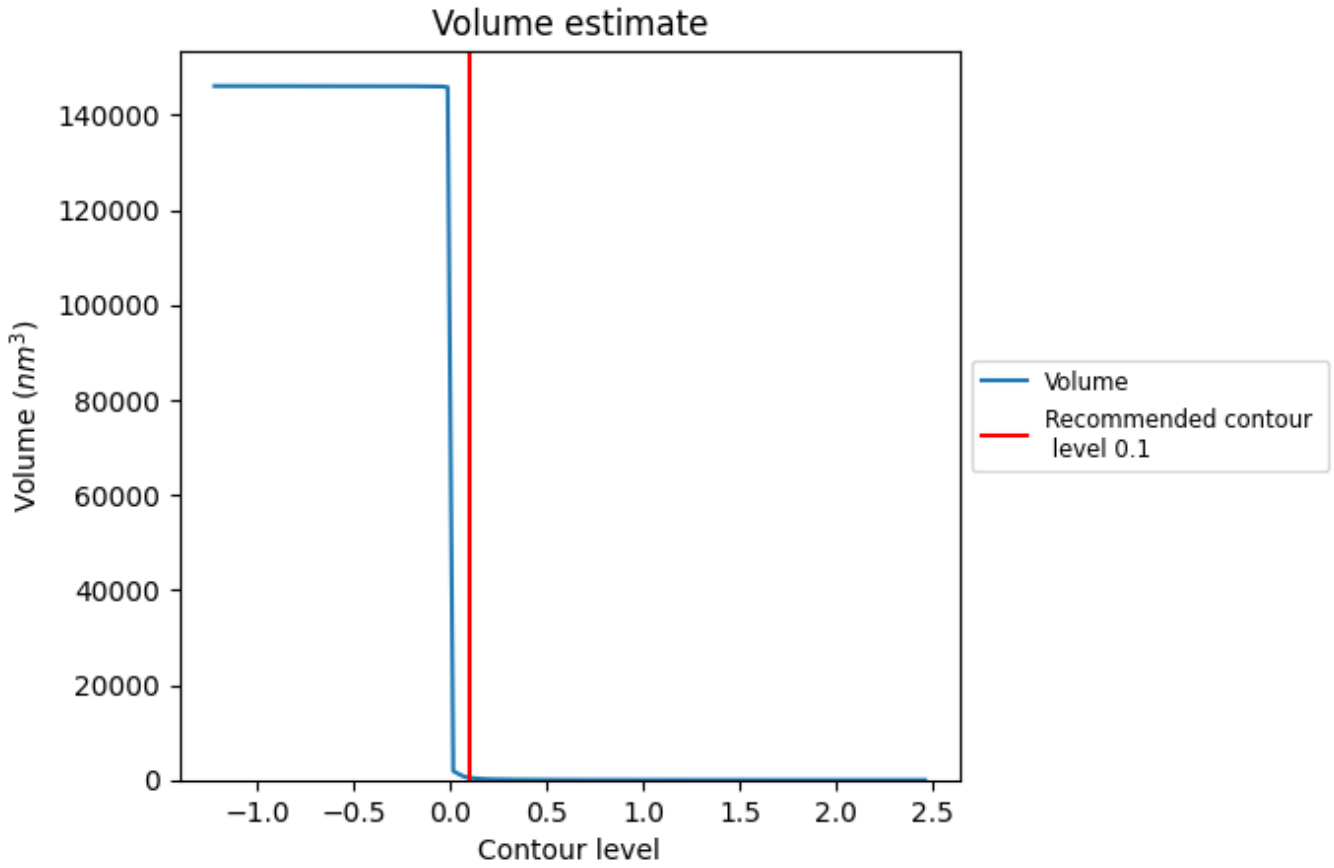
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

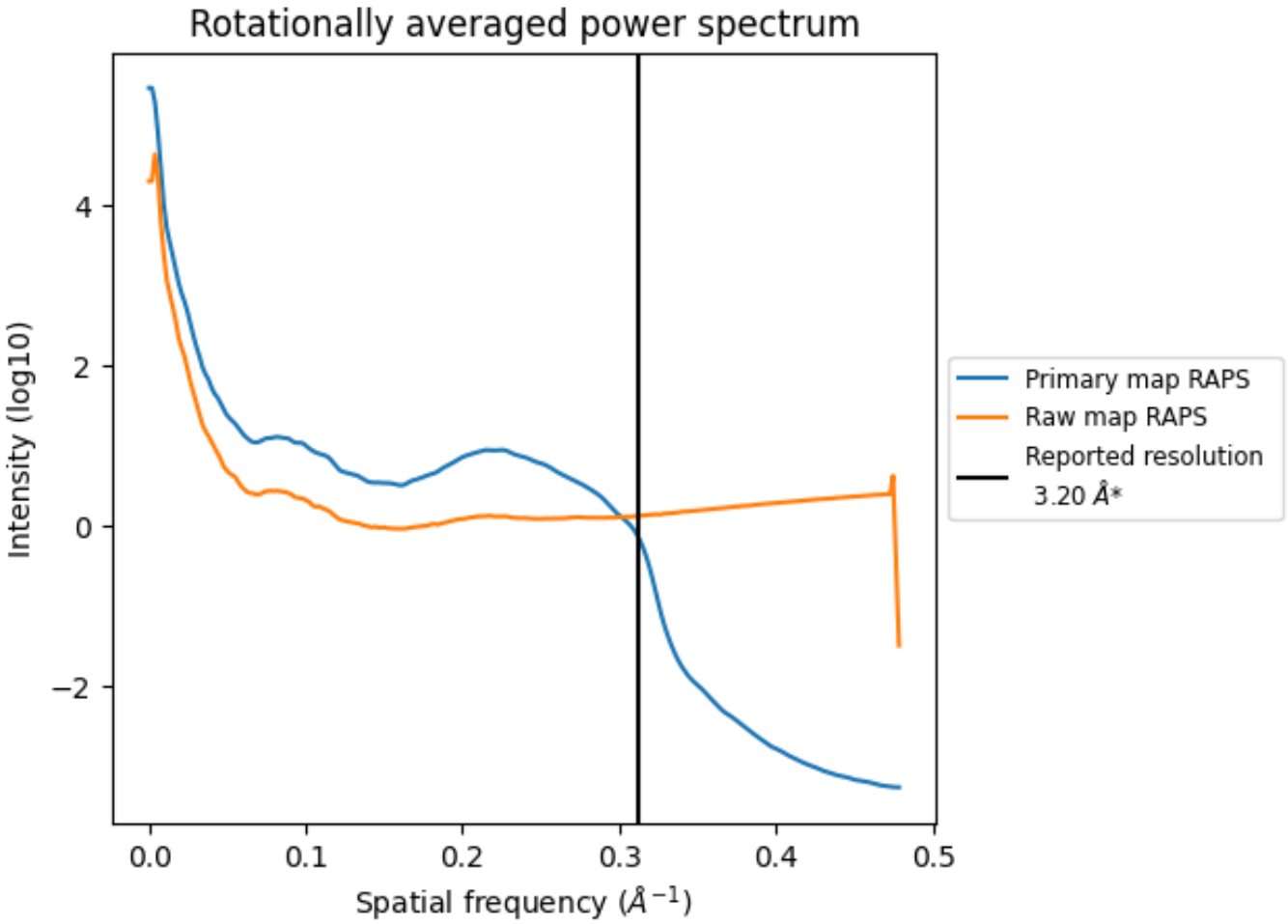
7.2 Volume estimate



The volume at the recommended contour level is 456 nm^3; this corresponds to an approximate mass of 412 kDa.

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

7.3 Rotationally averaged power spectrum (i)

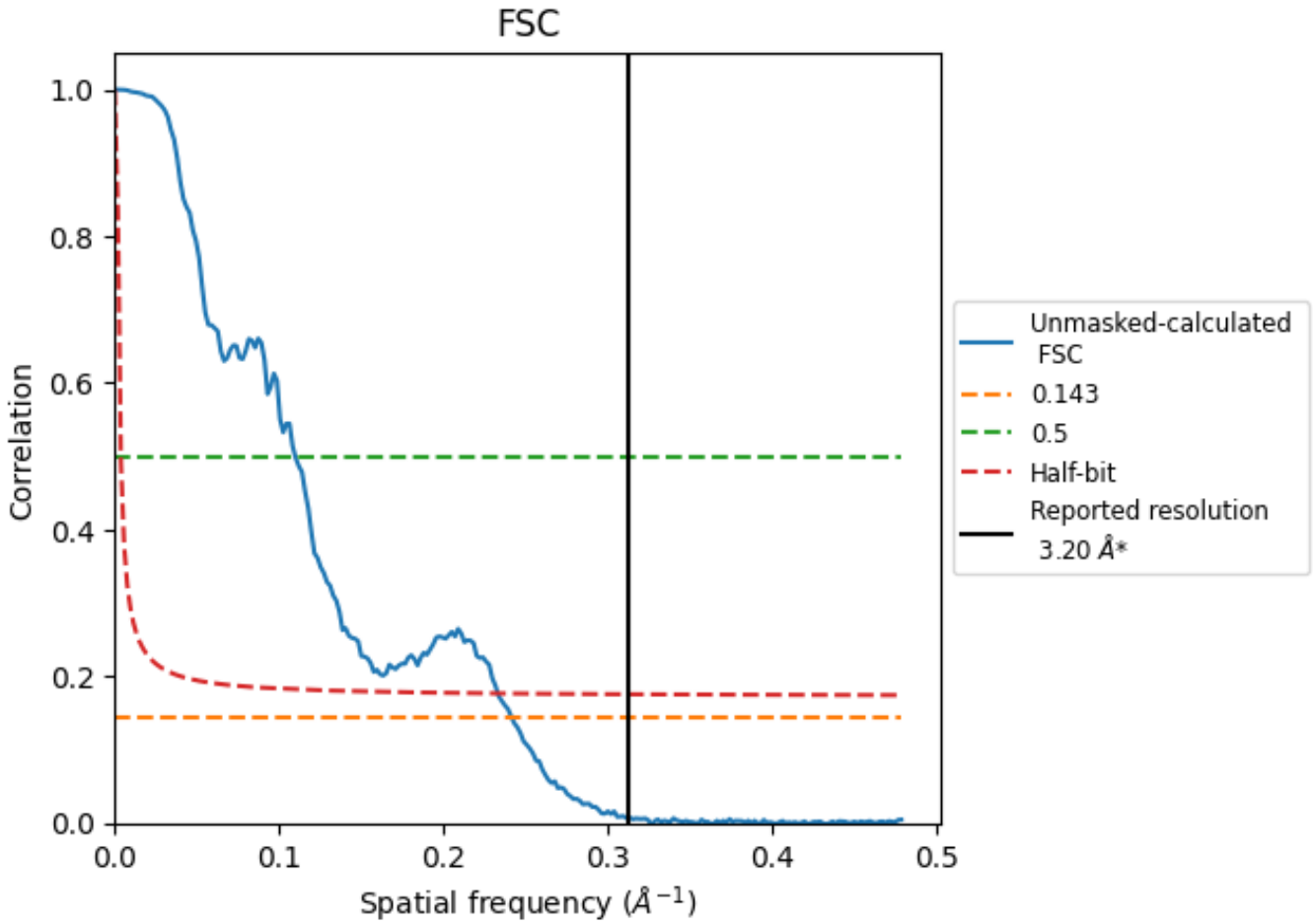


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

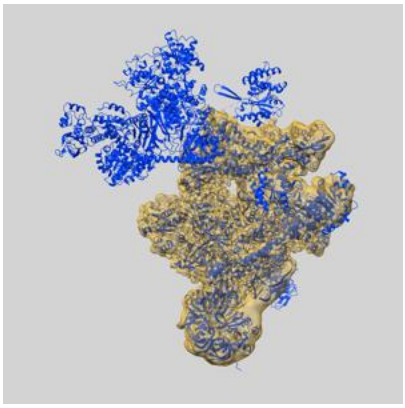
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	9.11	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.2 by more than 10 %

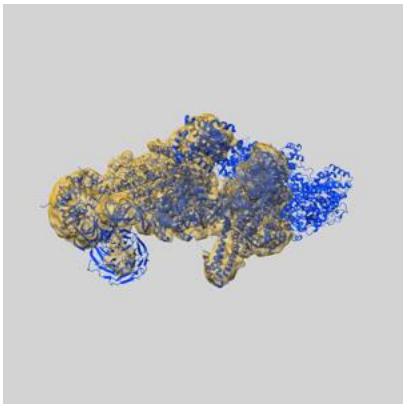
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19041 and PDB model 8RC0. Per-residue inclusion information can be found in section 3 on page 7.

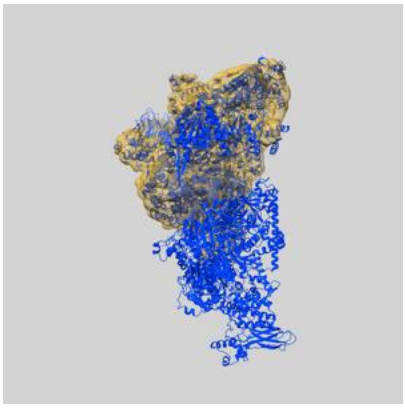
9.1 Map-model overlay



X



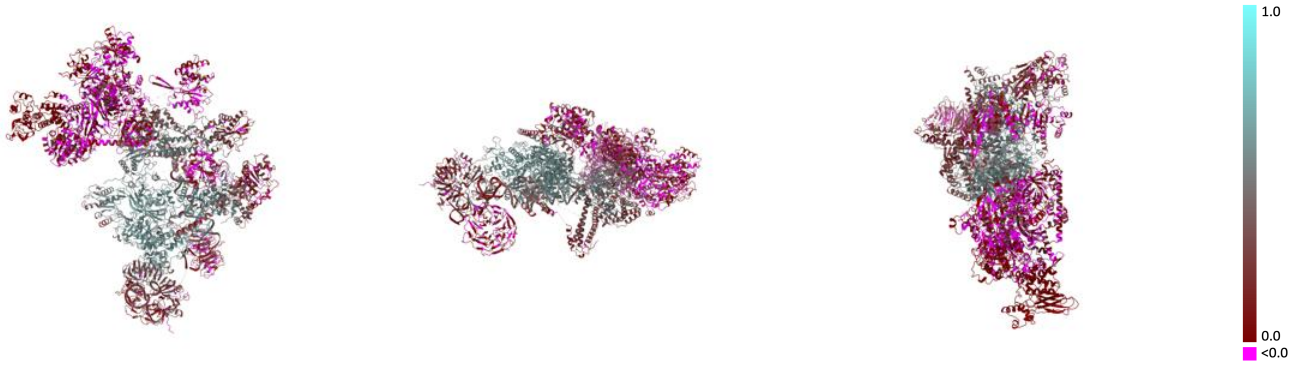
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

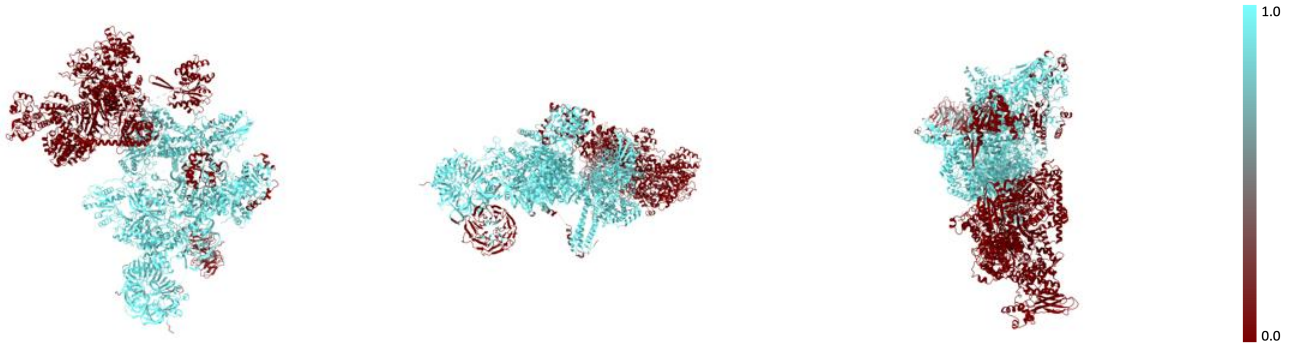
9.2 Q-score mapped to coordinate model



X Y Z

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

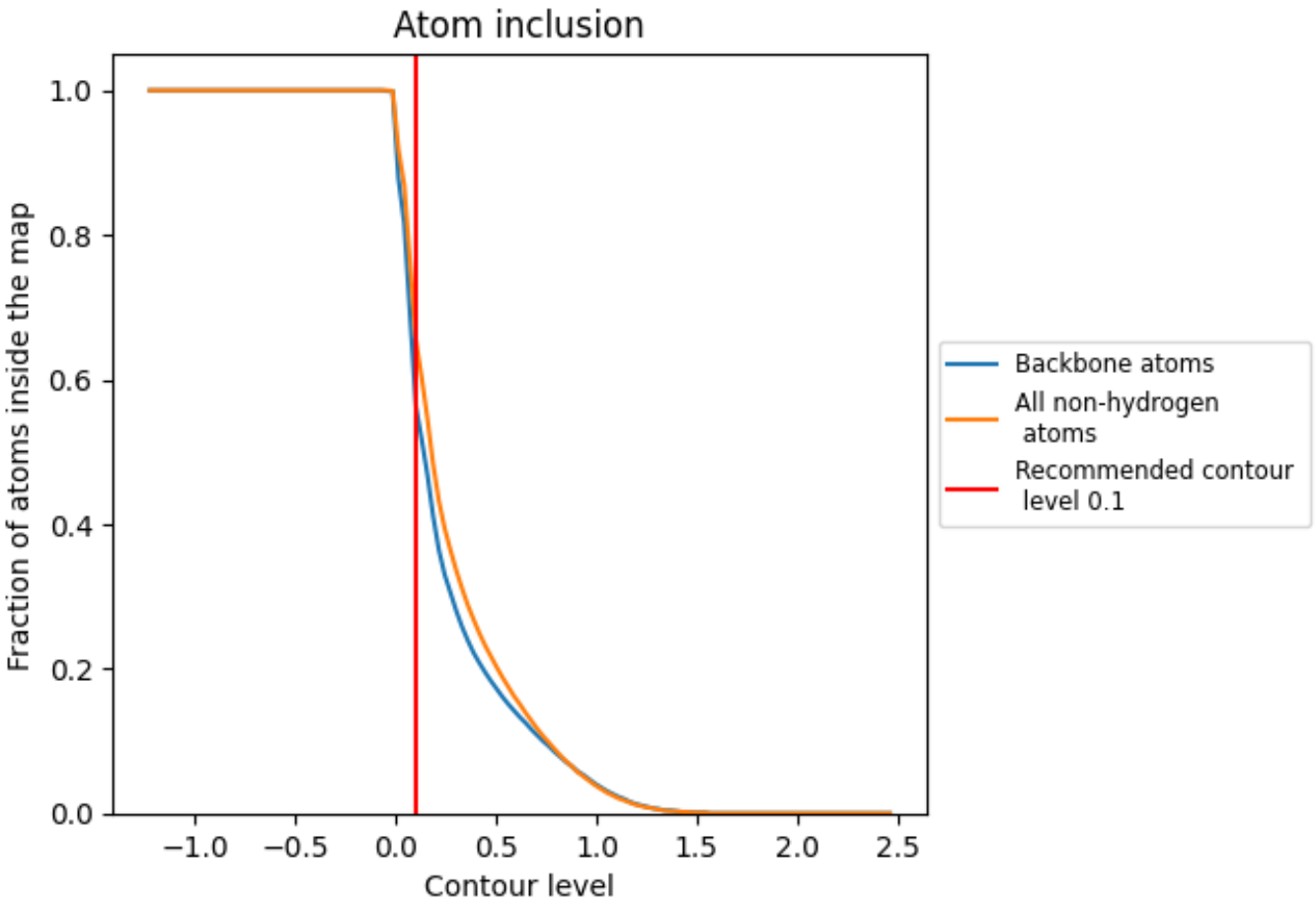
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6570	0.3090
5	0.9510	0.2970
A	0.7610	0.3710
B	0.0150	0.0280
C	0.9810	0.5600
D	0.6320	0.2220
E	0.5840	0.1820
F	0.9410	0.3760
G	0.1360	0.0540
h	0.9760	0.3080
i	0.9970	0.2900
j	0.8800	0.1940
k	0.9760	0.4080
l	1.0000	0.2280
m	0.9760	0.1970
n	0.8990	0.3060