wwPDB EM Validation Summary Report (i)

Mar 26, 2025 – 04:42 PM JST

PDB ID	:	9IZ0
EMDB ID	:	EMD-61006
Title	:	ATM/Tel1 bound to CHK2 peptide
Authors	:	Wang, P.
Deposited on	:	2024-07-31
Resolution	:	3.63 Å(reported)

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

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

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

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

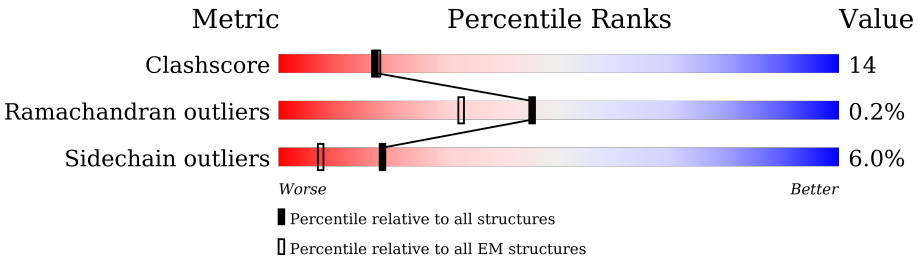
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 3.63 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	8	12% 62% 25% 12%
2	A	2812	23% 67% 18% • 14%
2	B	2812	19% 67% 18% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 32048 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.

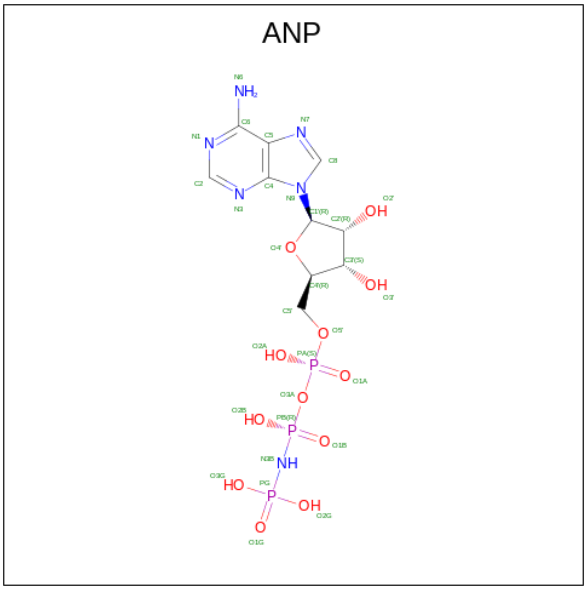
- Molecule 1 is a protein called VAL-SER-THR-GLN-GLU-LEU-TYR-SER.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	8	Total	C	N	O	0	0
			64	40	9	15		

- Molecule 2 is a protein called Serine/threonine-protein kinase tel1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2430	Total	C	N	O	S	0	0
			15929	10030	2839	3040	20		
2	B	2424	Total	C	N	O	S	0	0
			15993	10091	2847	3035	20		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

Continued on next page...

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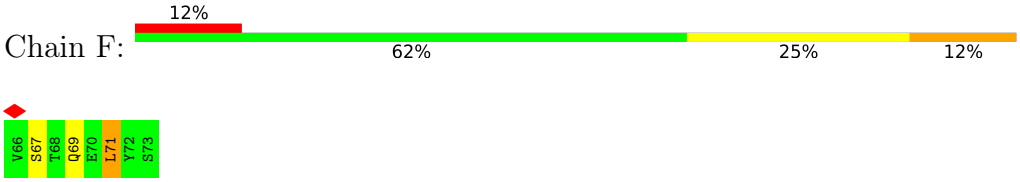
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

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.

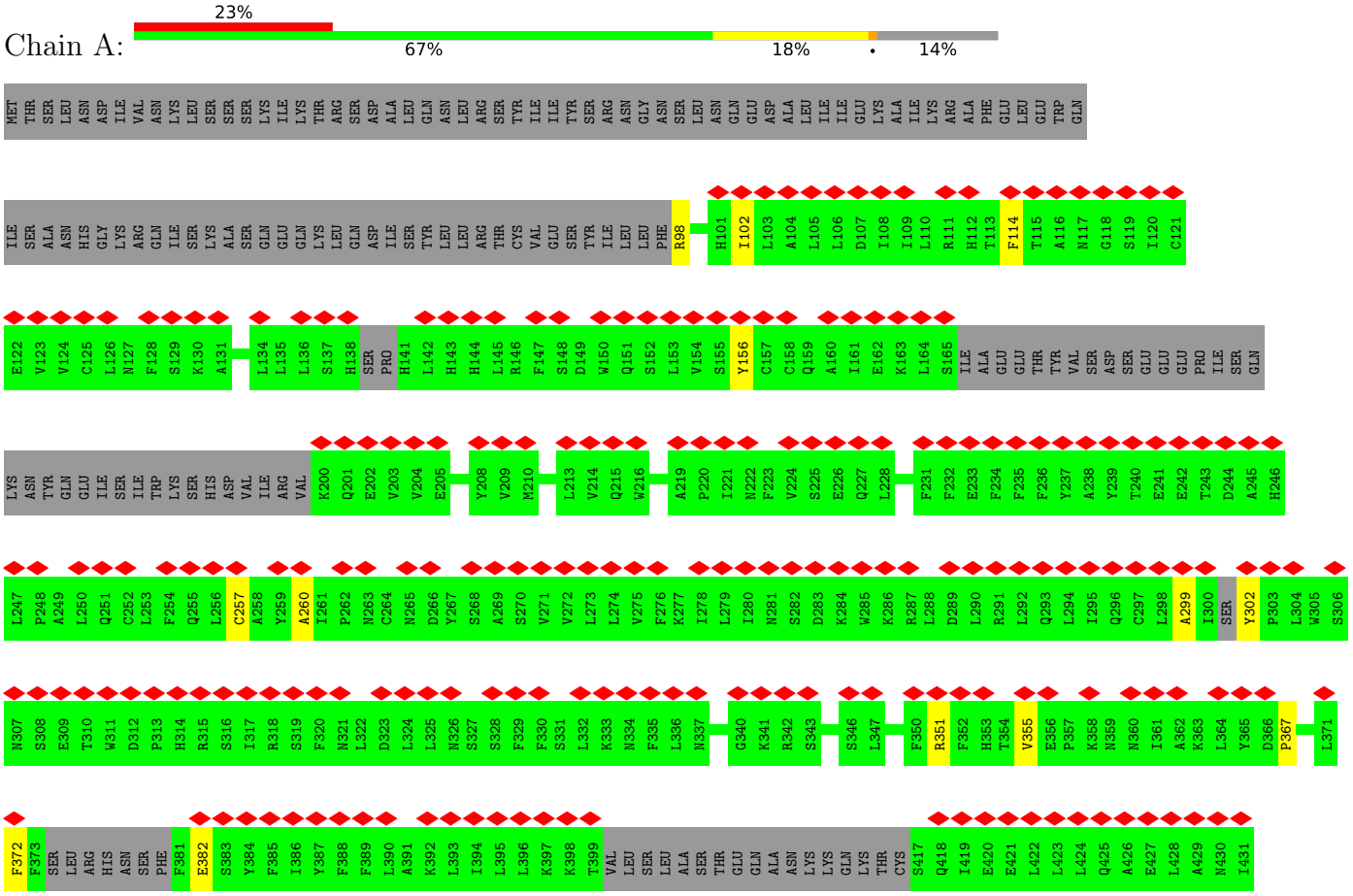
• Molecule 1: VAL-SER-THR-GLN-GLU-LEU-TYR-SER

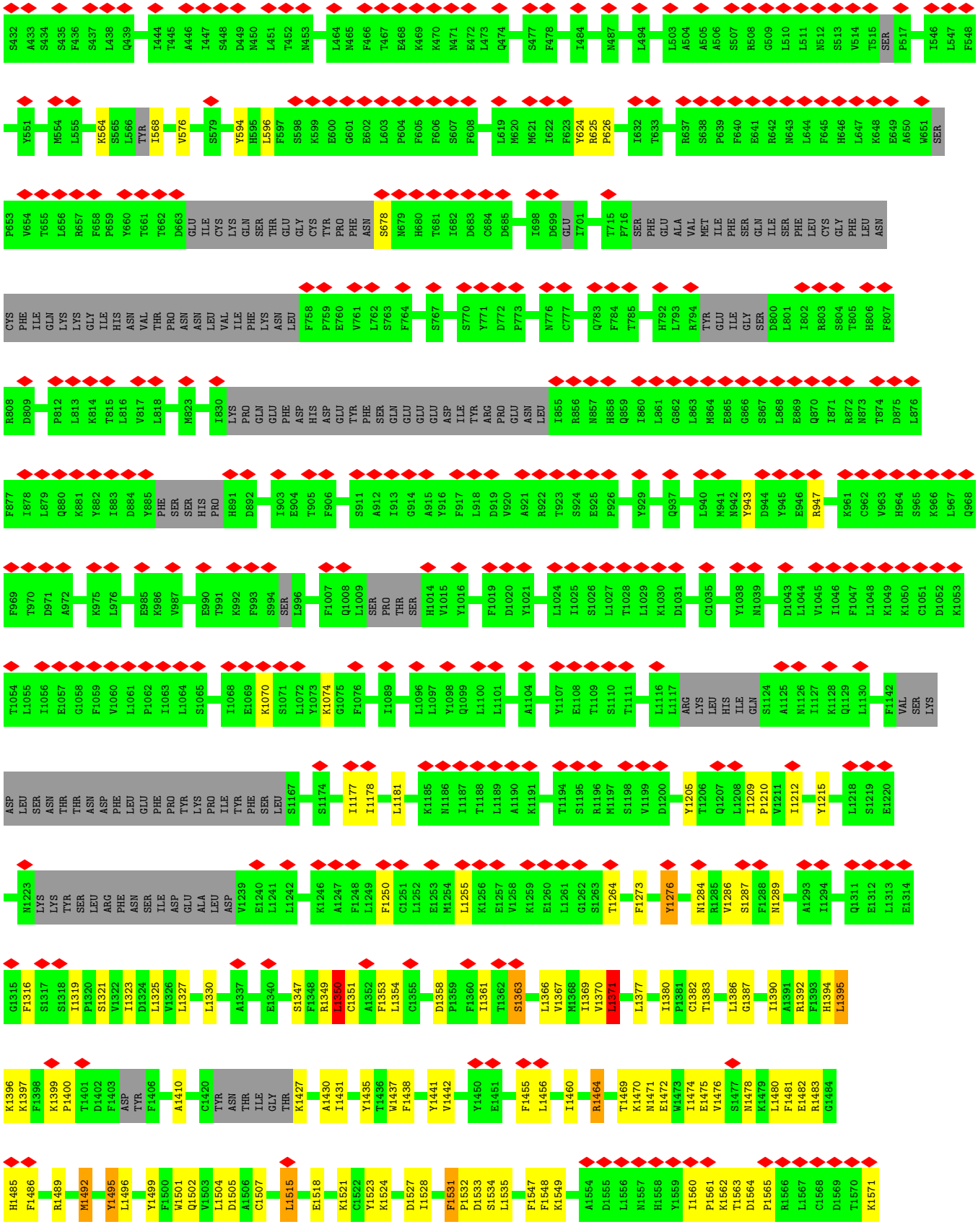
Chain F:

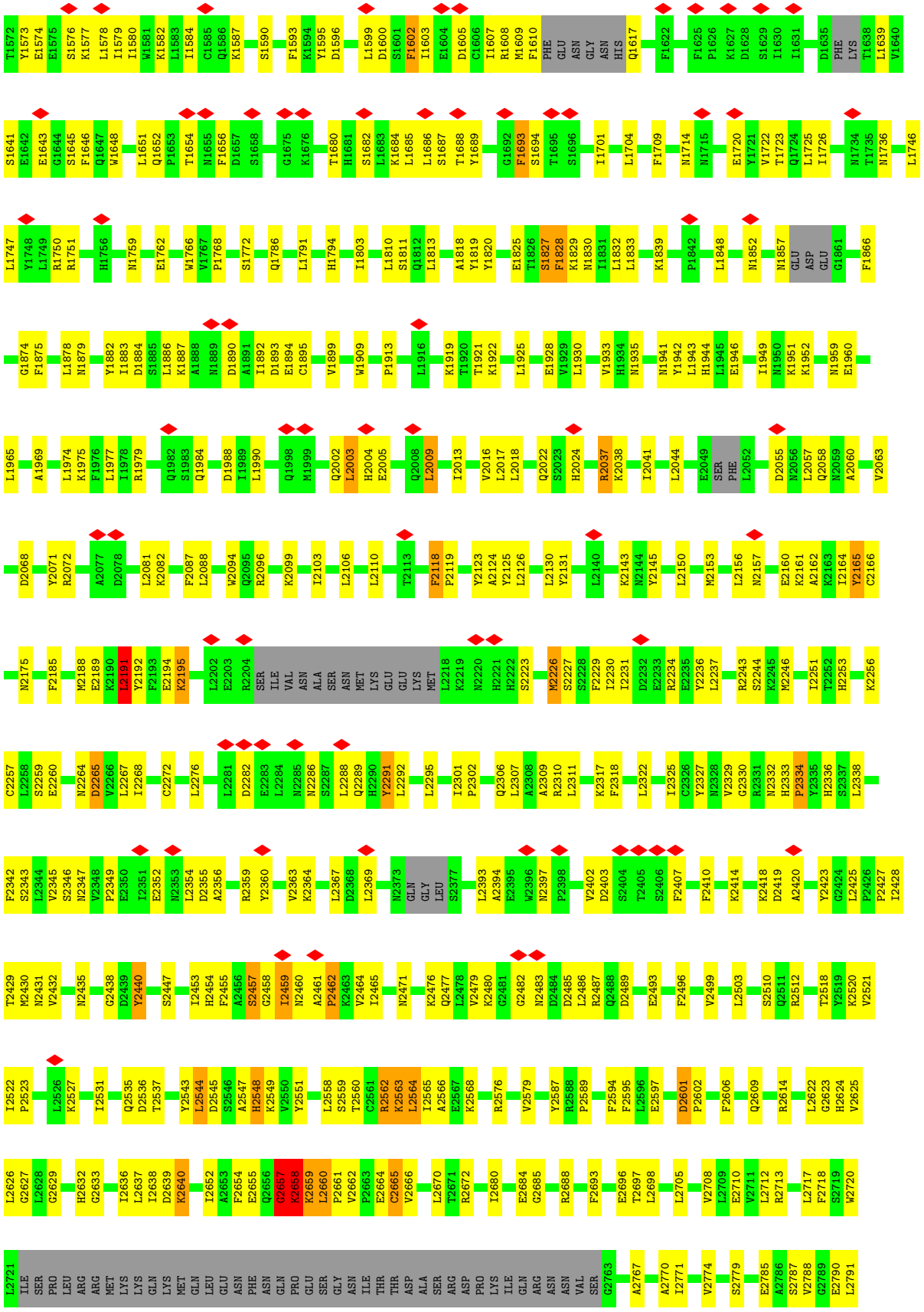


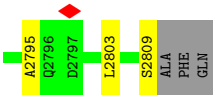
• Molecule 2: Serine/threonine-protein kinase tel1

Chain A:



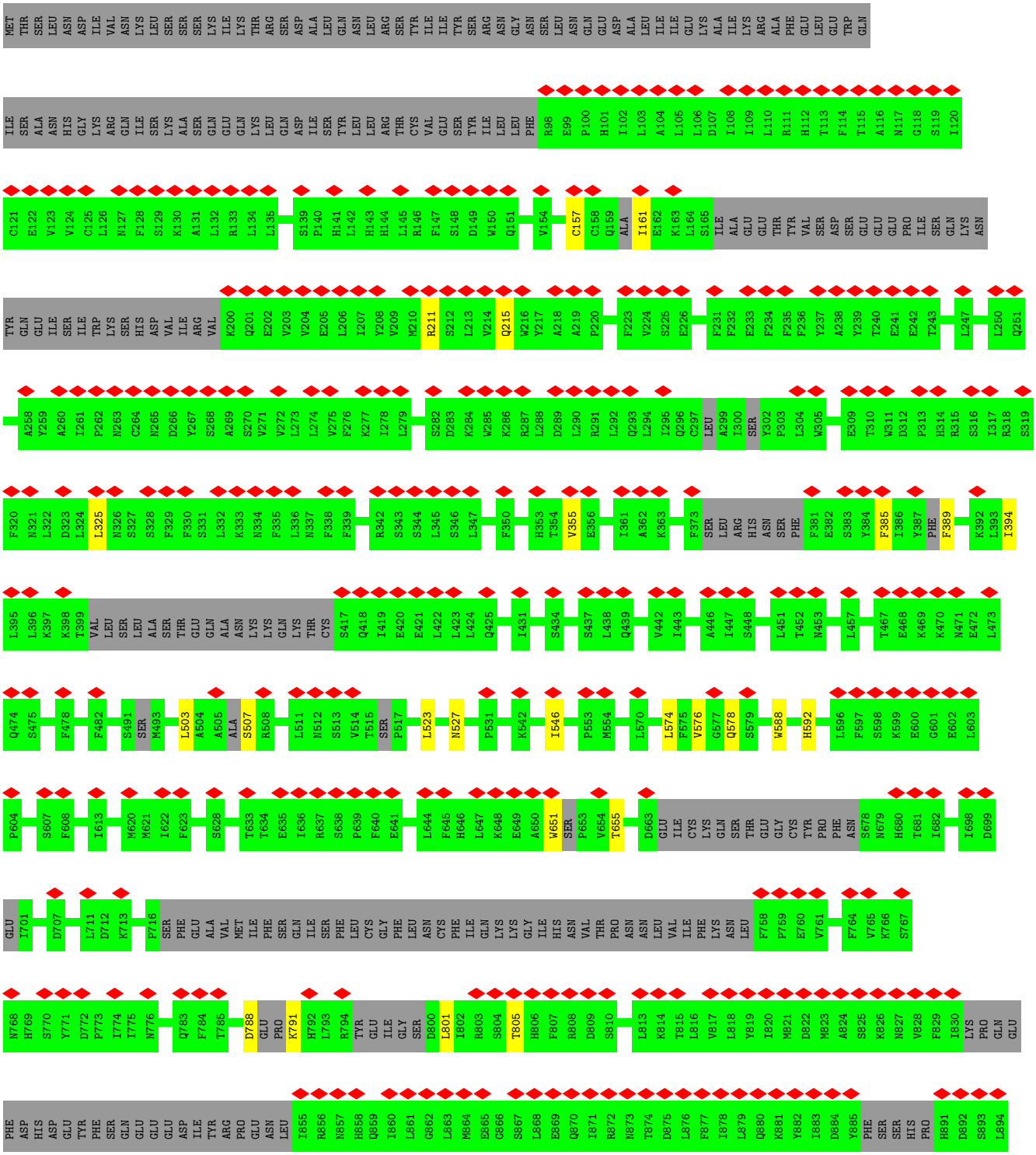

S432 A433 S434 S435 F436 S437 L438 Q439 I444 T445 A446 I447 S448 D449 N450 L451 T452 N453 L464 N465 F466 T467 E468 K469 K470 N471 E472 L473 Q474 S477 F478 I484 N487 L494 L503 A504 A505 A506 S507 R508 G509 L510 L511 N512 S513 V514 T515 SER P517 I546 L547 F548
Y551 M554 L555 K564 S565 L566 TYR I568 V576 S579 Y594 H595 L596 F597 S598 K599 E600 G601 E602 L603 P604 F605 F606 S607 F608 L619 M620 M621 I622 F623 Y624 R625 P626 I632 T633 R637 S638 P639 F640 E641 R642 N643 L644 F645 H646 L647 K648 E649 A650 W651 SER
P653 V654 T655 L656 R657 F658 P659 Y660 T661 T662 D663 GLU ILE CYS LYS GLN SER THR GLU GLY CYS TYR PRO PHE ASN S678 N679 H680 T681 I682 D683 C684 D685 I698 D699 GLU I701 T715 P716 SER PHE GLU ALA VAL MET ILE PHE SER GLN ILE SER PHE LEU CYS GLY PHE LEU ASN
CYS PHE ILE GLN LYS LYS GLY ILE HIS ASN VAL THR PRO ASN ASN ASN LEU VAL ILE PHE LYS ASN LEU F758 P759 E760 V761 L762 S763 F764 S767 S770 Y771 D772 P773 N776 C777 Q783 F784 T785 H792 L793 R794 TYR GLU ILE GLY SER D800 L801 I802 R803 S804 T805 H806 F807
R808 D809 P812 L813 K814 T815 L816 V817 L818 M823 I830 LYS PRO GLN GLU PHE ASP HIS ASP GLU TYR PHE SER GLN GLU GLU GLU ASP ILE TYR ARG PRO GLU ASN LEU I855 R856 N857 H858 Q859 I860 L861 G862 L863 M864 E865 G866 S867 L868 E869 Q870 I871 R872 N873 T874 D875 L876
F877 I878 L879 Q880 K881 Y882 I883 D884 Y885 PHE SER SER HIS PRO H891 D892 I903 E904 T905 F906 S911 A912 I913 G914 A915 Y916 F917 L918 D919 V920 A921 R922 T923 S924 E925 P926 Y929 Q937 L940 M941 N942 Y943 D944 Y945 E946 R947 K961 C962 V963 H964 S965 K966 L967 Q968
F969 T970 D971 A972 K975 L976 E985 K986 V987 E990 T991 K992 F993 S994 SER L996 F1007 Q1008 L1009 SER PRO THR SER H1014 V1015 Y1016 F1019 D1020 Y1021 L1024 I1025 S1026 L1027 T1028 L1029 K1030 D1031 C1035 Y1038 N1039 D1043 L1044 V1045 I1046 F1047 L1048 K1049 K1050 C1051 D1052 K1053
T1054 L1055 I1056 E1057 G1058 F1059 V1060 L1061 P1062 I1063 L1064 S1065 I1068 E1069 K1070 S1071 L1072 Y1073 K1074 G1075 F1076 I1089 L1096 L1097 Y1098 Q1099 L1100 L1101 A1104 Y1107 E1108 T1109 S1110 T1111 L1116 L1117 ARG LYS LEU HIS ILE GLN S1124 A1125 N1126 I1127 K1128 Q1129 L1130 F1142 VAL SER LYS
ASP LEU SER ASN THR THR ASN ASP PHE LEU GLU PHE PRO TYR LYS PRO ILE TYR PHE SER LEU S1167 S1174 I1177 I1178 L1181 K1185 N1186 I1187 T1188 L1189 A1190 K1191 T1194 S1195 R1196 M1197 S1198 V1199 D1200 Y1205 T1206 Q1207 L1208 I1209 P1210 V1211 I1212 Y1215 L1218 S1219 E1220
N1223 LYS LYS TYR SER LEU ARG PHE ASN SER ILE ASP GLU ALA LEU ASP V1239 E1240 L1241 L1242 K1246 A1247 F1248 L1249 F1250 C1251 L1252 E1253 M1254 L1255 K1256 E1257 V1258 K1259 E1260 L1261 G1262 S1263 T1264 F1273 Y1276 N1284 R1285 V1286 S1287 F1288 N1289 A1293 I1294 Q1311 E1312 L1313 E1314
G1315 F1316 S1317 S1318 I1319 P1320 S1321 V1322 I1323 D1324 L1325 V1326 L1327 L1330 A1337 E1340 S1347 F1348 R1349 L1350 C1351 A1352 F1353 L1354 C1355 D1358 P1359 F1360 I1361 T1362 S1363 L1366 V1367 M1368 I1369 V1370 L1371 L1377 I1380 P1381 C1382 T1383 L1386 G1387 I1390 A1391 R1392 F1393 H1394 L1396
K1396 K1397 F1398 K1399 P1400 T1401 D1402 F1403 ASP TYR F1406 A1410 C1420 TYR ASN THR ILE GLY THR K1427 A1430 I1431 Y1435 T1436 W1437 F1438 Y1441 V1442 Y1450 E1451 F1455 L1456 I1460 R1464 T1469 K1470 N1471 E1472 W1473 I1474 E1475 V1476 S1477 N1478 K1479 L1480 F1481 E1482 R1483 G1484
H1485 F1486 R1489 M1492 Y1495 L1496 Y1499 F1500 W1501 Q1502 V1503 L1504 D1505 A1506 C1507 L1515 E1518 K1521 C1522 Y1523 K1524 D1527 I1528 F1531 P1532 D1533 S1534 L1535 F1547 F1548 K1549 A1554 D1555 L1556 N1557 H1558 Y1559 I1560 P1561 K1562 T1563 D1564 P1565 R1566 L1567 C1568 D1569 T1570 K1571

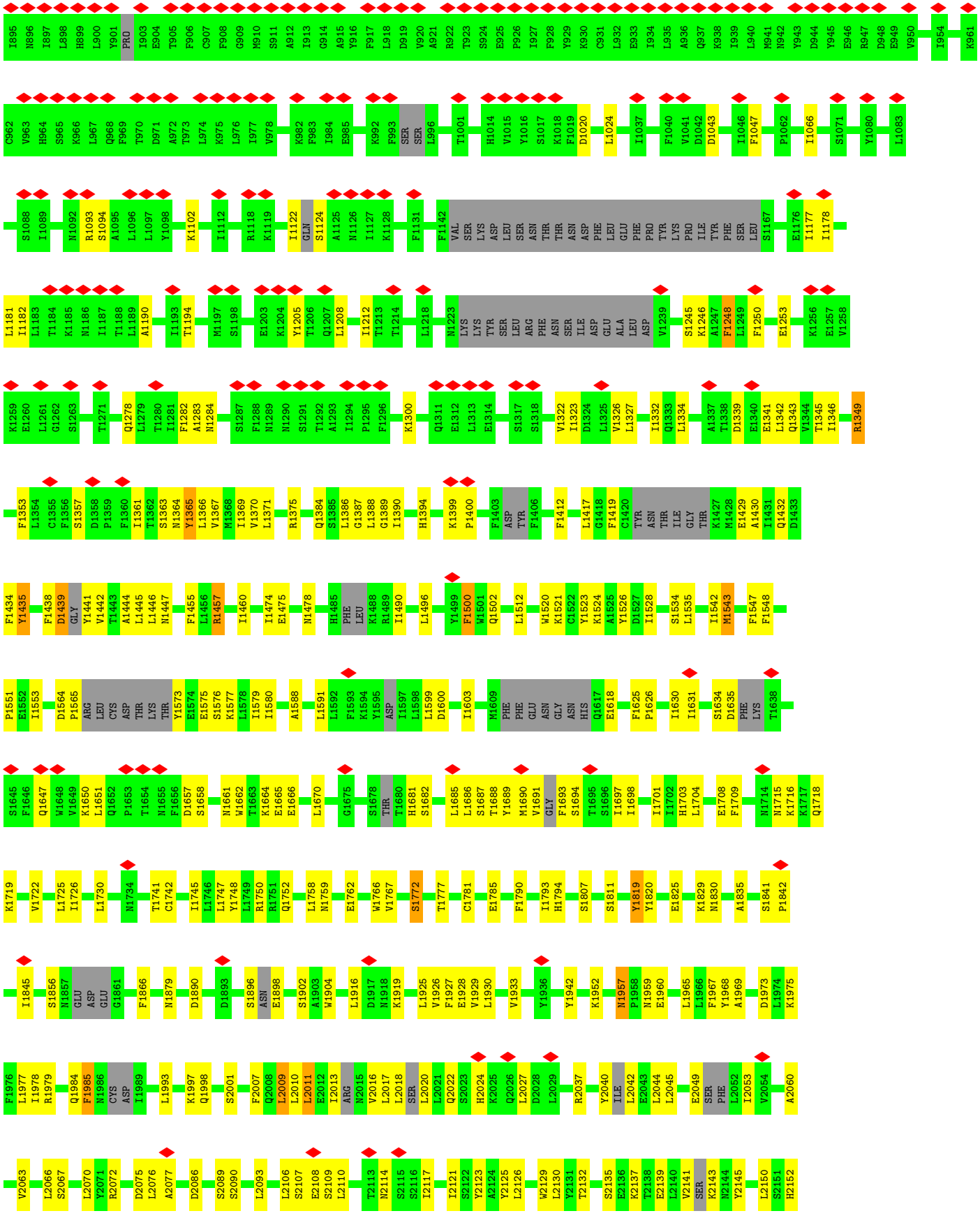




• Molecule 2: Serine/threonine-protein kinase tel1

Chain B:

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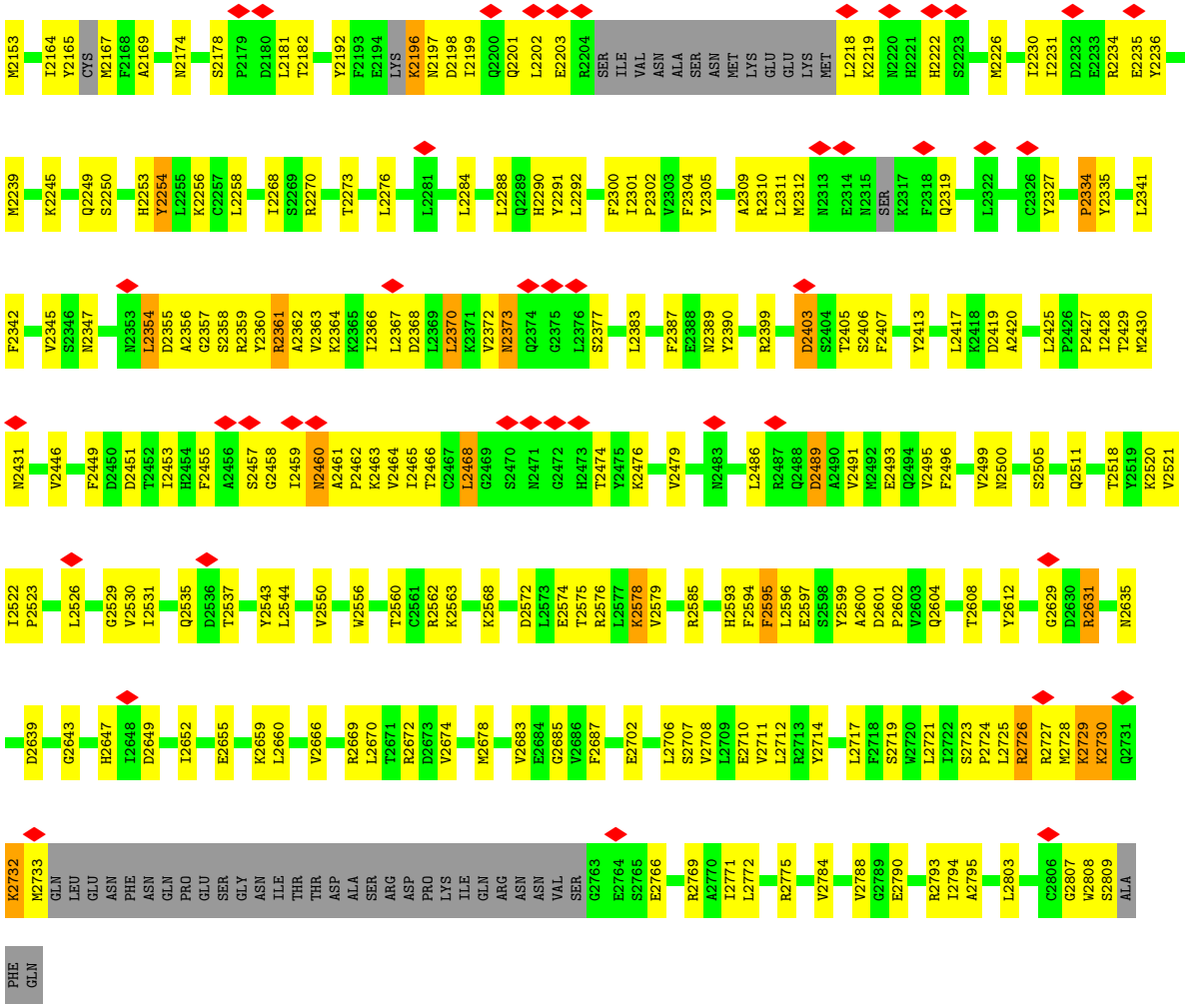
C962 V963 H964 S965 K966 L967 Q968 F969 T970 D971 A972 T973 L974 K975 L976 I977 V978 K982 F983 I984 E985 K992 F993 SER SER L996 T1001 H1014 V1015 Y1016 S1017 K1018 F1019 D1020 L1024 I1037 F1040 V1041 D1042 D1043 I1046 F1047 P1062 I1066 S1071 Y1080 L1083
S1088 I1089 N1092 R1093 S1094 A1095 L1096 L1097 Y1098 K1102 I1112 R1118 K1119 I1122 GLN S1124 A1125 N1126 I1127 K1128 F1131 F1142 VAL SER LYS ASP LEU SER ASN THR THR ASN ASP PHE LEU GLU PHE PRO TYR LYS PRO ILE TYR PHE SER LEU S1167 E1176 I1177 I1178
L1181 I1182 L1183 T1184 K1185 N1186 I1187 T1188 L1189 A1190 I1193 T1194 M1197 S1198 E1203 K1204 Y1205 T1206 Q1207 L1208 I1212 T1213 T1214 L1218 N1223 LYS LYS TYR SER LEU ARG PHE ASN SER ILE ASP GLU ALA LEU ASP V1239 S1245 K1246 A1247 F1248 L1249 F1250 E1253 K1256 E1257 V1258
K1259 E1260 L1261 G1262 S1263 T1271 Q1278 L1279 T1280 I1281 F1282 A1283 N1284 S1287 F1288 N1289 N1290 S1291 T1292 A1293 I1294 P1295 F1296 K1300 Q1311 E1312 L1313 E1314 S1317 S1318 V1322 I1323 D1324 L1325 V1326 L1327 I1332 Q1333 L1334 A1337 T1338 D1339 E1340 E1341 L1342 Q1343 Y1344 T1345 I1346 R1349
F1353 L1354 C1355 F1356 S1357 D1358 P1359 F1360 I1361 T1362 S1363 N1364 Y1365 L1366 V1367 M1368 I1369 V1370 L1371 R1375 Q1384 S1385 L1386 G1387 L1388 G1389 I1390 H1394 K1399 P1400 F1403 ASP TYR F1406 F1412 L1417 G1418 F1419 C1420 TYR ASN THR ILE GLY THR K1427 M1428 E1429 A1430 I1431 Q1432 D1433
F1434 Y1435 F1438 D1439 GLY Y1441 V1442 T1443 A1444 L1445 L1446 N1447 F1455 L1456 R1457 I1460 I1474 E1475 N1478 H1485 PHE LEU K1488 R1489 I1490 L1496 Y1499 F1500 W1501 Q1502 L1512 W1520 K1521 C1522 Y1523 K1524 A1525 Y1526 D1527 I1528 S1534 L1535 I1542 M1543 F1547 F1548
P1551 E1552 I1553 D1564 P1565 ARG LEU CYS ASP THR LYS THR Y1573 E1574 E1575 S1576 K1577 L1578 I1579 I1580 A1588 L1591 L1592 F1593 K1594 Y1595 ASP I1597 L1598 L1599 D1600 I1603 M1609 PHE PHE GLU ASN GLY ASN HIS Q1617 E1618 F1625 P1626 I1630 I1631 S1634 D1635 PHE LYS T1638
S1645 F1646 Q1647 W1648 V1649 K1650 L1651 Q1652 P1653 T1654 N1655 F1656 D1657 S1658 N1661 W1662 T1663 K1664 E1665 E1666 L1670 G1675 S1678 THR T1680 H1681 S1682 L1685 L1686 S1687 T1688 Y1689 M1690 V1691 GLY F1693 S1694 T1695 S1696 I1697 I1698 I1701 I1702 H1703 L1704 E1708 F1709 N1714 N1715 K1716 K1717 Q1718
K1719 V1722 L1725 I1726 L1730 N1734 T1741 C1742 I1745 L1746 L1747 Y1748 L1749 R1750 R1751 Q1752 L1758 N1759 E1762 W1766 V1767 S1772 T1777 C1781 E1785 F1790 I1793 H1794 S1807 S1811 Y1819 Y1820 E1825 K1829 N1830 A1835 S1841 P1842
T1845 S1856 N1857 GLU ASP GLU G1861 F1866 N1879 D1890 D1893 S1896 ASN E1898 S1902 A1903 W1904 L1916 D1917 N1918 K1919 L1925 V1926 F1927 E1928 V1929 L1930 V1933 Y1936 Y1942 K1952 N1957 P1958 N1959 E1960 L1965 L1966 F1967 Y1968 A1969 D1973 L1974 K1975
F1976 L1977 I1978 R1979 Q1984 F1985 N1986 CYS ASP I1989 L1993 K1997 Q1998 S2001 F2007 Q2008 L2009 L2010 L2011 E2012 I2013 ARG N2015 V2016 L2017 L2018 SER L2020 L2021 Q2022 S2023 H2024 K2025 Q2026 L2027 D2028 L2029 R2037 Y2040 ILE L2042 E2043 L2044 L2045 E2049 SER PHE L2052 I2053 V2054 A2060
V2063 L2066 S2067 L2070 Y2071 R2072 D2075 L2076 A2077 D2086 S2089 S2090 L2093 L2106 S2107 E2108 S2109 L2110 T2113 N2114 S2115 S2116 I2117 I2121 S2122 Y2123 A2124 Y2125 L2126 W2129 L2130 Y2131 T2132 S2135 E2136 K2137 T2138 E2139 L2140 V2141 SER K2143 N2144 Y2145 L2150 S2151 H2152


M2153 I2164 Y2165 CYS M2167 F2168 A2169 N2174 S2178 P2179 D2180 L2181 T2182 Y2192 F2193 E2194 LYS K2196 N2197 D2198 I2199 Q2200 Q2201 L2202 E2203 R2204 SER ILE VAL ASN ALA SER ASN MET LYS GLU GLU LYS MET L2218 K2219 N2220 H2221 H2222 S2223 M2226 I2230 I2231 D2232 E2233 R2234 E2235 Y2236
M2239 K2245 Q2249 S2250 H2253 Y2254 L2255 K2256 C2257 L2258 I2268 S2269 R2270 T2273 L2276 L2281 L2284 L2288 Q2289 H2290 Y2291 L2292 F2300 I2301 P2302 V2303 F2304 Y2305 A2309 R2310 L2311 M2312 N2313 E2314 N2315 SER K2317 F2318 Q2319 L2322 C2326 Y2327 P2334 Y2335 L2341
F2342 V2345 S2346 N2347 N2353 L2354 D2355 A2356 G2357 S2358 R2359 Y2360 R2361 A2362 V2363 K2364 K2365 I2366 L2367 D2368 L2369 L2370 K2371 V2372 N2373 Q2374 G2375 L2376 S2377 L2383 F2387 E2388 N2389 Y2390 R2399 D2403 S2404 T2405 S2406 F2407 Y2413 L2417 K2418 D2419 A2420 L2425 P2426 P2427 I2428 T2429 M2430
N2431 V2446 F2449 D2450 D2451 T2452 I2453 H2454 F2455 A2456 S2457 G2458 I2459 N2460 A2461 P2462 K2463 V2464 I2465 T2466 C2467 L2468 G2469 S2470 N2471 G2472 H2473 T2474 Y2475 K2476 V2479 N2483 L2486 R2487 Q2488 D2489 A2490 V2491 M2492 E2493 Q2494 V2495 F2496 V2499 N2500 S2505 Q2511 T2518 Y2519 K2520 V2521
I2522 P2523 L2526 G2529 V2530 I2531 Q2535 D2536 T2537 Y2543 L2544 V2550 W2556 T2560 C2561 R2562 K2563 K2568 D2572 L2573 E2574 T2575 R2576 L2577 K2578 V2579 R2585 H2593 F2594 F2595 L2596 E2597 S2598 Y2599 A2600 D2601 P2602 V2603 Q2604 T2608 Y2612 G2629 D2630 R2631 N2635
D2639 G2643 H2647 I2648 D2649 I2652 E2655 K2659 L2660 V2666 R2669 L2670 T2671 R2672 D2673 V2674 M2678 V2683 E2684 G2685 V2686 F2687 E2702 L2706 S2707 V2708 L2709 E2710 V2711 L2712 R2713 Y2714 L2717 F2718 S2719 W2720 L2721 I2722 S2723 P2724 L2725 R2726 R2727 M2728 K2729 K2730 Q2731
K2732 M2733 GLN LEU GLU ASN PHE ASN GLN PRO GLU SER GLY ASN ILE THR THR ASP ALA SER ARG ASP PRO LYS ILE GLN ARG ASN ASN VAL SER G2763 E2764 S2765 E2766 R2769 A2770 I2771 L2772 R2775 V2784 V2788 G2789 E2790 R2793 I2794 A2795 L2803 C2806 G2807 W2808 S2809 ALA
PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64713	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.494	Depositor
Minimum map value	-1.293	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	308.16, 308.16, 308.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.56	0/64	0.82	1/86 (1.2%)
2	A	0.27	1/16139 (0.0%)	0.50	13/22100 (0.1%)
2	B	0.25	0/16185	0.46	3/22124 (0.0%)
All	All	0.26	1/32388 (0.0%)	0.48	17/44310 (0.0%)

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
2	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2658	LYS	CA-C	-6.45	1.36	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2334	PRO	CA-N-CD	-9.50	98.20	111.50
2	A	1371	LEU	CA-CB-CG	7.96	133.61	115.30
2	A	2657	GLY	CA-C-N	-7.12	101.54	117.20
2	A	2003	LEU	CA-CB-CG	6.71	130.73	115.30
2	A	2563	LYS	CD-CE-NZ	6.61	126.89	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2657	GLY	Mainchain

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	64	0	59	6	0
2	A	15929	0	12395	401	0
2	B	15993	0	12577	368	0
3	A	31	0	13	3	0
3	B	31	0	13	4	0
All	All	32048	0	25057	771	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 14.

The worst 5 of 771 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)
2:A:2195:LYS:HD3	2:A:2229:PHE:HB2	1.56	0.88
2:A:2018:LEU:HB3	2:A:2037:ARG:HH22	1.38	0.88
2:B:2459:ILE:HG22	2:B:2459:ILE:O	1.73	0.86
2:A:1399:LYS:HG3	2:A:1400:PRO:HD3	1.59	0.84
2:A:2560:THR:O	2:A:2564:LEU:HB2	1.78	0.83

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	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	A	2372/2812 (84%)	2222 (94%)	142 (6%)	8 (0%)	37	66
2	B	2330/2812 (83%)	2190 (94%)	137 (6%)	3 (0%)	48	78
All	All	4708/5632 (84%)	4417 (94%)	280 (6%)	11 (0%)	45	72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1571	LYS
2	A	2640	LYS
2	A	2658	LYS
2	A	2462	PRO
2	A	2562	ARG

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	8/8 (100%)	8 (100%)	0	100	100
2	A	1106/2621 (42%)	1038 (94%)	68 (6%)	15	41
2	B	1126/2621 (43%)	1060 (94%)	66 (6%)	16	42
All	All	2240/5250 (43%)	2106 (94%)	134 (6%)	18	42

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2373	ASN
2	B	2457	SER
2	B	2728	MET
2	A	2265	ASP
2	A	2257	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2454	HIS
2	B	1759	ASN
2	B	1957	ASN
2	A	1752	GLN
2	A	1703	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	$\#\|Z\| > 2$
3	ANP	B	2901	-	29,33,33	1.09	4 (13%)	31,52,52	1.05	2 (6%)
3	ANP	A	2901	-	29,33,33	1.09	4 (13%)	31,52,52	1.10	2 (6%)

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
3	ANP	B	2901	-	-	7/14/38/38	0/3/3/3
3	ANP	A	2901	-	-	5/14/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2901	ANP	PG-N3B	2.47	1.69	1.63
3	B	2901	ANP	PG-O1G	2.45	1.50	1.46
3	A	2901	ANP	PG-N3B	2.44	1.69	1.63
3	A	2901	ANP	PG-O1G	2.39	1.49	1.46
3	A	2901	ANP	PB-O3A	-2.36	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2901	ANP	PB-O3A-PA	-3.84	119.09	132.62
3	B	2901	ANP	PB-O3A-PA	-3.61	119.91	132.62
3	A	2901	ANP	C5-C6-N6	2.29	123.83	120.35
3	B	2901	ANP	C5-C6-N6	2.28	123.81	120.35

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2901	ANP	PB-N3B-PG-O1G
3	A	2901	ANP	O4'-C4'-C5'-O5'
3	B	2901	ANP	PB-N3B-PG-O1G
3	B	2901	ANP	C5'-O5'-PA-O3A
3	A	2901	ANP	C3'-C4'-C5'-O5'

There are no ring outliers.

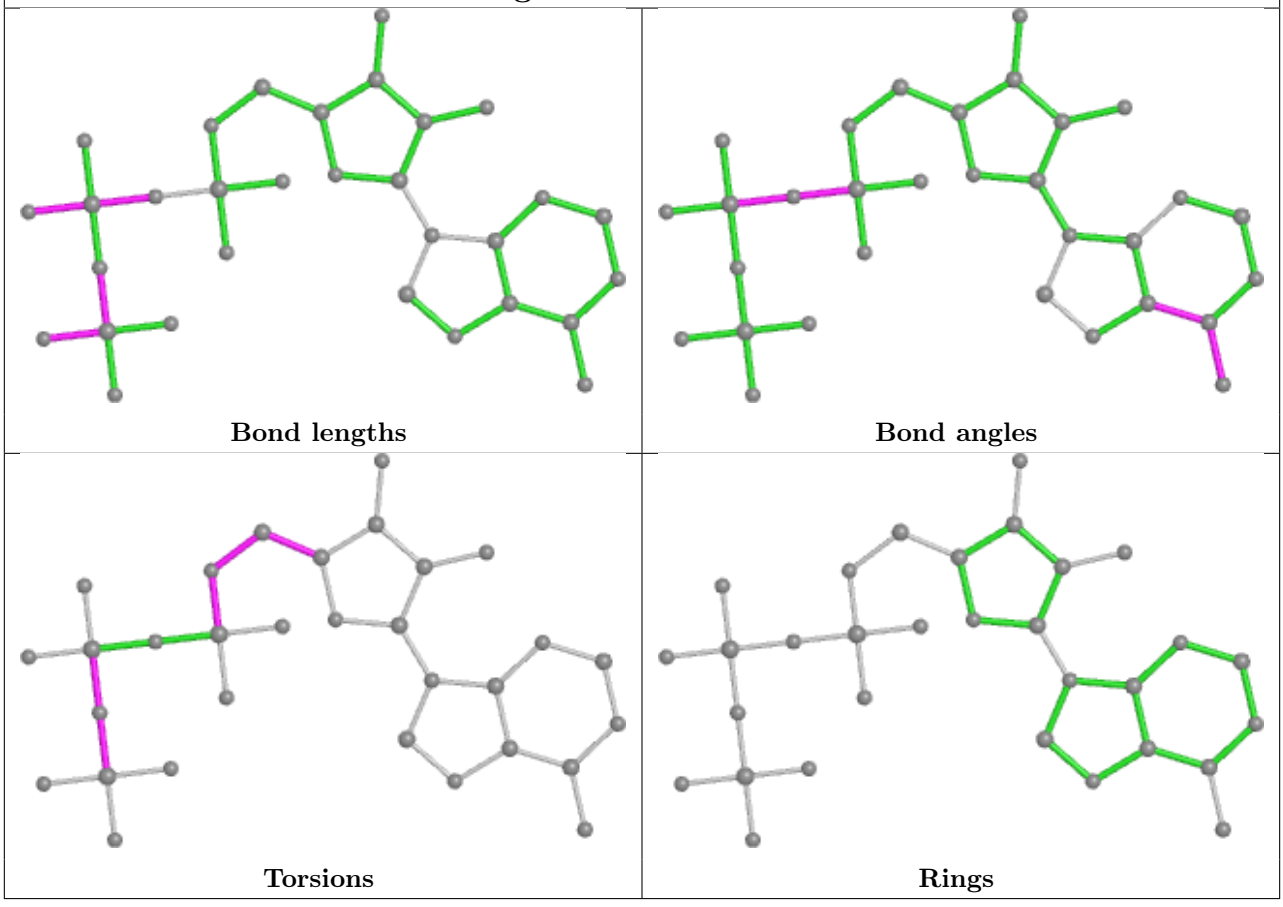
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2901	ANP	4	0
3	A	2901	ANP	3	0

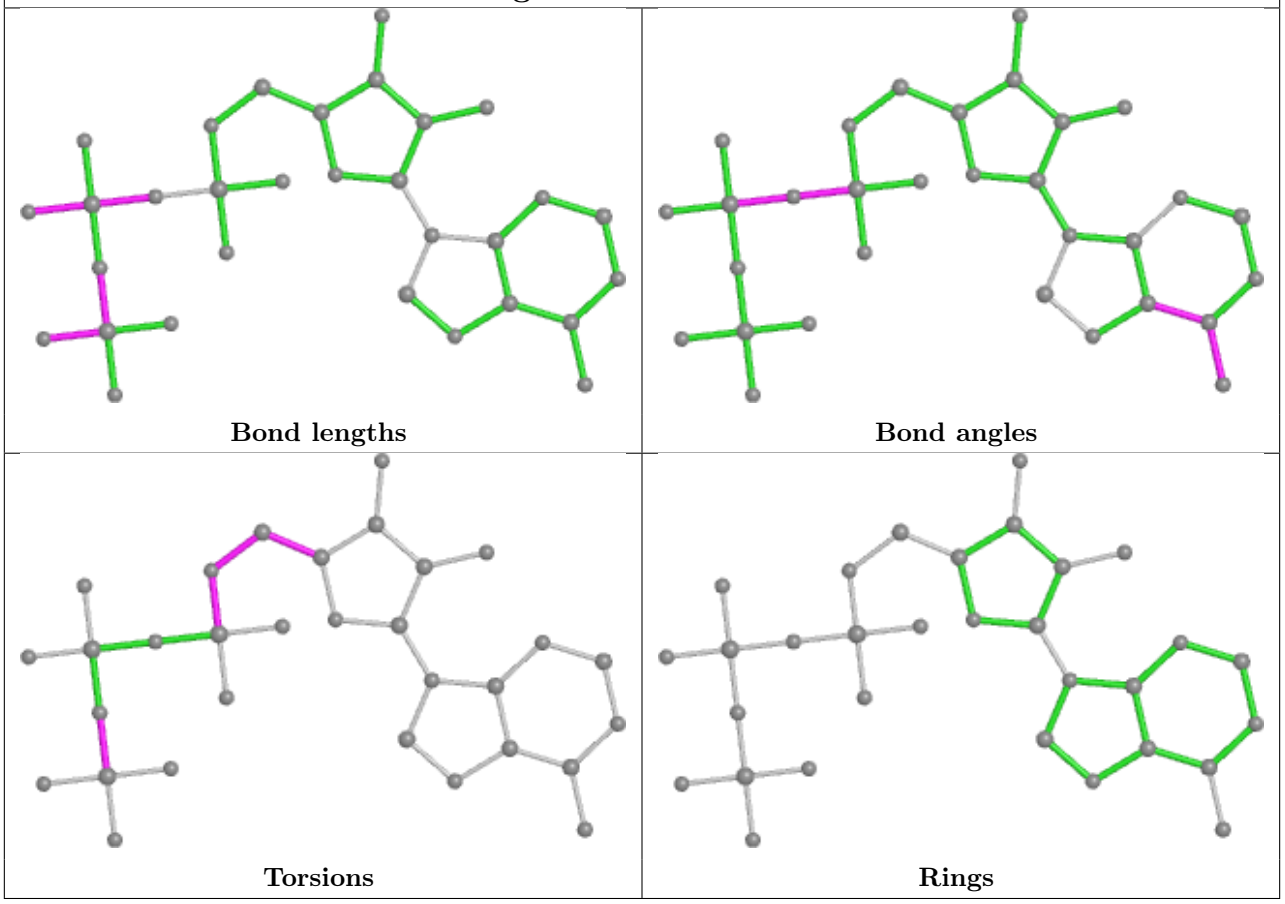
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ANP B 2901



Ligand ANP A 2901



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.

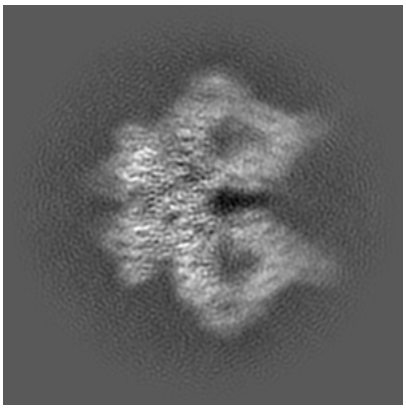
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61006. These allow visual inspection of the internal detail of the map and identification of artifacts.

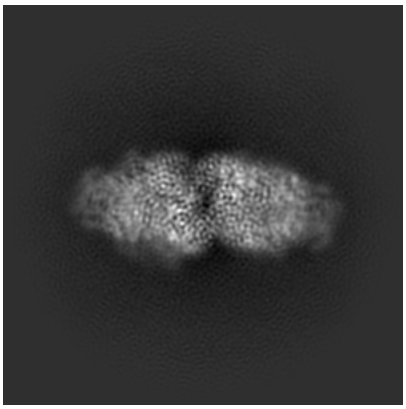
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

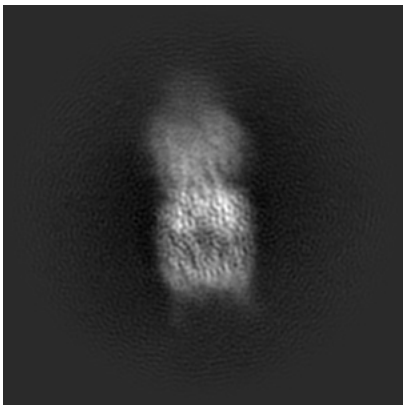
6.1.1 Primary map



X

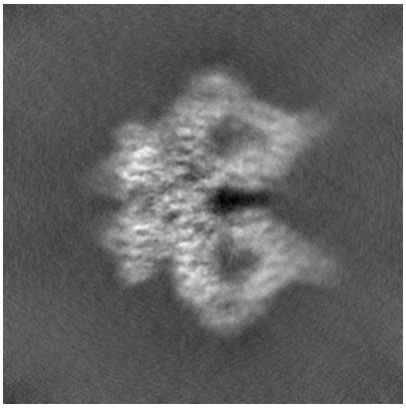


Y

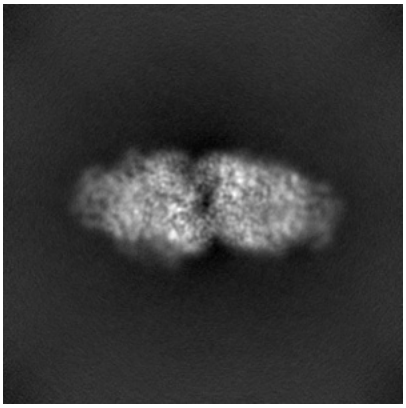


Z

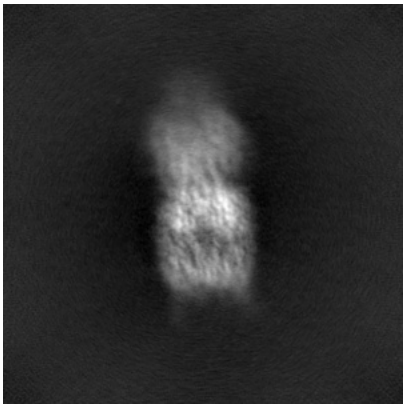
6.1.2 Raw map



X



Y

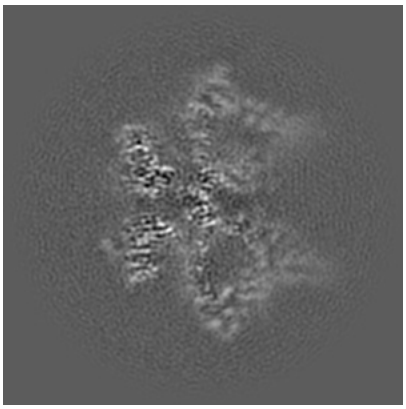


Z

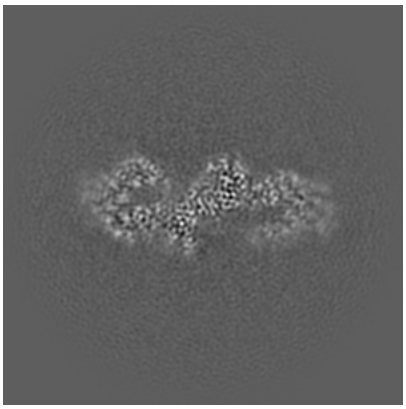
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

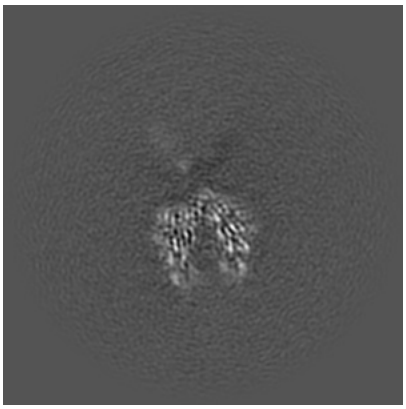
6.2.1 Primary map



X Index: 144

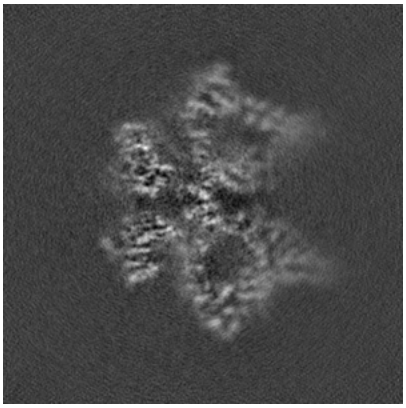


Y Index: 144

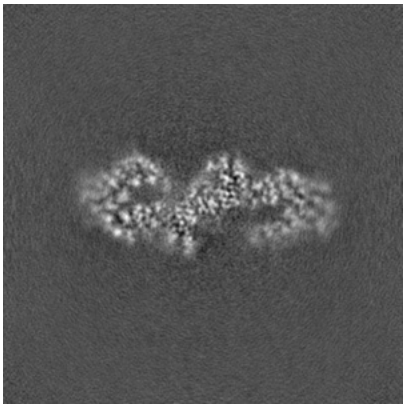


Z Index: 144

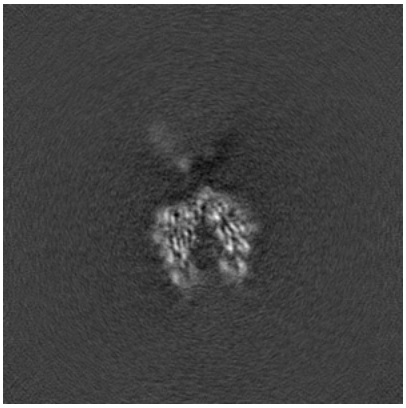
6.2.2 Raw map



X Index: 144



Y Index: 144

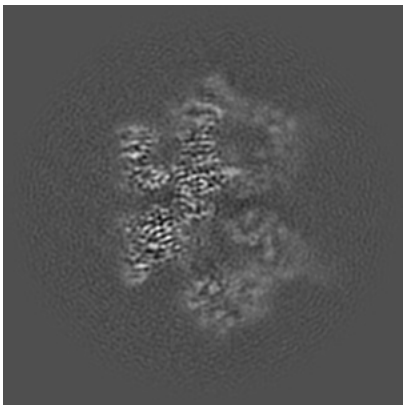


Z Index: 144

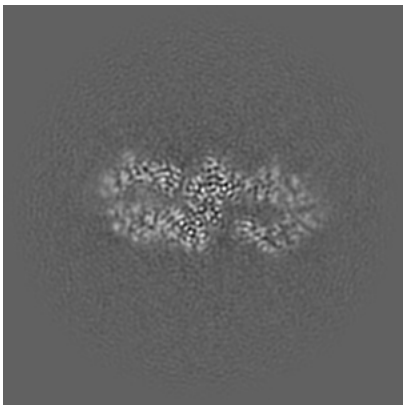
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

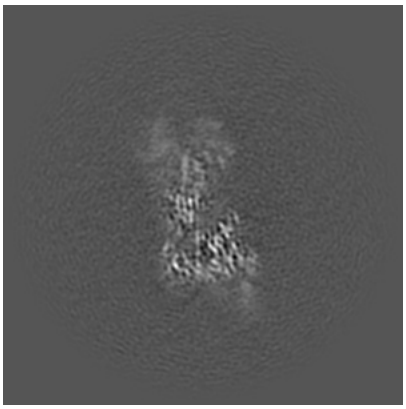
6.3.1 Primary map



X Index: 152

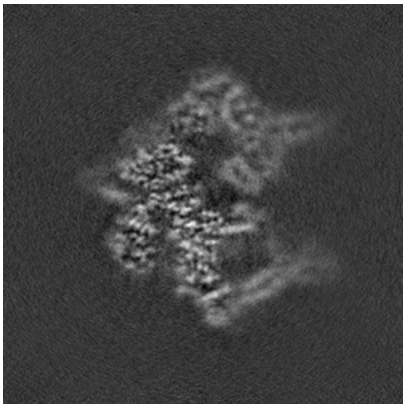


Y Index: 133

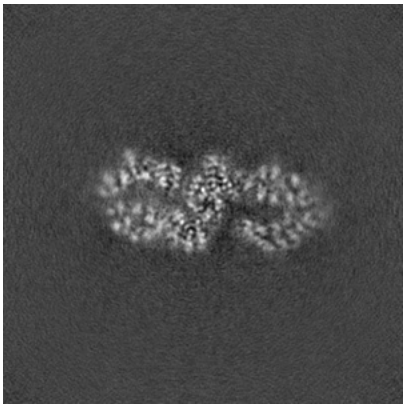


Z Index: 127

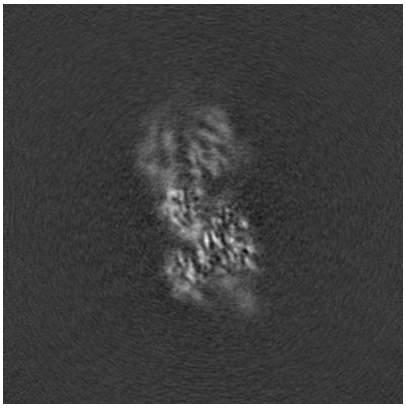
6.3.2 Raw map



X Index: 131



Y Index: 134

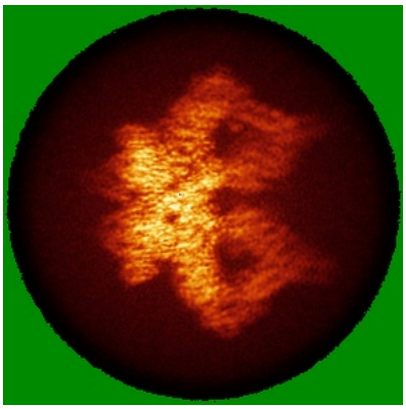


Z Index: 120

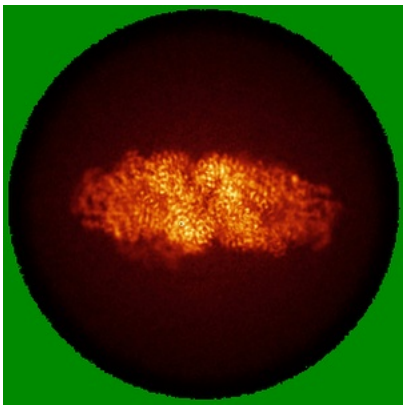
The images above show the largest variance slices of the map in three orthogonal directions.

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

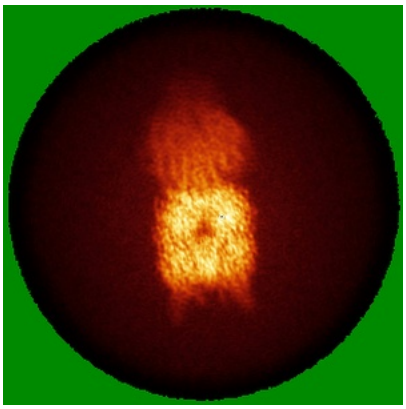
6.4.1 Primary map



X

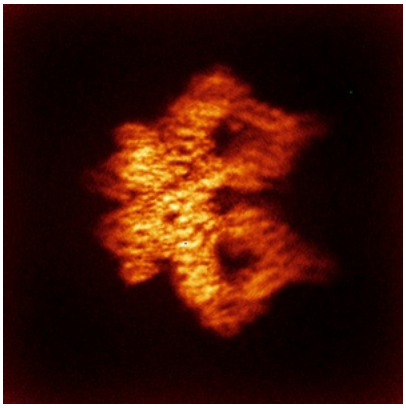


Y

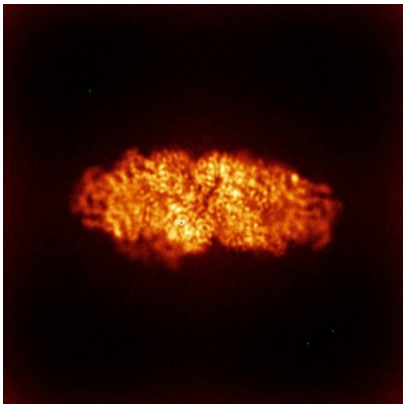


Z

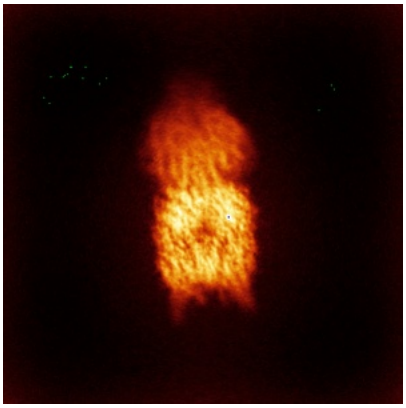
6.4.2 Raw map



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.

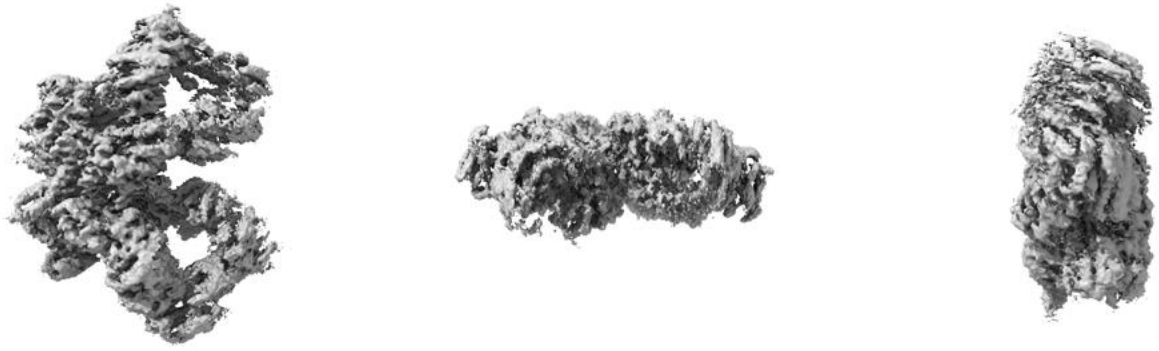
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. 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.

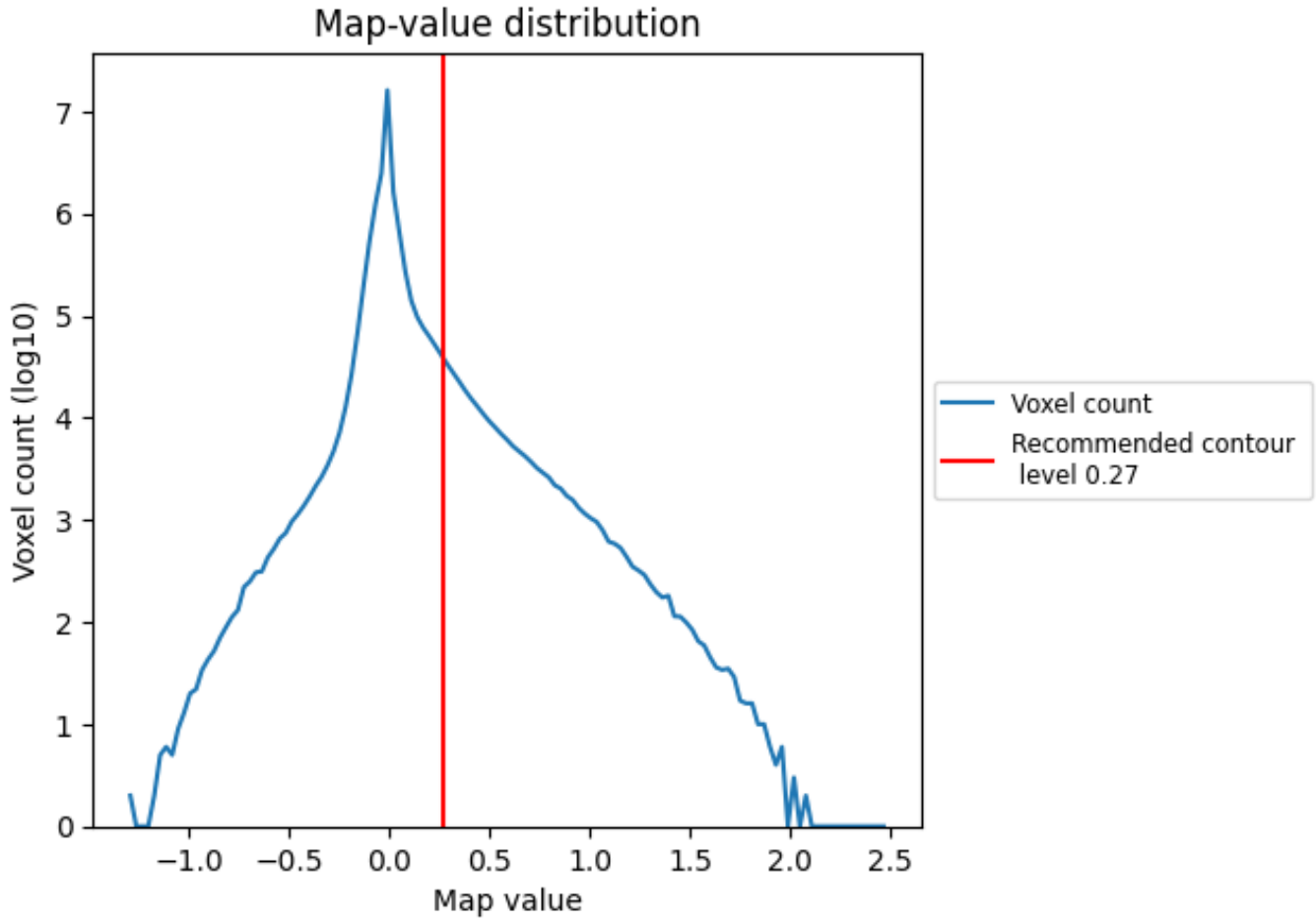
6.6 Mask visualisation (i)

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

7 Map analysis

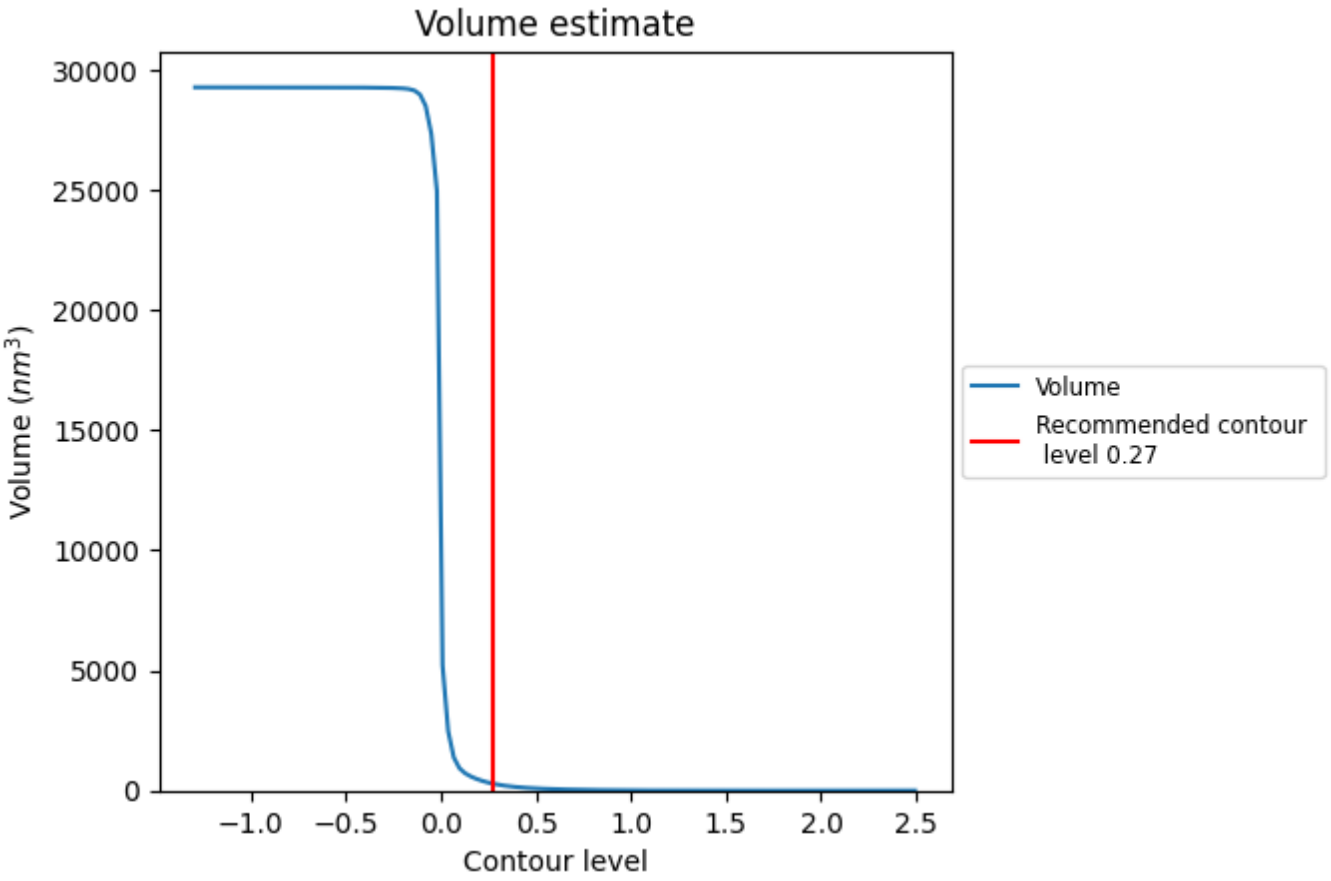
This section contains the results of statistical analysis of the map.

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.

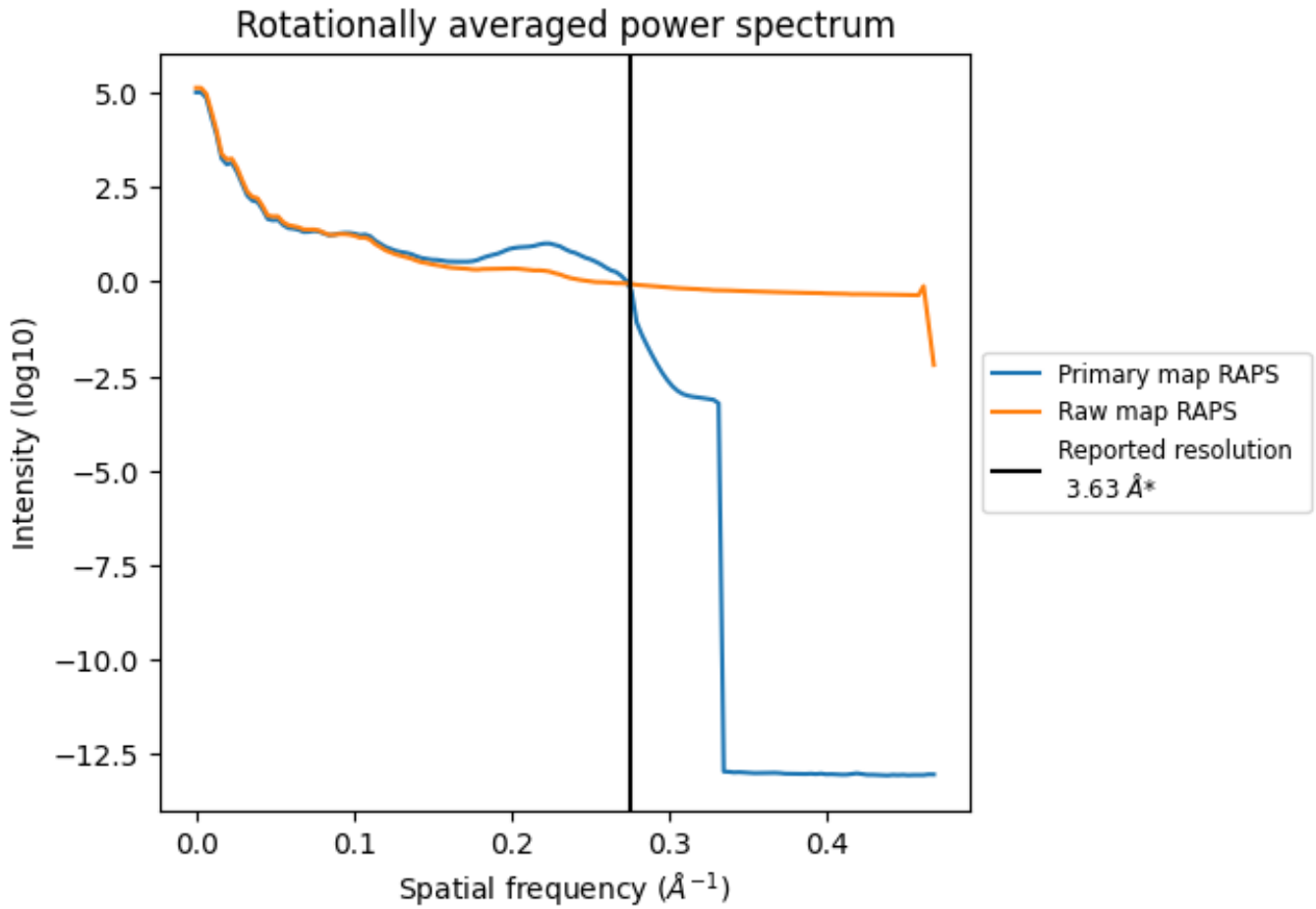
7.2 Volume estimate (i)



The volume at the recommended contour level is 294 nm^3; this corresponds to an approximate mass of 265 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)

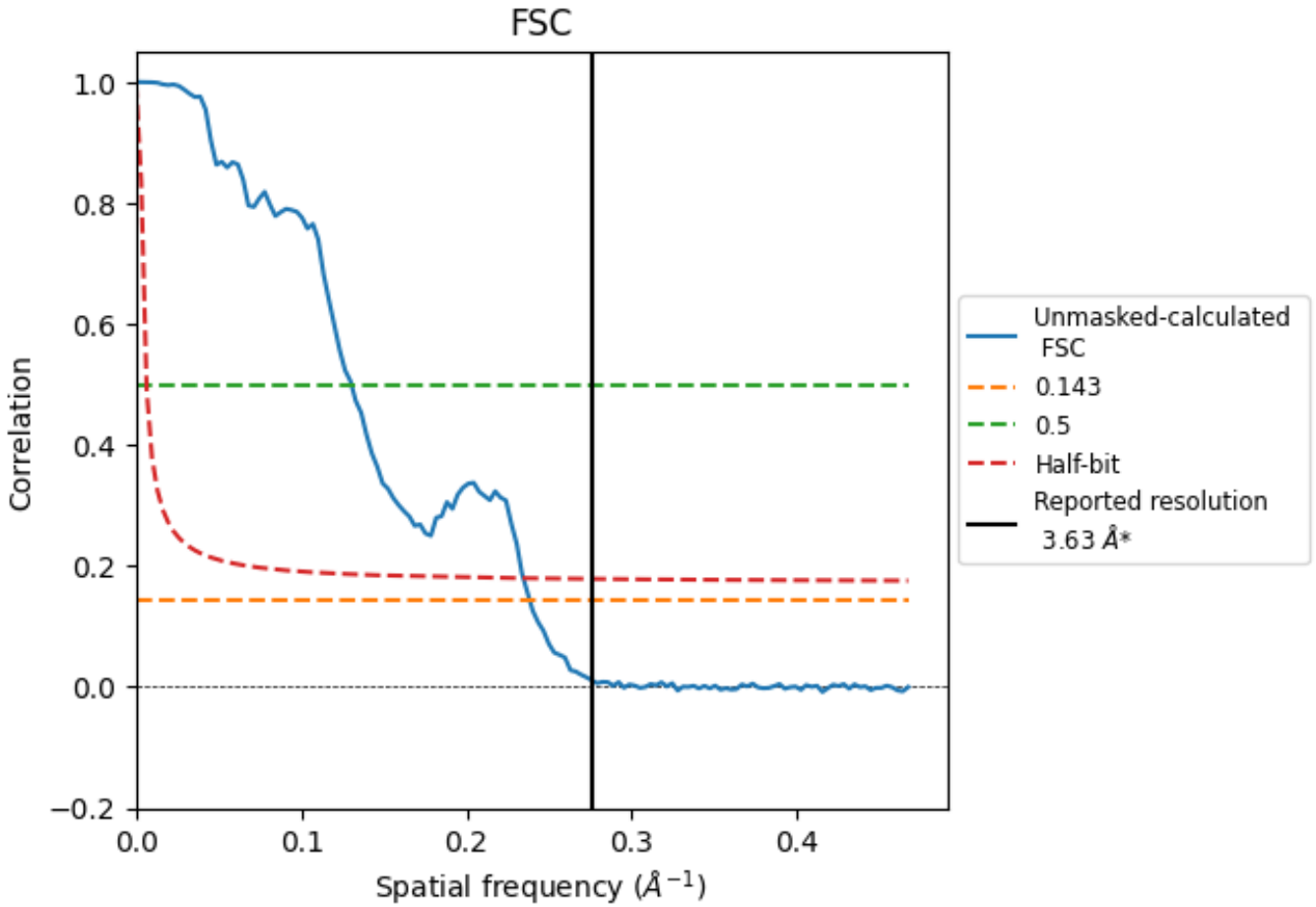


*Reported resolution corresponds to spatial frequency of 0.275 $Å^{-1}$

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 0.275 Å^{-1}

8.2 Resolution estimates (i)

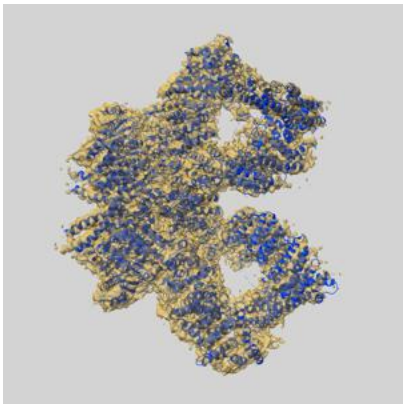
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	7.67	4.27

*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 4.20 differs from the reported value 3.63 by more than 10 %

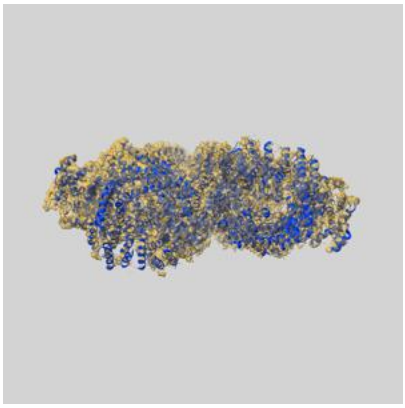
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61006 and PDB model 9IZ0. Per-residue inclusion information can be found in section 3 on page 5.

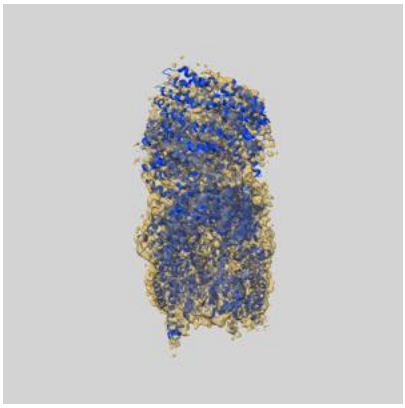
9.1 Map-model overlay



X



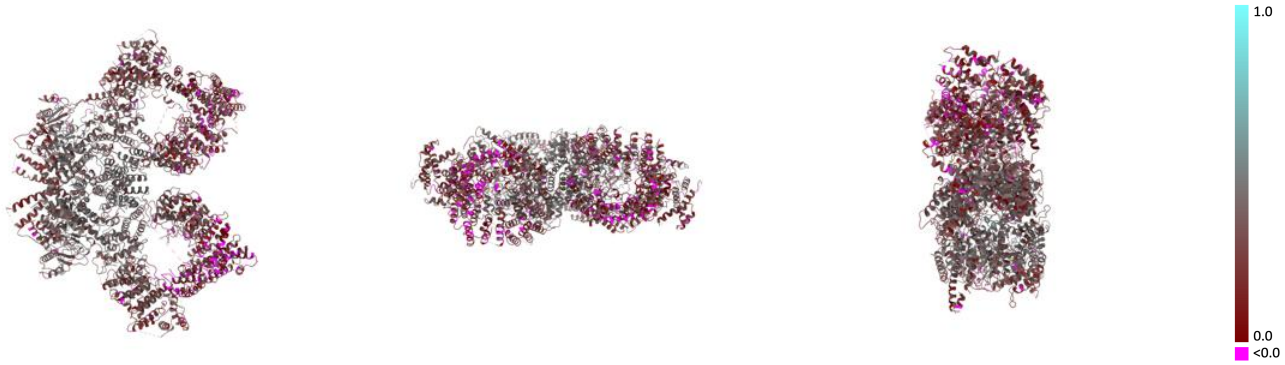
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

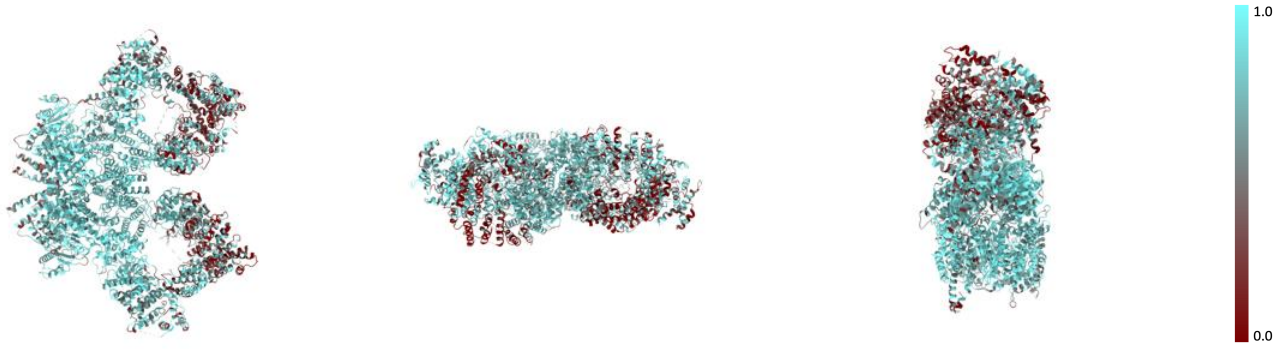
9.2 Q-score mapped to coordinate model (i)



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.

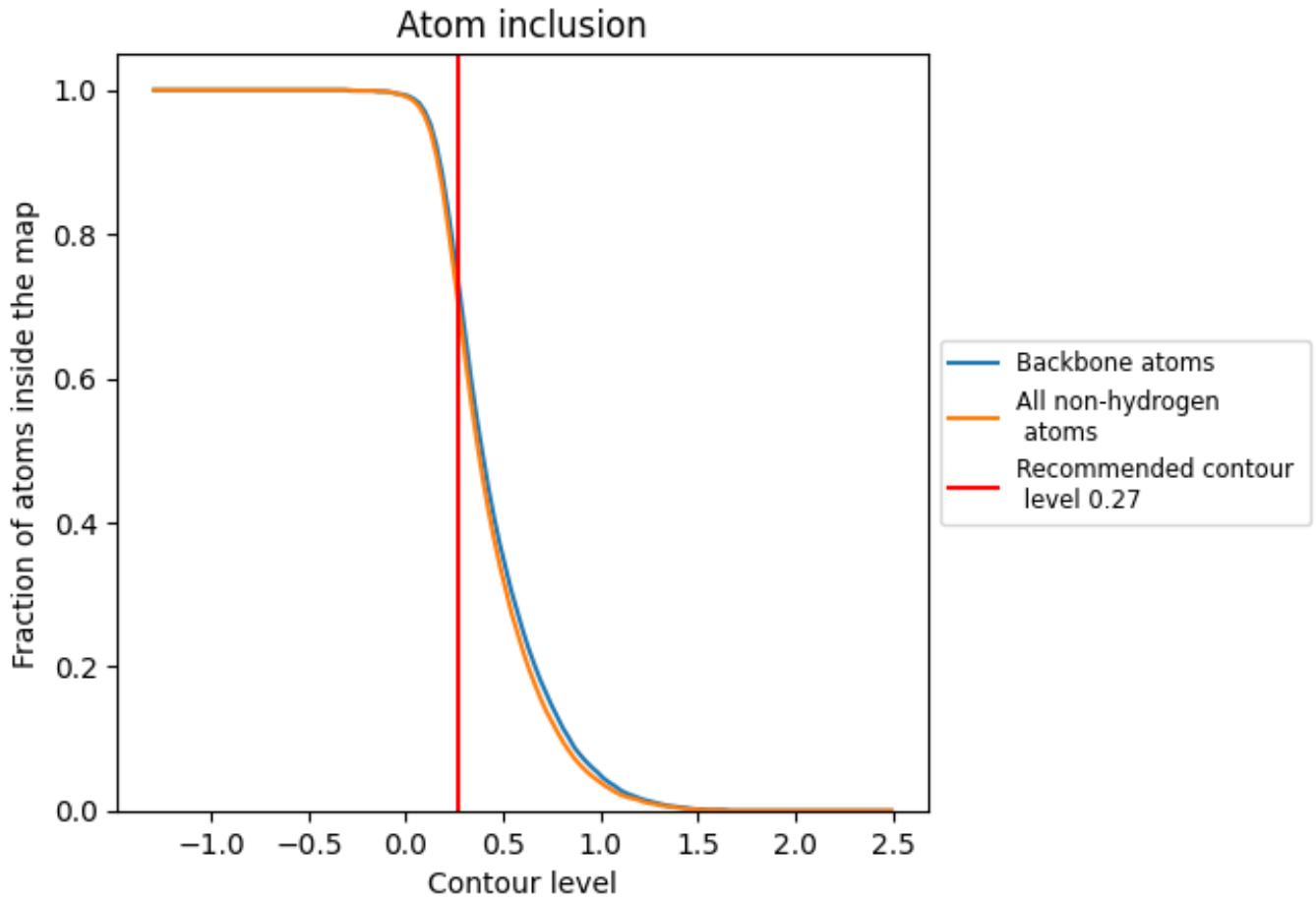
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.27).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7020	0.3170
A	0.6830	0.3180
B	0.7190	0.3170
F	0.8410	0.3680