wwPDB EM Validation Summary Report

Sep 23, 2026 – 07:26 am BST

PDB ID	:	9TU9 / pdb_00009tu9
EMDB ID	:	EMD-56253
Title	:	CryoEM structure of DruE:ATPgammaS:DNA from Druantia type III - dimer 2
Authors	:	Grass, L.M.; Himpich, S.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on	:	2026-01-08
Resolution	:	3.60 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 ⓘ 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:

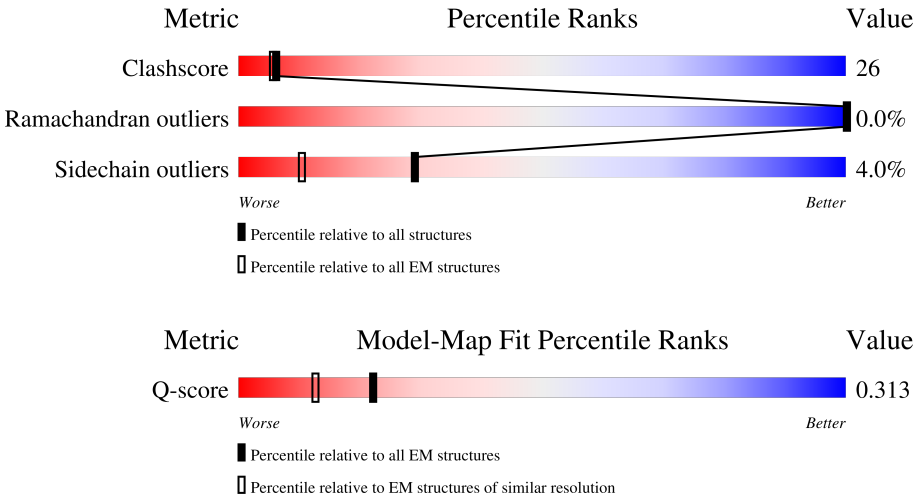
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	Y	2108	50% 46%
1	y	2108	13% 48% 48%
2	G	30	17% 63% 20%
3	I	30	13% 43% 43%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33663 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 DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	2075	Total	C	N	O	S	0	0
			16471	10380	2939	3080	72		
1	y	2050	Total	C	N	O	S	0	0
			16275	10265	2912	3026	72		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
Y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
Y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
Y	0	PHE	-	expression tag	UNP A0A4P8BDA5
y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
y	0	PHE	-	expression tag	UNP A0A4P8BDA5

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*AP*CP*CP*GP*TP*CP*GP*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*CP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	24	Total	C	N	O	P	0	0
			497	235	98	140	24		

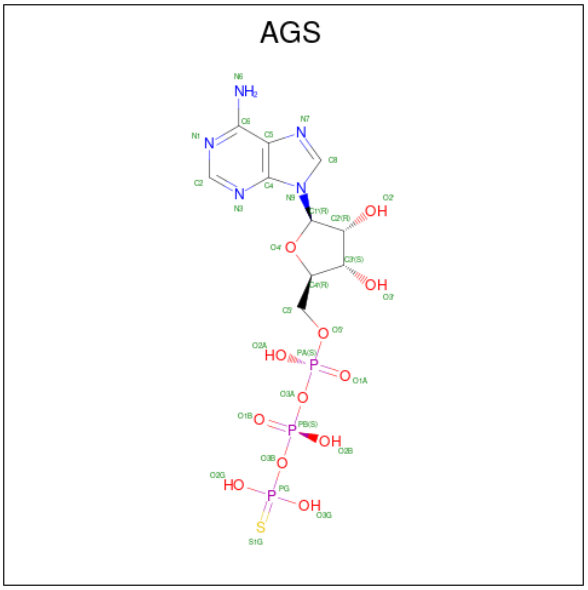
- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	17	Total	C	N	O	P	0	0
			348	166	62	103	17		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	Y	5	Total Zn 5 5	0
4	y	5	Total Zn 5 5	0

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



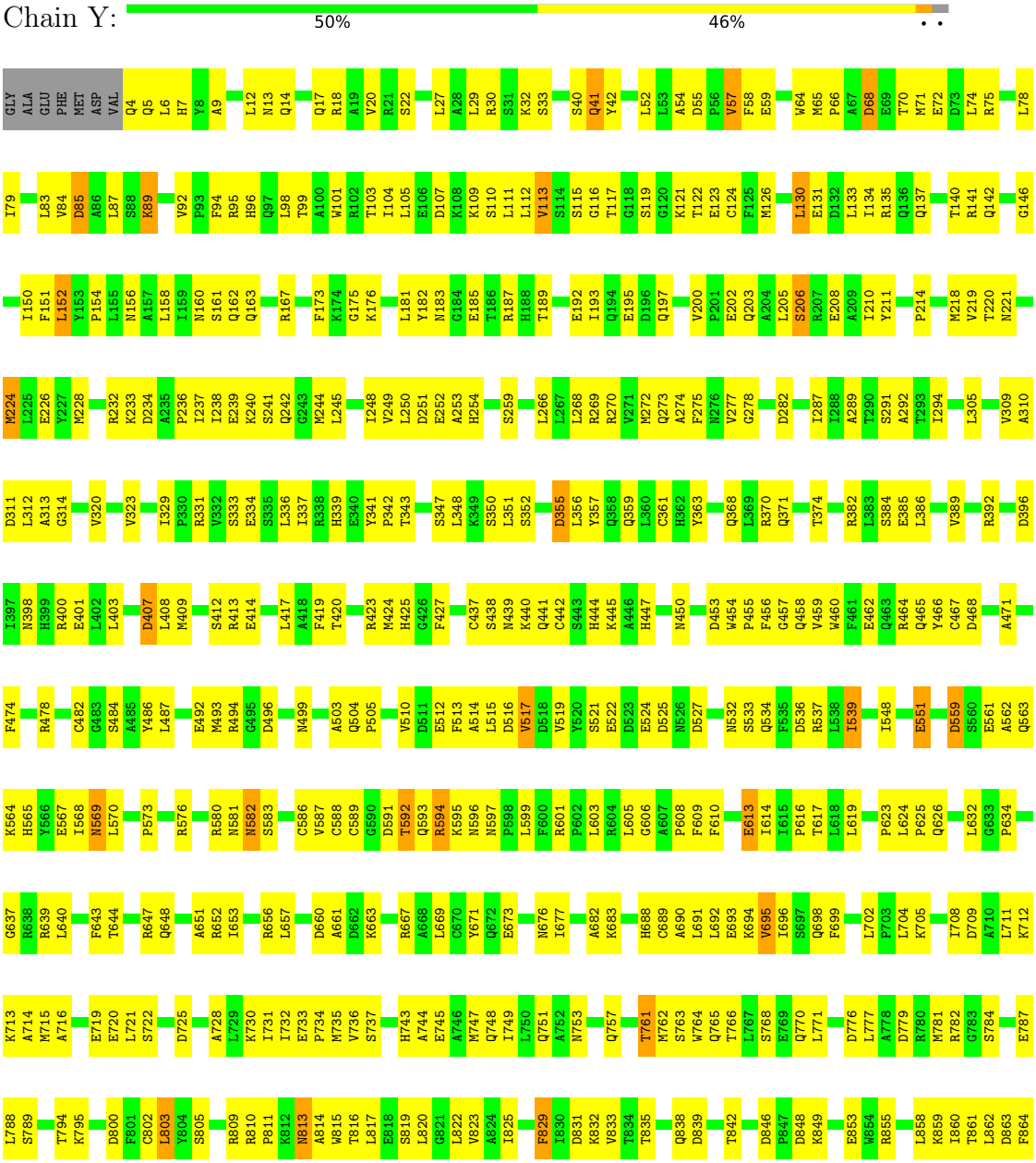
Mol	Chain	Residues	Atoms	AltConf
5	Y	1	Total C N O P S 31 10 5 12 3 1	0
5	y	1	Total C N O P S 31 10 5 12 3 1	0

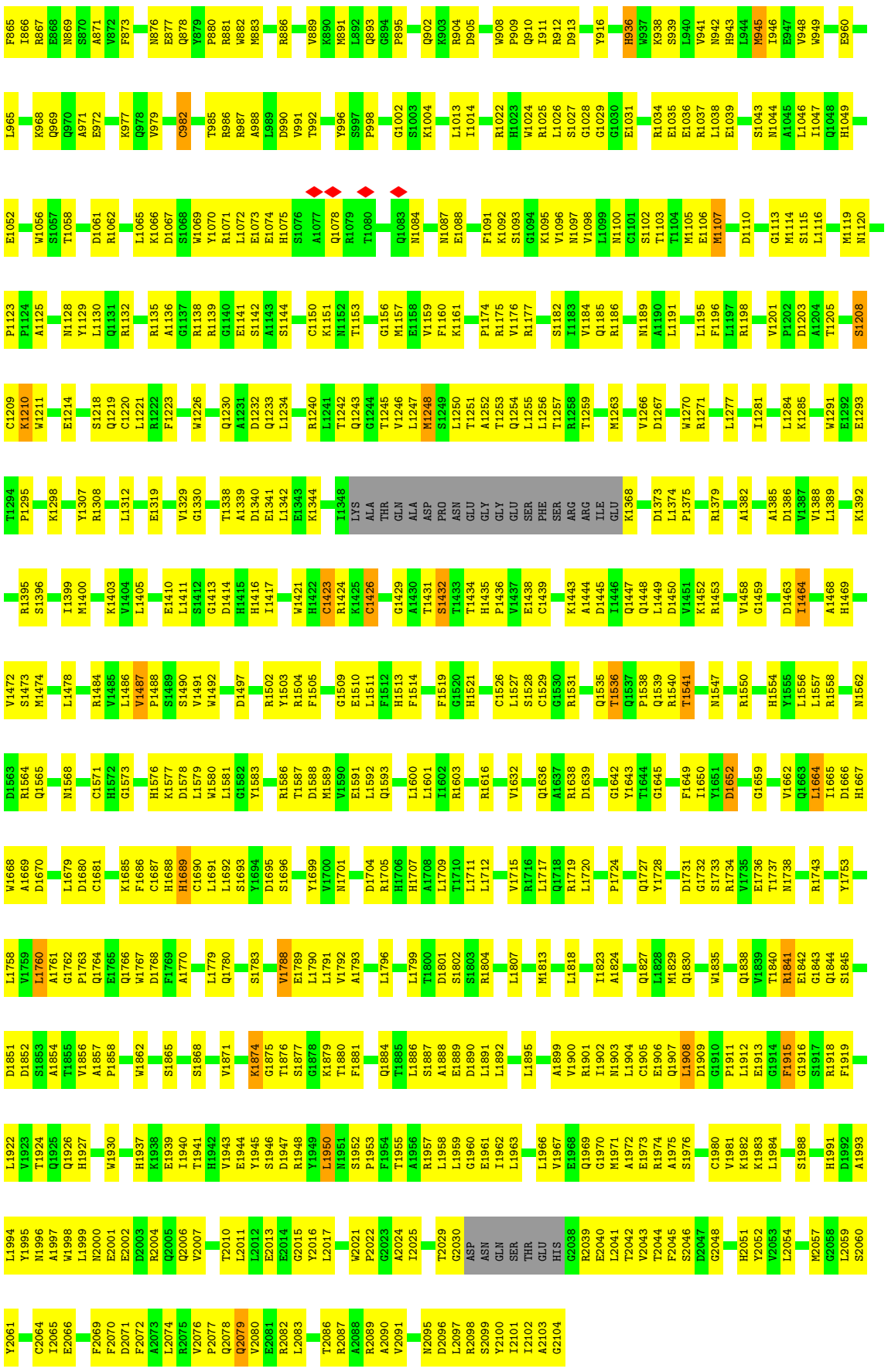
3 Residue-property plots (i)

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: DEAD/DEAH box helicase

Chain Y:

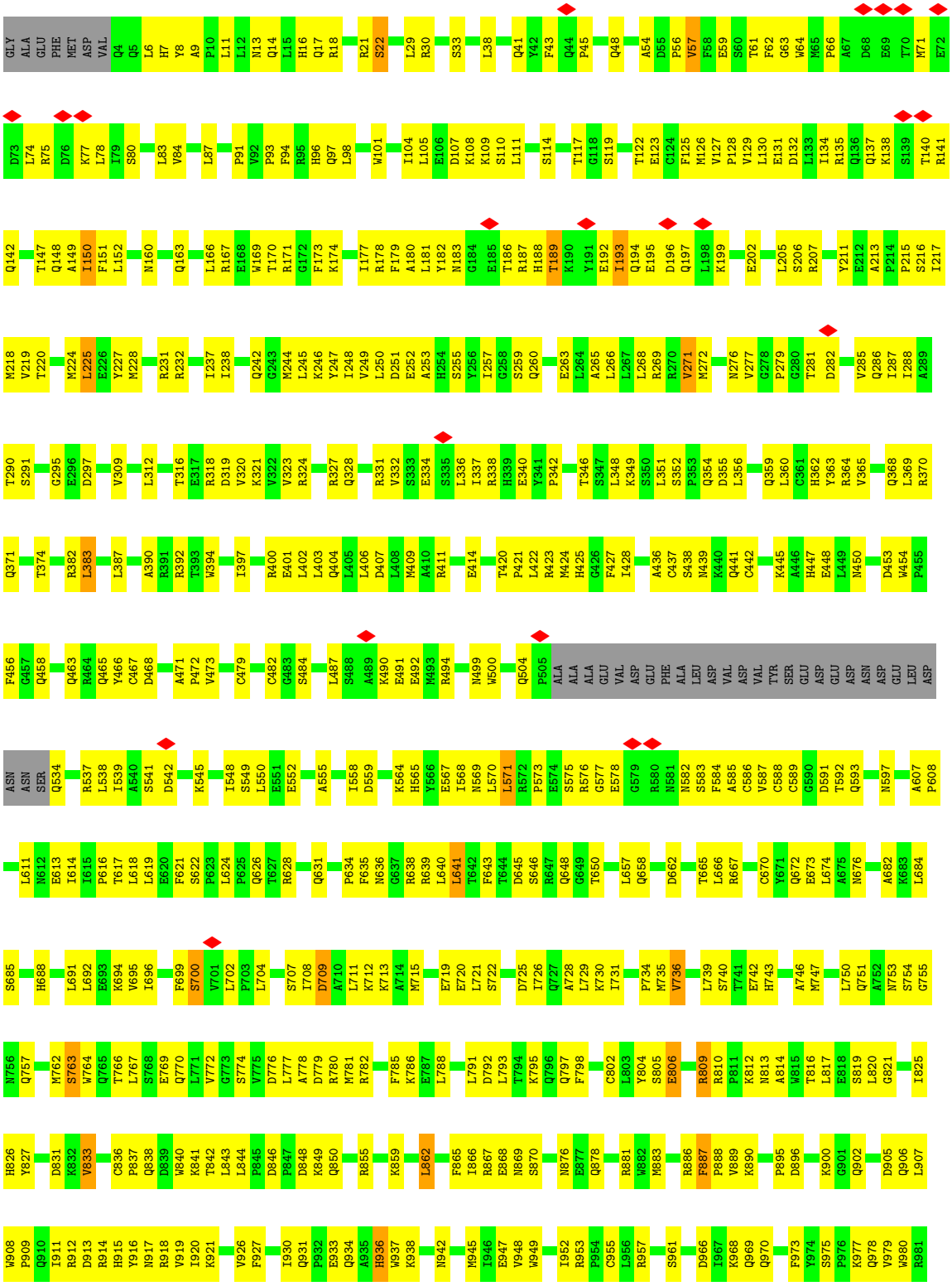


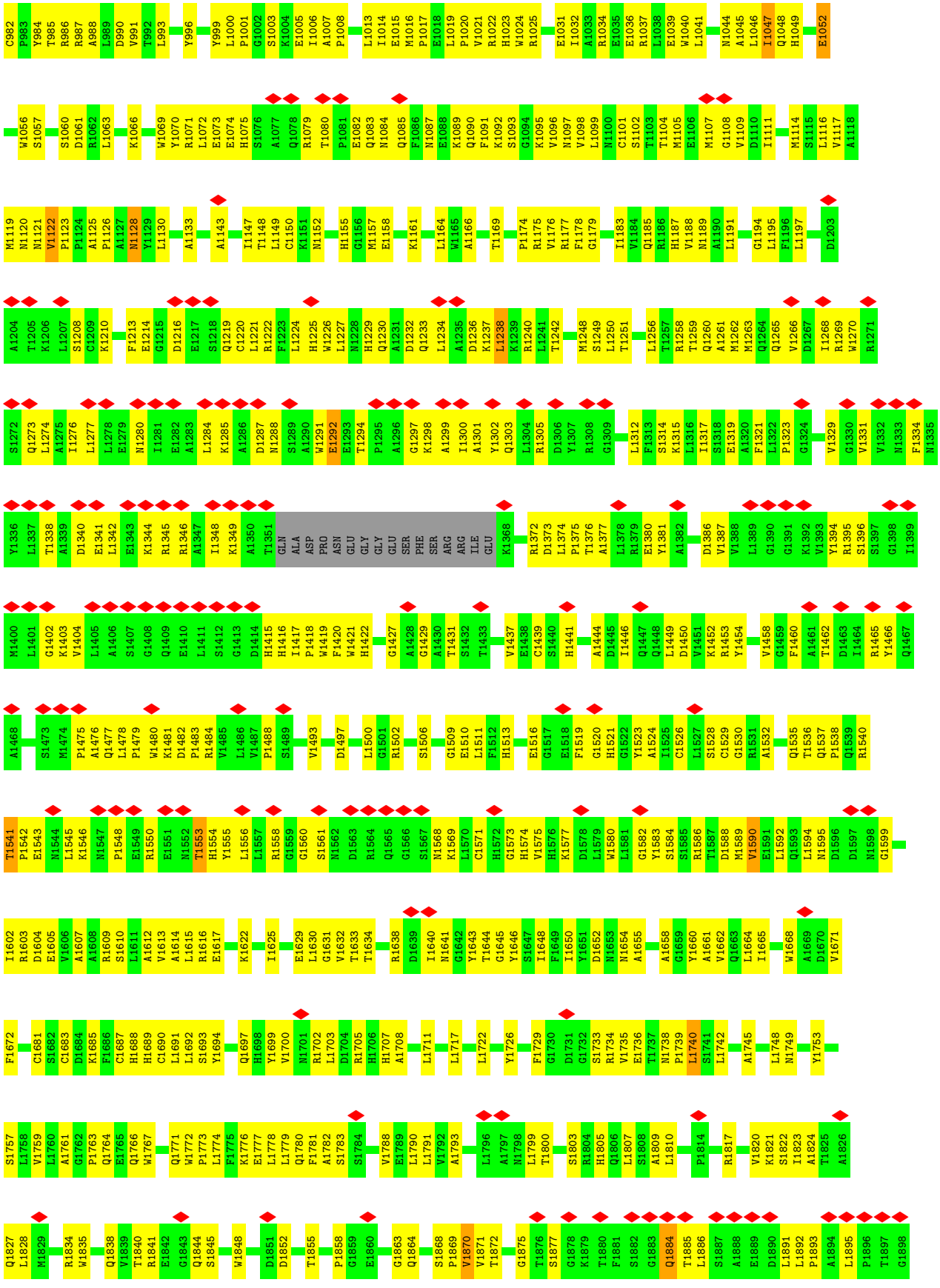

F865 I866 R867 E868 N869 S870 A871 V872 F873 N876 E877 Q878 Y879 P880 R881 W882 M883 R886 V889 K890 M891 L892 Q893 G894 P895 Q902 K903 R904 D905 W908 P909 Q910 I911 R912 D913 Y916 H936 W937 K938 S939 L940 V941 N942 H943 L944 M945 I946 E947 V948 W949 E960
L965 K968 Q969 Q970 A971 E972 K977 Q978 V979 C982 T985 R986 R987 A988 L989 D990 V991 T992 Y996 S997 P998 G1002 S1003 K1004 L1013 I1014 R1022 H1023 W1024 R1025 L1026 S1027 G1028 G1029 G1030 E1031 R1034 E1035 E1036 R1037 L1038 E1039 S1043 N1044 A1045 L1046 I1047 Q1048 H1049
E1052 W1056 S1057 T1058 D1061 R1062 L1065 K1066 D1067 S1068 W1069 Y1070 R1071 L1072 E1073 E1074 H1075 S1076 A1077 Q1078 R1079 T1080 Q1083 N1084 N1087 E1088 F1091 K1092 S1093 G1094 K1095 V1096 N1097 V1098 L1099 N1100 C1101 S1102 T1103 T1104 M1105 E1106 M1107 D1110 G1113 M1114 S1115 L1116 M1119 N1120
P1123 P1124 A1125 N1128 Y1129 L1130 Q1131 R1132 R1135 A1136 G1137 R1138 R1139 G1140 E1141 S1142 A1143 S1144 C1150 K1151 N1152 T1153 G1156 M1157 E1158 V1159 F1160 K1161 P1174 R1175 V1176 R1177 S1182 I1183 V1184 Q1185 R1186 N1189 A1190 L1191 L1195 F1196 L1197 R1198 V1201 P1202 D1203 A1204 T1205 S1208
C1209 K1210 W1211 E1214 S1218 Q1219 C1220 L1221 R1222 F1223 W1226 Q1230 A1231 D1232 Q1233 L1234 R1240 L1241 T1242 Q1243 G1244 T1245 V1246 L1247 M1248 S1249 L1250 T1251 A1252 T1253 Q1254 L1255 L1256 T1257 R1258 T1259 M1263 V1266 D1267 W1270 R1271 L1277 I1281 L1284 K1286 W1291 E1292 E1293
T1294 P1295 K1298 Y1307 R1308 L1312 E1319 V1329 G1330 T1338 A1339 D1340 E1341 L1342 E1343 K1344 I1348 LYS ALA THR GLN ALA ASP PRO ASN GLU GLY GLY GLU SER PHE SER ARG ARG ILE GLU K1368 D1373 L1374 P1375 R1379 A1382 A1385 D1386 V1387 V1388 L1389 K1392
R1395 S1396 I1399 M1400 K1403 V1404 L1405 E1410 L1411 S1412 G1413 D1414 H1415 H1416 I1417 W1421 H1422 C1423 R1424 K1425 C1426 G1429 A1430 T1431 S1432 T1433 T1434 H1435 P1436 V1437 E1438 C1439 K1443 A1444 D1445 I1446 Q1447 Q1448 L1449 D1450 V1451 K1452 R1453 V1458 G1459 D1463 I1464 A1468 H1469
V1472 S1473 M1474 L1478 R1484 V1485 L1486 V1487 P1488 S1489 S1490 V1491 W1492 D1497 R1502 Y1503 R1504 F1505 G1509 E1510 L1511 F1512 H1513 F1514 F1519 G1520 H1521 C1526 L1527 S1528 C1529 G1530 R1531 Q1535 T1536 Q1537 P1538 Q1539 R1540 T1541 N1547 R1550 H1554 Y1555 L1556 L1557 R1558 N1562
D1563 R1564 Q1565 N1568 C1571 H1572 G1573 H1576 K1577 D1578 L1579 W1580 L1581 G1582 Y1583 R1586 T1587 D1588 M1589 V1590 E1591 L1592 Q1593 L1600 L1601 I1602 R1603 R1616 V1632 Q1636 A1637 R1638 D1639 G1642 Y1643 T1644 G1645 F1649 I1650 Y1651 D1652 G1659 V1662 Q1663 L1664 I1665 D1666 H1667
W1668 A1669 D1670 L1679 D1680 C1681 K1685 F1686 C1687 H1688 H1689 C1690 L1691 L1692 S1693 Y1694 D1695 S1696 Y1699 V1700 N1701 D1704 R1705 H1706 H1707 A1708 L1709 T1710 L1711 L1712 V1715 R1716 L1717 Q1718 R1719 L1720 P1724 Q1727 Y1728 D1731 G1732 S1733 R1734 E1735 E1736 T1737 N1738 R1743 Y1753
L1758 V1759 L1760 A1761 G1762 P1763 Q1764 E1765 Q1766 W1767 D1768 F1769 A1770 L1779 Q1780 S1783 V1788 E1789 L1790 L1791 V1792 A1793 L1796 L1799 T1800 D1801 S1802 S1803 R1804 L1807 M1813 L1818 I1823 A1824 Q1827 L1828 M1829 Q1830 W1835 Q1838 V1839 T1840 R1841 E1842 G1843 Q1844 S1845
D1851 D1852 S1853 A1854 T1855 V1856 A1857 P1858 W1862 S1865 S1868 V1871 K1874 G1875 T1876 S1877 G1878 K1879 T1880 F1881 Q1884 T1885 L1886 S1887 A1888 E1889 D1890 L1891 L1892 L1895 A1899 V1900 R1901 I1902 N1903 L1904 C1905 E1906 Q1907 L1908 D1909 G1910 P1911 L1912 E1913 G1914 F1915 G1916 S1917 R1918 F1919
L1922 V1923 T1924 Q1925 Q1926 H1927 W1930 H1937 K1938 E1939 I1940 T1941 H1942 V1943 E1944 Y1945 S1946 D1947 R1948 Y1949 L1950 N1951 S1952 P1953 F1954 T1955 A1956 R1957 L1958 L1959 G1960 E1961 I1962 L1963 L1966 V1967 E1968 Q1969 G1970 M1971 A1972 E1973 R1974 A1975 S1976 C1980 V1981 K1982 K1983 L1984 S1988 H1991 D1992 A1993
L1994 Y1995 N1996 A1997 W1998 L1999 N2000 E2001 E2002 D2003 R2004 Q2005 Q2006 V2007 T2010 L2011 L2012 E2013 E2014 G2015 Y2016 L2017 W2021 P2022 G2023 A2024 I2025 T2029 G2030 ASP ASN GLN SER THR GLU HIS G2038 R2039 E2040 L2041 T2042 V2043 T2044 F2045 S2046 D2047 G2048 H2051 Y2052 V2053 L2054 M2057 G2058 L2059 S2060
Y2061 C2064 I2065 E2066 F2069 F2070 D2071 F2072 A2073 L2074 R2075 V2076 P2077 Q2078 Q2079 V2080 E2081 R2082 L2083 T2086 R2087 A2088 R2089 A2090 V2091 N2095 D2096 L2097 R2098 S2099 Y2100 I2101 I2102 A2103 G2104

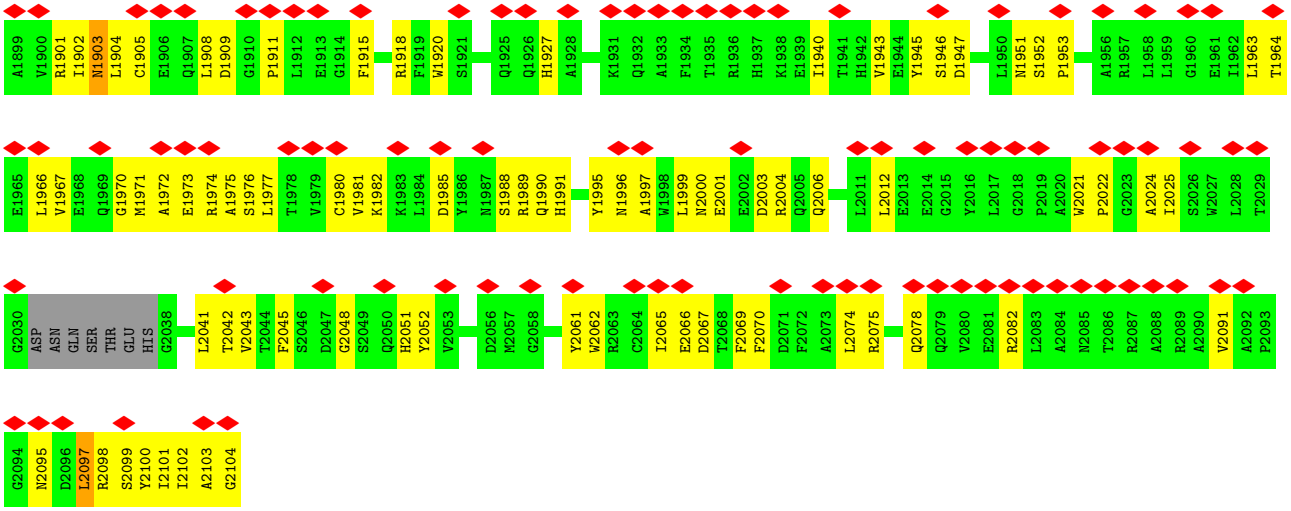
• Molecule 1: DEAD/DEAH box helicase

Chain y:



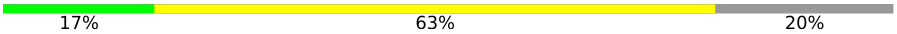


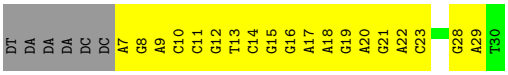

C982 P983 Y984 T985 R986 R987 A988 L989 D990 V991 T992 L993 Y996 Y999 L1000 P1001 G1002 S1003 K1004 E1005 I1006 A1007 P1008 L1013 I1014 E1015 M1016 P1017 E1018 L1019 P1020 V1021 R1022 H1023 W1024 R1025 E1031 I1032 A1033 R1034 E1035 E1036 R1037 L1038 E1039 W1040 L1041 N1044 A1045 L1046 I1047 Q1048 H1049 E1052
W1056 S1057 S1060 D1061 R1062 L1063 K1066 W1069 Y1070 R1071 L1072 E1073 E1074 H1075 S1076 A1077 Q1078 R1079 T1080 P1081 E1082 Q1083 N1084 Q1085 F1086 N1087 E1088 K1089 Q1090 F1091 K1092 S1093 G1094 K1095 V1096 N1097 V1098 L1099 N1100 C1101 S1102 T1103 T1104 M1105 E1106 M1107 G1108 D1110 I1111 M1114 S1115 L1116 V1117 A1118
M1119 N1120 N1121 V1122 P1123 P1124 A1125 P1126 A1127 N1128 Y1129 L1130 A1133 A1143 I1147 T1148 L1149 C1150 K1151 N1152 H1155 G1156 M1157 E1158 K1161 L1164 W1165 A1166 T1169 P1174 R1175 V1176 R1177 F1178 G1179 I1183 V1184 Q1185 R1186 H1187 V1188 N1189 A1190 L1191 G1194 L1195 F1196 L1197 D1203
A1204 T1205 K1206 L1207 S1208 C1209 K1210 F1213 E1214 G1215 D1216 E1217 S1218 Q1219 C1220 L1221 R1222 F1223 L1224 H1225 W1226 L1227 N1228 H1229 Q1230 A1231 D1232 Q1233 L1234 A1235 D1236 K1237 L1238 K1239 R1240 L1241 T1242 M1248 S1249 L1250 T1251 L1256 T1257 R1258 T1259 Q1260 A1261 M1262 M1263 Q1264 Q1265 V1266 D1267 I1268 R1269 W1270 R1271
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Y1336 L1337 T1338 A1339 D1340 E1341 L1342 E1343 K1344 R1345 R1346 A1347 I1348 K1349 A1350 T1351 GLN ALA ASP PRO ASN GLU GLY GLY GLU SER PHE SER ARG ARG ILE GLU K1368 R1372 D1373 L1374 P1375 T1376 A1377 L1378 R1379 E1380 Y1381 A1382 D1386 V1387 V1388 L1389 G1390 G1391 K1392 V1393 Y1394 R1395 S1396 S1397 G1398 I1399
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F1672 C1681 S1682 C1683 D1684 K1685 F1686 C1687 H1688 H1689 C1690 L1691 L1692 S1693 Y1694 Q1697 H1698 Y1699 V1700 N1701 R1702 L1703 D1704 R1705 H1706 H1707 A1708 L1711 L1717 L1722 Y1726 F1729 G1730 D1731 G1732 S1733 R1734 V1735 E1736 T1737 N1738 P1739 L1740 S1741 L1742 A1745 L1748 N1749 Y1753
S1757 L1758 V1759 L1760 A1761 G1762 P1763 Q1764 E1765 Q1766 W1767 F1775 K1776 E1777 L1778 L1779 Q1780 F1781 A1782 S1783 S1784 V1788 E1789 L1790 L1791 V1792 A1793 L1796 A1797 N1798 L1799 T1800 S1803 R1804 H1805 Q1806 L1807 S1808 A1809 L1810 P1814 R1817 V1820 K1821 S1822 I1823 A1824 T1825 A1826
Q1827 L1828 M1829 R1834 W1835 Q1838 V1839 T1840 R1841 E1842 G1843 Q1844 S1845 W1848 D1851 D1852 T1855 P1858 G1859 E1860 G1863 Q1864 S1868 P1869 V1870 V1871 T1872 G1875 T1876 S1877 G1878 K1879 T1880 F1881 S1882 G1883 Q1884 T1885 L1886 S1887 A1888 E1889 D1890 L1891 L1892 P1893 A1894 L1895 P1896 T1897 G1898



• Molecule 2: DNA (5'-D(P*AP*GP*AP*CP*CP*GP*TP*CP*GP*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*CP*GP*AP*T)-3')

Chain G:





• Molecule 3: DNA (5'-D(P*AP*TP*CP*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*C)-3')

Chain I:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27507	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.374	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1093334, 1.1093334, 1.1093334	Depositor

5 Model quality

5.1 Standard geometry

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

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	Y	0.33	0/16840	0.42	0/22830
1	y	0.17	0/16641	0.35	0/22555
2	G	0.29	0/559	0.45	0/861
3	I	0.25	0/389	0.41	0/598
All	All	0.26	0/34429	0.39	0/46844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	16471	0	16231	822	0
1	y	16275	0	16083	867	0
2	G	497	0	269	39	0
3	I	348	0	193	23	0
4	Y	5	0	0	0	0
4	y	5	0	0	0	0
5	Y	31	0	12	6	0
5	y	31	0	12	3	0
All	All	33663	0	32800	1721	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 26.

The worst 5 of 1721 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1529:CYS:SG	1:Y:1554:HIS:CD2	2.49	1.05
1:y:1622:LYS:HZ3	1:y:1671:VAL:HA	1.29	0.96
2:G:21:DG:N2	3:I:10:DC:O2	2.00	0.92
1:Y:65:MET:HE3	1:Y:66:PRO:HD2	1.51	0.92
2:G:21:DG:N1	3:I:10:DC:N3	2.19	0.90

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	Y	2069/2108 (98%)	1919 (93%)	149 (7%)	1 (0%)	100	100
1	y	2042/2108 (97%)	1934 (95%)	108 (5%)	0	100	100
All	All	4111/4216 (98%)	3853 (94%)	257 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	1208	SER

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	Y	1768/1795 (98%)	1683 (95%)	85 (5%)	23	50
1	y	1746/1795 (97%)	1691 (97%)	55 (3%)	34	58
All	All	3514/3590 (98%)	3374 (96%)	140 (4%)	29	54

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	1169	THR
1	y	1251	THR
1	y	1574	HIS
1	Y	1201	VAL
1	Y	1153	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	y	1083	GLN
1	y	1688	HIS
1	y	1128	ASN
1	y	1576	HIS
1	y	1805	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)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
5	AGS	y	2206	-	29,33,33	0.47	1 (3%)	39,52,52	0.75	1 (2%)
5	AGS	Y	2206	-	29,33,33	0.46	0	39,52,52	0.75	1 (2%)

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
5	AGS	y	2206	-	-	7/21/38/38	0/3/3/3
5	AGS	Y	2206	-	-	6/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	y	2206	AGS	PG-S1G	2.09	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	2206	AGS	PA-O3A-PB	-3.90	119.45	132.83
5	y	2206	AGS	PA-O3A-PB	-3.76	119.93	132.83

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

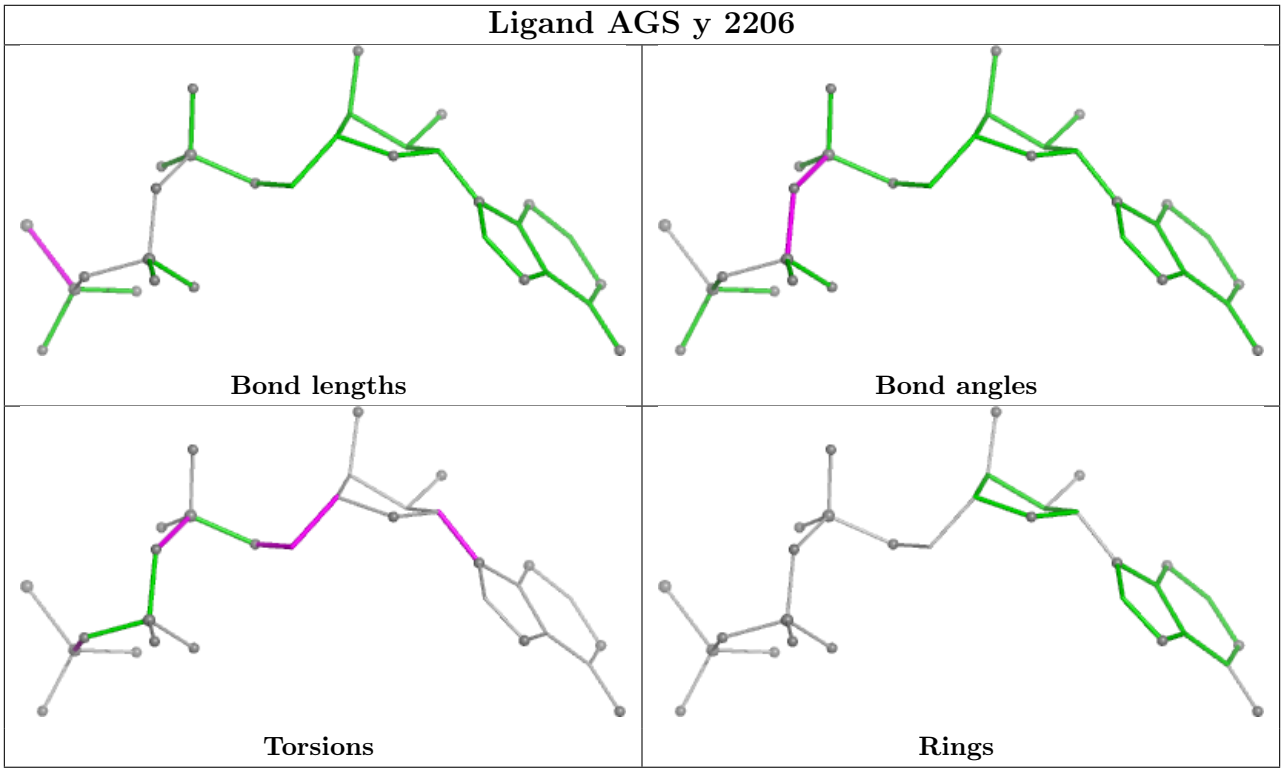
Mol	Chain	Res	Type	Atoms
5	Y	2206	AGS	C5'-O5'-PA-O2A
5	y	2206	AGS	PB-O3B-PG-O2G
5	y	2206	AGS	PB-O3B-PG-O3G
5	Y	2206	AGS	O4'-C4'-C5'-O5'
5	y	2206	AGS	O4'-C4'-C5'-O5'

There are no ring outliers.

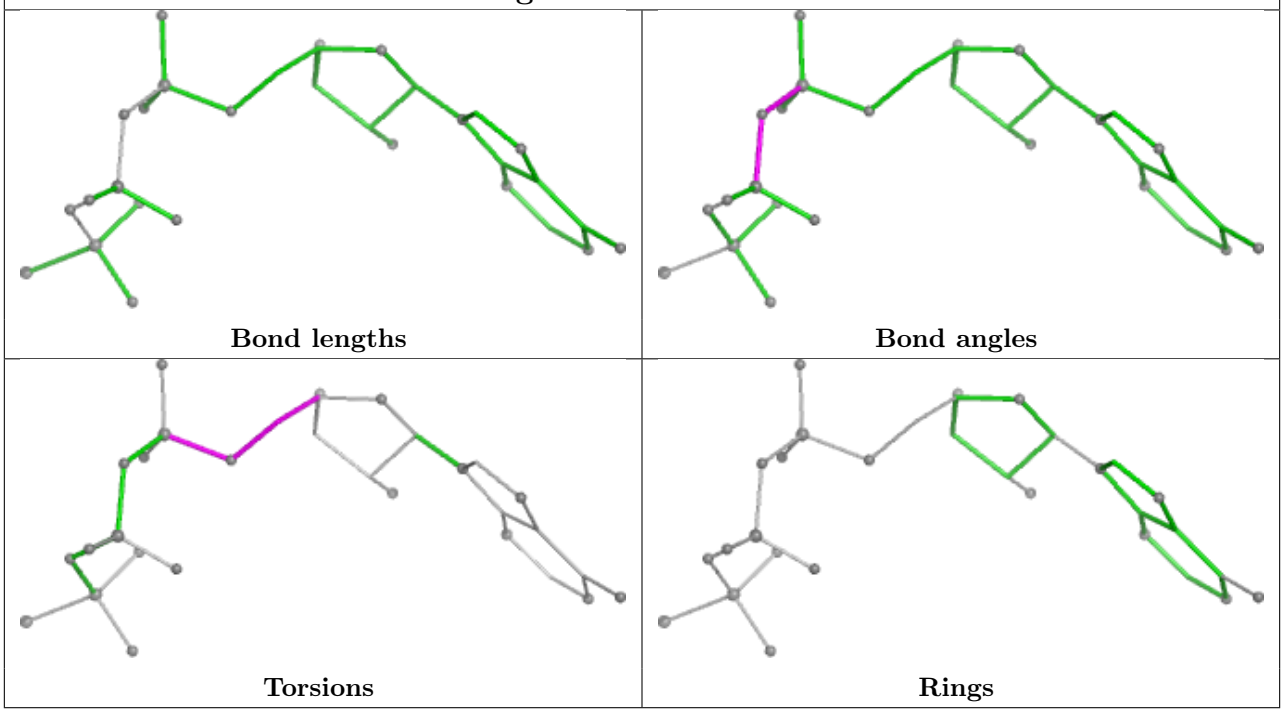
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	y	2206	AGS	3	0
5	Y	2206	AGS	6	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 AGS Y 2206



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.

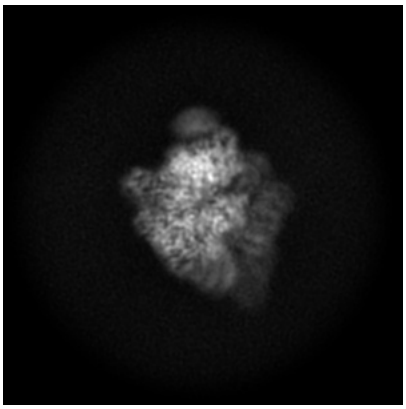
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56253. These allow visual inspection of the internal detail of the map and identification of artifacts.

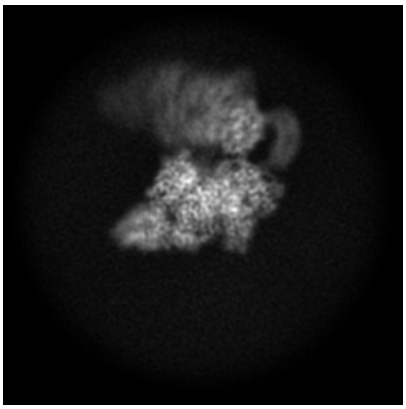
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

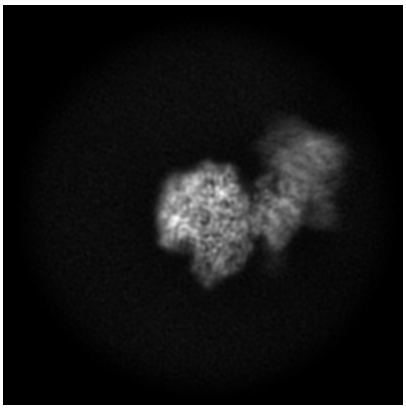
6.1.1 Primary map



X

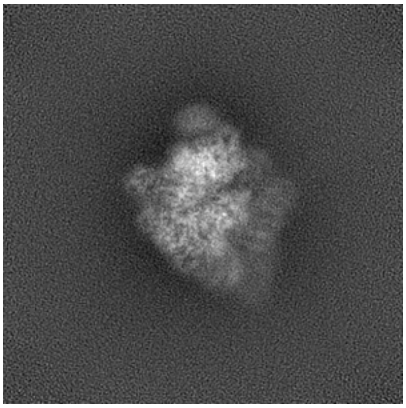


Y

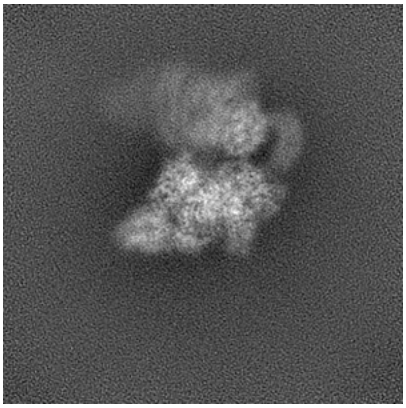


Z

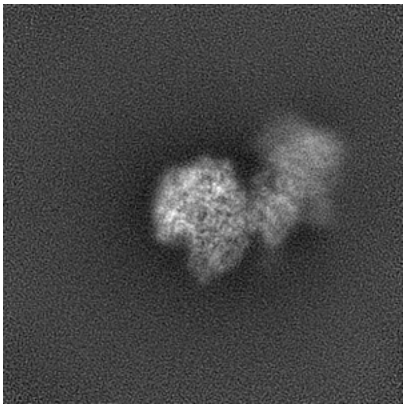
6.1.2 Raw map



X



Y

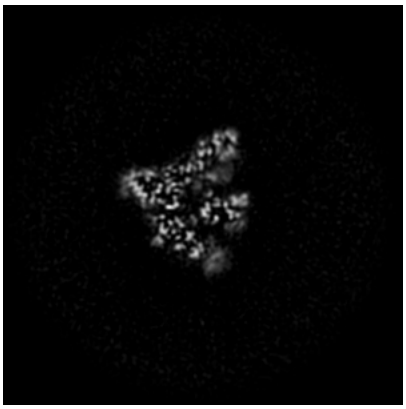


Z

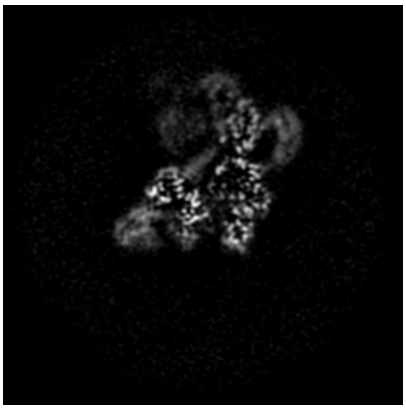
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

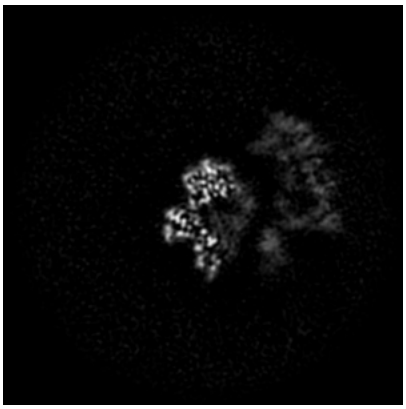
6.2.1 Primary map



X Index: 144

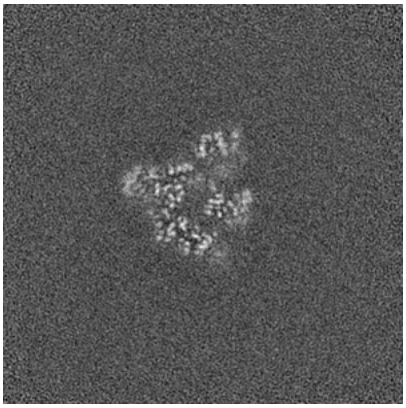


Y Index: 144

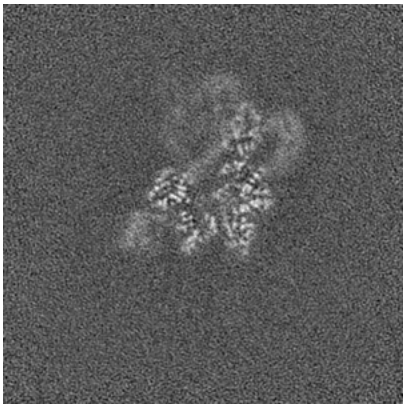


Z Index: 144

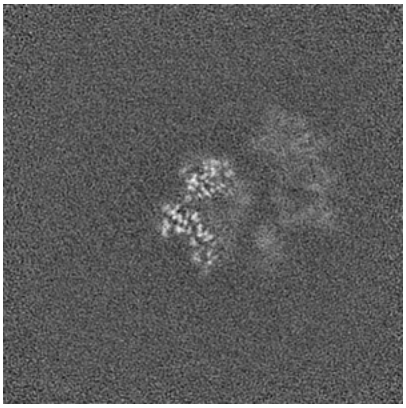
6.2.2 Raw map



X Index: 144



Y Index: 144

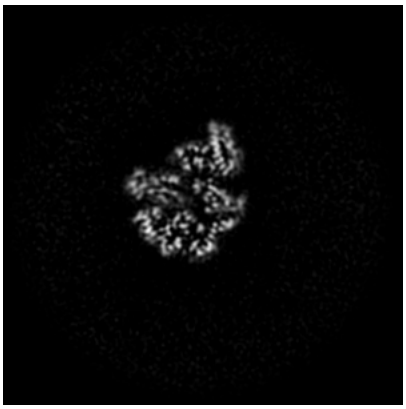


Z Index: 144

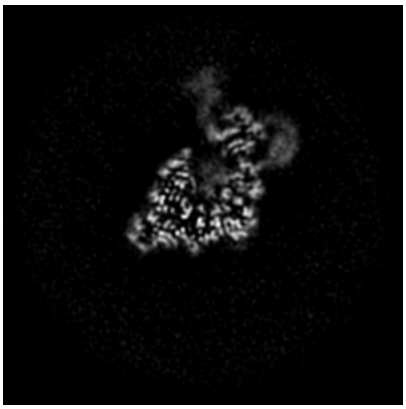
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

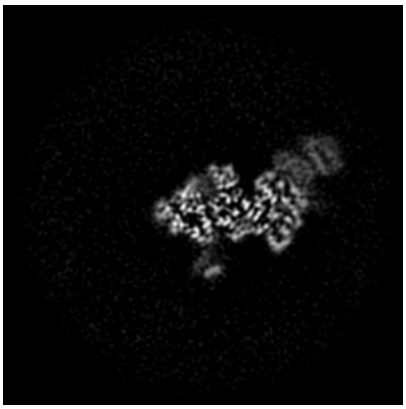
6.3.1 Primary map



X Index: 157

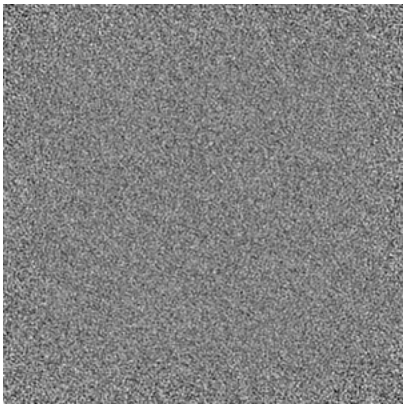


Y Index: 129

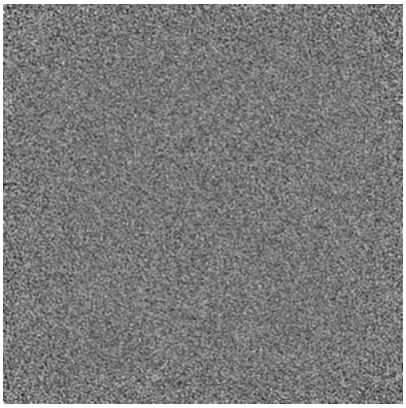


Z Index: 170

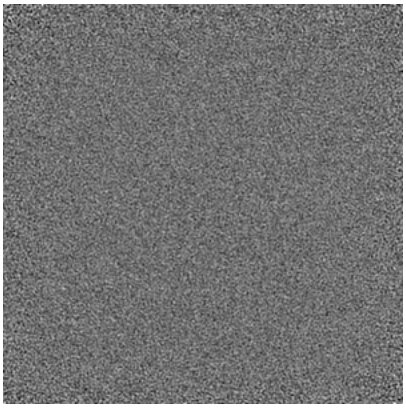
6.3.2 Raw map



X Index: 0



Y Index: 0

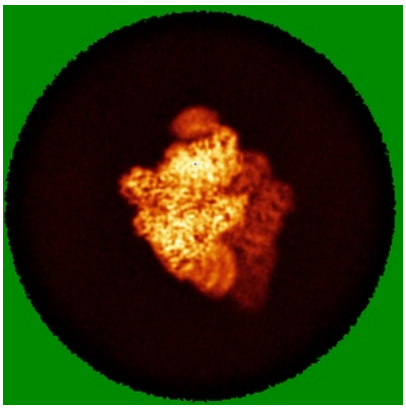


Z Index: 0

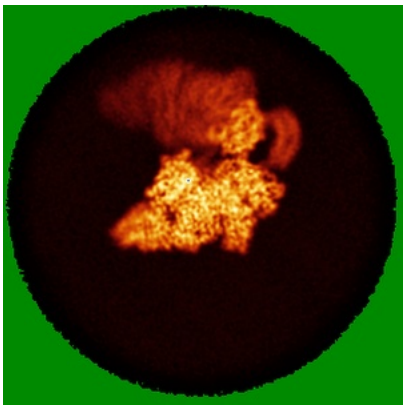
The images above show the largest variance slices of the map in three orthogonal directions.

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

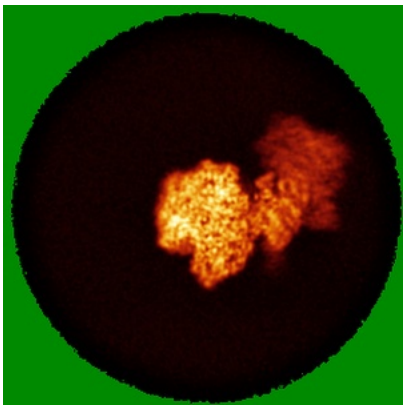
6.4.1 Primary map



X

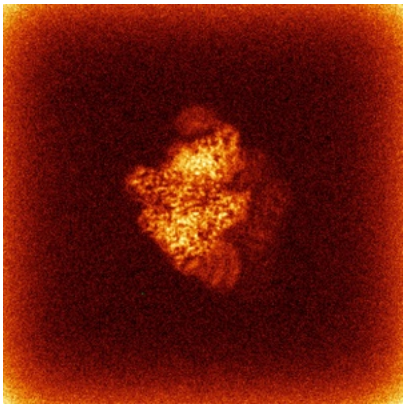


Y

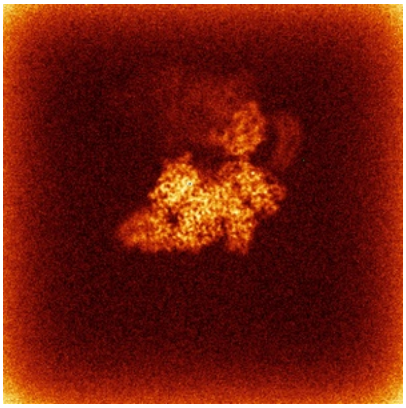


Z

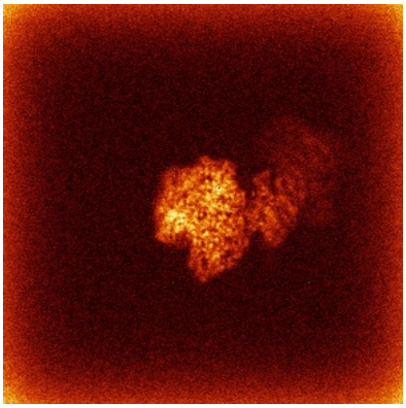
6.4.2 Raw map



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)

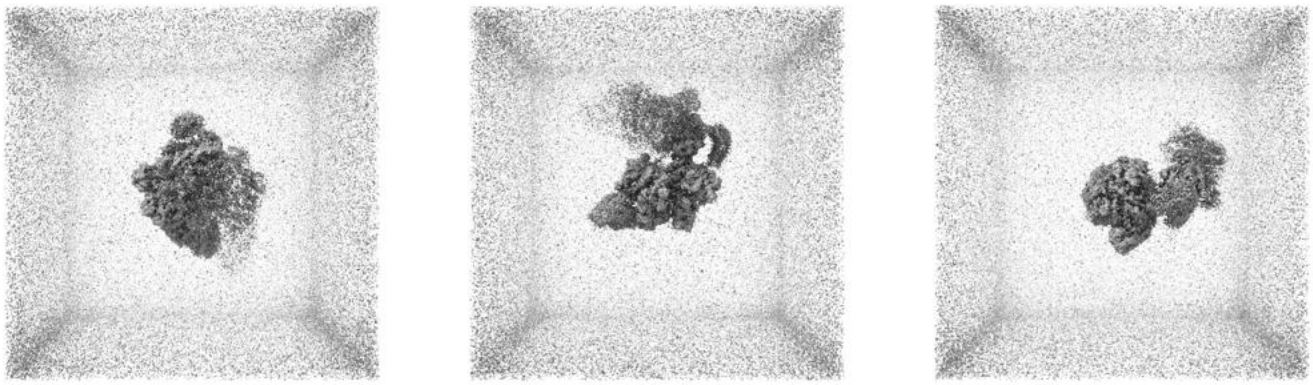
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

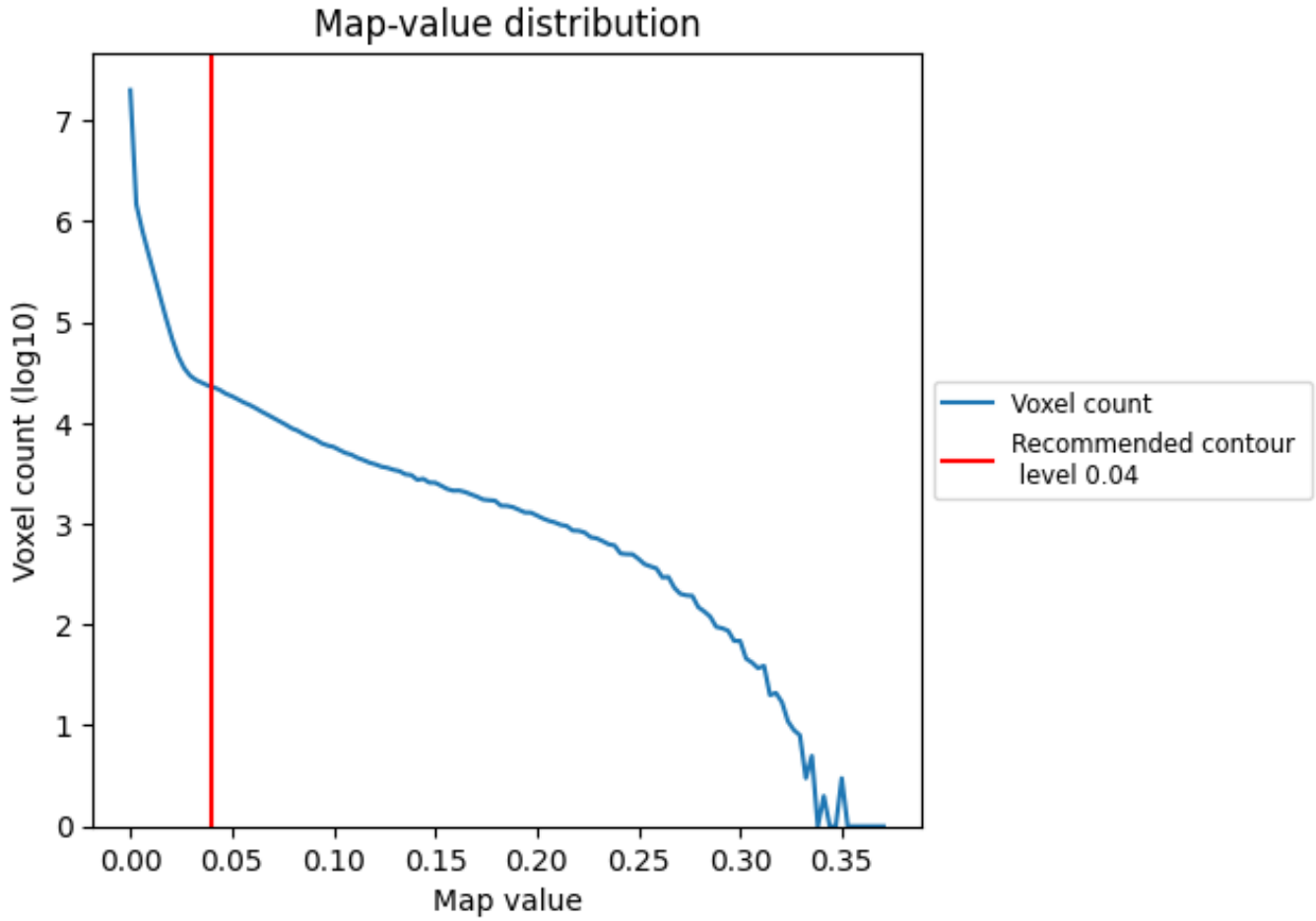
6.6 Mask visualisation (i)

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

7 Map analysis

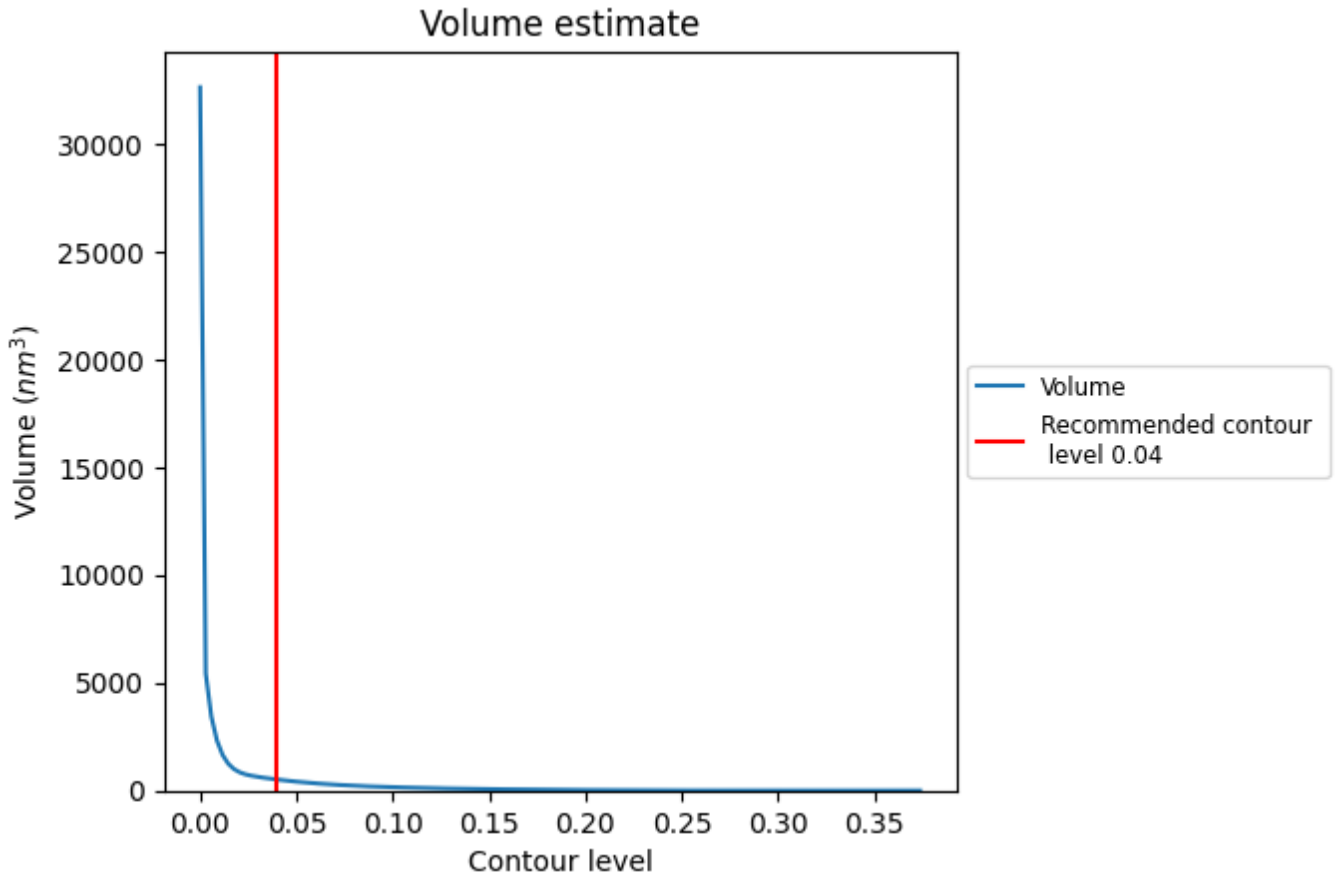
This section contains the results of statistical analysis of the map.

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.

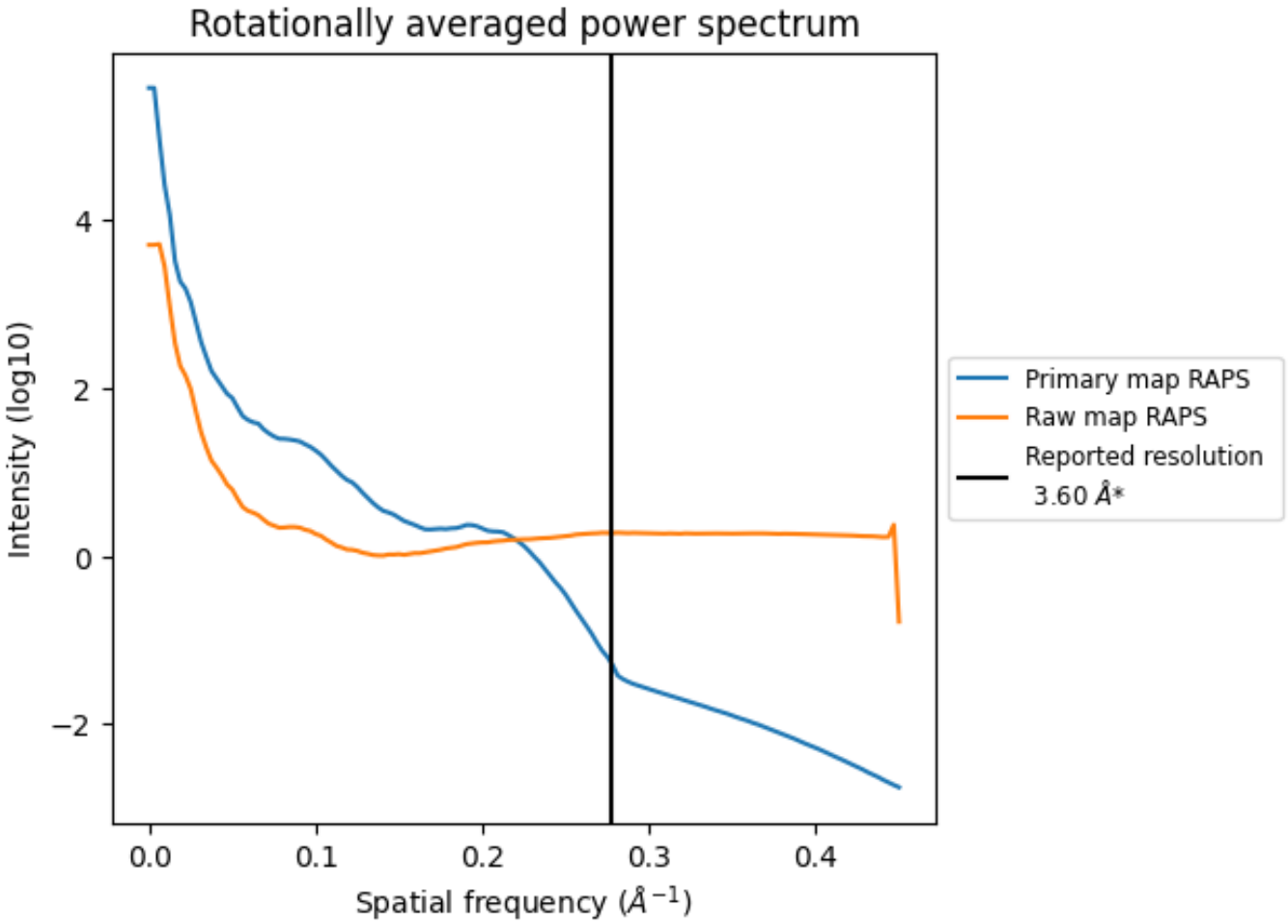
7.2 Volume estimate (i)



The volume at the recommended contour level is 512 nm^3; this corresponds to an approximate mass of 463 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)

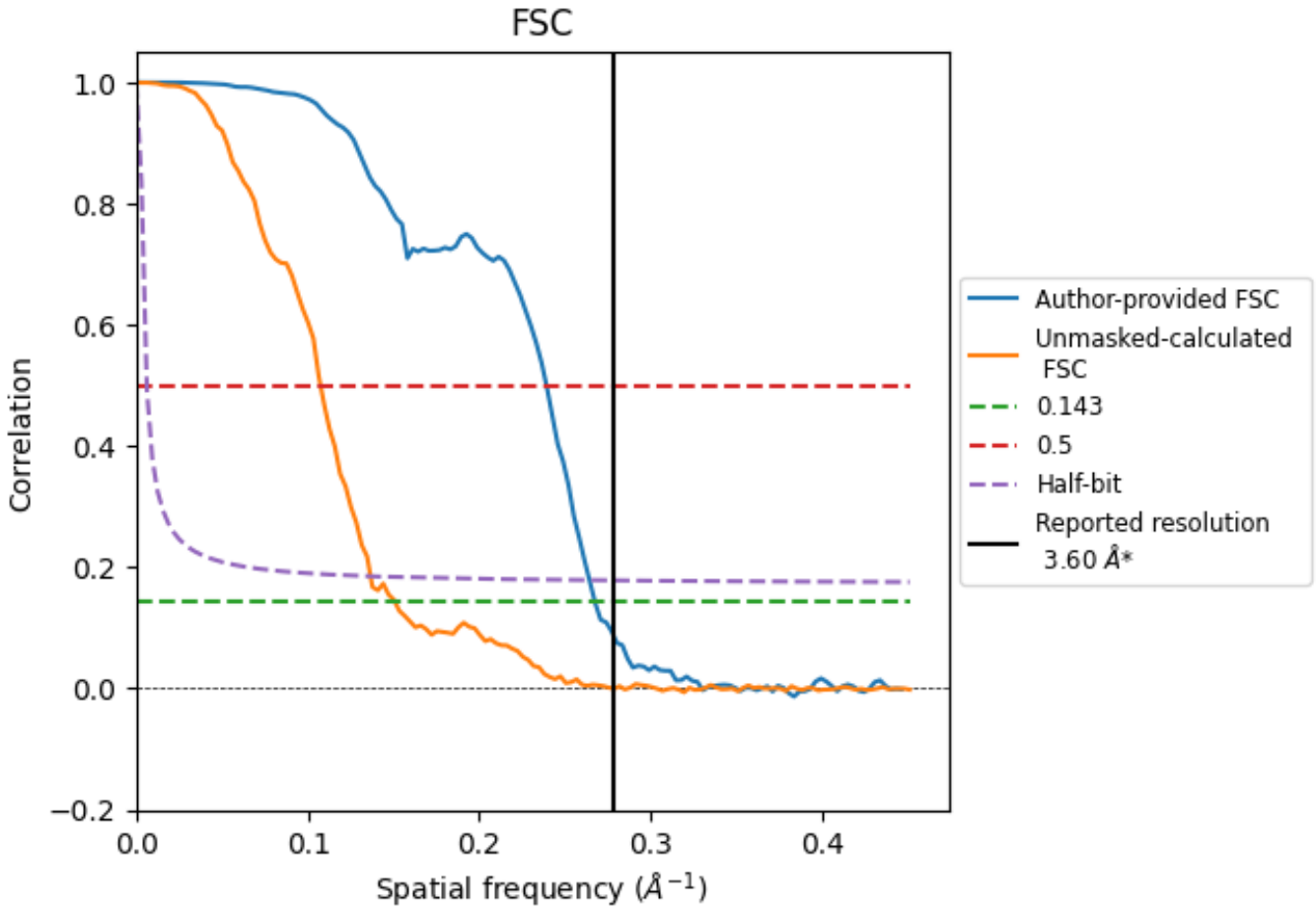


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

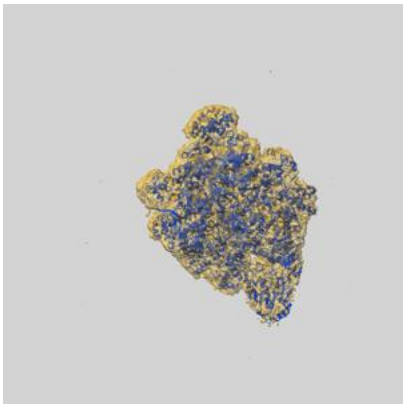
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.74	4.18	3.79
Unmasked-calculated*	6.63	9.31	7.32

*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 6.63 differs from the reported value 3.6 by more than 10 %

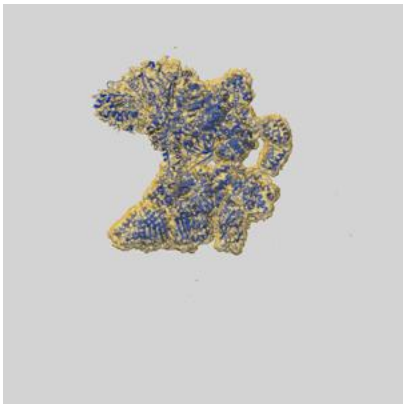
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56253 and PDB model 9TU9. Per-residue inclusion information can be found in section 3 on page 5.

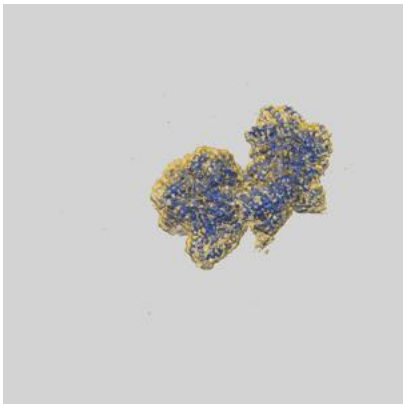
9.1 Map-model overlay



X



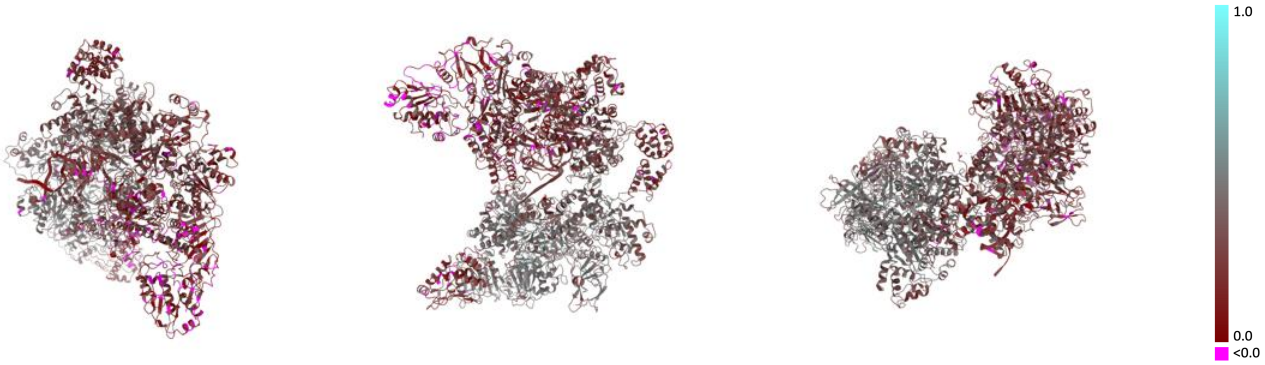
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

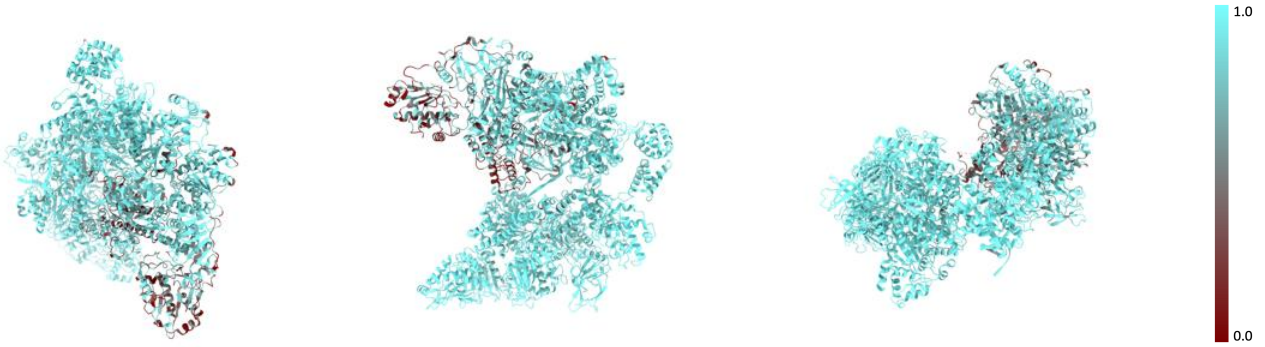
9.2 Q-score mapped to coordinate model (i)



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.

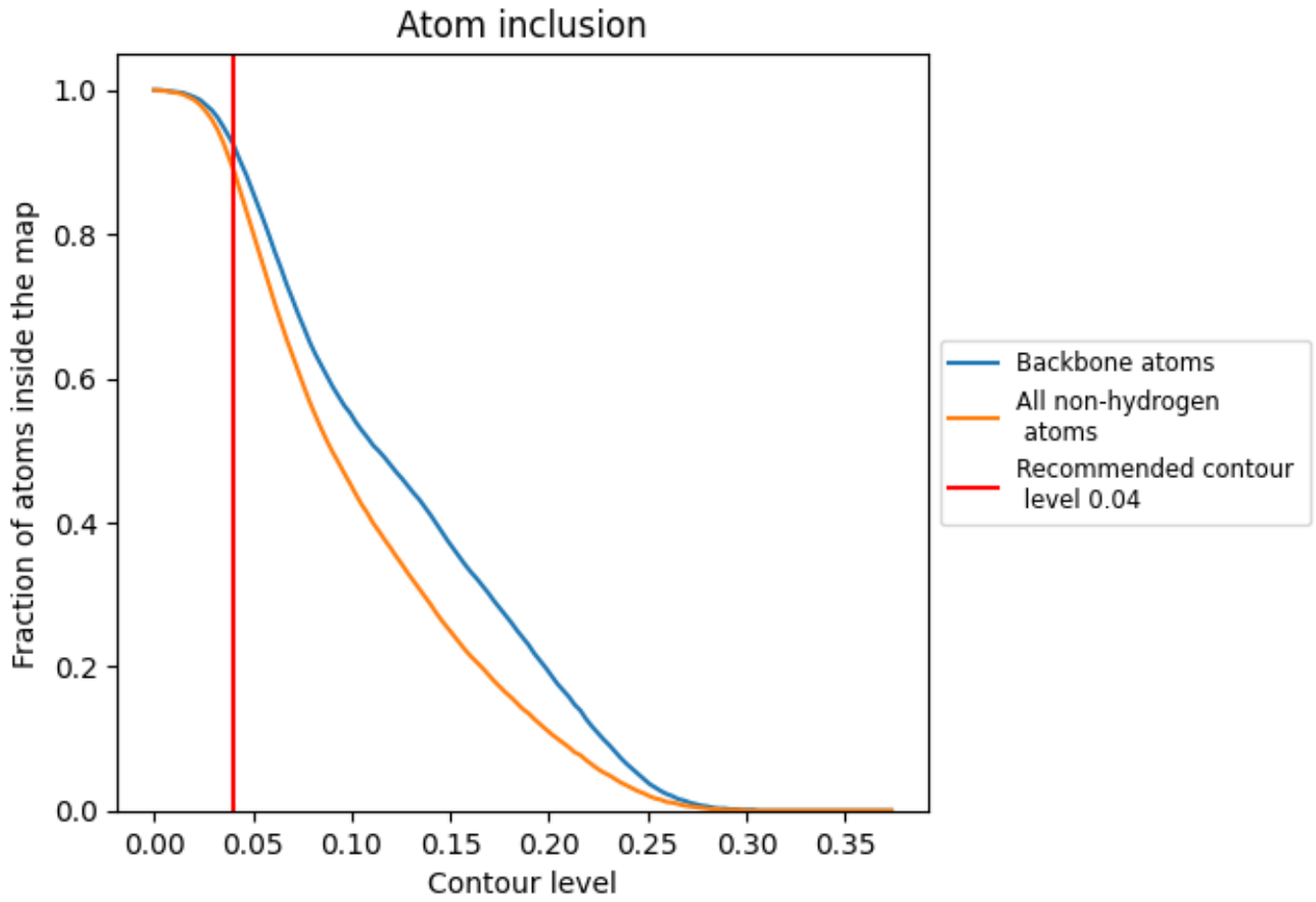
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.3130
G	0.9380	0.2590
I	0.9400	0.2340
Y	0.9890	0.3870
y	0.7890	0.2420

