wwPDB EM Validation Summary Report (i)

Oct 6, 2024 – 12:06 AM JST

PDB ID	:	5YZ0
EMDB ID	:	EMD-6862
Title	:	Cryo-EM Structure of human ATR-ATRIP complex
Authors	:	Rao, Q.; Liu, M.; Tian, Y.; Wu, Z.; Wang, H.; Wang, J.; Xu, Y.
Deposited on	:	2017-12-11
Resolution	:	4.70 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:

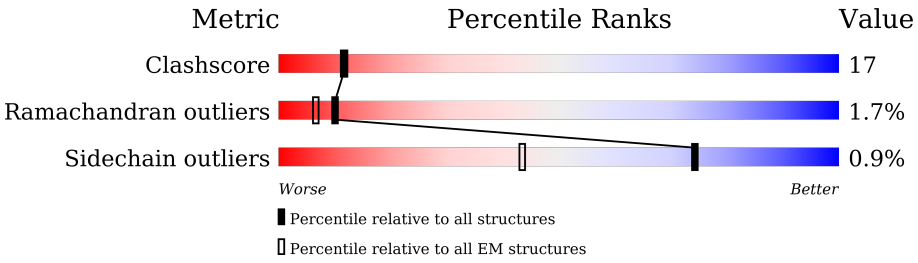
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.70 Å.

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



Metric	Whole archive (#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	A	2644	59% 29% 11%
1	B	2644	57% 30% 11%
2	C	791	32% 11% 54%
2	D	791	6% 30% 8% 60%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 33371 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 Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2362	Total 15007	C 9318	N 2785	O 2842	S 62	0	0
1	B	2362	Total 15007	C 9318	N 2785	O 2842	S 62	0	0

- Molecule 2 is a protein called ATR-interacting protein.

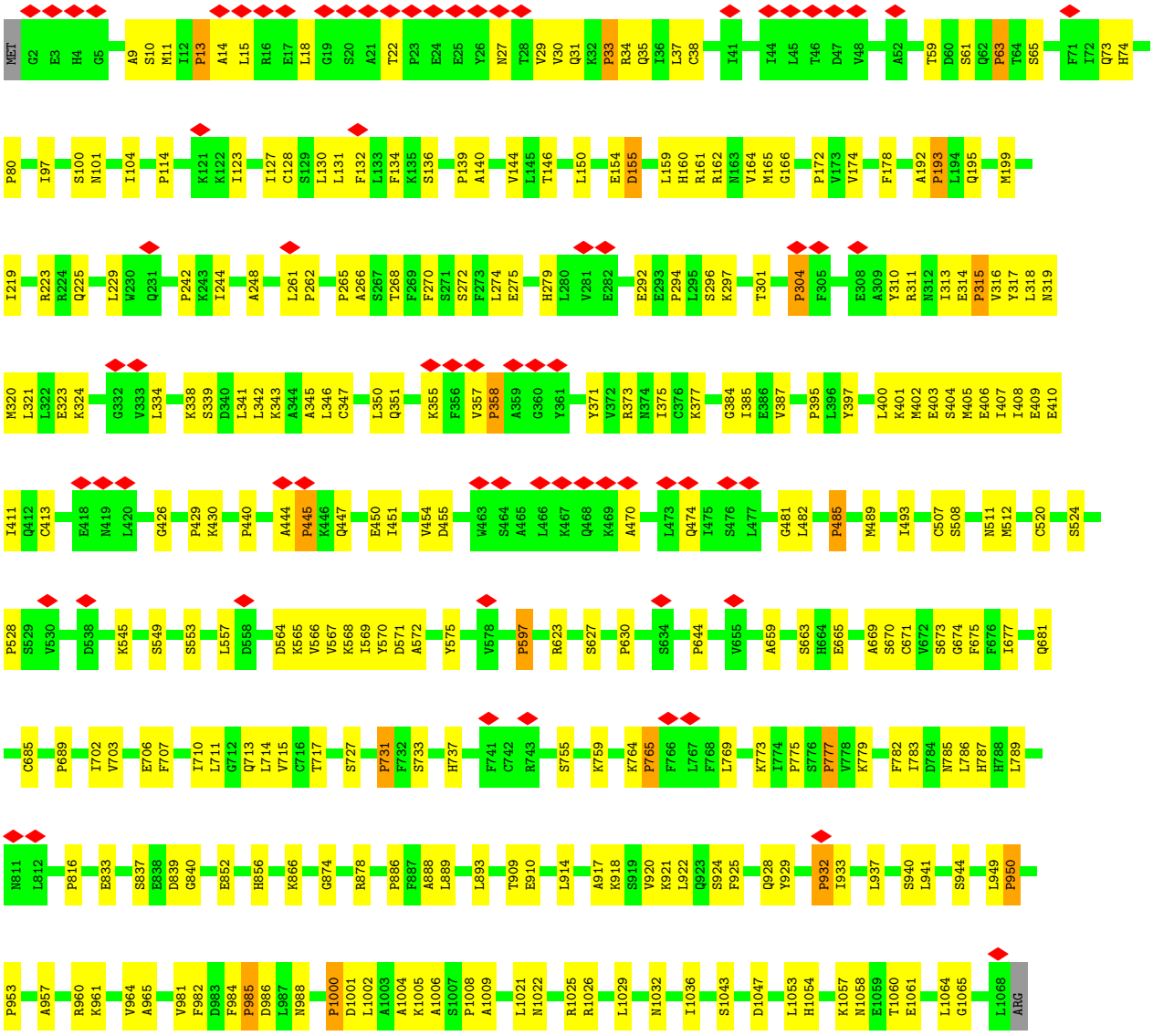
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	362	Total 1785	C 1061	N 362	O 362	0	0
2	D	318	Total 1572	C 936	N 318	O 318	0	0

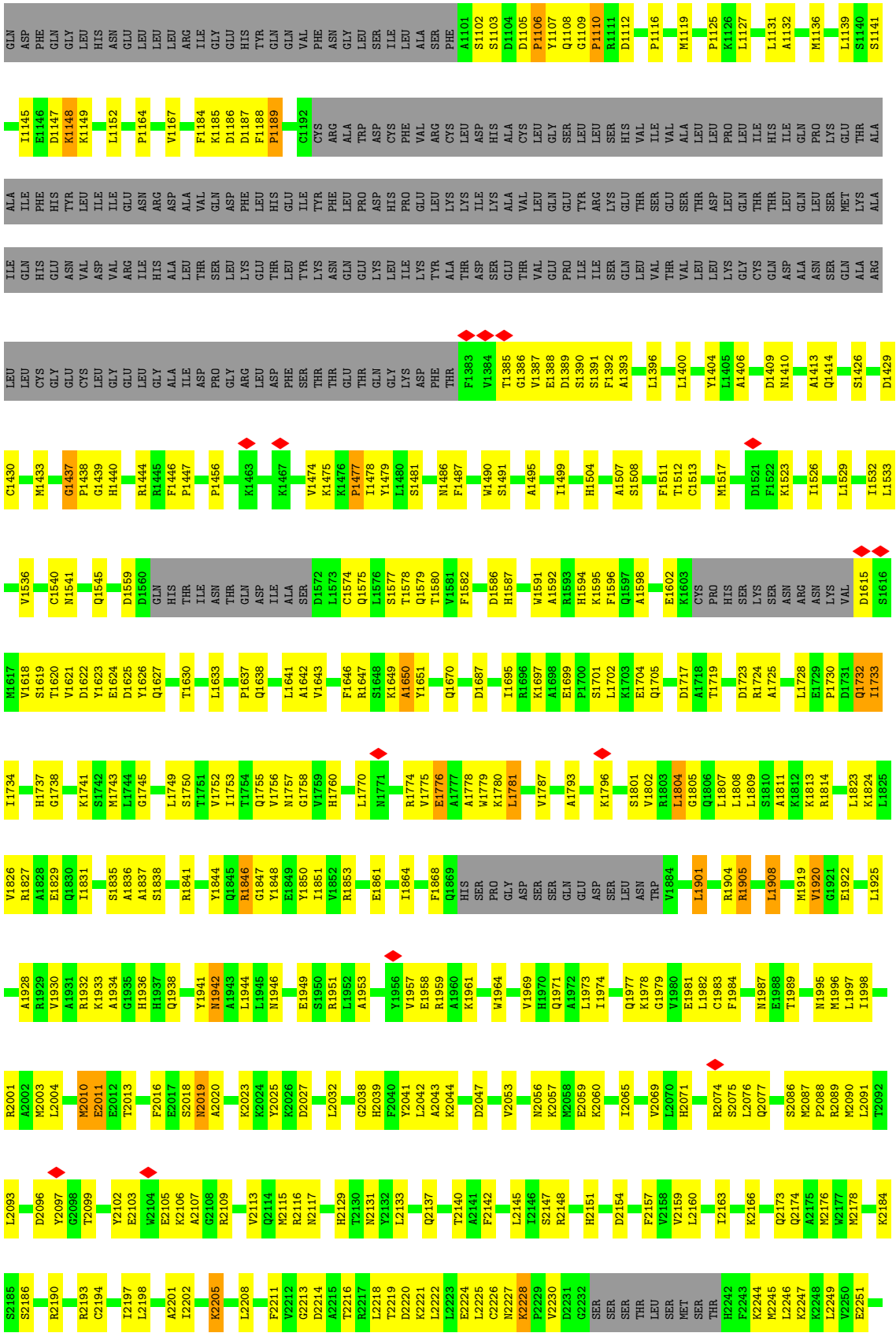
3 Residue-property plots (i)

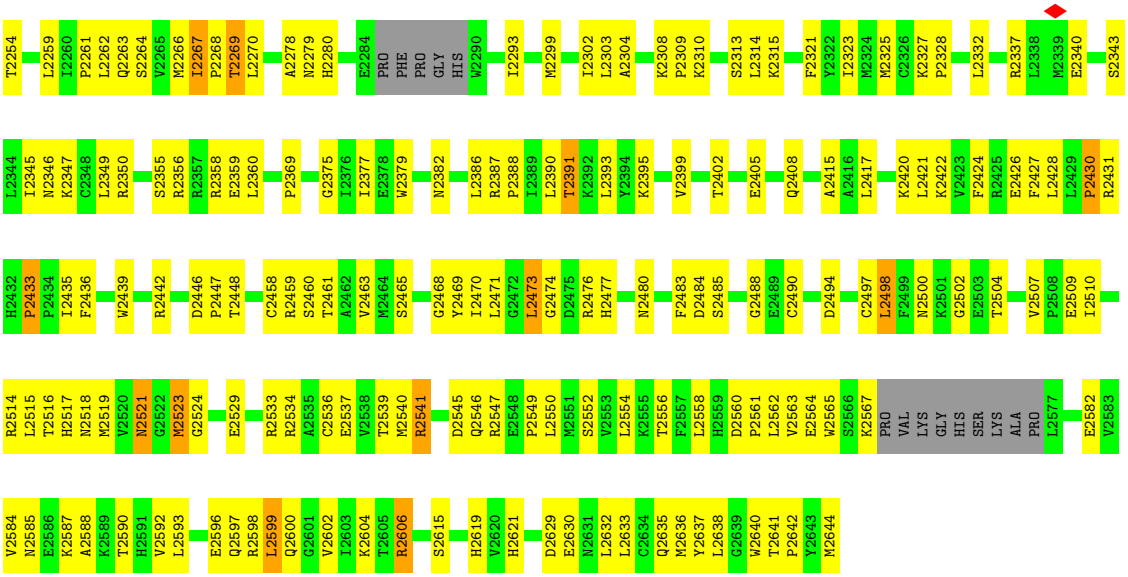
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Serine/threonine-protein kinase ATR

Chain A:

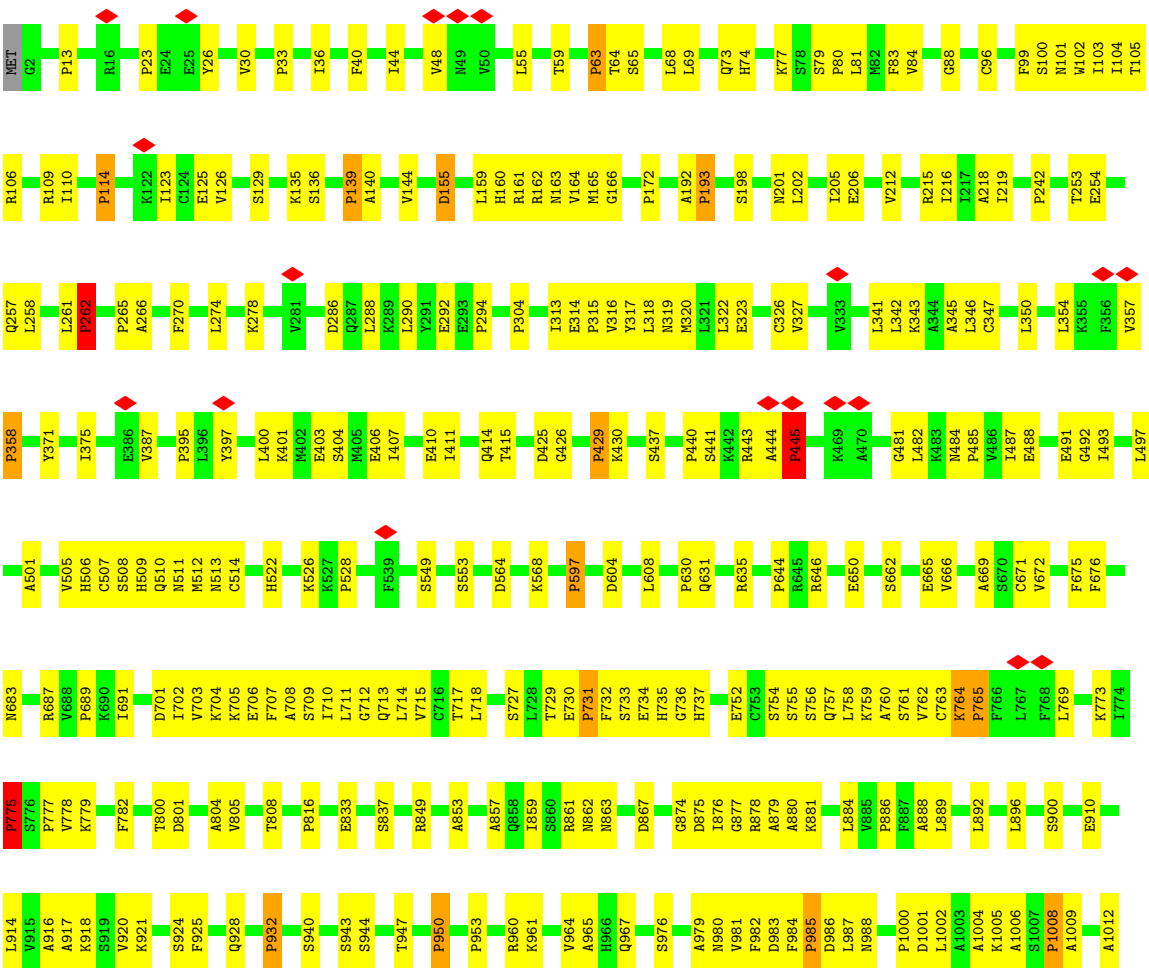


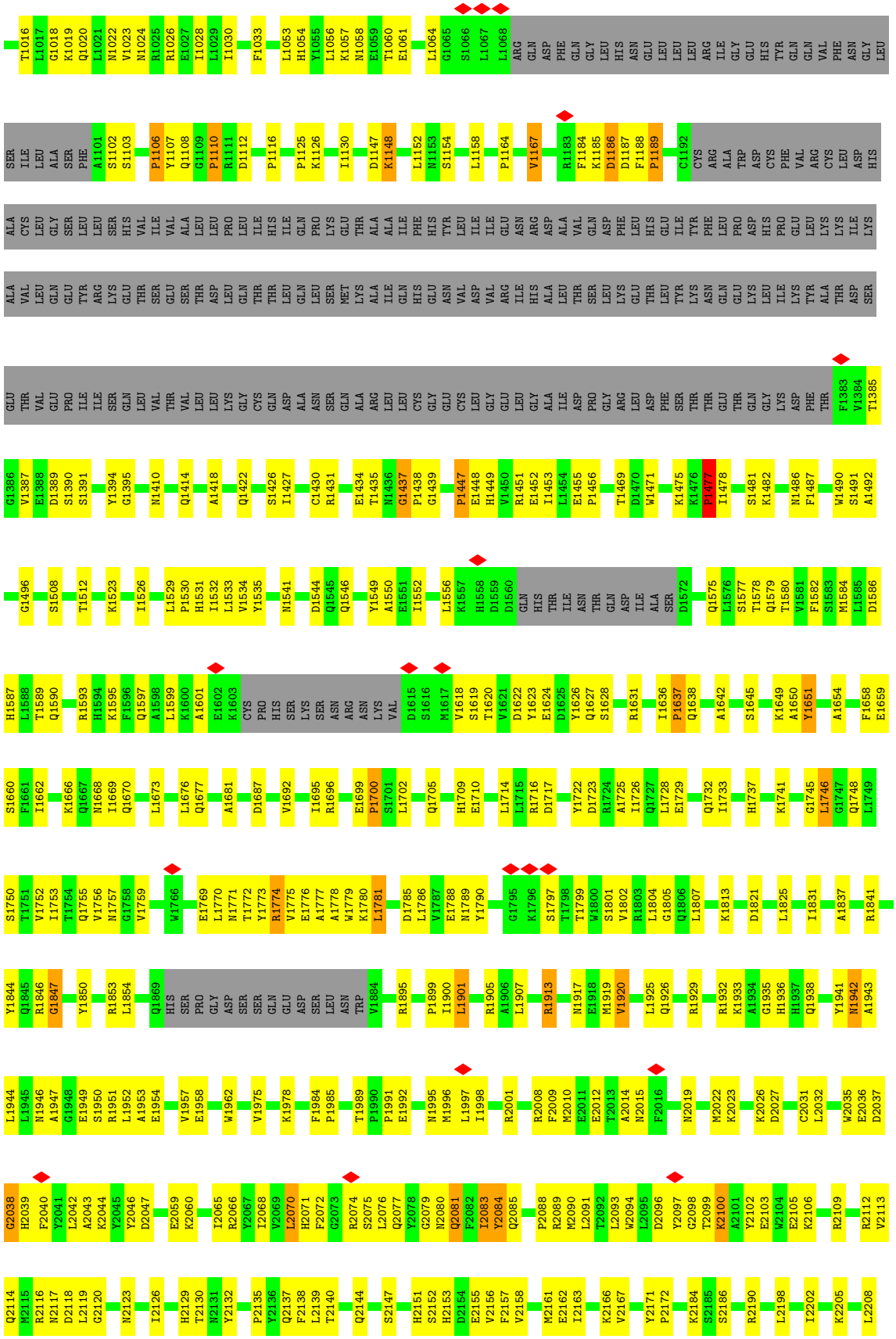


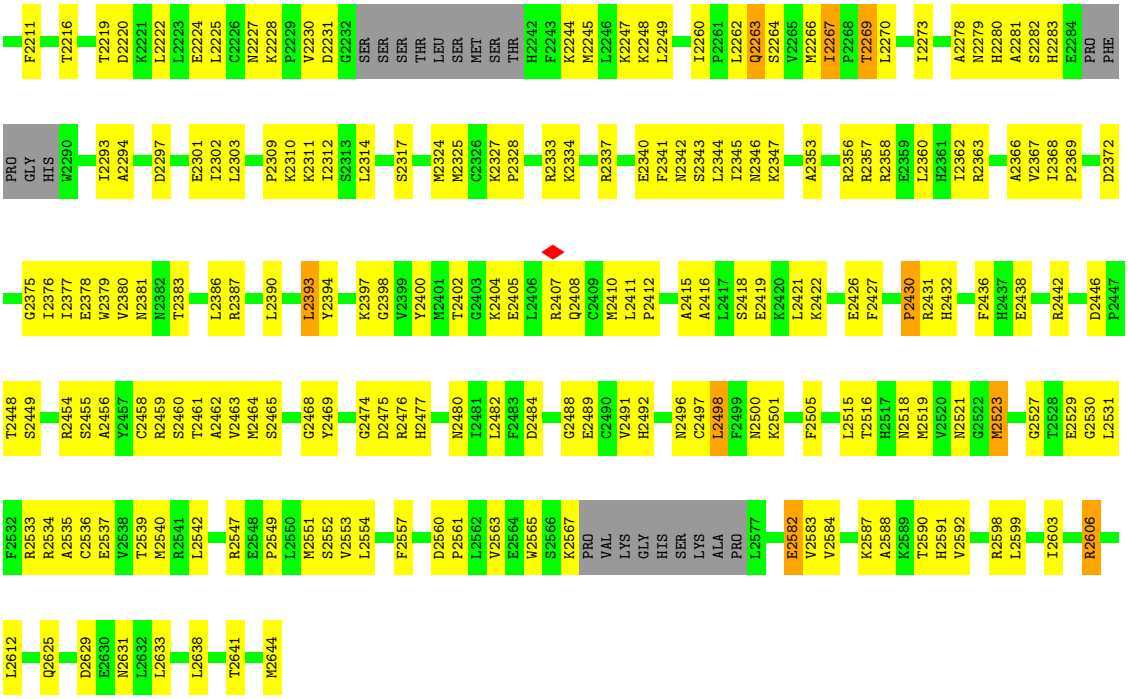


• Molecule 1: Serine/threonine-protein kinase ATR

Chain B:

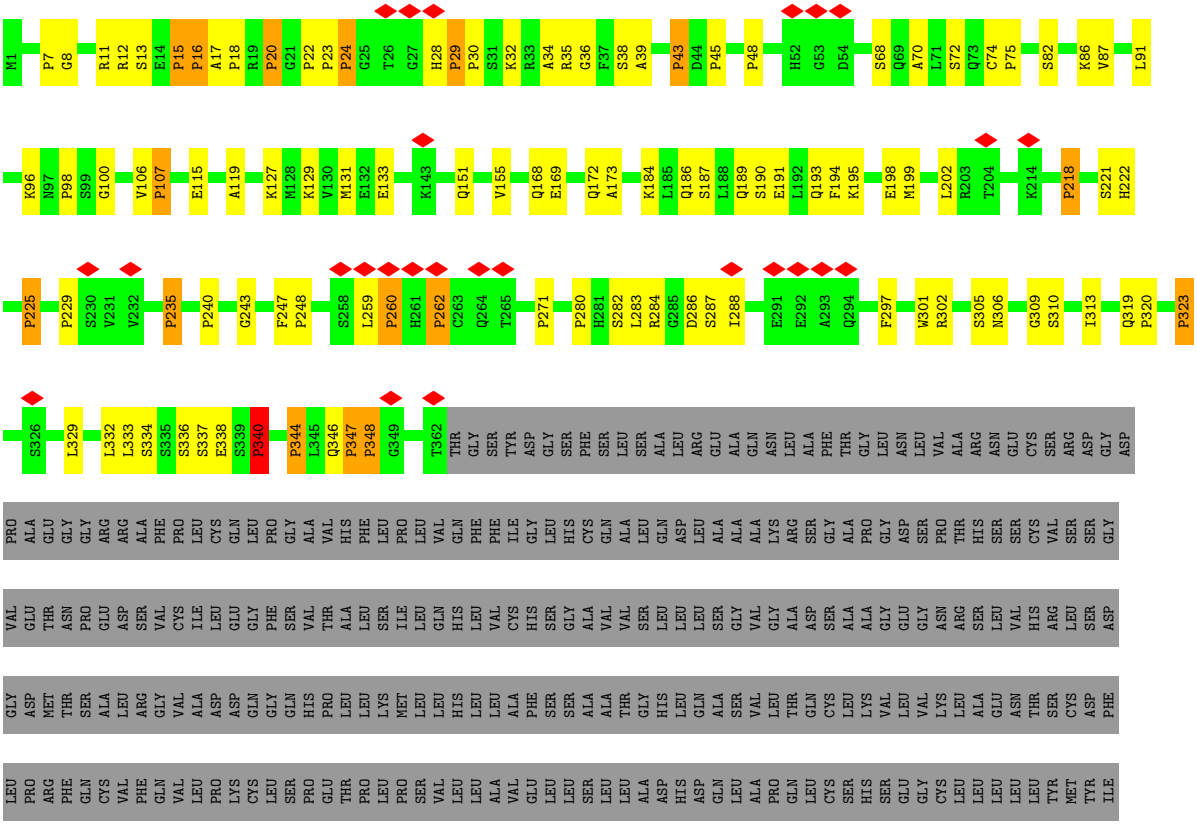


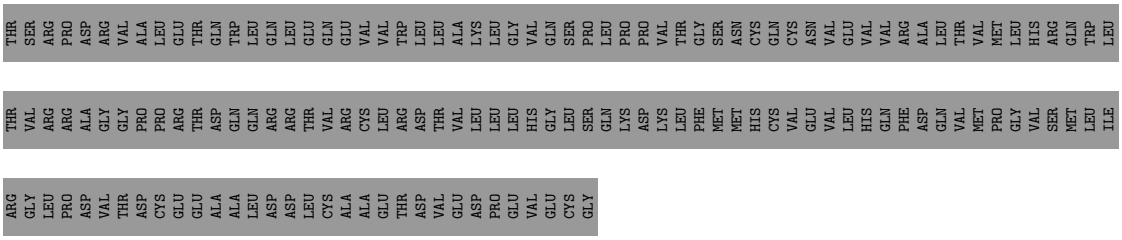

T1016 L1017 G1018 K1019 Q1020 L1021 N1022 V1023 N1024 R1025 R1026 E1027 I1028 L1029 I1030 F1033 L1053 H1054 Y1055 L1056 K1057 N1058 E1059 T1060 E1061 L1064 G1065 S1066 L1067 L1068
SER ILE LEU ALA SER PHE A1101 S1102 S1103 P1106 Y1107 Q1108 G1109 P1110 R1111 D1112 P1116 P1125 K1126 I1130 D1147 K1148 L1152 N1153 S1154 L1158 P1164 V1167 R1183 F1184 K1185 D1186 D1187 F1188 P1189 C1192 CYS ARG ALA TRP ASP CYS PHE VAL ARG CYS LEU ASP HIS
ALA CYS LEU GLY SER LEU LEU SER HIS VAL ILE VAL ALA LEU LEU PRO LEU ILE HIS ILE GLN PRO LYS GLU THR ALA ALA ILE PHE HIS TYR LEU ILE ILE GLU ASN ARG ASP ALA VAL GLN ASP PHE LEU HIS GLU ILE TYR PHE LEU PRO ASP HIS PRO GLU LEU LYS LYS ILE LYS
ALA VAL LEU GLN GLU TYR ARG LYS GLU THR SER GLU SER THR ASP LEU GLN THR THR LEU GLN LEU SER MET LYS ALA ILE GLN HIS GLU ASN VAL ASP VAL ARG ILE HIS ALA LEU THR SER LEU LYS GLU THR LEU TYR LYS ASN GLN GLU LYS LEU ILE LYS TYR ALA THR ASP SER
GLU THR VAL GLU PRO ILE ILE SER GLN LEU VAL THR VAL LEU LEU LYS GLY CYS GLN ASP ALA ASN SER GLN ALA ARG LEU LEU CYS GLY GLU CYS LEU GLY GLU LEU GLY ALA ILE ASP PRO GLY ARG LEU ASP PHE SER THR THR GLU THR GLN GLY LYS ASP PHE THR F1383 V1384 T1385
G1386 V1387 E1388 D1389 S1390 S1391 Y1394 G1395 N1410 Q1414 A1418 Q1422 S1426 I1427 C1430 R1431 E1434 T1435 N1436 G1437 P1438 G1439 P1447 E1448 H1449 V1450 R1451 E1452 I1453 L1454 E1455 P1456 T1469 D1470 W1471 K1475 K1476 P1477 I1478 S1481 K1482 N1486 F1487 W1490 S1491 A1492
G1496 S1508 T1512 K1523 I1526 L1529 P1530 H1531 I1532 L1533 V1534 Y1535 N1541 D1544 Q1545 Q1546 Y1549 A1550 E1551 I1552 L1556 K1557 H1558 D1559 D1560 GLN HIS THR ILE ASN THR GLN ASP ILE ALA SER D1572 Q1575 L1576 S1577 T1578 Q1579 T1580 V1581 F1582 S1583 M1584 L1585 D1586
H1587 L1588 T1589 Q1590 R1593 H1594 K1595 F1596 Q1597 A1598 L1599 K1600 A1601 E1602 K1603 CYS PRO HIS SER LYS SER ASN ARG ASN LYS VAL D1615 S1616 M1617 V1618 S1619 T1620 V1621 D1622 Y1623 E1624 D1625 Y1626 Q1627 S1628 R1631 I1636 P1637 Q1638 A1642 S1645 K1649 A1650 Y1651 A1654 F1658 E1659
S1660 F1661 I1662 K1666 Q1667 N1668 I1669 Q1670 L1673 L1676 Q1677 A1681 D1687 V1692 I1695 R1696 E1699 P1700 S1701 L1702 Q1705 H1709 E1710 L1714 L1715 R1716 D1717 Y1722 D1723 R1724 A1725 I1726 Q1727 L1728 E1729 Q1732 I1733 H1737 K1741 G1745 L1746 G1747 Q1748 L1749
S1750 T1751 V1752 I1753 T1754 Q1755 V1756 N1757 G1758 V1759 W1766 E1769 L1770 N1771 T1772 Y1773 R1774 V1775 E1776 A1777 A1778 W1779 K1780 L1781 D1785 L1786 V1787 E1788 N1789 Y1790 G1795 K1796 S1797 T1798 T1799 W1800 S1801 V1802 R1803 L1804 G1805 Q1806 L1807 K1813 D1821 L1825 I1831 A1837 R1841
Y1844 Q1845 R1846 G1847 Y1850 R1853 L1854 Q1869 HIS SER PRO GLY ASP SER SER GLN GLU ASP SER LEU ASN TRP V1884 R1895 P1899 I1900 L1901 R1905 A1906 L1907 R1913 N1917 E1918 M1919 V1920 L1925 Q1926 R1929 R1932 K1933 A1934 G1935 H1936 H1937 Q1938 Y1941 N1942 A1943
L1944 L1945 N1946 A1947 G1948 E1949 S1950 R1951 L1952 A1953 E1954 V1957 E1958 W1962 V1975 K1978 F1984 P1985 T1989 P1990 P1991 E1992 N1995 M1996 L1997 I1998 R2001 R2008 F2009 M2010 E2011 E2012 T2013 A2014 N2015 F2016 N2019 M2022 K2023 K2026 D2027 C2031 L2032 W2035 E2036 D2037
G2038 H2039 F2040 Y2041 I2042 A2043 K2044 Y2045 Y2046 D2047 E2059 K2060 I2065 R2066 Y2067 I2068 V2069 L2070 H2071 F2072 G2073 R2074 S2075 L2076 Q2077 Y2078 G2079 N2080 Q2081 F2082 I2083 Y2084 Q2085 P2088 R2089 M2090 L2091 T2092 L2093 W2094 L2095 D2096 Y2097 G2098 T2099 K2100 A2101 Y2102 E2103 W2104 E2105 K2106 R2109 R2112 Y2113
Q2114 M2115 R2116 N2117 D2118 L2119 G2120 N2123 I2126 H2129 T2130 N2131 Y2132 P2135 Y2136 Q2137 F2138 L2139 T2140 Q2144 S2147 H2151 S2152 H2153 D2154 E2155 V2156 F2157 V2158 M2161 E2162 I2163 K2166 V2167 Y2171 P2172 K2184 S2185 S2186 R2190 L2198 I2202 K2205 L2208



• Molecule 2: ATR-interacting protein

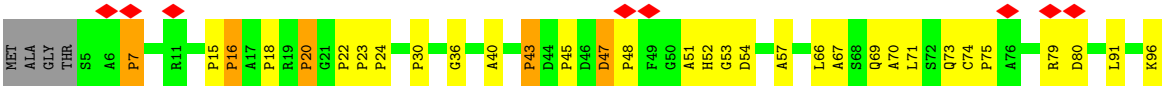
Chain C:

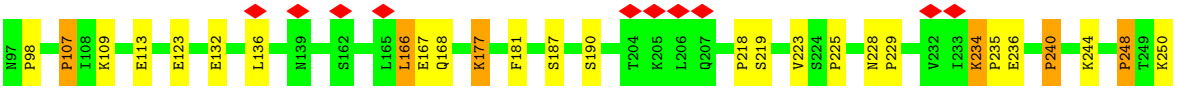


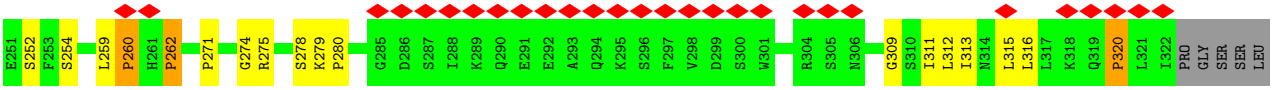


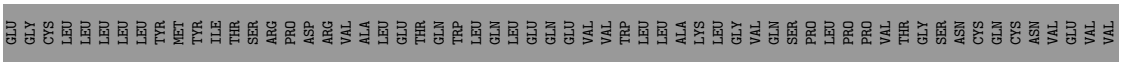
• Molecule 2: ATR-interacting protein

Chain D:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/15191	0.70	57/20804 (0.3%)
1	B	0.44	0/15191	0.71	51/20804 (0.2%)
2	C	0.28	0/1784	0.84	32/2481 (1.3%)
2	D	0.29	0/1571	0.84	26/2187 (1.2%)
All	All	0.42	0/33737	0.72	166/46276 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	48
1	B	0	59
2	C	0	3
2	D	0	3
All	All	0	113

There are no bond length outliers.

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	PRO	N-CA-CB	7.24	111.99	103.30
1	A	1189	PRO	N-CA-CB	7.15	111.88	103.30
2	D	107	PRO	N-CA-CB	7.12	111.85	103.30
2	C	24	PRO	N-CA-CB	6.96	111.66	103.30
2	C	323	PRO	N-CA-CB	6.90	111.58	103.30

There are no chirality outliers.

5 of 113 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1032	ASN	Peptide
1	A	22	THR	Peptide
1	A	384	GLY	Peptide
1	A	866	LYS	Peptide
1	A	933	ILE	Peptide

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	A	15007	0	11392	455	0
1	B	15007	0	11392	484	0
2	C	1785	0	791	44	0
2	D	1572	0	689	26	0
All	All	33371	0	24264	1003	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 17.

The worst 5 of 1003 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1637:PRO:HB2	1:A:1638:GLN:HG2	1.62	0.78
1:B:2333:ARG:HH11	1:B:2337:ARG:HH21	1.36	0.74
1:A:1964:TRP:HE1	1:A:2010:MET:HG3	1.51	0.74
1:A:1559:ASP:HB3	1:A:1574:CYS:HB3	1.71	0.72
1:A:1670:GLN:HE22	1:A:1697:LYS:HE3	1.56	0.71

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	A	2344/2644 (89%)	1962 (84%)	350 (15%)	32 (1%)	9 40
1	B	2344/2644 (89%)	1953 (83%)	358 (15%)	33 (1%)	9 40
2	C	360/791 (46%)	284 (79%)	63 (18%)	13 (4%)	3 20
2	D	316/791 (40%)	240 (76%)	64 (20%)	12 (4%)	2 19
All	All	5364/6870 (78%)	4439 (83%)	835 (16%)	90 (2%)	10 36

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	192	ALA
1	A	193	PRO
1	A	357	VAL
1	A	444	ALA

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	A	924/2363 (39%)	914 (99%)	10 (1%)	70 80
1	B	924/2363 (39%)	918 (99%)	6 (1%)	84 88
All	All	1848/4726 (39%)	1832 (99%)	16 (1%)	74 83

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2521	ASN
1	B	1951	ARG
1	A	2523	MET
1	B	1913	ARG
1	A	2521	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2153	HIS
1	B	2280	HIS
1	A	2199	ASN
1	A	2174	GLN
1	B	2480	ASN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

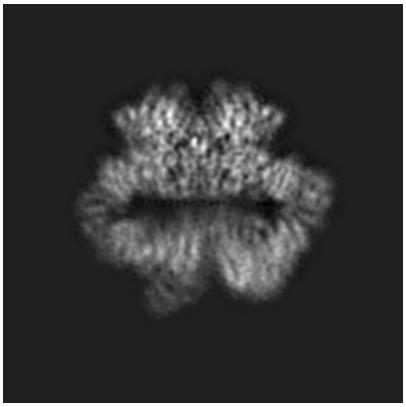
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6862. These allow visual inspection of the internal detail of the map and identification of artifacts.

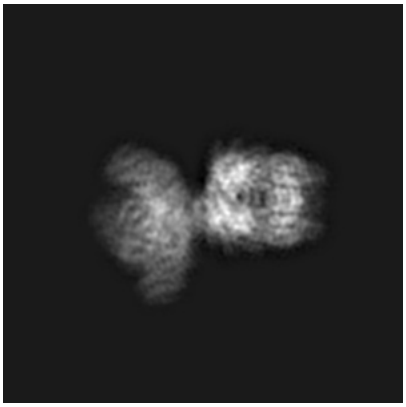
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

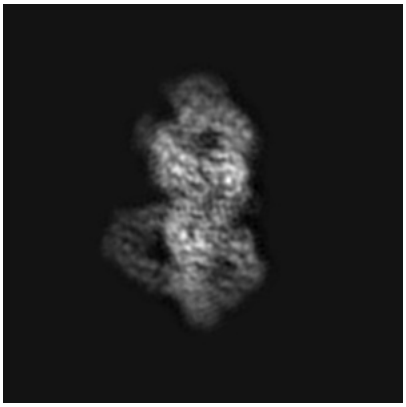
6.1.1 Primary map



X



Y

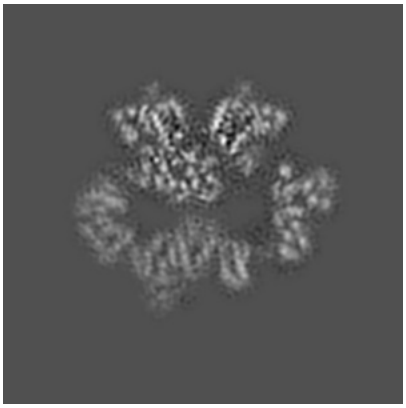


Z

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

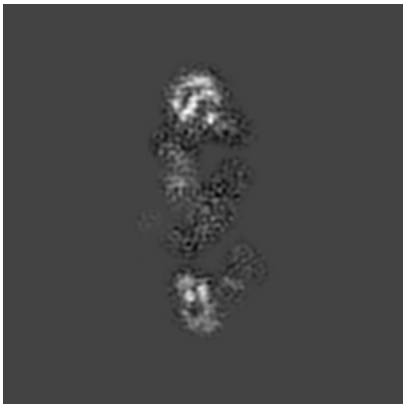
6.2 Central slices

6.2.1 Primary map



X Index: 120

Y Index: 120

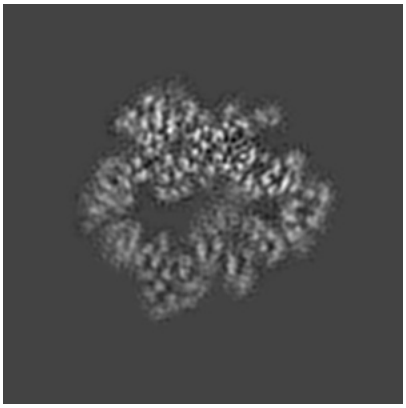


Z Index: 120

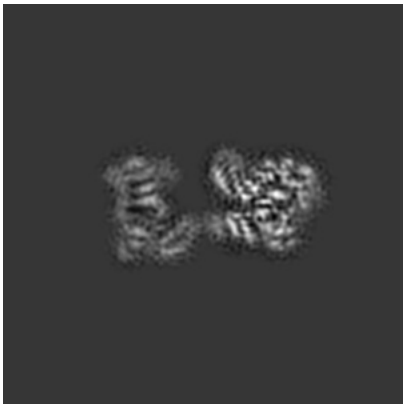
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

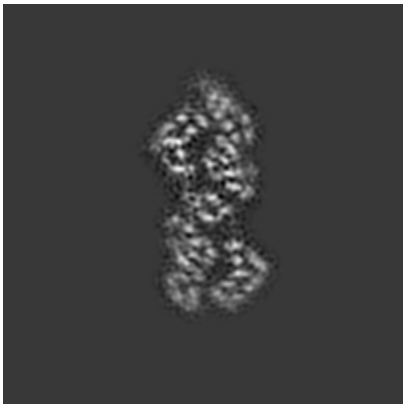
6.3.1 Primary map



X Index: 110



Y Index: 140

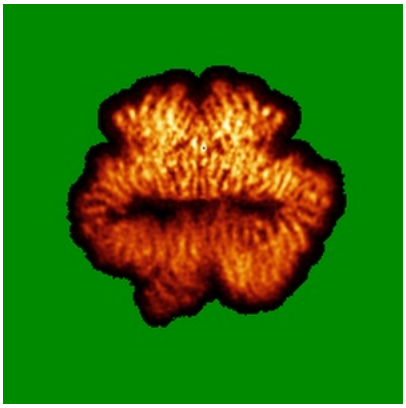


Z Index: 138

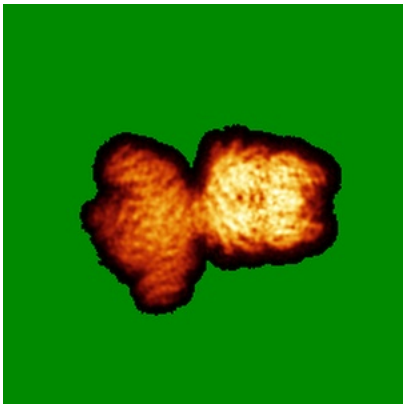
The images above show the largest variance slices of the map in three orthogonal directions.

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

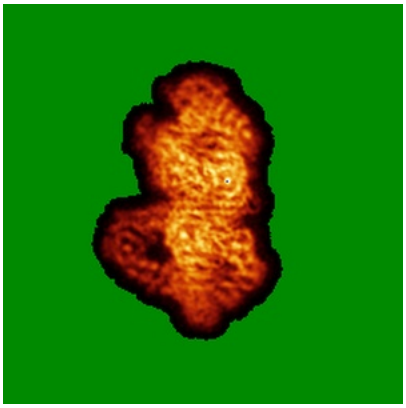
6.4.1 Primary map



X



Y



Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

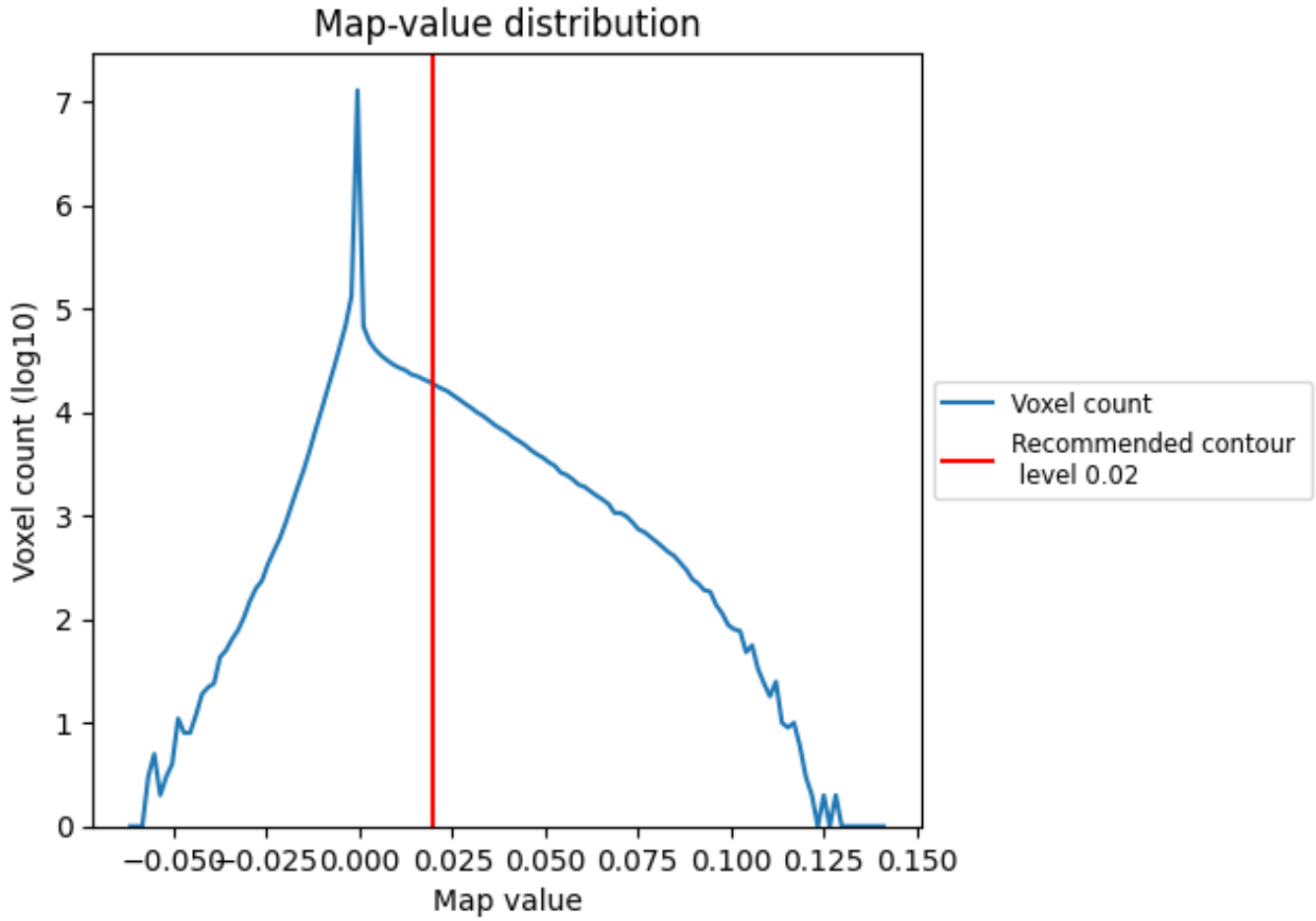
6.6 Mask visualisation (i)

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

7 Map analysis

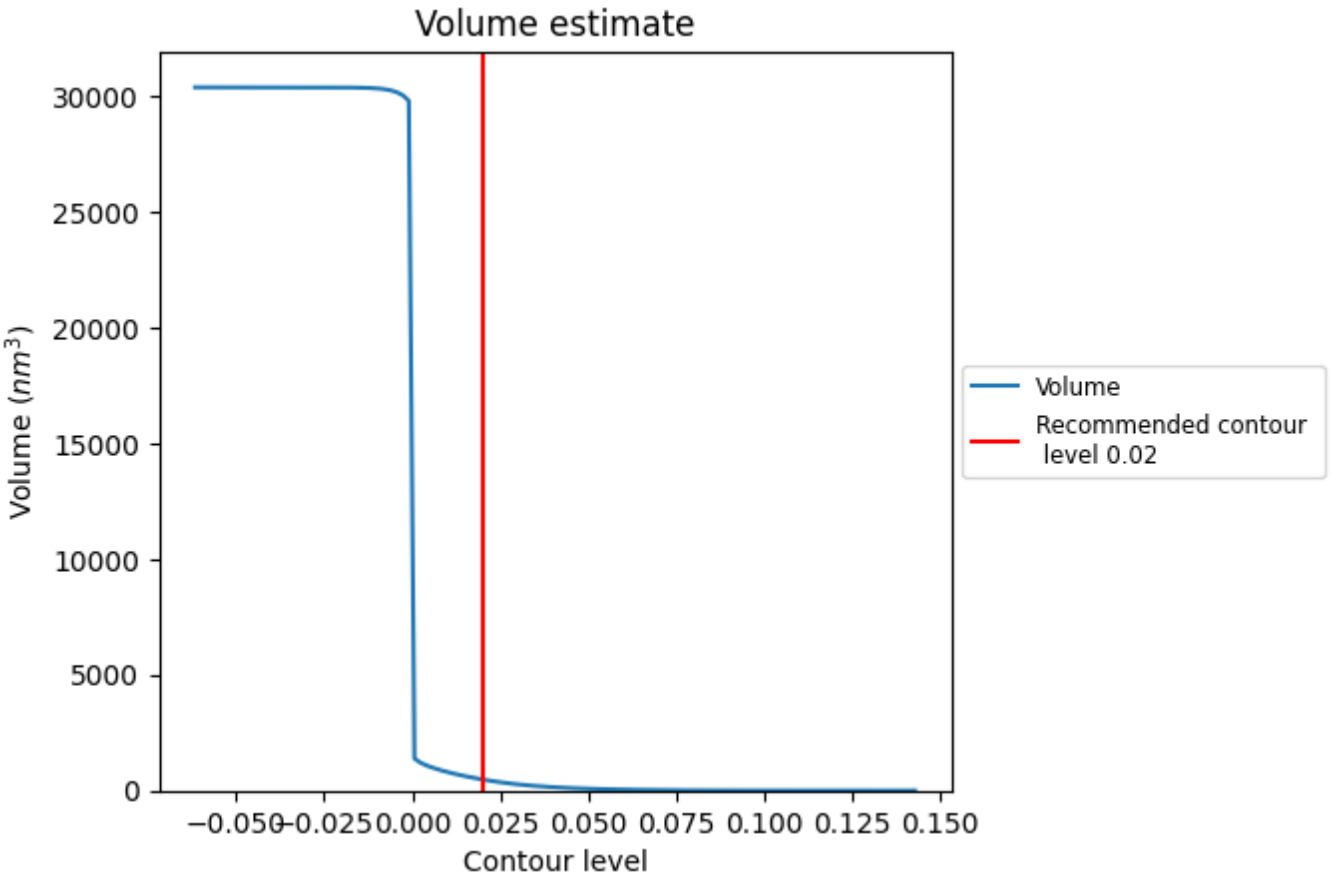
This section contains the results of statistical analysis of the map.

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.

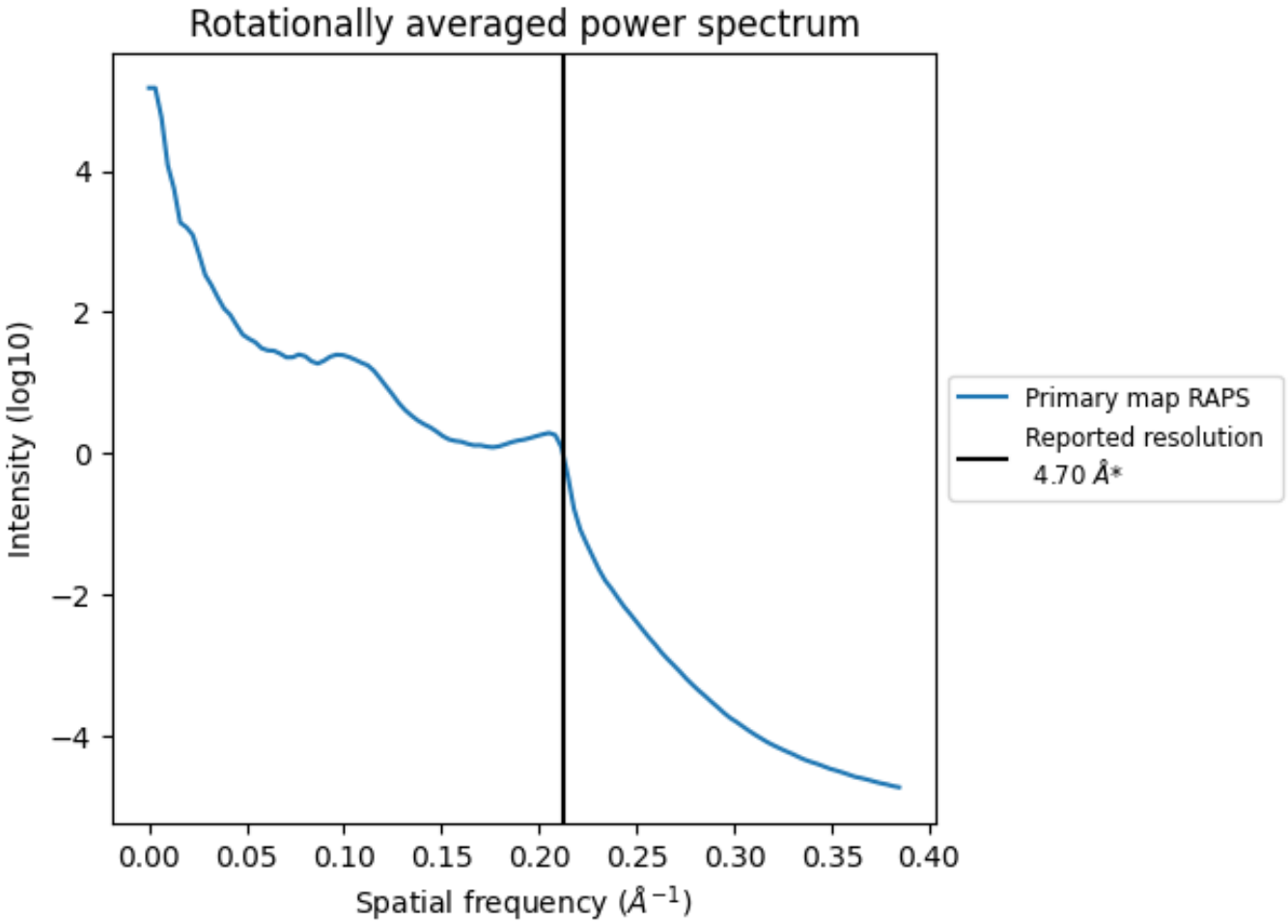
7.2 Volume estimate (i)



The volume at the recommended contour level is 477 nm^3; this corresponds to an approximate mass of 431 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)

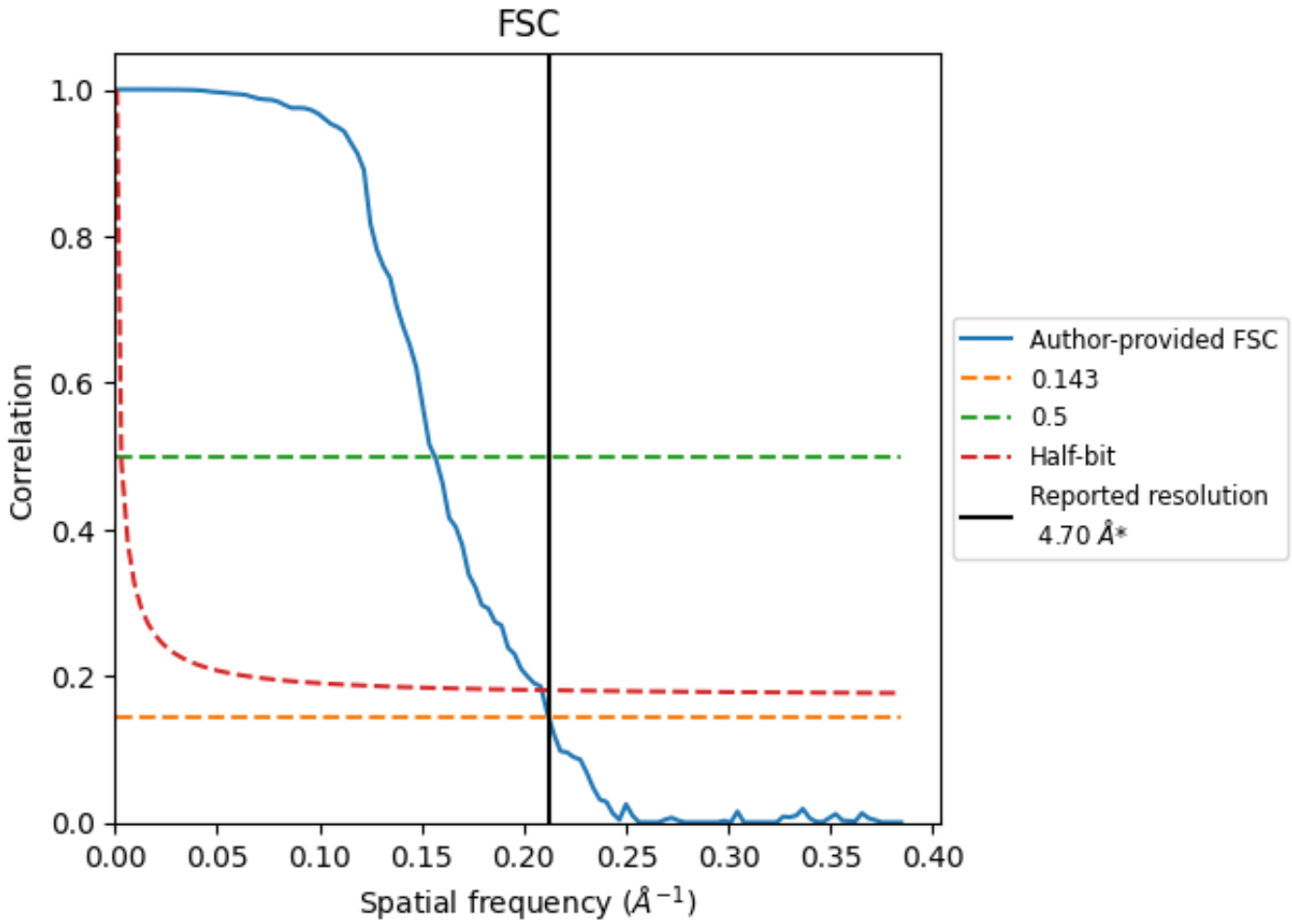


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

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 0.213 Å^{-1}

8.2 Resolution estimates (i)

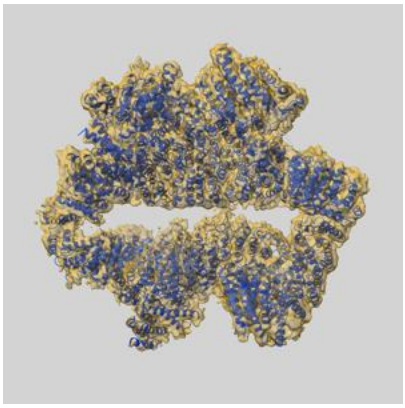
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.71	6.40	4.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

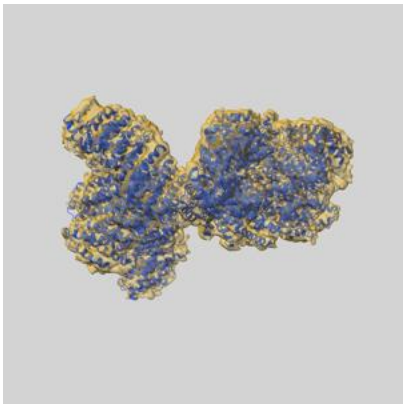
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6862 and PDB model 5YZ0. Per-residue inclusion information can be found in section 3 on page 4.

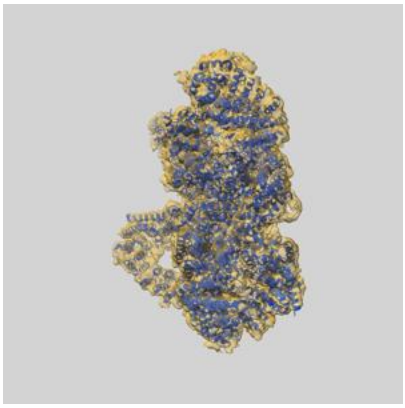
9.1 Map-model overlay



X



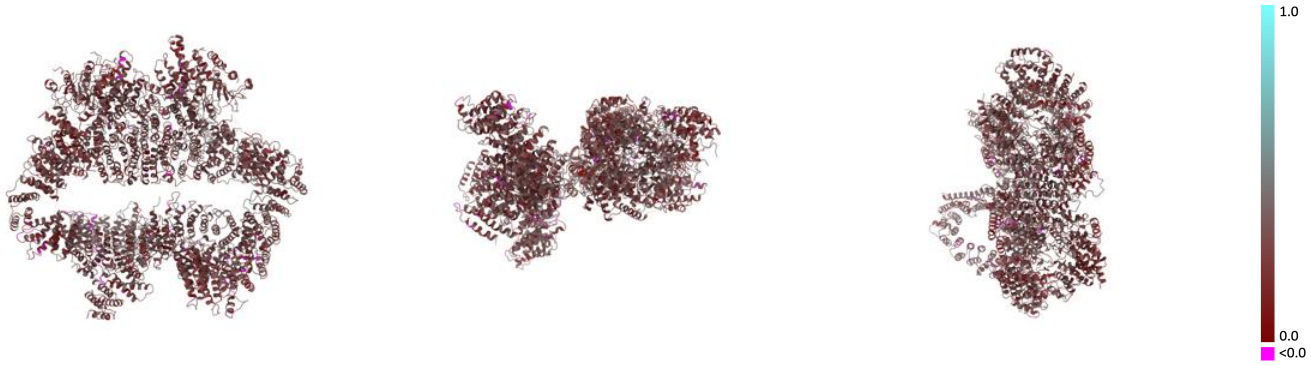
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

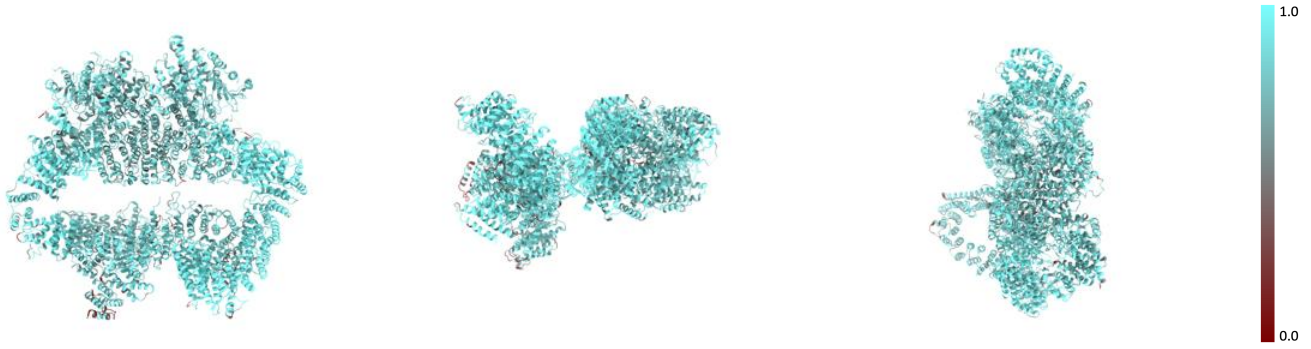
9.2 Q-score mapped to coordinate model



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.

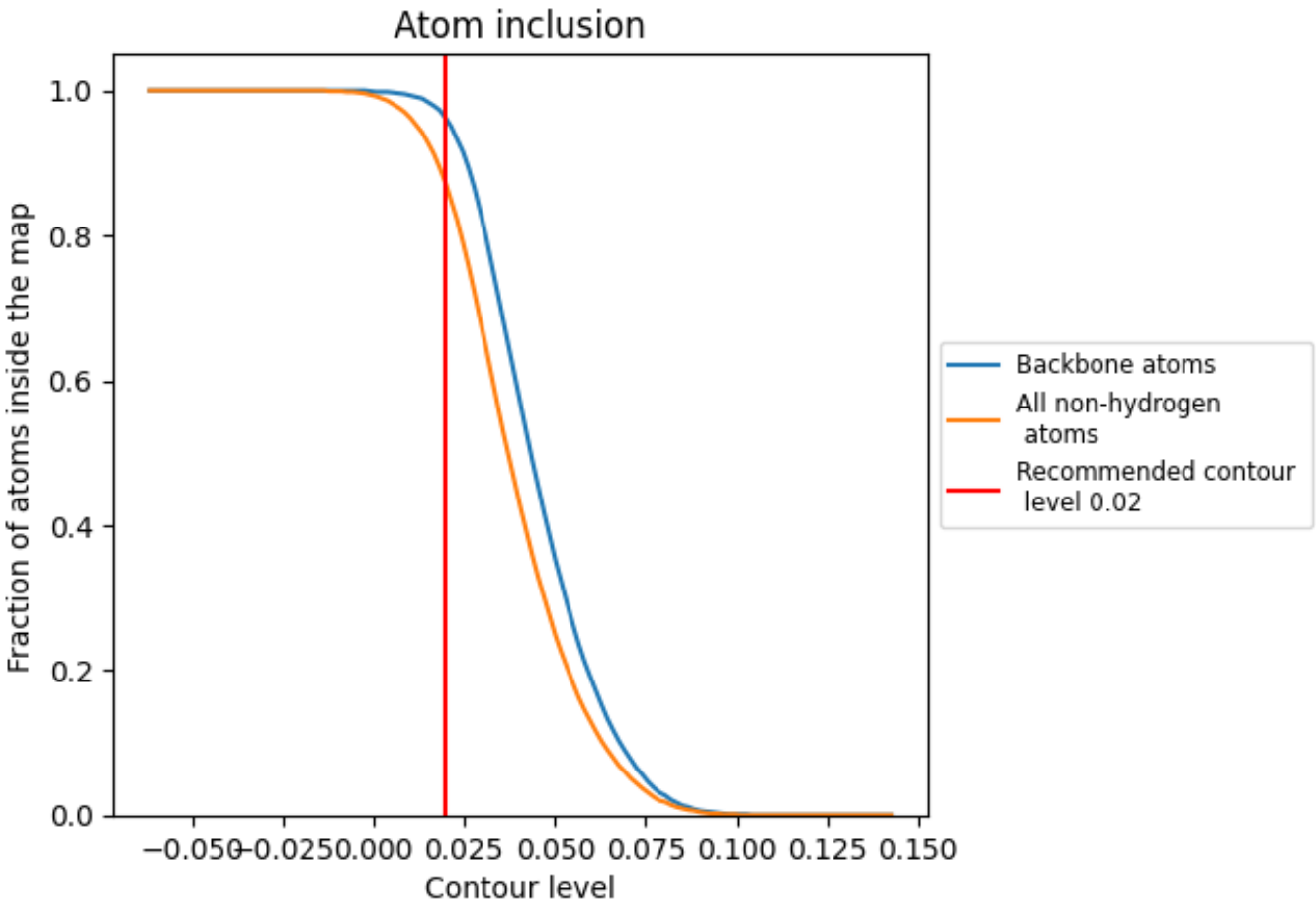
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 87% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8700	0.2810
A	0.8570	0.2760
B	0.8900	0.2880
C	0.8500	0.2820
D	0.8220	0.2630