wwPDB EM Validation Summary Report

Nov 8, 2022 – 04:25 pm GMT

PDB ID	:	7YYN
EMDB ID	:	EMD-14384
Title	:	Mammalian Dicer in the dicing state with pre-miR-15a substrate
Authors	:	Zanova, M.; Zapletal, D.; Kubicek, K.; Stefl, R.; Pinkas, M.; Novacek, J.
Deposited on	:	2022-02-18
Resolution	:	6.21 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:

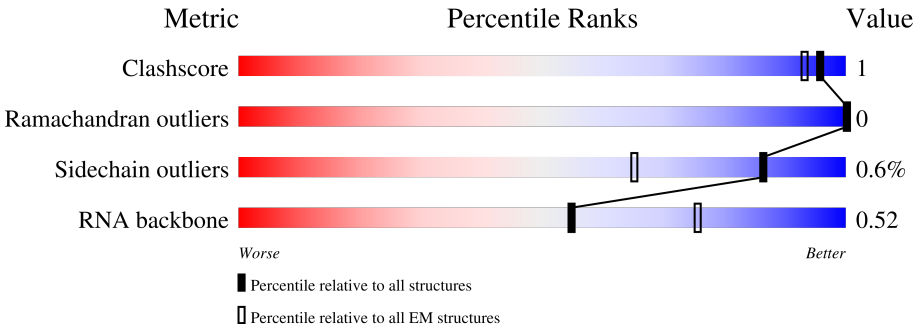
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 6.21 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	59	34% 8% 53% 25% 7% 7%
2	A	1765	18% 37% 60%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13111 atoms, of which 6287 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 59-nt precursor of miR-15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	B	55	1763	523	590	205	390	55	0	0

- Molecule 2 is a protein called Isoform 2 of Endoribonuclease Dicer.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	A	705	11348	3643	5697	954	1026	28	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-51	MET	-	initiating methionine	UNP Q8R418
A	-50	VAL	-	expression tag	UNP Q8R418
A	-49	TRP	-	expression tag	UNP Q8R418
A	-48	SER	-	expression tag	UNP Q8R418
A	-47	HIS	-	expression tag	UNP Q8R418
A	-46	PRO	-	expression tag	UNP Q8R418
A	-45	GLN	-	expression tag	UNP Q8R418
A	-44	PHE	-	expression tag	UNP Q8R418
A	-43	GLU	-	expression tag	UNP Q8R418
A	-42	LYS	-	expression tag	UNP Q8R418
A	-41	GLY	-	expression tag	UNP Q8R418
A	-40	GLY	-	expression tag	UNP Q8R418
A	-39	GLY	-	expression tag	UNP Q8R418
A	-38	SER	-	expression tag	UNP Q8R418
A	-37	GLY	-	expression tag	UNP Q8R418
A	-36	GLY	-	expression tag	UNP Q8R418
A	-35	GLY	-	expression tag	UNP Q8R418
A	-34	SER	-	expression tag	UNP Q8R418
A	-33	GLY	-	expression tag	UNP Q8R418
A	-32	GLY	-	expression tag	UNP Q8R418
A	-31	SER	-	expression tag	UNP Q8R418

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	ALA	-	expression tag	UNP Q8R418
A	-29	TRP	-	expression tag	UNP Q8R418
A	-28	SER	-	expression tag	UNP Q8R418
A	-27	HIS	-	expression tag	UNP Q8R418
A	-26	PRO	-	expression tag	UNP Q8R418
A	-25	GLN	-	expression tag	UNP Q8R418
A	-24	PHE	-	expression tag	UNP Q8R418
A	-23	GLU	-	expression tag	UNP Q8R418
A	-22	LYS	-	expression tag	UNP Q8R418
A	-21	GLY	-	expression tag	UNP Q8R418
A	-20	ASP	-	expression tag	UNP Q8R418
A	-19	TYR	-	expression tag	UNP Q8R418
A	-18	PRO	-	expression tag	UNP Q8R418
A	-17	TYR	-	expression tag	UNP Q8R418
A	-16	ASP	-	expression tag	UNP Q8R418
A	-15	VAL	-	expression tag	UNP Q8R418
A	-14	PRO	-	expression tag	UNP Q8R418
A	-13	ASP	-	expression tag	UNP Q8R418
A	-12	TYR	-	expression tag	UNP Q8R418
A	-11	ALA	-	expression tag	UNP Q8R418
A	-10	GLY	-	expression tag	UNP Q8R418
A	-9	THR	-	expression tag	UNP Q8R418
A	-8	GLU	-	expression tag	UNP Q8R418
A	-7	ASN	-	expression tag	UNP Q8R418
A	-6	LEU	-	expression tag	UNP Q8R418
A	-5	TYR	-	expression tag	UNP Q8R418
A	-4	PHE	-	expression tag	UNP Q8R418
A	-3	GLN	-	expression tag	UNP Q8R418
A	-2	GLY	-	expression tag	UNP Q8R418
A	-1	LEU	-	expression tag	UNP Q8R418
A	0	VAL	-	expression tag	UNP Q8R418
A	1	ASP	-	expression tag	UNP Q8R418
A	872	SER	THR	conflict	UNP Q8R418
A	1322	ALA	GLU	engineered mutation	UNP Q8R418
A	1381	SER	ALA	conflict	UNP Q8R418
A	1569	ALA	GLU	engineered mutation	UNP Q8R418
A	1679	GLY	-	expression tag	UNP Q8R418
A	1680	ARG	-	expression tag	UNP Q8R418
A	1681	GLY	-	expression tag	UNP Q8R418
A	1682	GLU	-	expression tag	UNP Q8R418
A	1683	ASN	-	expression tag	UNP Q8R418
A	1684	LEU	-	expression tag	UNP Q8R418

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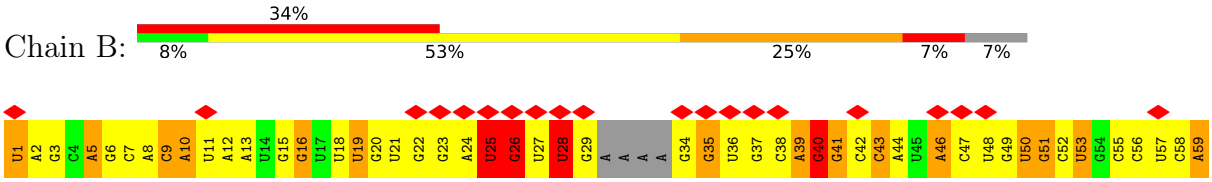
Chain	Residue	Modelled	Actual	Comment	Reference
A	1685	TYR	-	expression tag	UNP Q8R418
A	1686	PHE	-	expression tag	UNP Q8R418
A	1687	GLN	-	expression tag	UNP Q8R418
A	1688	GLY	-	expression tag	UNP Q8R418
A	1689	ALA	-	expression tag	UNP Q8R418
A	1690	SER	-	expression tag	UNP Q8R418
A	1691	ASP	-	expression tag	UNP Q8R418
A	1692	TYR	-	expression tag	UNP Q8R418
A	1693	LYS	-	expression tag	UNP Q8R418
A	1694	ASP	-	expression tag	UNP Q8R418
A	1695	HIS	-	expression tag	UNP Q8R418
A	1696	ASP	-	expression tag	UNP Q8R418
A	1697	GLY	-	expression tag	UNP Q8R418
A	1698	ASP	-	expression tag	UNP Q8R418
A	1699	TYR	-	expression tag	UNP Q8R418
A	1700	LYS	-	expression tag	UNP Q8R418
A	1701	ASP	-	expression tag	UNP Q8R418
A	1702	HIS	-	expression tag	UNP Q8R418
A	1703	ASP	-	expression tag	UNP Q8R418
A	1704	GLY	-	expression tag	UNP Q8R418
A	1705	SER	-	expression tag	UNP Q8R418
A	1706	HIS	-	expression tag	UNP Q8R418
A	1707	HIS	-	expression tag	UNP Q8R418
A	1708	HIS	-	expression tag	UNP Q8R418
A	1709	HIS	-	expression tag	UNP Q8R418
A	1710	HIS	-	expression tag	UNP Q8R418
A	1711	HIS	-	expression tag	UNP Q8R418
A	1712	HIS	-	expression tag	UNP Q8R418
A	1713	HIS	-	expression tag	UNP Q8R418

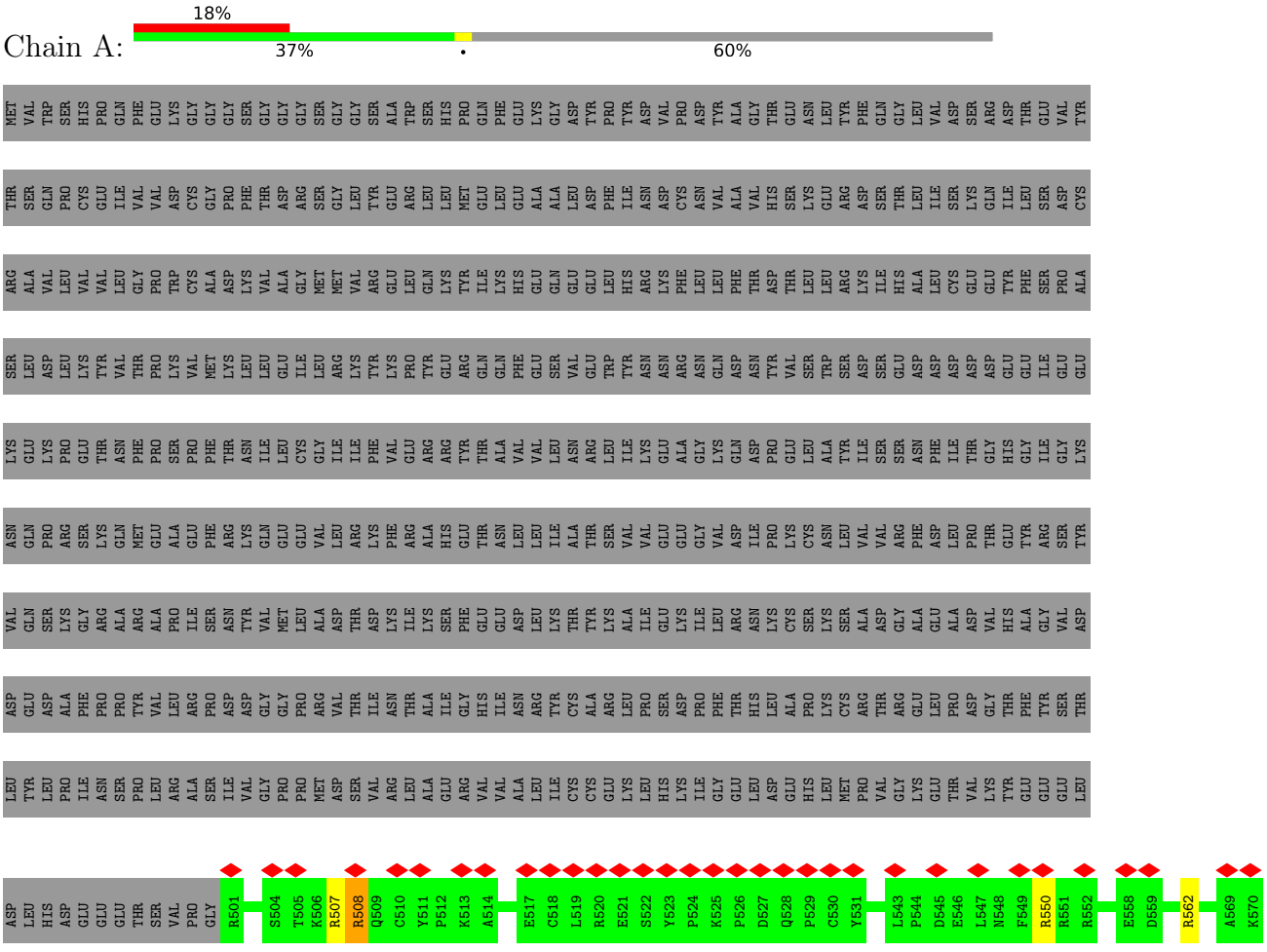
3 Residue-property plots (i)

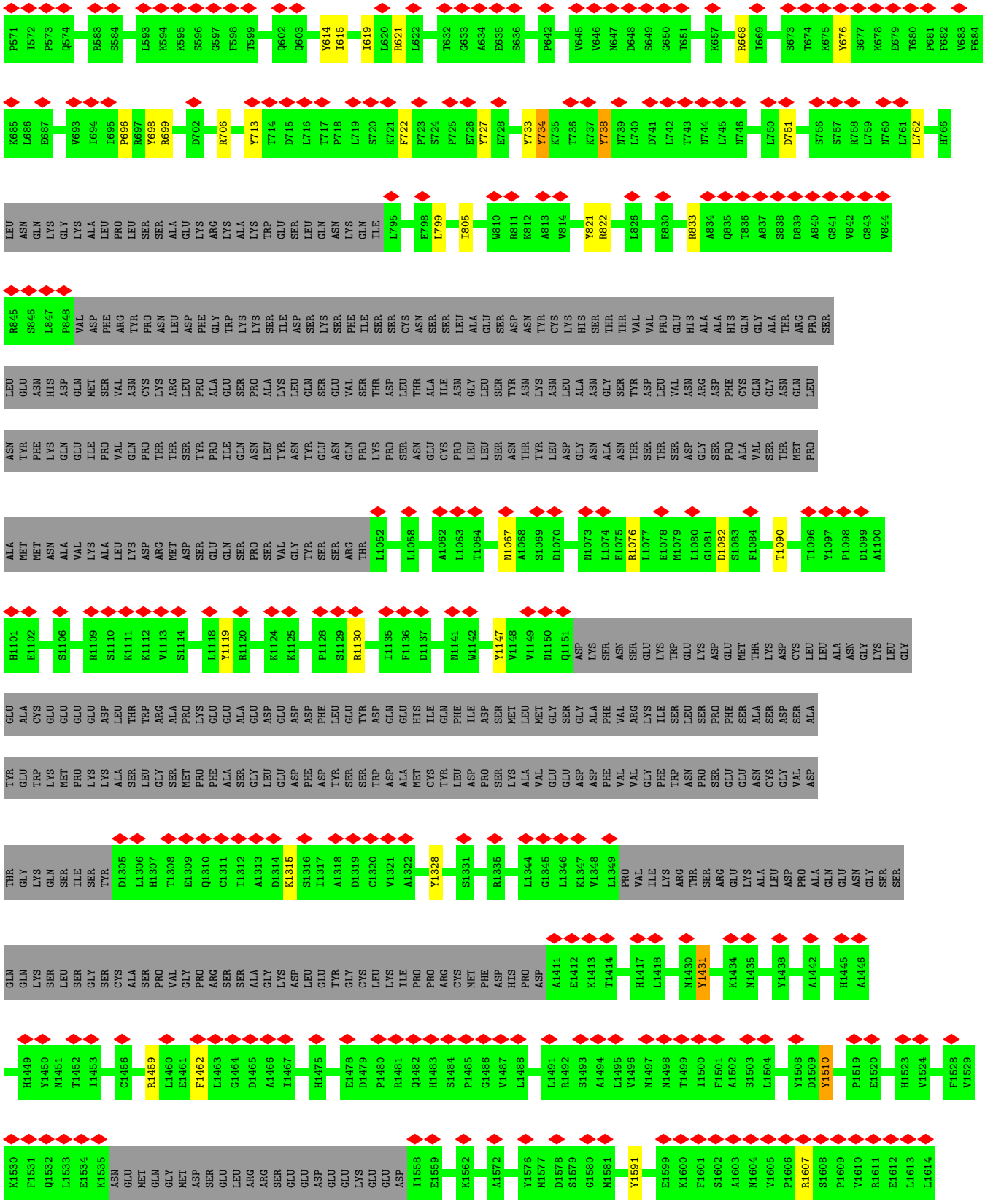
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

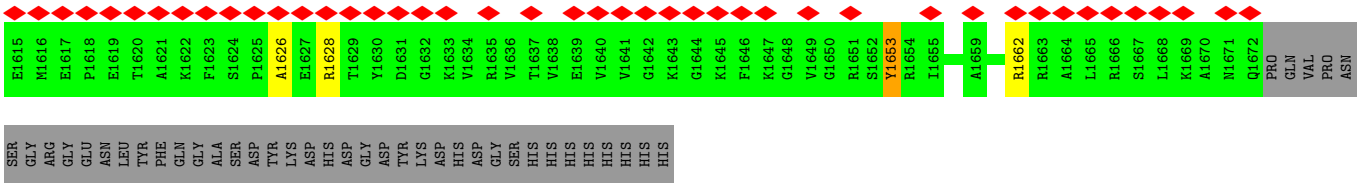
- Molecule 1: 59-nt precursor of miR-15a



- Molecule 2: Isoform 2 of Endoribonuclease Dicer




P571 I572 P573 Q574 R583 S584 L593 K594 K595 S596 G597 F598 T599 Q602 Q603 Y614 I615 I619 L620 R621 L622 T632 G633 A634 E635 S636 P642 V645 V646 N647 D648 S649 G650 T651 K657 R668 I669 S673 T674 K675 Y676 S677 K678 E679 T680 P681 F682 V683 F684
K685 L686 E687 V693 I694 I695 P696 R697 Y698 R699 D702 R706 Y713 T714 D715 L716 T717 P718 L719 S720 K721 F722 P723 S724 P725 E726 Y727 E728 Y733 Y734 K735 T736 K737 Y738 N739 L740 D741 L742 T743 N744 L745 N746 L750 D751 S756 S757 R758 L759 N760 L761 L762 H766
LEU ASN GLN LYS GLY LYS ALA LEU PRO LEU SER SER ALA GLU LYS ARG LYS ALA LYS TRP GLU SER LEU GLN ASN LYS GLN ILE L795 E798 L799 I805 W810 R811 K812 A813 V814 Y821 R822 L826 E830 R833 A834 Q835 T836 A837 S838 D839 A840 G841 V842 G843 V844
R845 S846 L847 P848 VAL ASP PHE ARG TYR PRO ASN LEU ASP PHE GLY TRP LYS LYS SER ILE ASP SER LYS SER PHE ILE SER SER CYS ASN SER SER LEU ALA GLU SER ASP ASN TYR CYS LYS HIS SER THR THR VAL VAL PRO GLU HIS ALA ALA HIS GLN GLY GLY ALA THR ARG PRO SER
LEU GLU ASN HIS ASP GLN MET SER VAL ASN CYS LYS ARG LEU PRO ALA GLU SER PRO ALA LYS LEU GLN SER GLU VAL SER THR ASP LEU THR ALA ILE ASN GLY LEU SER TYR ASN LYS ASN LEU ALA ASN GLY SER TYR ASP LEU VAL ASN ARG ASP PHE CYS GLN GLY ASN GLN LEU
ASN TYR PHE LYS GLN GLU ILE PRO VAL GLN PRO THR THR SER TYR PRO ILE GLN ASN LEU TYR ASN TYR GLU ASN GLN PRO LYS PRO SER ASN GLU CYS PRO LEU LEU LEU SER ASN THR TYR LEU ASP GLY ASN ALA ASN THR SER THR SER ASP GLY SER PRO ALA VAL SER THR MET PRO
ALA MET MET ASN ALA VAL LYS ALA LEU LYS ASP ARG MET ASP SER GLU GLN SER PRO SER VAL GLY TYR SER SER ARG THR L1052 L1058 A1062 L1063 T1064 N1067 A1068 S1069 D1070 N1073 L1074 E1075 R1076 L1077 E1078 M1079 L1080 G1081 D1082 S1083 F1084 T1090 T1096 Y1097 P1098 D1099 A1100
H1101 E1102 S1106 R1109 S1110 K1111 K1112 V1113 S1114 L1118 Y1119 R1120 K1124 K1125 P1128 S1129 R1130 I1135 F1136 D1137 N1141 W1142 Y1147 V1148 V1149 N1150 Q1151 ASP LYS SER ASN SER GLU LYS TRP GLU LYS ASP GLU MET THR LYS ASP CYS LEU LEU ALA ASN GLY LYS LEU GLY
GLU ALA CYS GLU GLU GLU GLU ASP LEU THR TRP ARG ALA PRO LYS GLU GLU ALA GLU ASP GLU ASP ASP PHE LEU GLU GLY TYR ASP GLN GLU HIS ILE GLN PHE ILE ASP SER MET LEU MET GLY SER GLY ALA PHE VAL ARG LYS ILE SER LEU SER PRO PHE SER ALA SER ASP SER ALA
TYR GLU TRP LYS MET PRO LYS LYS ALA SER LEU GLY SER MET PRO PHE ALA SER GLY LEU GLU ASP PHE ASP TYR SER SER TRP ASP ALA MET CYS TYR LEU ASP PRO SER LYS ALA VAL GLU GLU ASP ASP PHE VAL VAL GLY PHE TRP ASN PRO SER GLU GLU ASN CYS GLY VAL ASP
THR GLY LYS GLN SER ILE SER TYR D1305 L1306 H1307 T1308 E1309 Q1310 C1311 I1312 A1313 D1314 K1315 S1316 I1317 A1318 D1319 C1320 V1321 A1322 Y1328 S1331 R1335 L1344 G1345 L1346 K1347 V1348 L1349 PRO VAL ILE LYS ARG THR SER ARG GLU LYS ALA LEU ASP PRO ALA GLN GLU ASN GLY SER SER
GLN GLN LYS SER LEU SER GLY CYS ALA SER PRO VAL GLY PRO ARG SER SER ALA GLY CYS LEU LYS ILE PRO PRO ARG CYS MET PHE ASP HIS PRO ASP A1411 E1412 K1413 T1414 H1417 L1418 N1430 Y1431 K1434 N1435 Y1438 A1442 H1445 A1446
H1449 Y1450 N1451 T1452 I1453 C1456 R1459 L1460 E1461 F1462 L1463 G1464 D1465 A1466 I1467 H1475 E1478 D1479 P1480 R1481 Q1482 H1483 S1484 P1485 G1486 V1487 L1488 L1491 R1492 S1493 A1494 L1495 V1496 N1497 N1498 T1499 I1500 F1501 A1502 S1503 L1504 Y1508 D1509 Y1610 P1519 E1520 H1523 V1524 F1528 V1529
K1530 F1531 Q1532 L1533 E1534 K1535 ASN GLU MET GLN GLY MET ASP SER GLU LEU ARG ARG SER GLU GLU ASP GLU GLU LYS GLU GLU ASP I1558 E1559 K1562 A1572 Y1576 M1577 D1578 S1579 G1580 M1581 Y1591 E1599 K1600 F1601 S1602 A1603 N1604 V1605 P1606 R1607 S1608 P1609 V1610 R1611 E1612 L1613 L1614


E1615 M1616 E1617 P1618 E1619 T1620 A1621 K1622 F1623 S1624 P1625 A1626 E1627 R1628 T1629 Y1630 D1631 G1632 K1633 V1634 R1635 V1636 T1637 V1638 E1639 V1640 V1641 G1642 K1643 G1644 K1645 F1646 K1647 G1648 V1649 G1650 R1651 S1652 Y1653 R1654 I1655 A1659 R1662 R1663 A1664 L1665 R1666 S1667 L1668 K1669 A1670 N1671 Q1672 PRO GLN VAL PRO ASN
SER GLY ARG GLY GLU ASN LEU TYR PHE GLN GLY ALA SER ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP GLY SER HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84697	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.141	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.112	Depositor
Map size (Å)	317.952, 317.952, 317.952	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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	B	1.49	6/1309 (0.5%)	2.22	82/2036 (4.0%)
2	A	0.69	0/5790	1.03	23/7851 (0.3%)
All	All	0.89	6/7099 (0.1%)	1.37	105/9887 (1.1%)

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	B	0	17
2	A	0	10
All	All	0	27

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	C	C4-N4	-7.37	1.27	1.33
1	B	29	G	C2-N2	-7.25	1.27	1.34
1	B	8	A	C5-C4	-5.30	1.35	1.38
1	B	26	G	C2-N2	-5.08	1.29	1.34
1	B	29	G	N1-C2	-5.05	1.33	1.37

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	U	O4'-C1'-N1	14.24	119.60	108.20
1	B	40	G	P-O3'-C3'	9.83	131.50	119.70
1	B	52	C	N3-C4-C5	8.71	125.39	121.90
1	B	40	G	C4'-C3'-O3'	8.42	129.84	113.00
1	B	58	C	N3-C2-O2	-8.18	116.18	121.90

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	25	U	Sidechain
1	B	26	G	Sidechain
1	B	28	U	Sidechain
1	B	5	A	Sidechain
1	B	6	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1173	590	583	3	0
2	A	5651	5697	5696	10	0
All	All	6824	6287	6279	12	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 1.

The worst 5 of 12 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:698:TYR:CD1	2:A:738:TYR:CE2	2.97	0.53
1:B:1:U:H5"	2:A:621:ARG:HH11	1.79	0.47
2:A:1090:THR:HG23	2:A:1462:PHE:CE2	2.51	0.45
1:B:18:U:H2'	1:B:19:U:C6	2.53	0.43
2:A:619:ILE:HD11	2:A:805:ILE:CD1	2.50	0.42

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
2	A	693/1765 (39%)	684 (99%)	9 (1%)	0	100 100

There are no Ramachandran outliers to report.

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
2	A	625/1561 (40%)	621 (99%)	4 (1%)	86 92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	706	ARG
2	A	1067	ASN
2	A	1082	ASP
2	A	1315	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	53/59 (89%)	9 (16%)	1 (1%)

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	16	G
1	B	25	U
1	B	26	G

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Mol	Chain	Res	Type
1	B	27	U
1	B	28	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	40	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

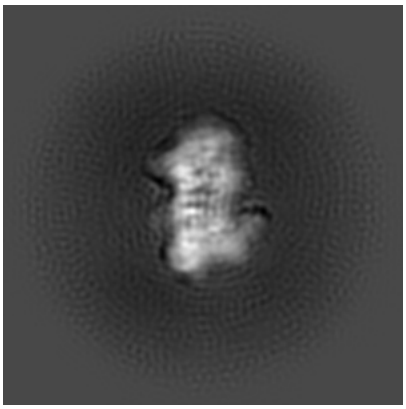
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14384. These allow visual inspection of the internal detail of the map and identification of artifacts.

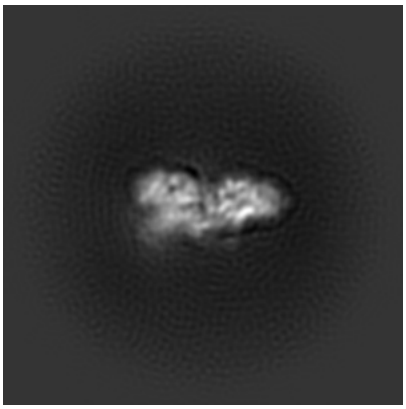
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

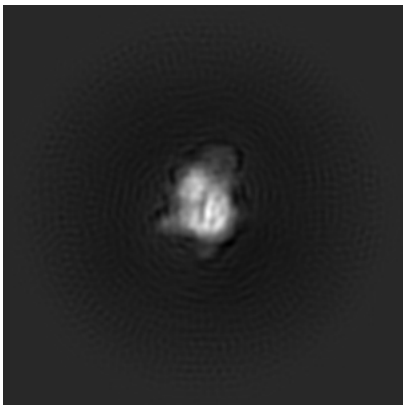
6.1.1 Primary map



X

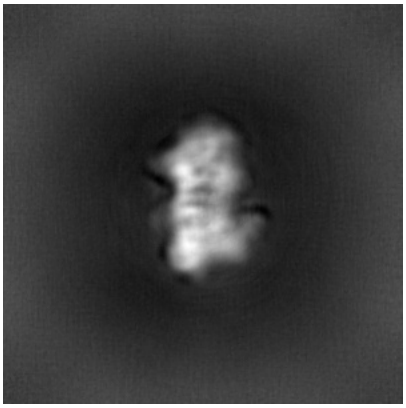


Y

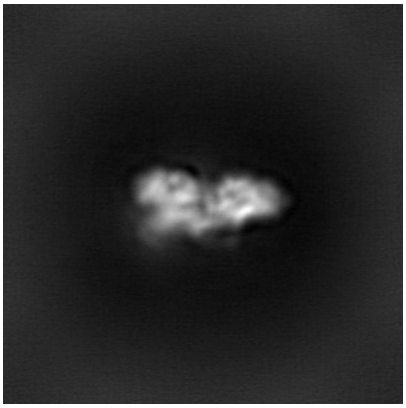


Z

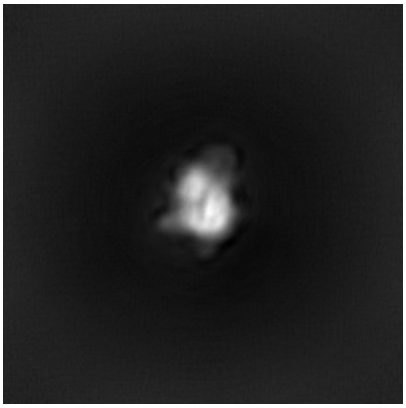
6.1.2 Raw map



X



Y

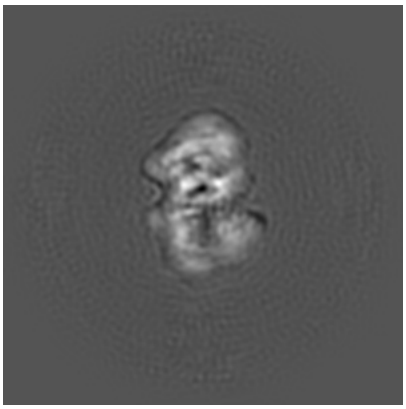


Z

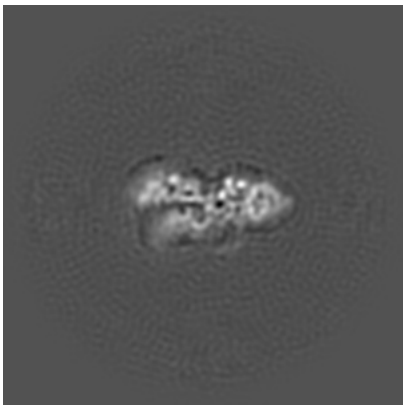
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

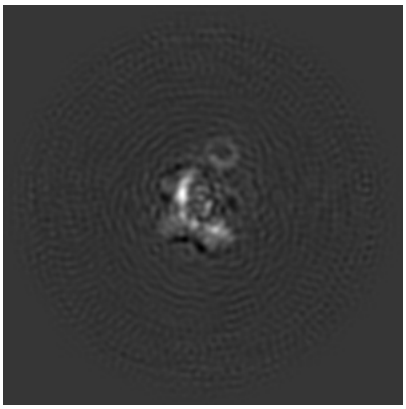
6.2.1 Primary map



X Index: 192

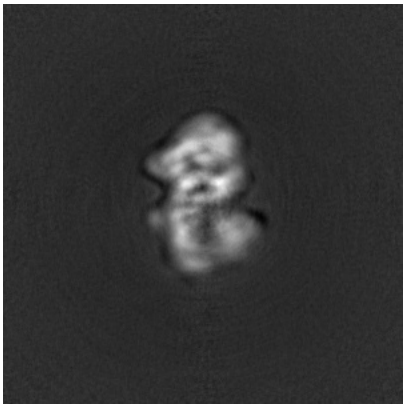


Y Index: 192

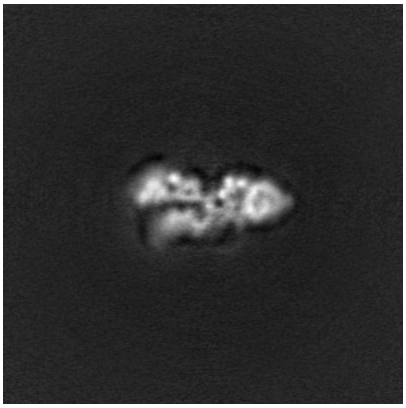


Z Index: 192

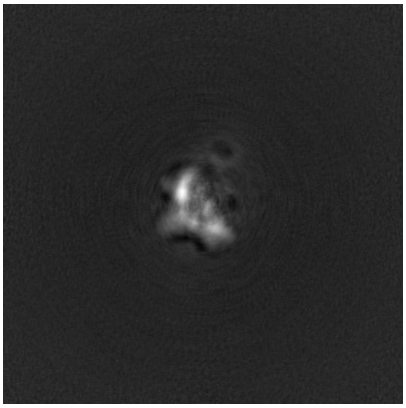
6.2.2 Raw map



X Index: 192



Y Index: 192

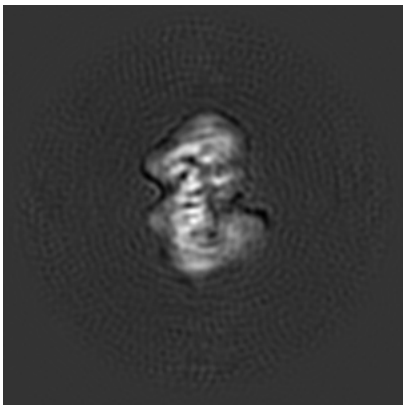


Z Index: 192

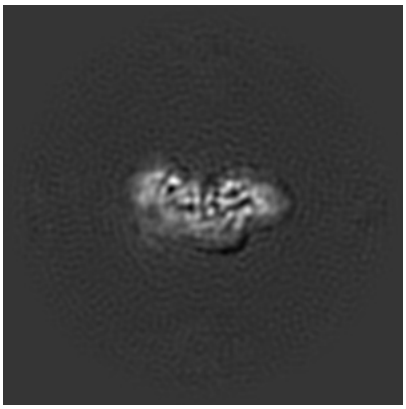
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

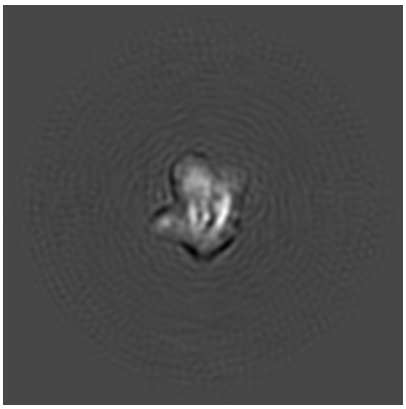
6.3.1 Primary map



X Index: 196

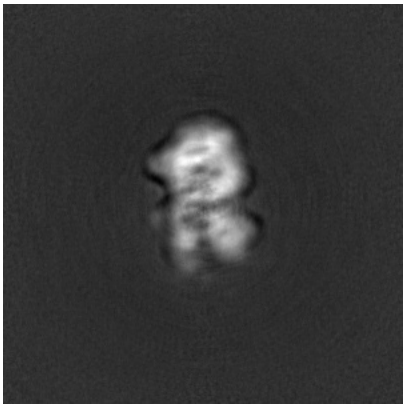


Y Index: 182

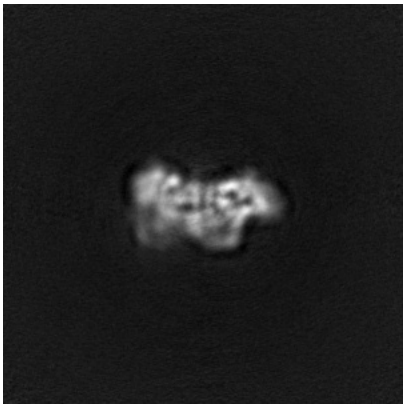


Z Index: 217

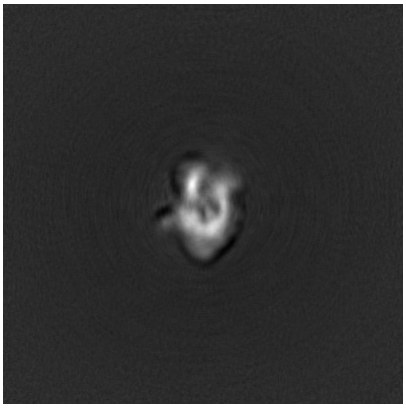
6.3.2 Raw map



X Index: 186



Y Index: 177

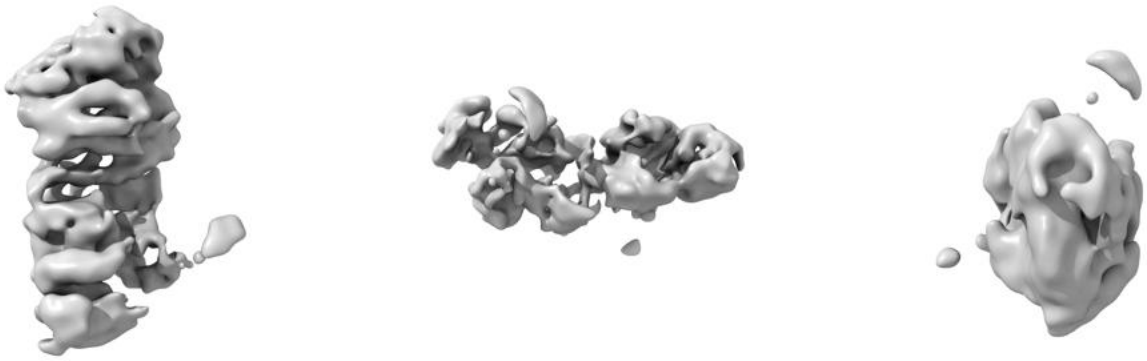


Z Index: 226

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

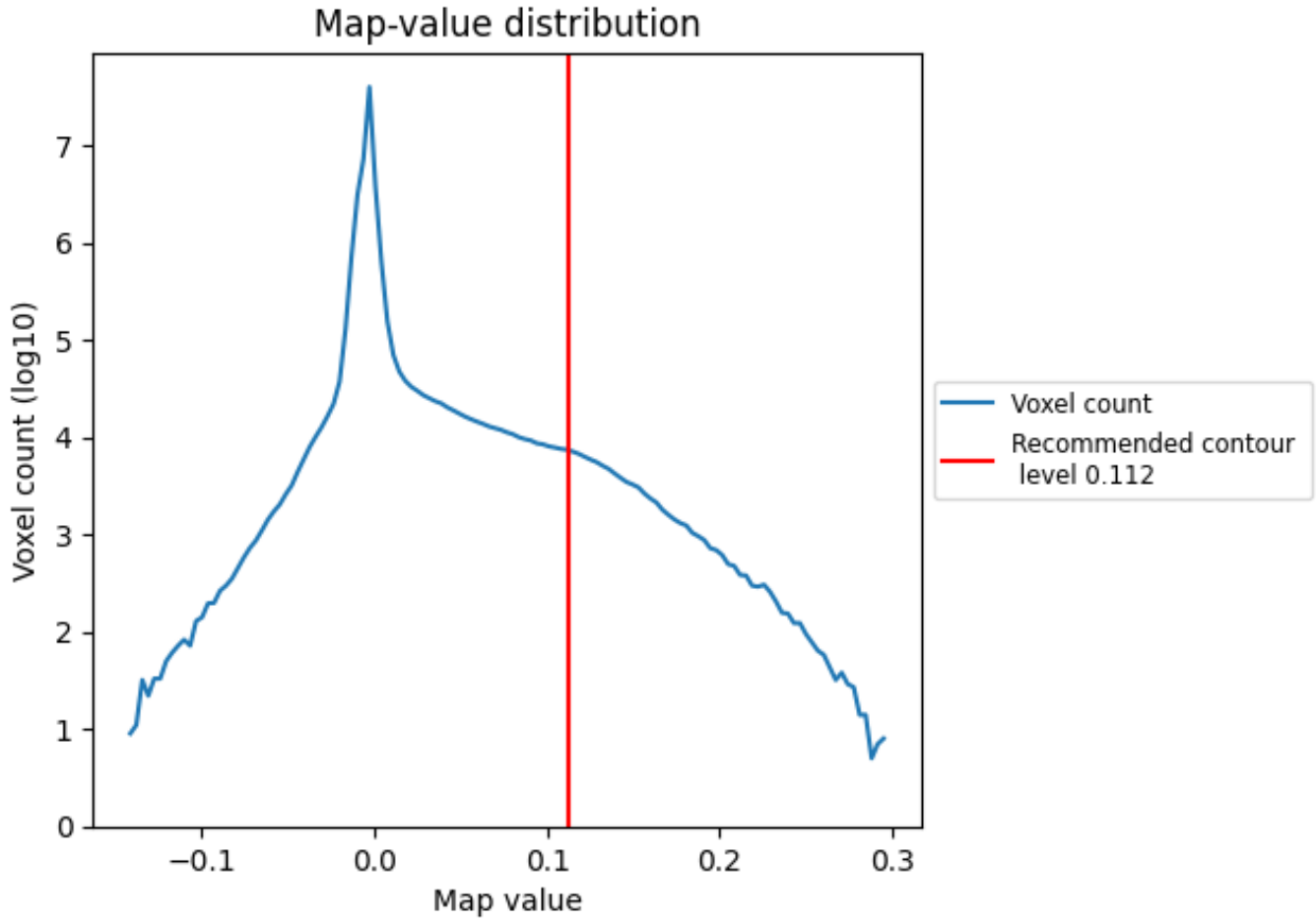
6.5 Mask visualisation (i)

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

7 Map analysis

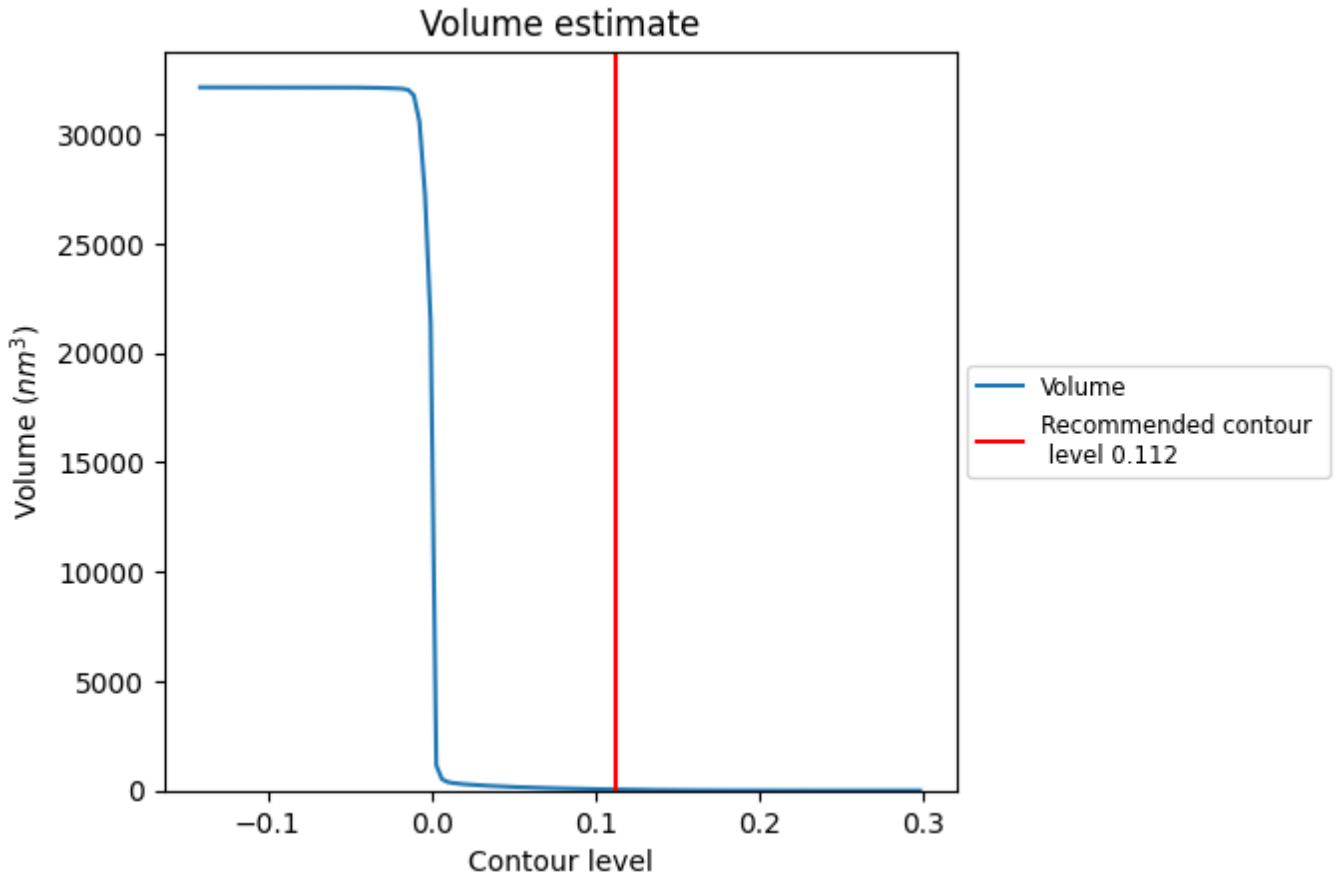
This section contains the results of statistical analysis of the map.

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.

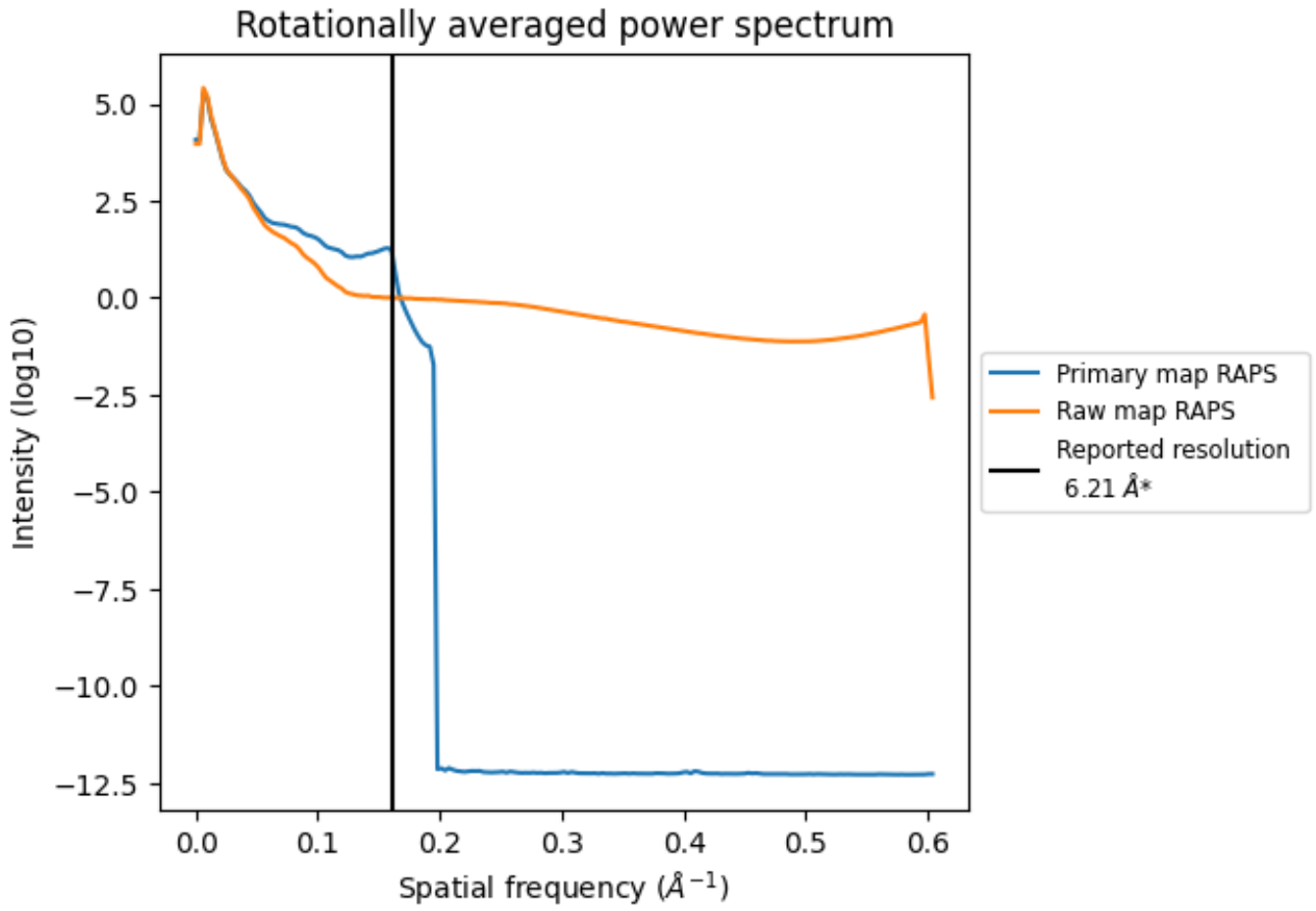
7.2 Volume estimate (i)



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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)

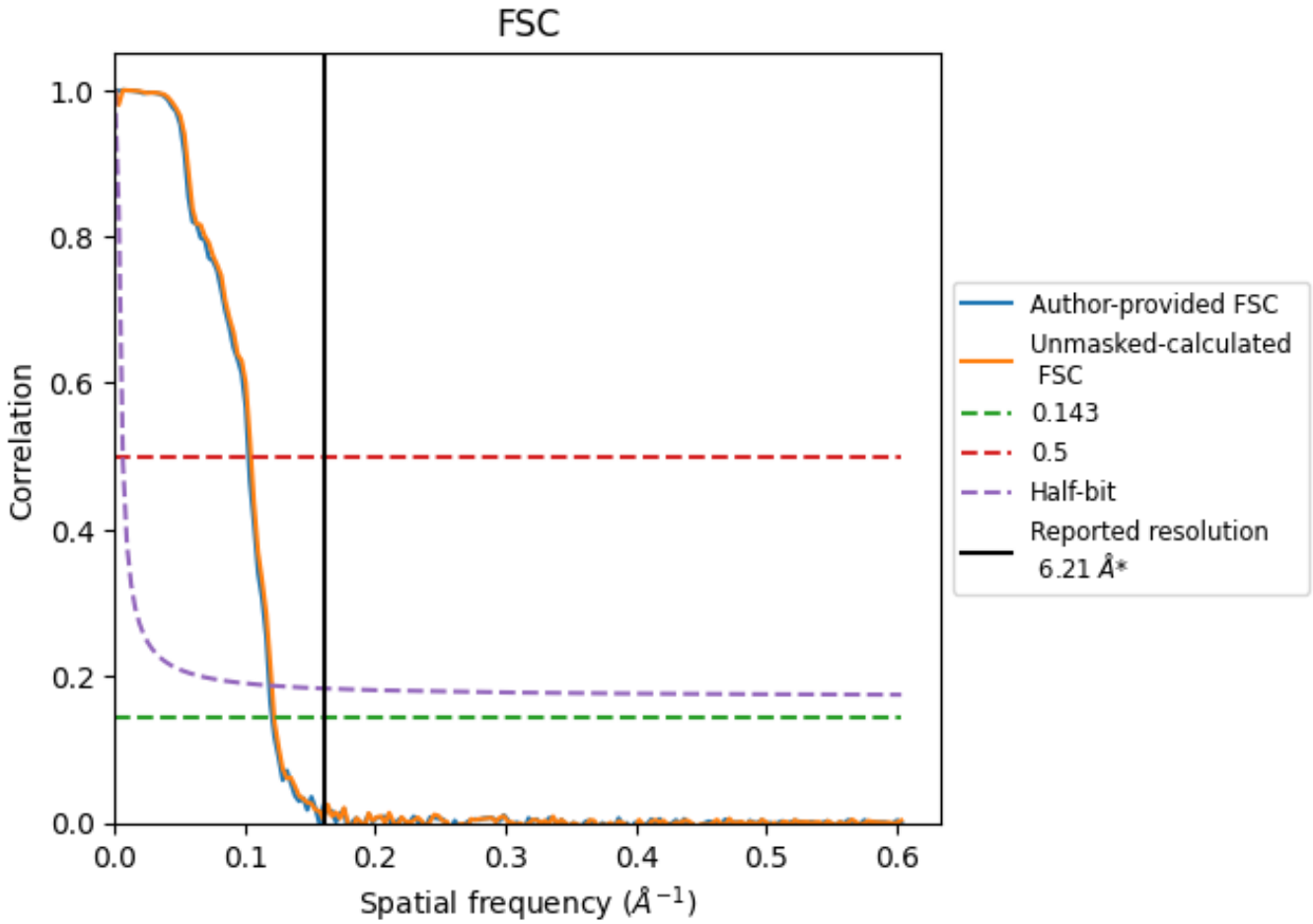


*Reported resolution corresponds to spatial frequency of 0.161 Å^{-1}

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 0.161 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.21	-	-
Author-provided FSC curve	8.27	9.74	8.42
Unmasked-calculated*	8.17	9.56	8.29

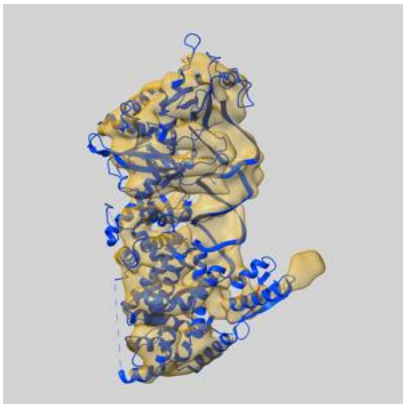
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.27 differs from the reported value 6.21 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.17 differs from the reported value 6.21 by more than 10 %

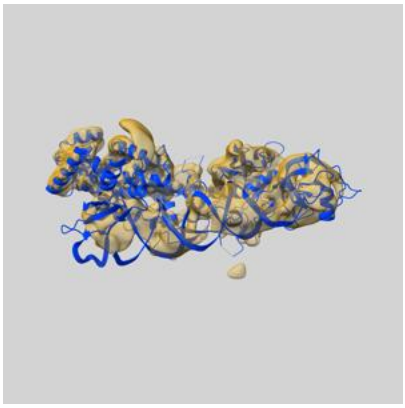
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14384 and PDB model 7YYN. Per-residue inclusion information can be found in section 3 on page 6.

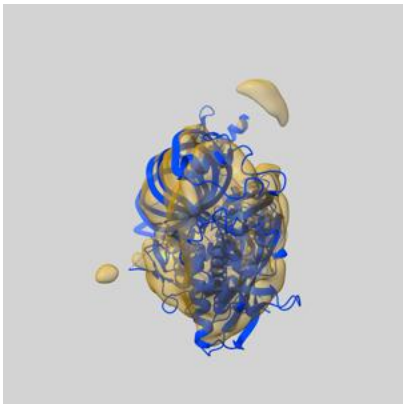
9.1 Map-model overlay



X



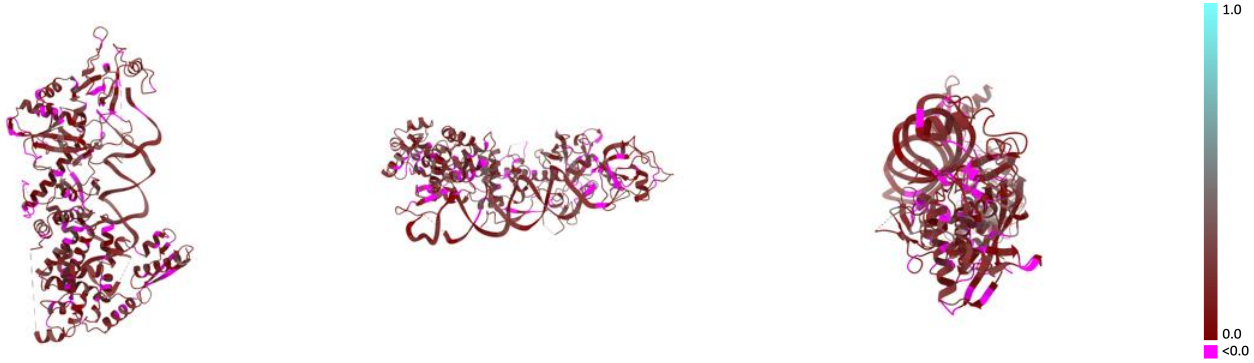
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.112 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.

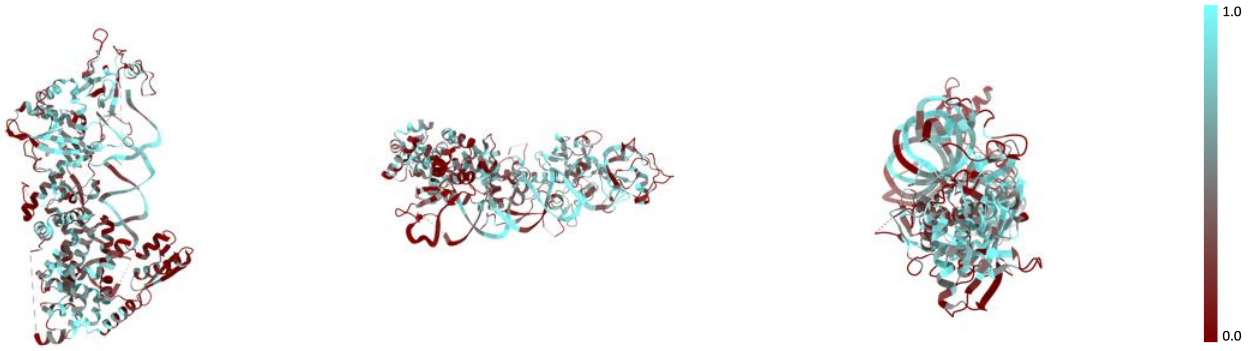
9.2 Q-score mapped to coordinate model



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.

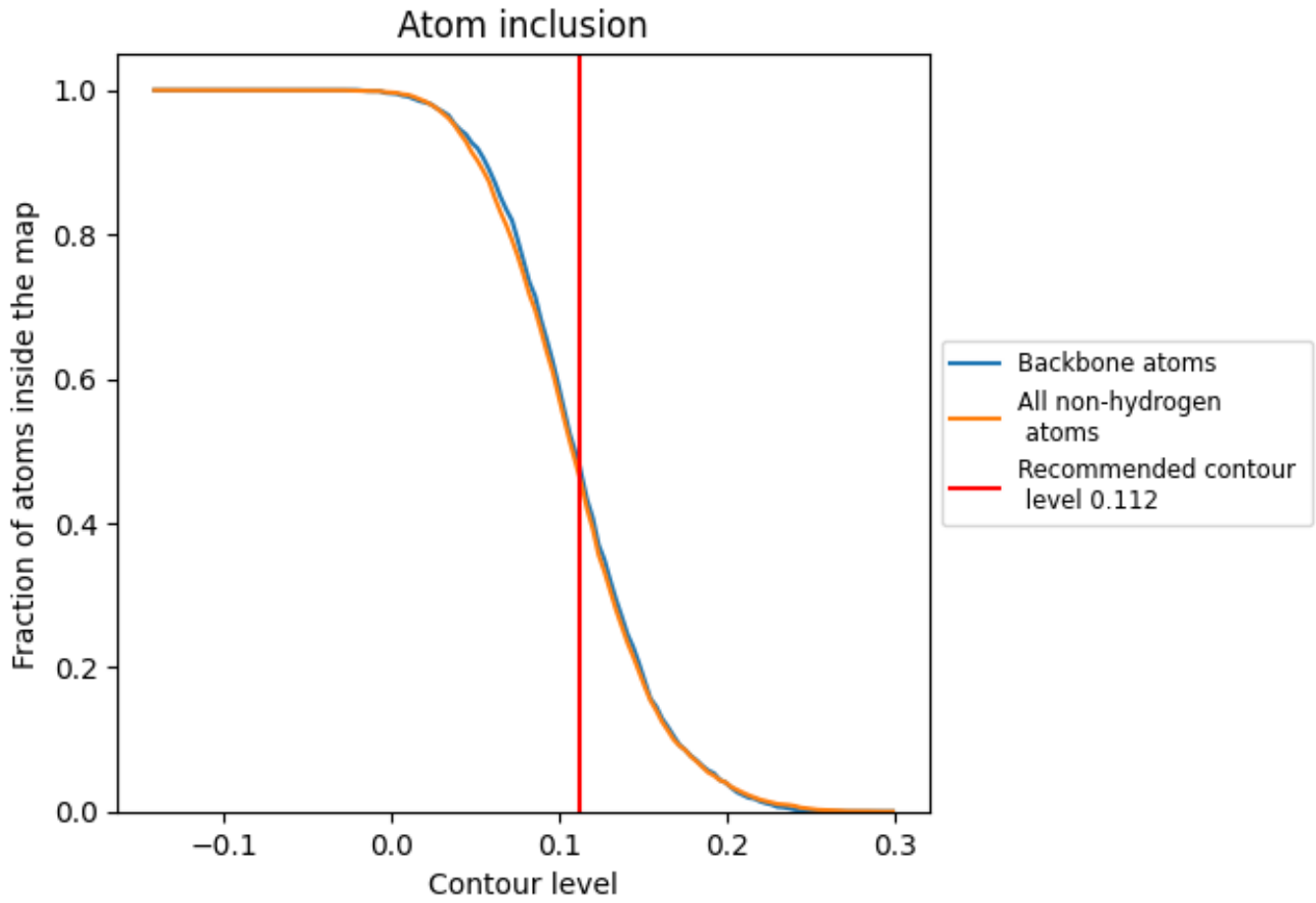
9.3 Atom inclusion mapped to coordinate model



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 (0.112).

9.4 Atom inclusion (i)



At the recommended contour level, 48% of all backbone atoms, 46% 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 (0.112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4630	0.1330
A	0.4487	0.1320
B	0.5217	0.1410