wwPDB EM Validation Summary Report

Nov 22, 2022 – 02:27 PM JST

PDB ID	:	7EJU
EMDB ID	:	EMD-31163
Title	:	Junin virus(JUNV) RNA polymerase L complexed with Z protein
Authors	:	Chen, Y.
Deposited on	:	2021-04-02
Resolution	:	3.50 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:

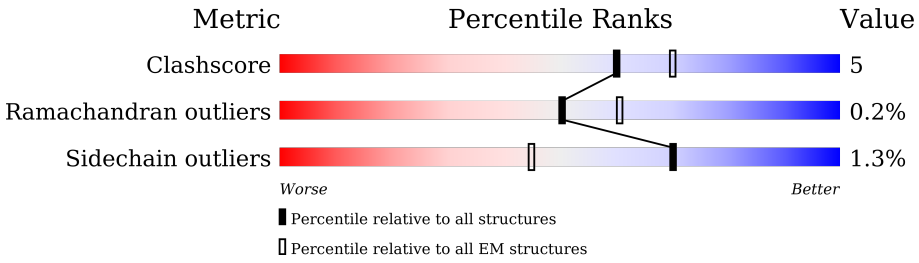
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.50 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

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	2210	23% 63% 11% 25%
2	B	94	22% 44% 11% · 45%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13713 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1648	13287	8496	2247	2449	95	0	0

- Molecule 2 is a protein called RING finger protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	52	423	265	75	74	9	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0
3	B	1	Total	Zn	0
			1	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

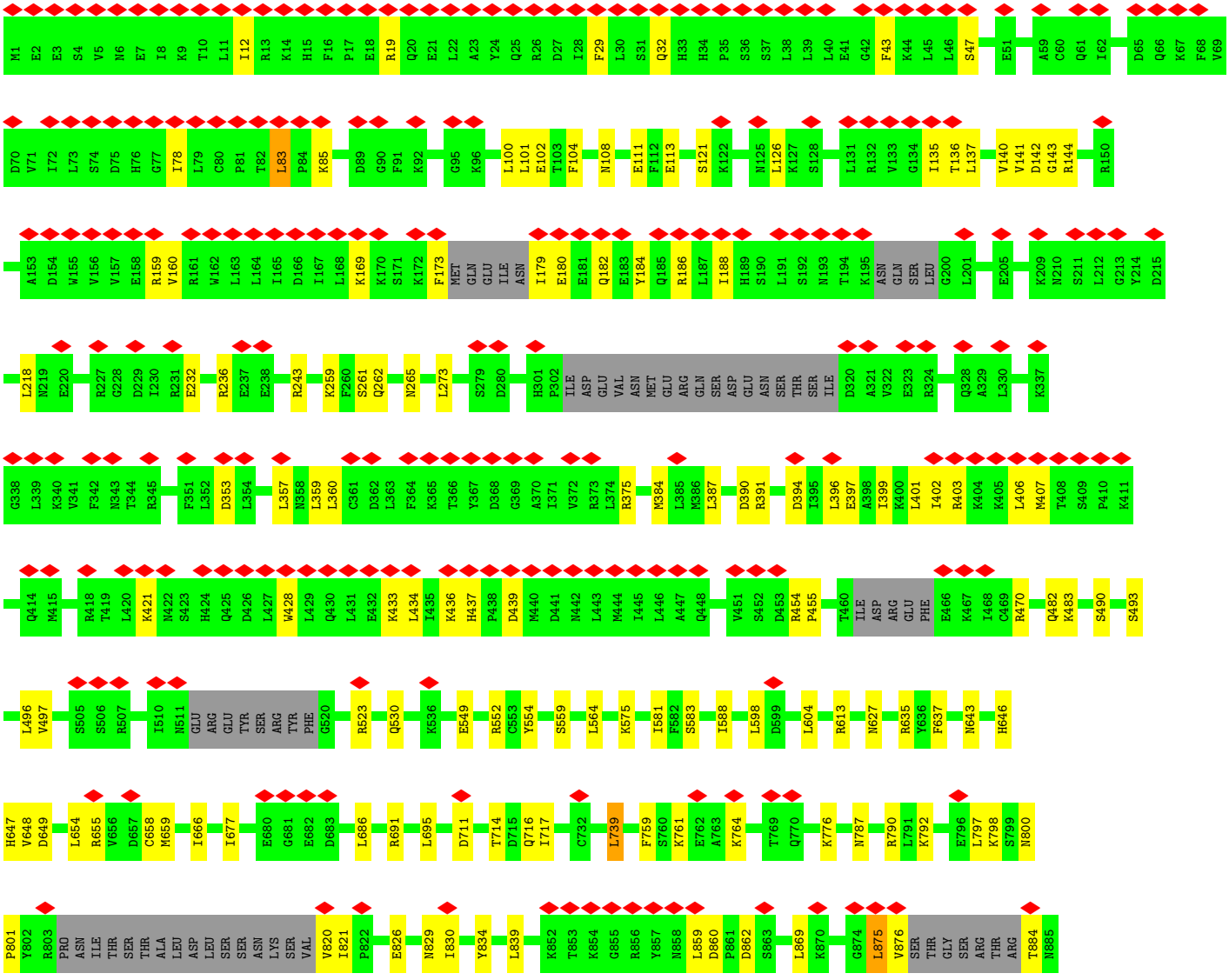
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0

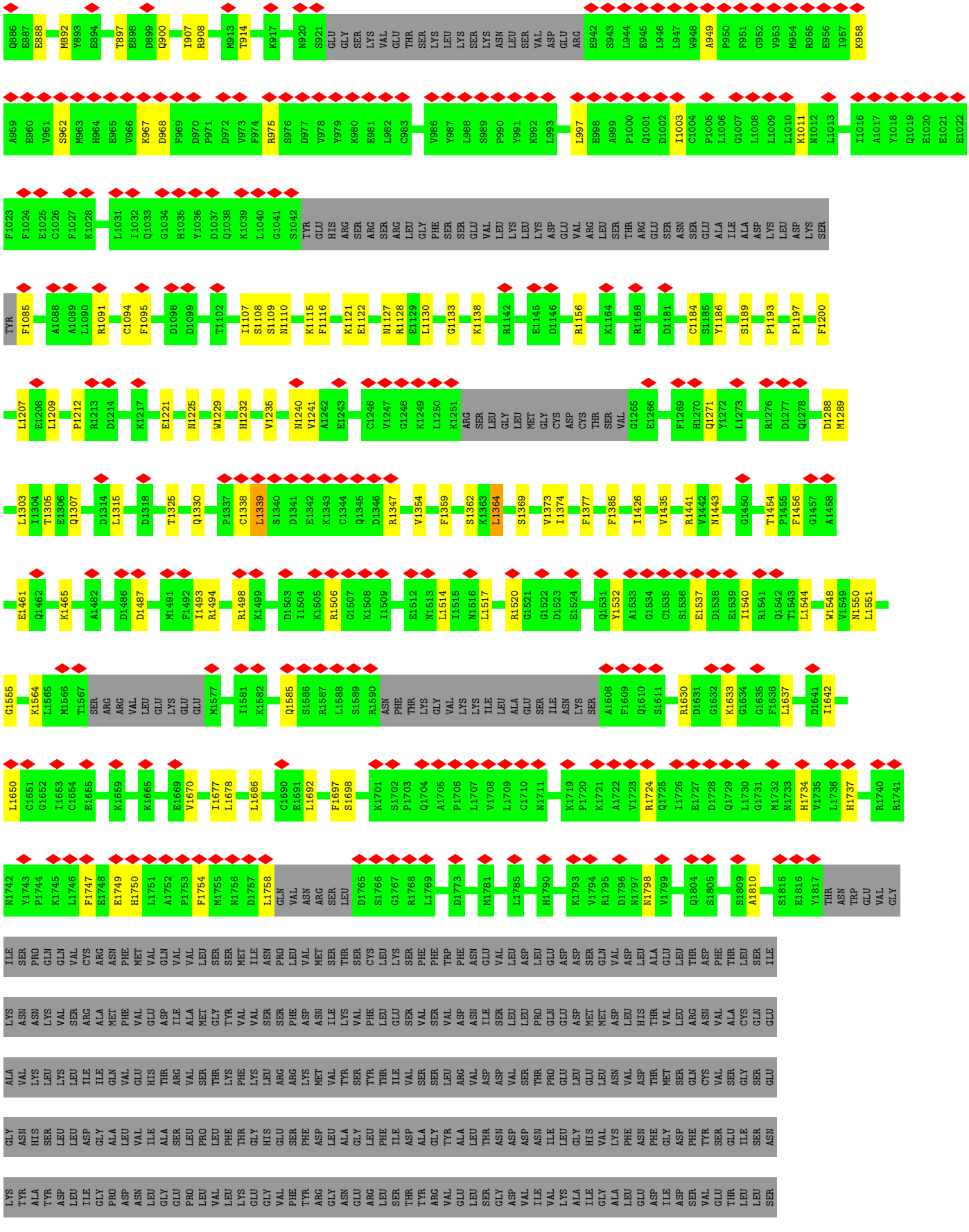
3 Residue-property plots (i)

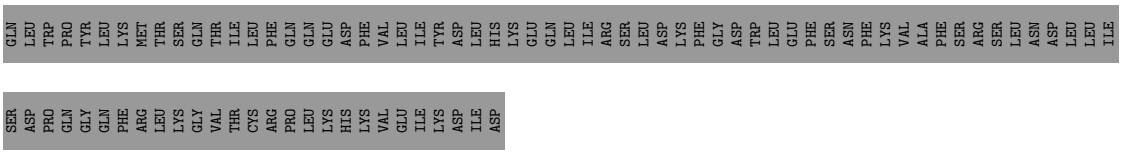
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

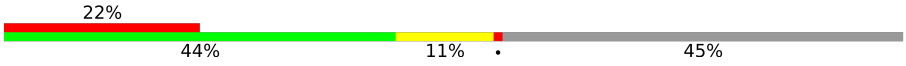


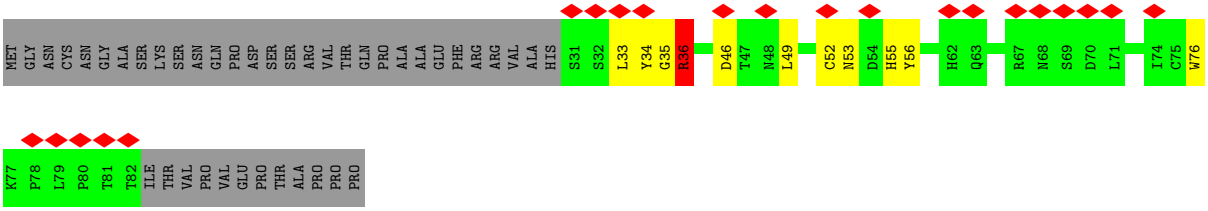

Q886 E887 E888 M892 Y893 E894 T897 E898 D899 Q900 I907 R908 M913 T914 K917 N920 S921 GLU GLY SER LYS VAL GLU THR SER LYS LEU LYS SER LYS ASN LEU SER VAL ASP GLU ARG E942 S943 L944 E945 L946 L947 W948 A949 P950 F951 G952 V953 M954 R955 E956 I957 K958
A959 E960 V961 S962 M963 H964 E965 V966 K967 D968 F969 D970 P971 D972 V973 F974 R975 S976 D977 V978 Y979 K980 E981 L982 C983 V986 Y987 L988 S989 P990 Y991 K992 L993 L997 E998 A999 P1000 Q1001 D1002 I1003 C1004 P1005 L1006 G1007 L1008 L1009 L1010 K1011 N1012 L1013 I1016 A1017 Y1018 Q1019 E1020 E1021 E1022
F1023 F1024 E1025 C1026 F1027 K1028 L1031 I1032 Q1033 G1034 H1035 Y1036 D1037 Q1038 K1039 L1040 G1041 S1042 TYR GLU HIS ARG SER ARG SER ARG LEU GLY PHE SER SER GLU VAL LEU LYS LEU LYS ASP GLU VAL ARG LEU SER THR ARG GLU SER ASN SER GLU ALA ILE ALA ASP LYS LEU ASP LYS SER
TYR F1085 A1088 A1089 L1090 R1091 C1094 F1095 D1098 D1099 T1102 I1107 S1108 S1109 N1110 K1115 F1116 K1121 E1122 N1127 R1128 E1129 L1130 G1133 K1138 R1142 E1145 D1146 R1156 K1164 R1168 D1181 C1184 S1185 Y1186 S1189 P1193 P1197 F1200
L1207 E1208 L1209 P1212 R1213 D1214 K1217 E1221 N1225 W1229 H1232 V1235 N1240 V1241 A1242 E1243 C1246 V1247 G1248 K1249 L1250 K1251 ARG SER LEU GLY LEU MET GLY CYS ASP CYS THR SER VAL G1265 E1266 F1269 H1270 Q1271 Y1272 L1273 R1276 D1277 Q1278 D1288 M1289
L1303 I1304 T1305 E1306 Q1307 D1314 L1315 D1318 T1325 Q1330 P1337 C1338 L1339 S1340 D1341 E1342 K1343 C1344 Q1345 D1346 R1347 V1354 F1359 S1362 K1363 L1364 S1369 V1373 I1374 F1377 F1385 I1426 V1435 R1441 V1442 N1443 G1450 T1454 P1455 F1456 G1457 A1458
E1461 Q1462 K1465 A1482 D1486 D1487 M1491 F1492 I1493 R1494 R1498 K1499 D1503 I1504 K1505 R1506 G1507 K1508 I1509 E1512 N1513 L1514 I1515 N1516 L1517 R1520 G1521 G1522 D1523 E1524 Q1531 Y1532 A1533 G1534 C1535 S1536 E1537 D1538 E1539 I1540 R1541 Q1542 T1543 L1544 W1548 V1549 N1550 L1551
G1555 K1564 L1565 M1566 T1567 SER ARG ARG VAL LEU GLU LYS GLU GLU M1577 I1581 K1582 Q1585 S1586 R1587 L1588 S1589 R1590 ASN PHE THR LYS GLY VAL LYS LYS ILE LEU ALA GLU SER ILE ASN LYS SER A1608 F1609 Q1610 S1611 R1630 D1631 G1632 K1633 G1634 G1635 F1636 L1637 D1641 I1642
L1650 C1651 G1652 I1653 C1654 E1665 K1659 K1665 E1669 V1670 I1677 L1678 L1686 C1690 E1691 L1692 F1697 S1698 K1701 S1702 P1703 Q1704 A1705 P1706 L1707 V1708 L1709 C1710 N1711 K1719 P1720 K1721 A1722 V1723 R1724 Q1725 I1726 E1727 D1728 Q1729 L1730 G1731 M1732 N1733 H1734 V1735 L1736 H1737 R1740 R1741
N1742 Y1743 P1744 K1745 L1746 F1747 E1748 E1749 H1750 L1751 A1752 P1753 F1754 M1755 N1756 D1757 L1758 GLN VAL ASN ARG SER LEU D1765 S1766 G1767 R1768 L1769 D1773 M1781 L1785 H1790 K1793 V1794 R1795 D1796 N1797 N1798 V1799 Q1804 S1805 S1809 A1810 S1815 E1816 Y1817 THR ASN TRP GLU VAL GLY
ILE SER PRO GLN GLN VAL CYS ARG ASN PHE MET VAL GLN VAL VAL LEU SER SER MET ILE ASN PRO LEU VAL MET SER THR SER CYS LEU LYS SER PHE PHE TRP PHE ASN GLU VAL LEU ASP LEU GLU ASP ASP SER GLN VAL ASP LEU LEU THR ASP PHE THR LEU SER ILE
LYS ASN ASN LYS VAL SER ARG ALA MET PHE VAL GLU ASP ILE ALA MET GLY TYR VAL VAL SER SER PHE ASP ASN ILE LYS VAL PHE LEU GLU SER VAL SER VAL ASP ASN ILE SER LEU LEU PRO GLN GLU ASP MET MET ASP LEU HIS THR VAL LEU LEU ARG ASN VAL ALA CYS GLN GLU
ALA VAL LYS LEU LYS LEU ILE GLN VAL GLU HIS THR ARG VAL SER THR LYS PHE LYS LEU ARG ARG LYS MET VAL TYR SER TYR THR ILE VAL SER SER LEU ARG VAL ASP ASP VAL SER THR PRO GLU LEU GLU LEU ASN VAL ASP THR MET SER GLN CYS VAL SER GLY SER GLU
GLY ASN HIS SER LEU LEU ASP GLY ALA LEU VAL ILE ALA SER LEU PRO LEU PHE THR GLY HIS GLU SER PHE ASP LEU ALA GLY LEU PHE ILE ASP ALA GLY TYR ALA LEU THR ASN ASP ASP ASN ILE LEU GLY HIS VAL LYS PHE ASN PHE ASP GLY PHE GLY ASP PHE TYR SER GLU ILE SER ASN
LYS TYR ALA TYR ASP LEU ILE GLY PRO ASP ASN LEU GLY GLU PRO LEU VAL LEU LYS GLY GLY VAL PHE TYR ARG GLY ASN GLU ARG LEU SER THR TYR ARG VAL GLU LEU SER GLY ASP VAL ILE VAL LYS ALA ILE GLY ALA LEU GLU ASP ILE ASP SER VAL GLU THR LEU LEU SER



• Molecule 2: RING finger protein Z

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	362657	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	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	0.067	Depositor
Minimum map value	-0.048	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0123	Depositor
Map size (Å)	166.4, 166.4, 166.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	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, MG

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	0.44	0/13530	0.71	10/18230 (0.1%)
2	B	0.45	0/434	0.71	0/590
All	All	0.44	0/13964	0.71	10/18820 (0.1%)

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	A	0	4
2	B	0	3
All	All	0	7

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	434	LEU	CA-CB-CG	6.95	131.27	115.30
1	A	1544	LEU	CA-CB-CG	6.25	129.66	115.30
1	A	353	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	1692	LEU	CA-CB-CG	5.95	128.98	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1364	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	1506	ARG	Peptide
1	A	19	ARG	Peptide
1	A	949	ALA	Peptide
2	B	35	GLY	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	13287	0	13459	124	0
2	B	423	0	403	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
All	All	13713	0	13862	129	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 5.

The worst 5 of 129 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:B:52:CYS:HB3	2:B:55:HIS:O	1.92	0.69
1:A:716:GLN:HE22	1:A:1240:ASN:HD22	1.42	0.67
1:A:101:LEU:HA	1:A:140:VAL:O	1.94	0.67
1:A:169:LYS:HD3	1:A:188:ILE:HD11	1.76	0.67
1:A:677:ILE:O	1:A:691:ARG:NH1	2.28	0.66

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	1620/2210 (73%)	1353 (84%)	265 (16%)	2 (0%)	51 84
2	B	50/94 (53%)	30 (60%)	19 (38%)	1 (2%)	7 39
All	All	1670/2304 (72%)	1383 (83%)	284 (17%)	3 (0%)	50 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	ARG
1	A	862	ASP
1	A	1798	ASN

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	1514/2034 (74%)	1494 (99%)	20 (1%)	69 86
2	B	50/85 (59%)	50 (100%)	0	100 100
All	All	1564/2119 (74%)	1544 (99%)	20 (1%)	70 86

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1271	GLN
1	A	1633	LYS
1	A	1724	ARG
1	A	1686	LEU
1	A	686	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1127	ASN
1	A	1232	HIS
1	A	1790	HIS
1	A	1585	GLN
1	A	1734	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

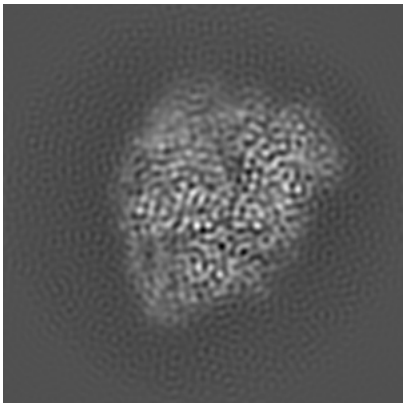
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31163. These allow visual inspection of the internal detail of the map and identification of artifacts.

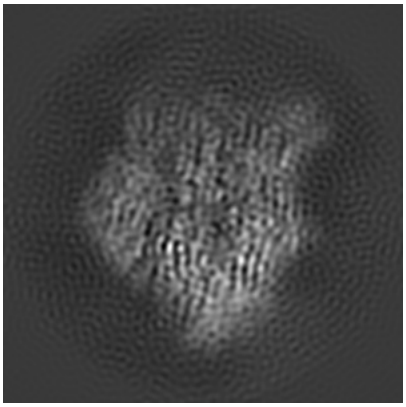
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

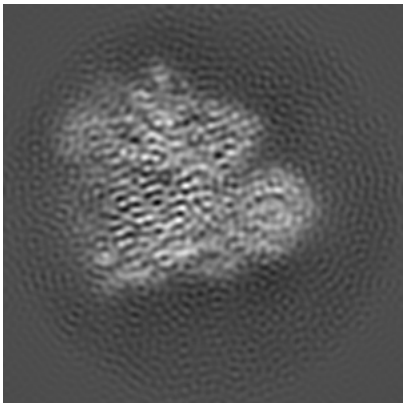
6.1.1 Primary map



X



Y

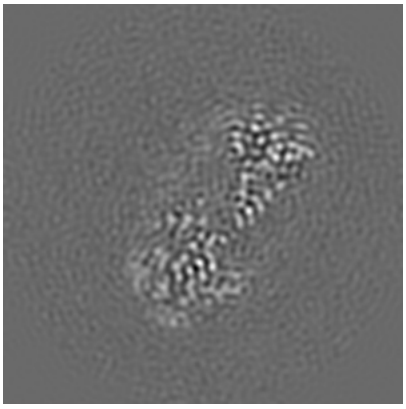


Z

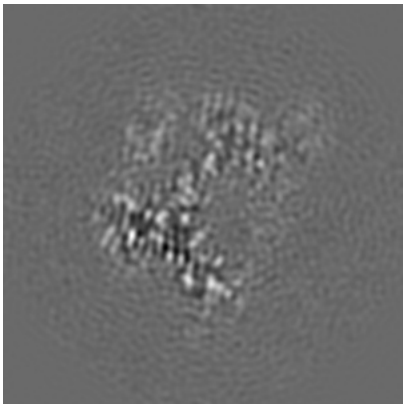
The images above show the map projected in three orthogonal directions.

6.2 Central slices

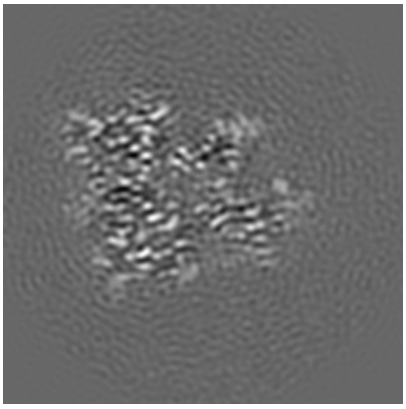
6.2.1 Primary map



X Index: 128



Y Index: 128

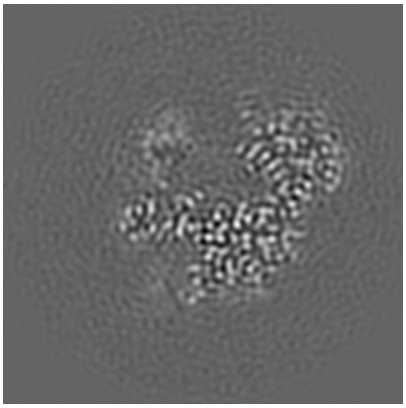


Z Index: 128

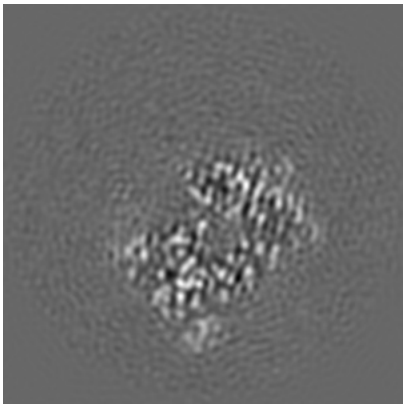
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

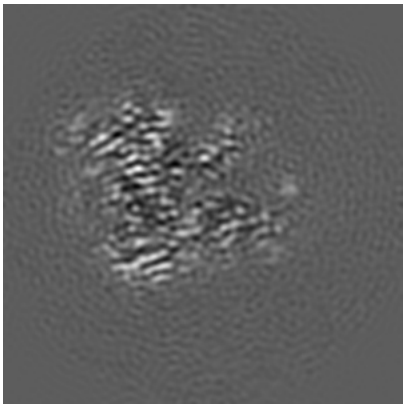
6.3.1 Primary map



X Index: 98



Y Index: 162



Z Index: 123

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 0.0123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

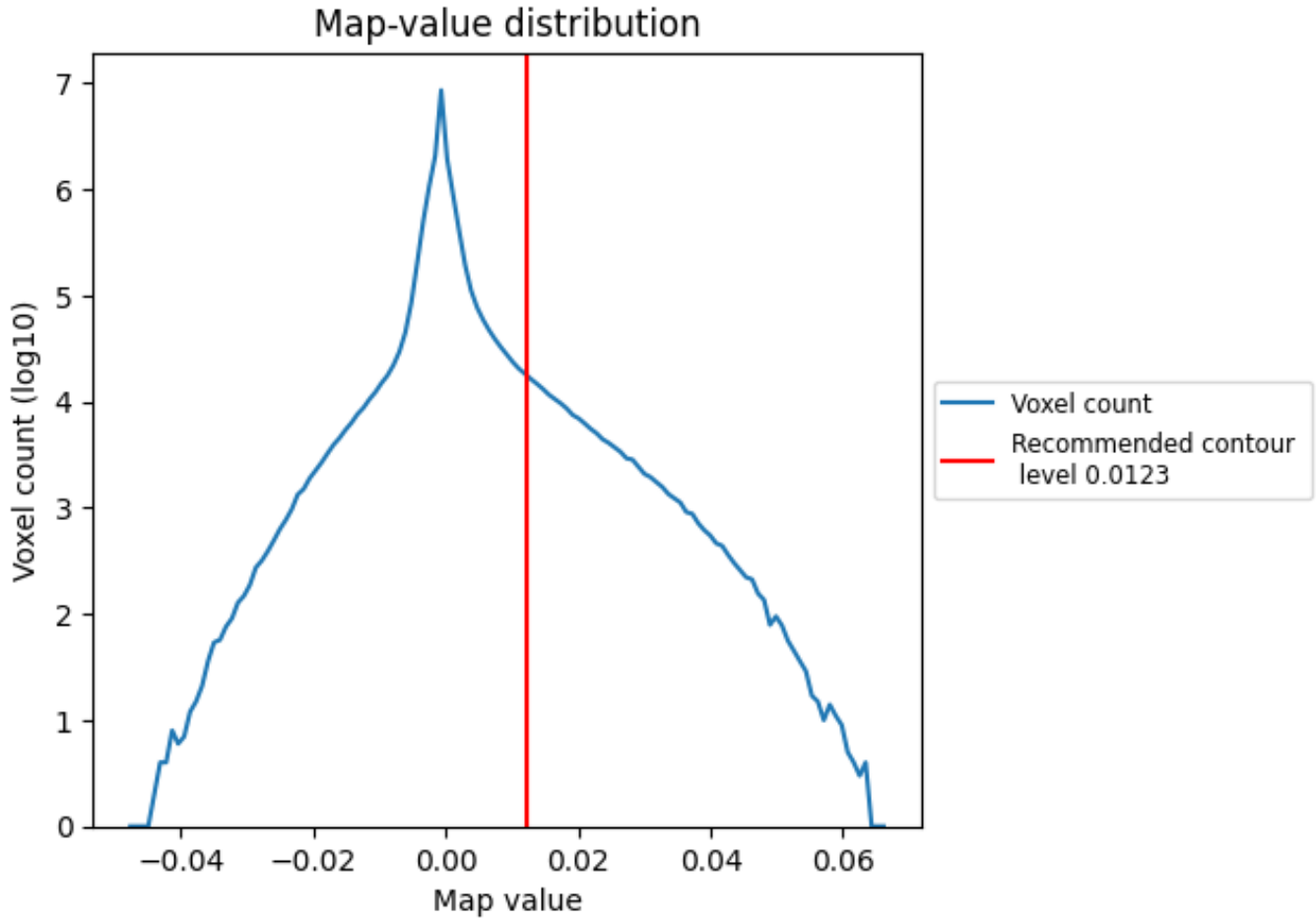
6.5 Mask visualisation (i)

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

7 Map analysis

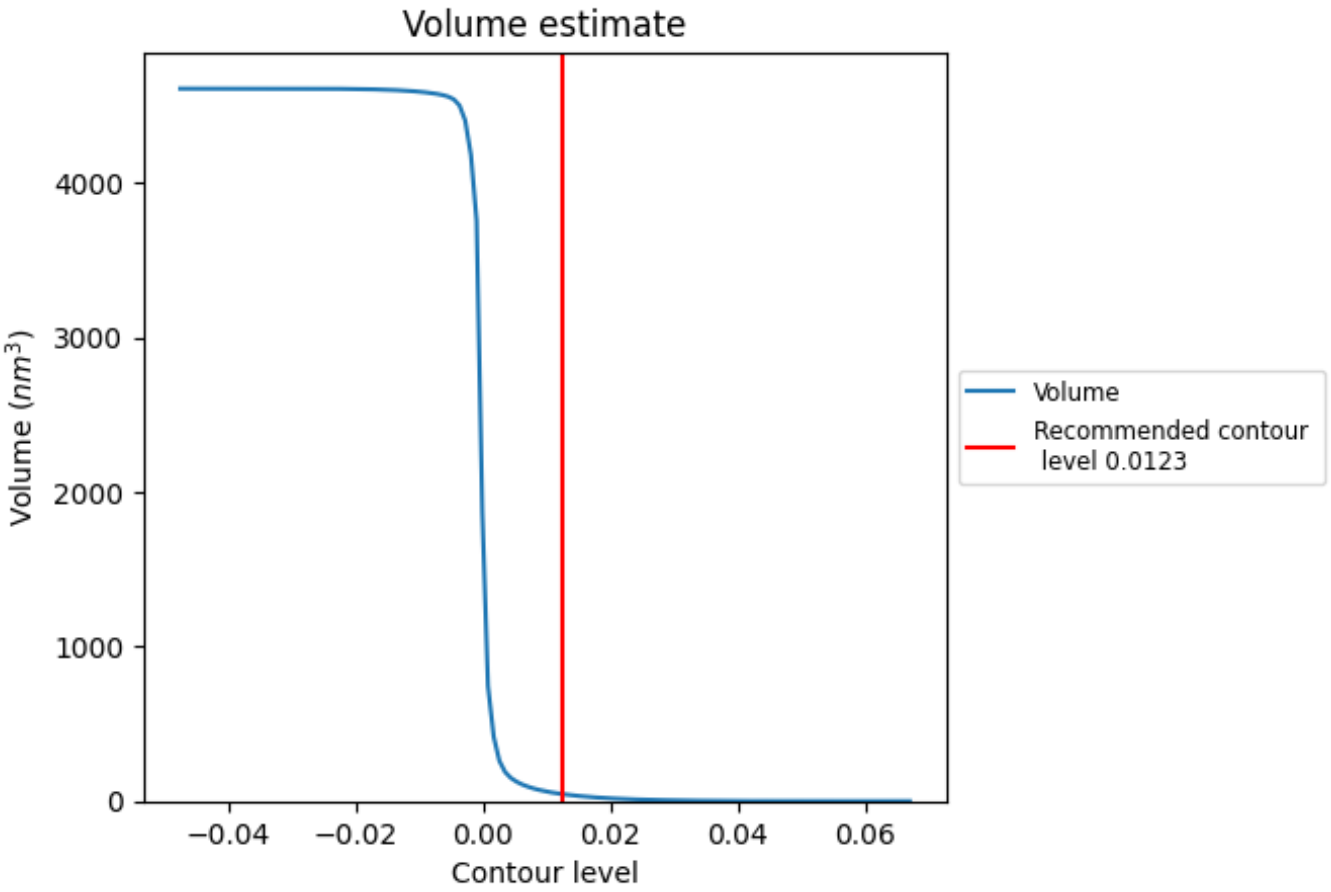
This section contains the results of statistical analysis of the map.

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.

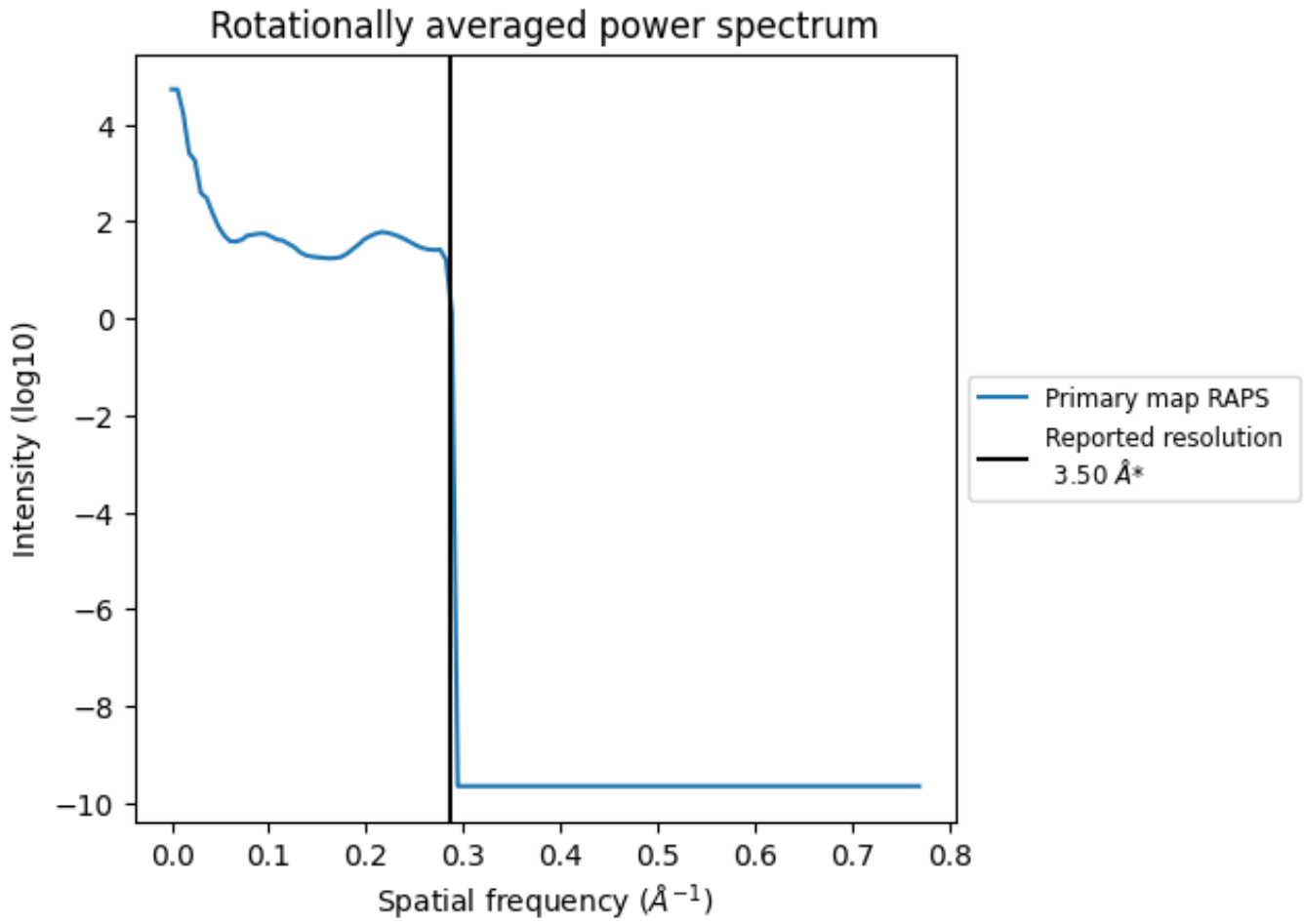
7.2 Volume estimate (i)



The volume at the recommended contour level is 46 nm^3; this corresponds to an approximate mass of 42 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 0.286 Å^{-1}

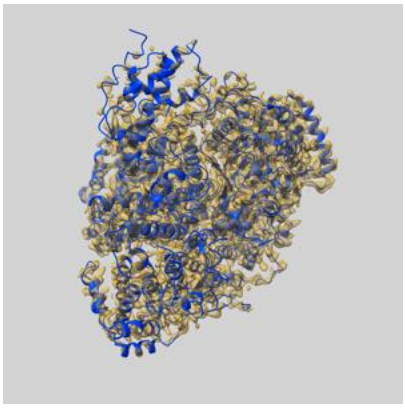
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

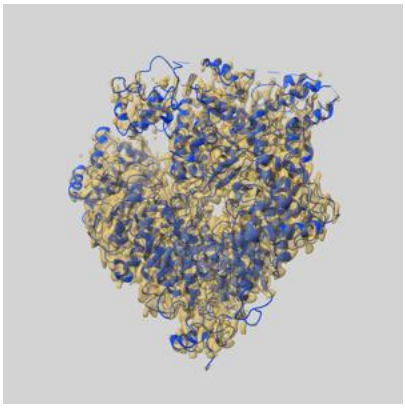
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31163 and PDB model 7EJU. Per-residue inclusion information can be found in section 3 on page 4.

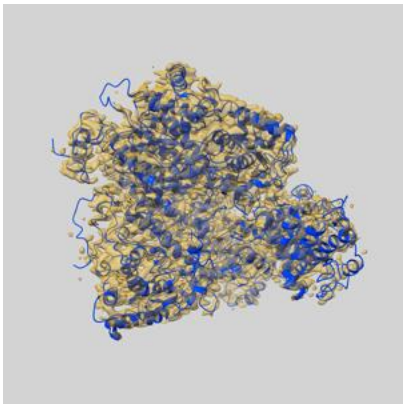
9.1 Map-model overlay



X



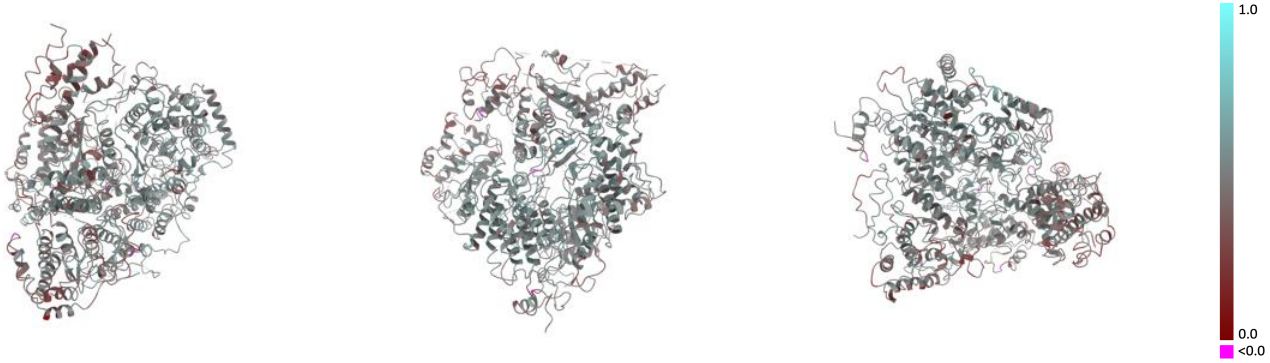
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0123 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.

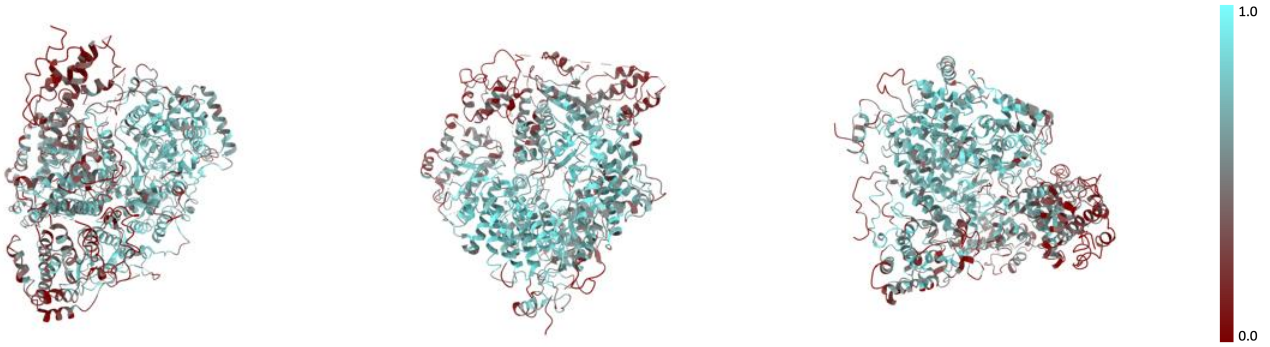
9.2 Q-score mapped to coordinate model (i)



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.

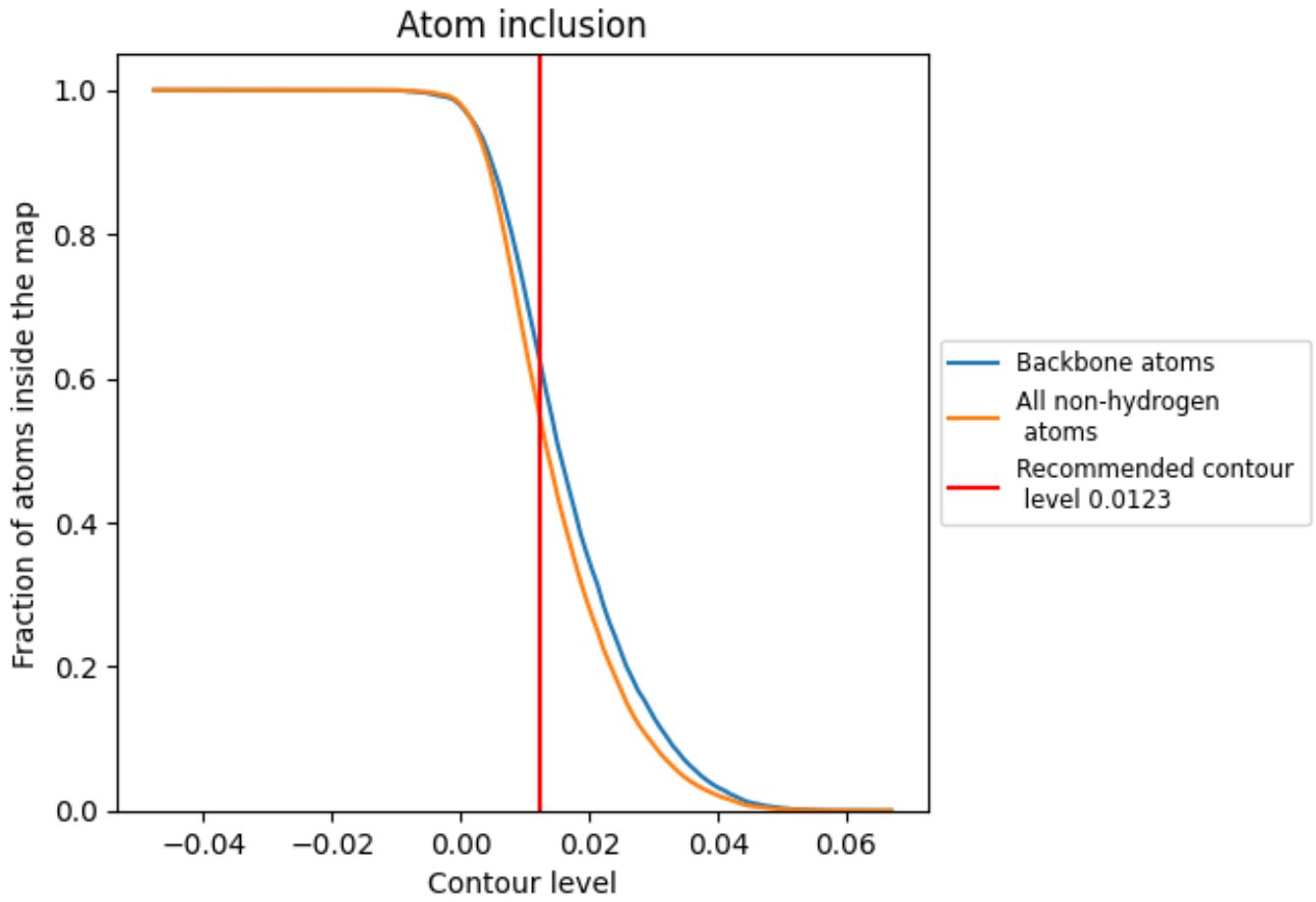
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0123).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 55% 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 (0.0123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5487	0.4730
A	0.5507	0.4740
B	0.4867	0.4520