wwPDB EM Validation Summary Report

Mar 13, 2024 – 12:42 PM JST

PDB ID	:	3J2C
EMDB ID	:	EMD-5504
Title	:	Dissecting the in vivo assembly of the 30S ribosomal subunit reveals the role of RimM
Authors	:	Guo, Q.; Goto, S.; Chen, Y.; Muto, A.; Himeno, H.; Deng, H.; Lei, J.; Gao, N.
Deposited on	:	2012-09-28
Resolution	:	13.20 Å(reported)
Based on initial model	:	3OFA

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:

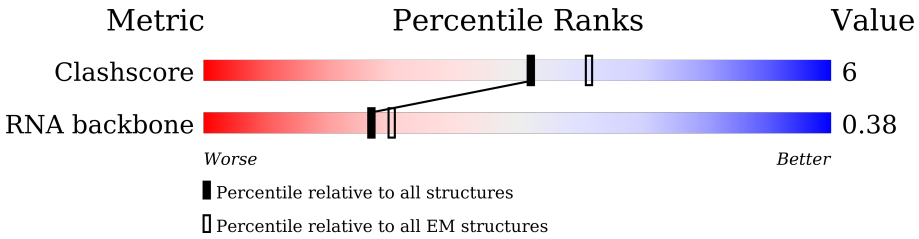
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 13.20 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
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	M	462	30% 29% 43% 29%
2	N	927	23% 44% 32%
3	O	144	43% 31% 48% 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 49444 atoms, of which 16558 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 16S rRNA head domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	M	462	14865	4410	4987	1793	3214	461	0	0

- Molecule 2 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	N	927	29941	8884	10017	3681	6433	926	0	0

- Molecule 3 is a RNA chain called 16S rRNA body domain.

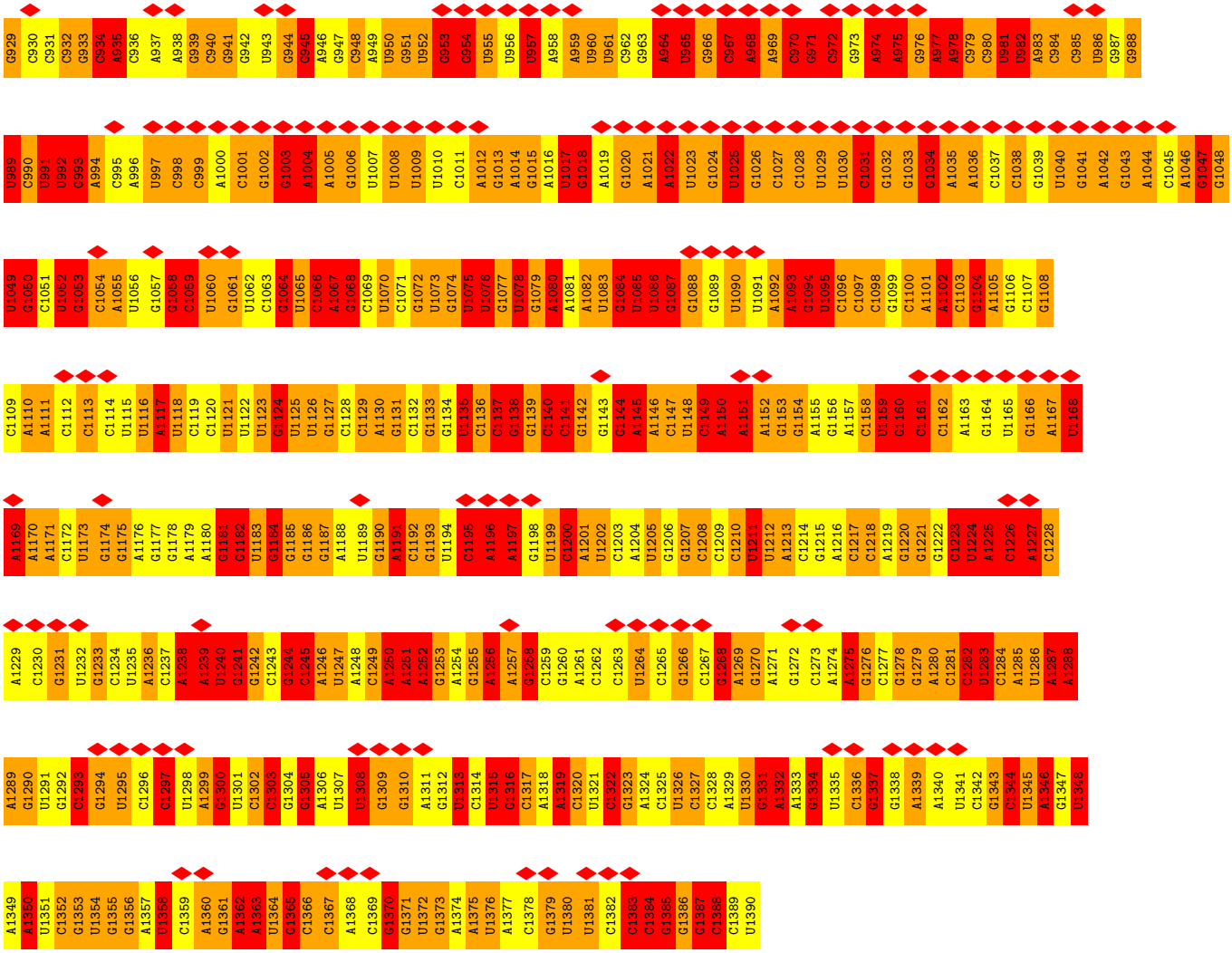
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
3	O	144	4638	1377	1554	562	1002	143	0	0

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.

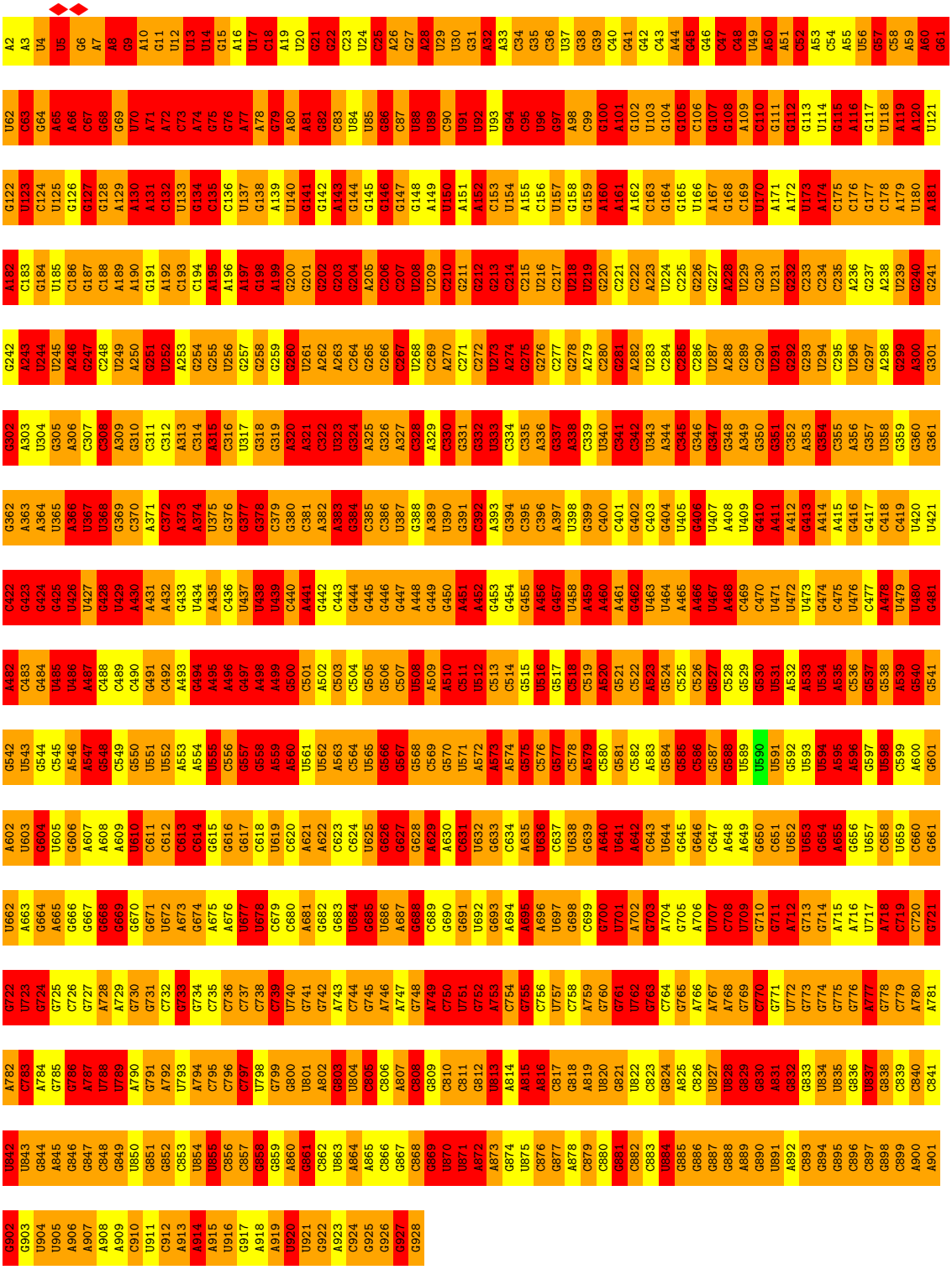
• Molecule 1: 16S rRNA head domain

Chain M:



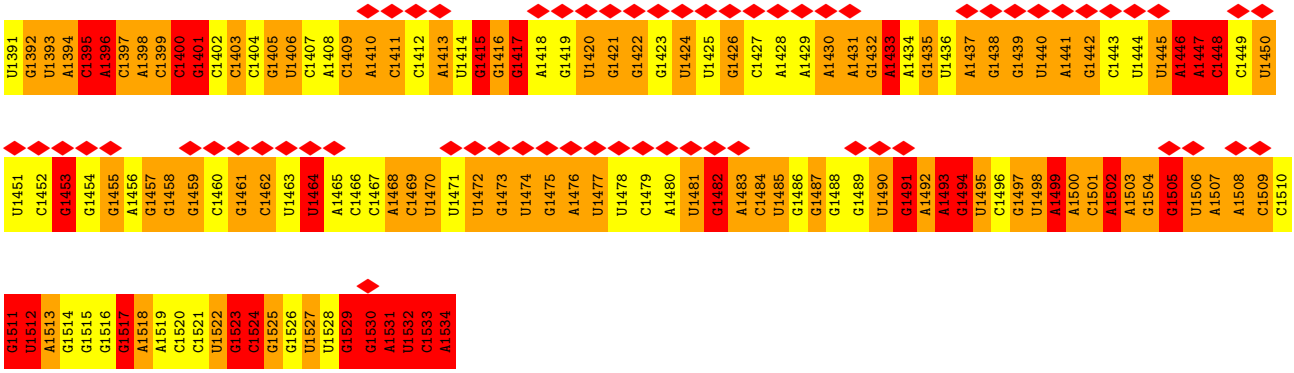
• Molecule 2: 16S rRNA body domain

Chain N:



• Molecule 3: 16S rRNA body domain

Chain O:


U1391 G1392 U1393 A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 A1408 C1409 A1410 C1411 C1412 A1413 U1414 G1415 G1416 G1417 A1418 G1419 U1420 G1421 G1422 G1423 U1424 U1425 G1426 C1427 A1428 A1429 A1430 A1431 G1432 A1433 A1434 G1435 U1436 A1437 G1438 G1439 U1440 A1441 G1442 C1443 U1444 U1445 A1446 A1447 C1448 C1449 U1450

U1451 C1452 G1453 G1454 G1455 A1456 G1457 G1458 G1459 C1460 G1461 C1462 U1463 U1464 A1465 C1466 C1467 A1468 C1469 U1470 U1471 U1472 G1473 U1474 G1475 A1476 U1477 U1478 C1479 A1480 U1481 G1482 A1483 C1484 U1485 G1486 G1487 G1488 G1489 U1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497 U1498 A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1507 A1508 C1509 C1510

G1511 U1512 A1513 G1514 G1515 G1516 G1517 A1518 A1519 C1520 C1521 U1522 G1523 C1524 G1525 G1526 U1527 U1528 G1529 G1530 A1531 U1532 C1533 A1534

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44392	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Weiner filter	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	80000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	4.325	Depositor
Minimum map value	-6.829	Depositor
Average map value	-4.406	Depositor
Map value standard deviation	0.508	Depositor
Recommended contour level	-3.2	Depositor
Map size (Å)	345.0, 345.0, 345.0	wwPDB
Map dimensions	125, 125, 125	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.76, 2.76, 2.76	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	M	3.43	1534/11053 (13.9%)	3.80	2624/17234 (15.2%)
2	N	3.44	3141/22318 (14.1%)	3.88	5510/34825 (15.8%)
3	O	3.32	455/3452 (13.2%)	3.95	849/5383 (15.8%)
All	All	3.43	5130/36823 (13.9%)	3.86	8983/57442 (15.6%)

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	M	0	236
2	N	0	522
3	O	0	78
All	All	0	836

The worst 5 of 5130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1502	A	N7-C5	-20.70	1.26	1.39
1	M	1251	A	N9-C4	18.33	1.48	1.37
2	N	124	C	N1-C6	-18.06	1.26	1.37
2	N	533	A	N7-C5	-17.64	1.28	1.39
2	N	350	G	C6-N1	17.60	1.51	1.39

The worst 5 of 8983 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	1253	G	N1-C6-O6	26.96	136.07	119.90
3	O	1455	G	N1-C6-O6	26.35	135.71	119.90
3	O	1458	G	N1-C6-O6	25.20	135.02	119.90
1	M	1362	A	P-O3'-C3'	24.79	149.44	119.70
3	O	1405	G	C5-C6-O6	-24.61	113.83	128.60

There are no chirality outliers.

5 of 836 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	929	G	Sidechain
1	M	933	G	Sidechain
1	M	934	C	Sidechain
1	M	935	A	Sidechain
1	M	939	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	M	9878	4987	4986	67	0
2	N	19924	10017	10006	206	0
3	O	3084	1554	1553	14	0
All	All	32886	16558	16545	281	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 6.

The worst 5 of 281 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:M:998:C:H42	1:M:1042:A:H61	1.38	0.71
2:N:50:A:H1'	2:N:52:C:C6	2.25	0.71
2:N:664:G:H22	2:N:741:G:H1	1.38	0.70
2:N:858:G:H1	2:N:869:G:H2'	1.55	0.70
2:N:411:A:H61	2:N:428:G:H1'	1.57	0.70

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	461/462 (99%)	152 (32%)	41 (8%)
2	N	926/927 (99%)	255 (27%)	84 (9%)
3	O	143/144 (99%)	31 (21%)	9 (6%)
All	All	1530/1533 (99%)	438 (28%)	134 (8%)

5 of 438 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	932	C
1	M	934	C
1	M	935	A
1	M	944	G
1	M	953	G

5 of 134 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	N	641	U
2	N	733	G
3	O	1513	A
2	N	65	A
2	N	60	A

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 (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.

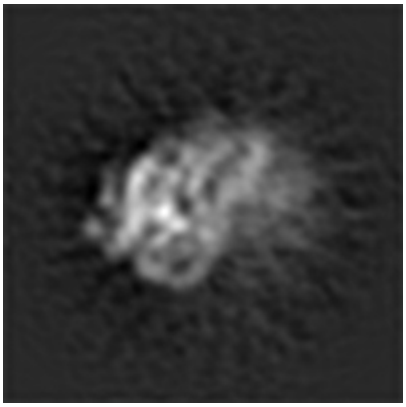
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5504. These allow visual inspection of the internal detail of the map and identification of artifacts.

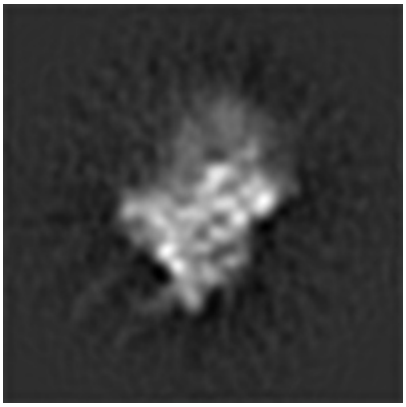
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

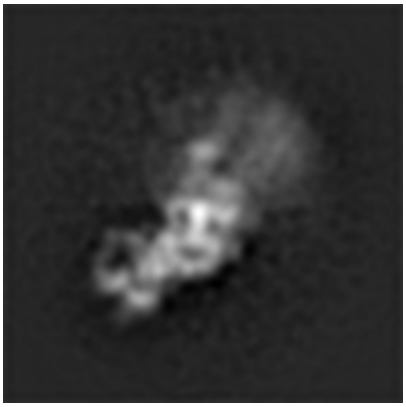
6.1.1 Primary map



X



Y

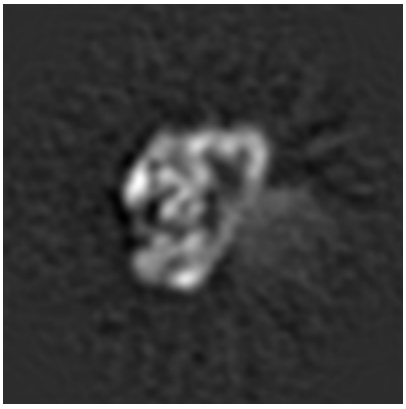


Z

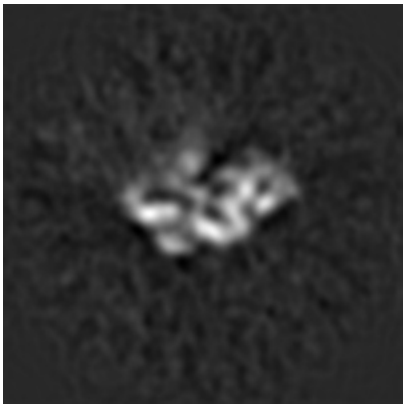
The images above show the map projected in three orthogonal directions.

6.2 Central slices

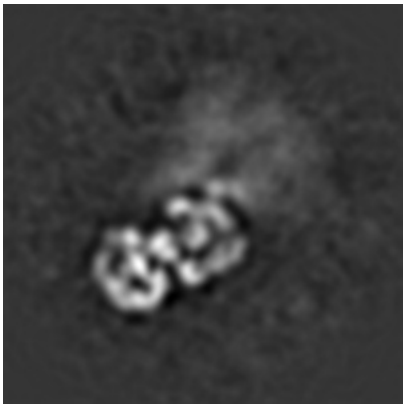
6.2.1 Primary map



X Index: 62



Y Index: 62

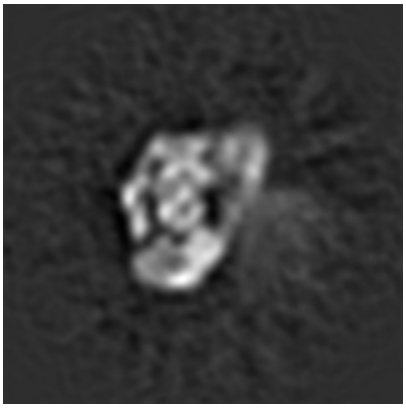


Z Index: 62

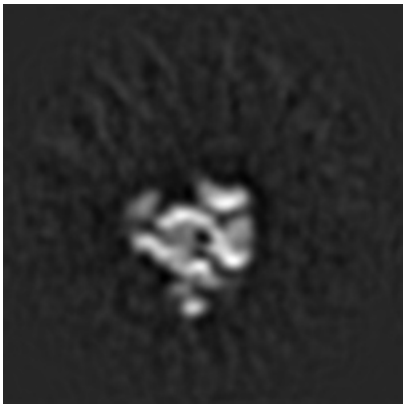
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

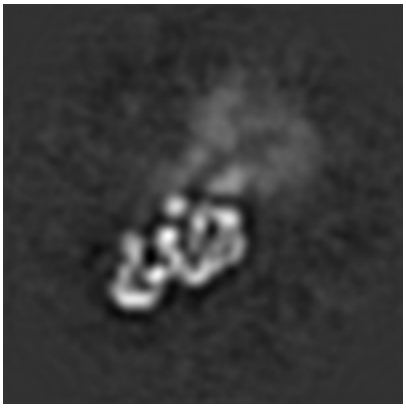
6.3.1 Primary map



X Index: 60



Y Index: 42

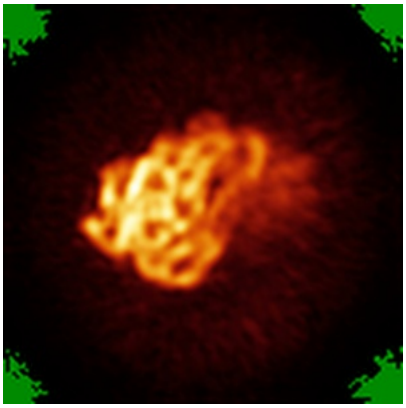


Z Index: 65

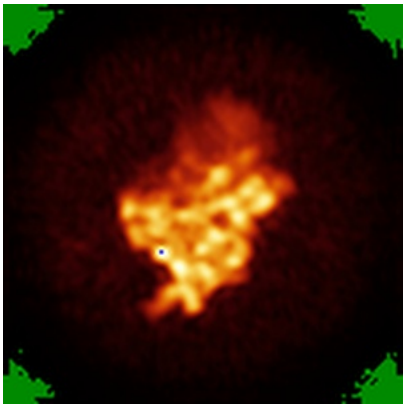
The images above show the largest variance slices of the map in three orthogonal directions.

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

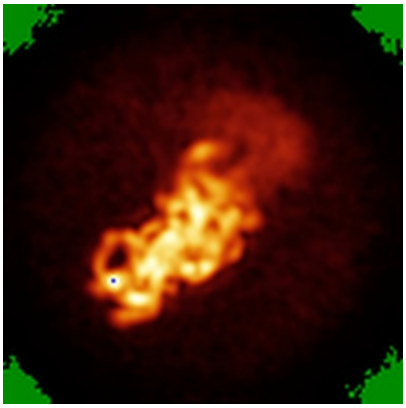
6.4.1 Primary map



X



Y

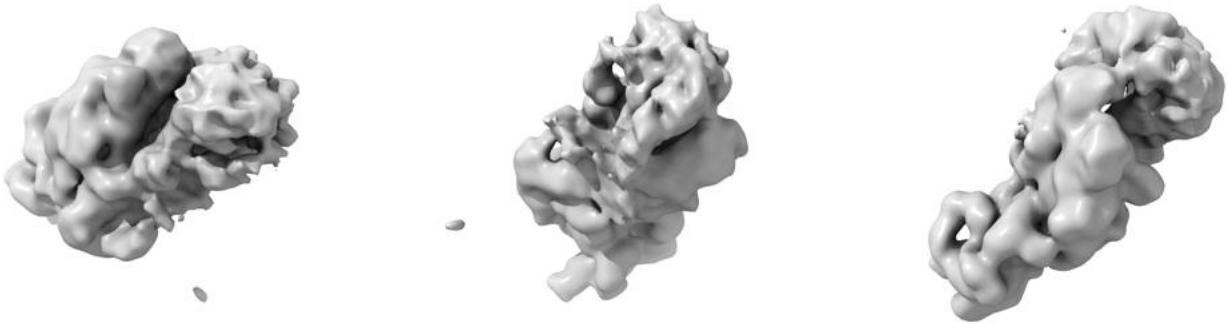


Z

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 -3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

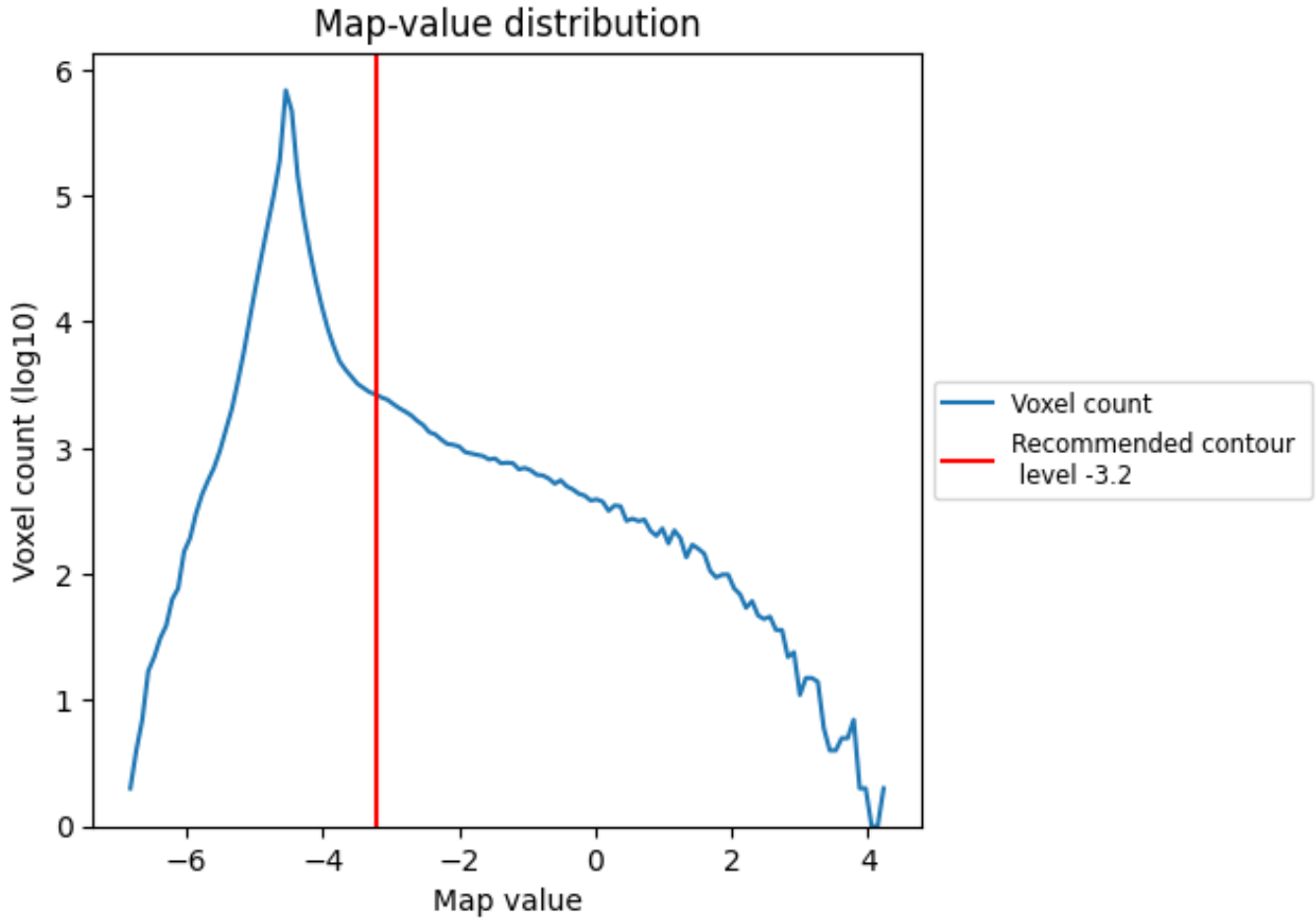
6.6 Mask visualisation (i)

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

7 Map analysis

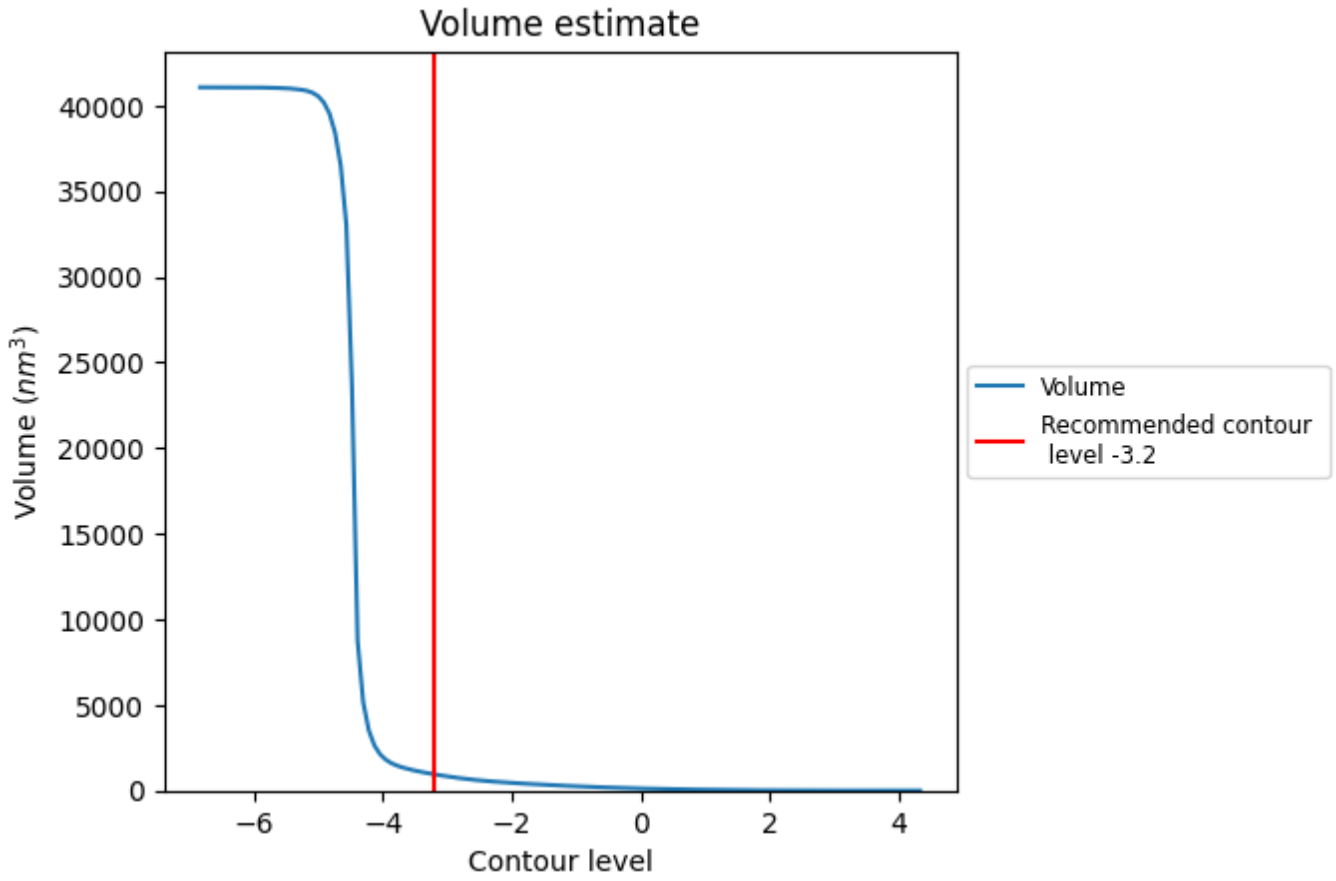
This section contains the results of statistical analysis of the map.

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.

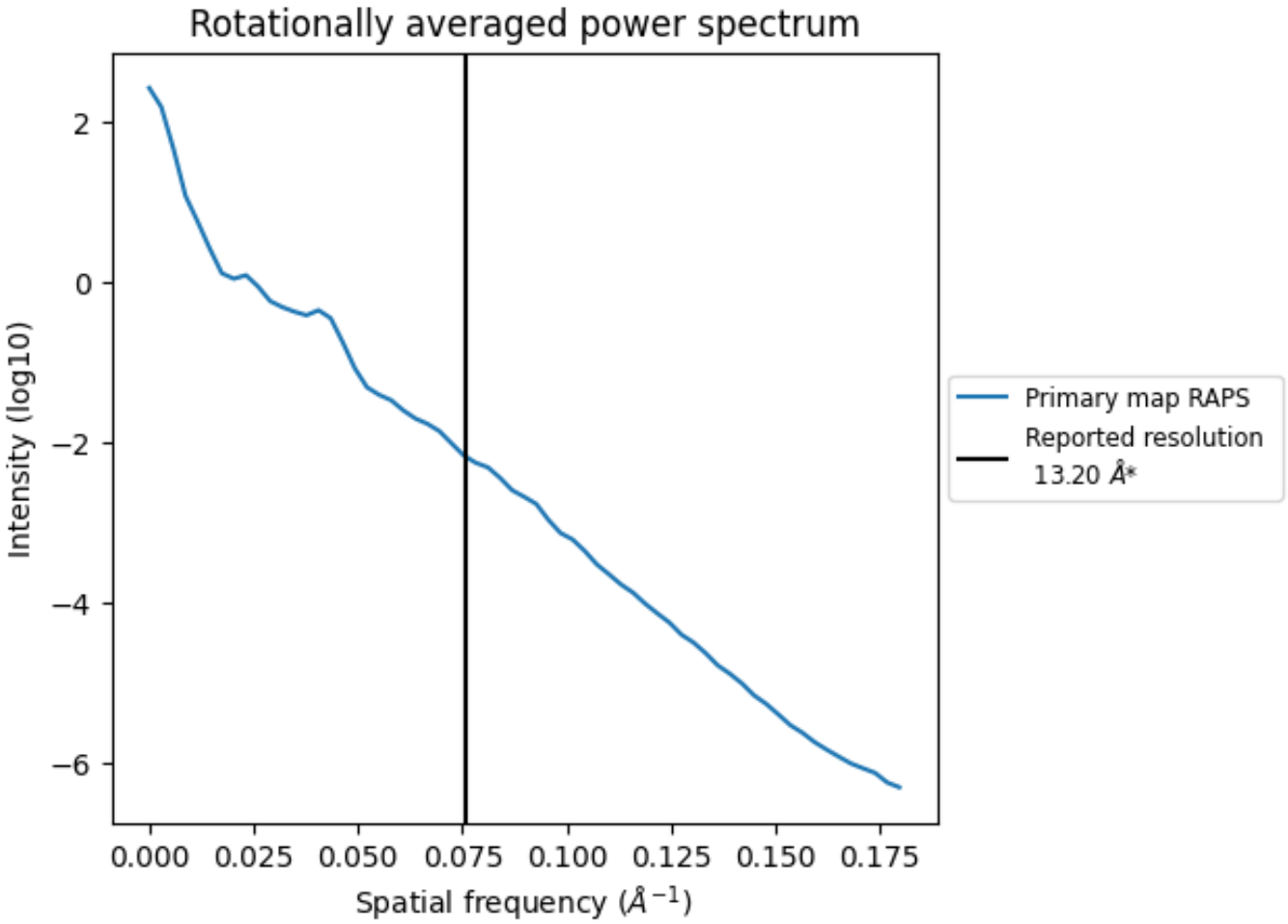
7.2 Volume estimate (i)



The volume at the recommended contour level is 949 nm^3; this corresponds to an approximate mass of 858 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 0.076 Å^{-1}

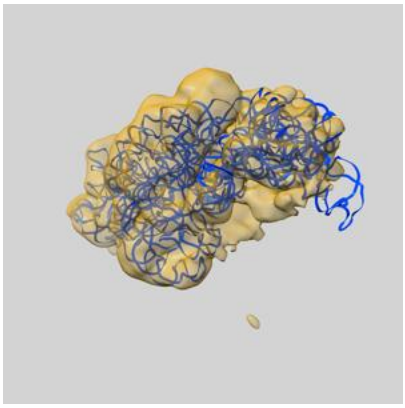
8 Fourier-Shell correlation (i)

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

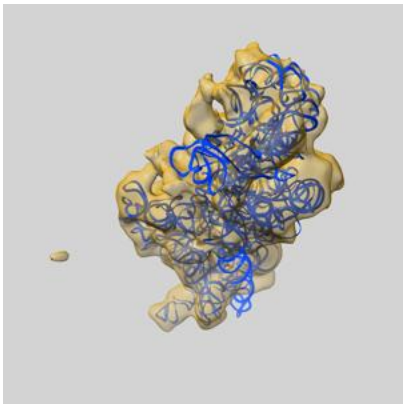
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-5504 and PDB model 3J2C. Per-residue inclusion information can be found in section 3 on page 4.

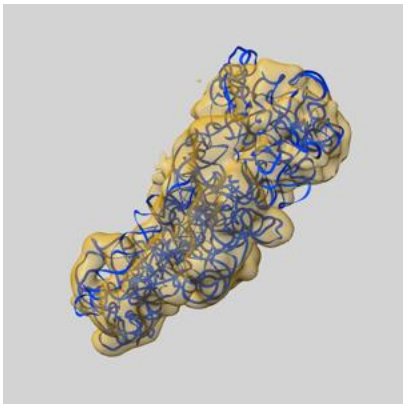
9.1 Map-model overlay



X



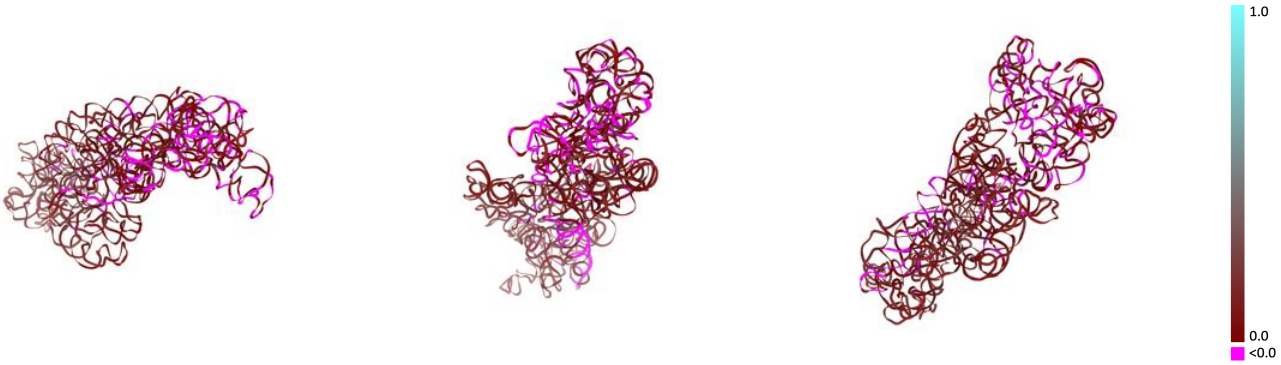
Y



Z

The images above show the 3D surface view of the map at the recommended contour level -3.2 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.

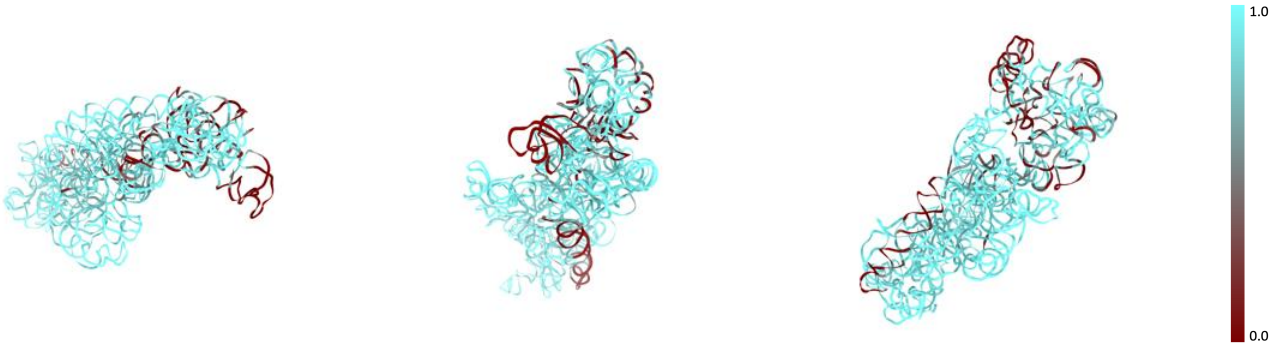
9.2 Q-score mapped to coordinate model



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.

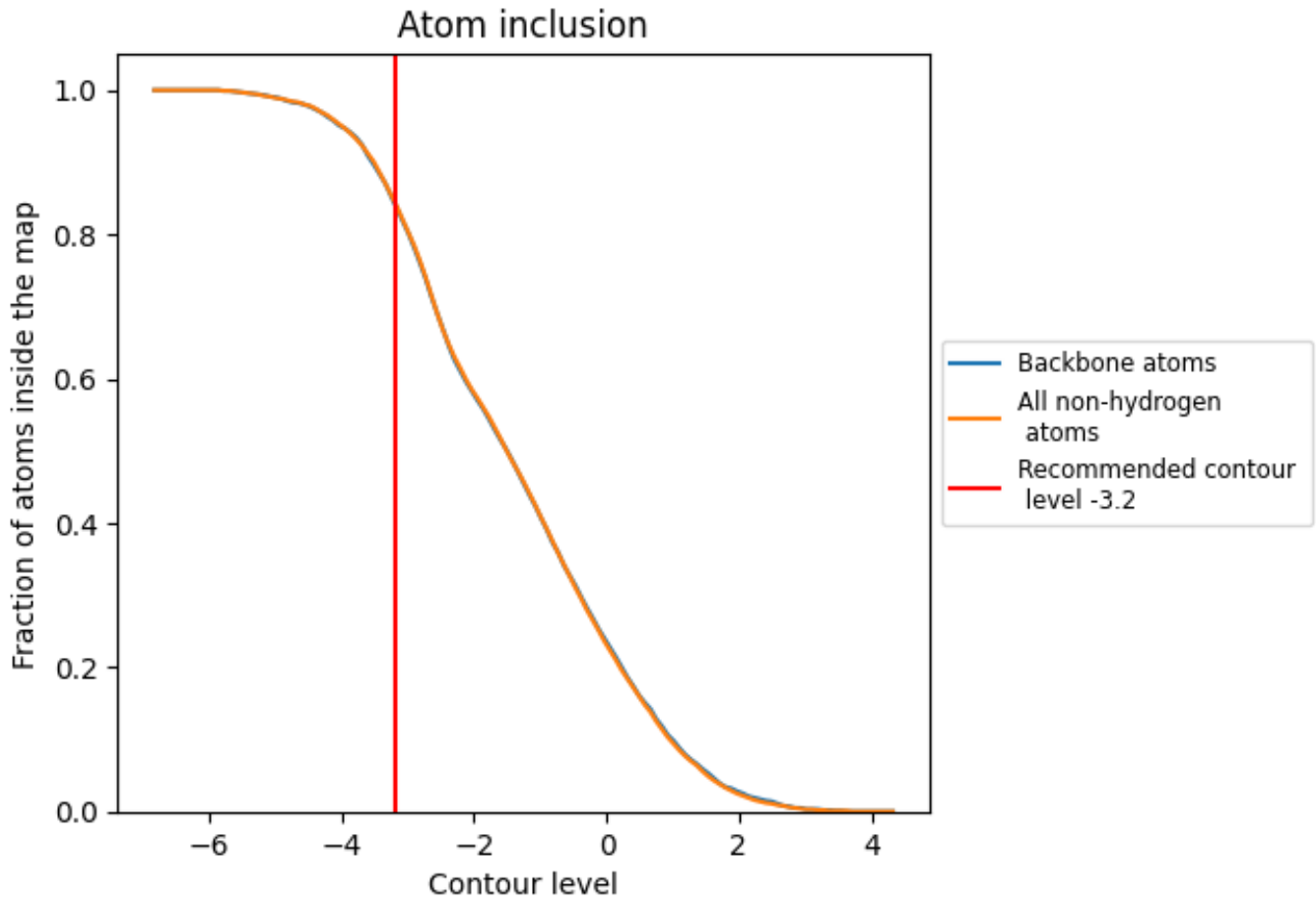
9.3 Atom inclusion mapped to coordinate model



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 (-3.2).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (-3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.0760
M	0.6650	0.0380
N	0.9860	0.1040
O	0.5350	0.0120