



wwPDB EM Validation Summary Report ⓘ

May 23, 2024 – 11:36 AM EDT

PDB ID : 7U0F
EMDB ID : EMD-26257
Title : HIV-1 Rev in complex with tubulin
Authors : Eren, E.
Deposited on : 2022-02-18
Resolution : 3.53 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92
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) : 2.36.2

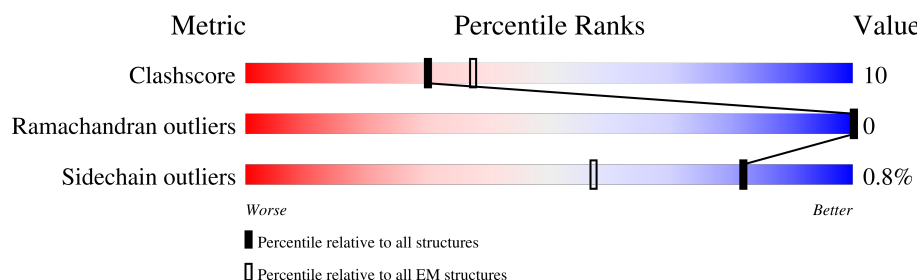
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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 $\leq 5\%$. 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	451	
1	C	451	
2	B	445	
2	D	445	
3	E	116	
3	F	116	
3	G	116	
3	H	116	

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Mol	Chain	Length	Quality of chain
3	I	116	 29% 18% 53%
3	J	116	 34% 10% 56%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16569 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 Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3419	2161	581	656	21		
1	C	450	Total	C	N	O	S	0	0
			3500	2208	589	682	21		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	428	Total	C	N	O	S	0	0
			3349	2100	575	648	26		
2	D	444	Total	C	N	O	S	0	0
			3482	2178	592	686	26		

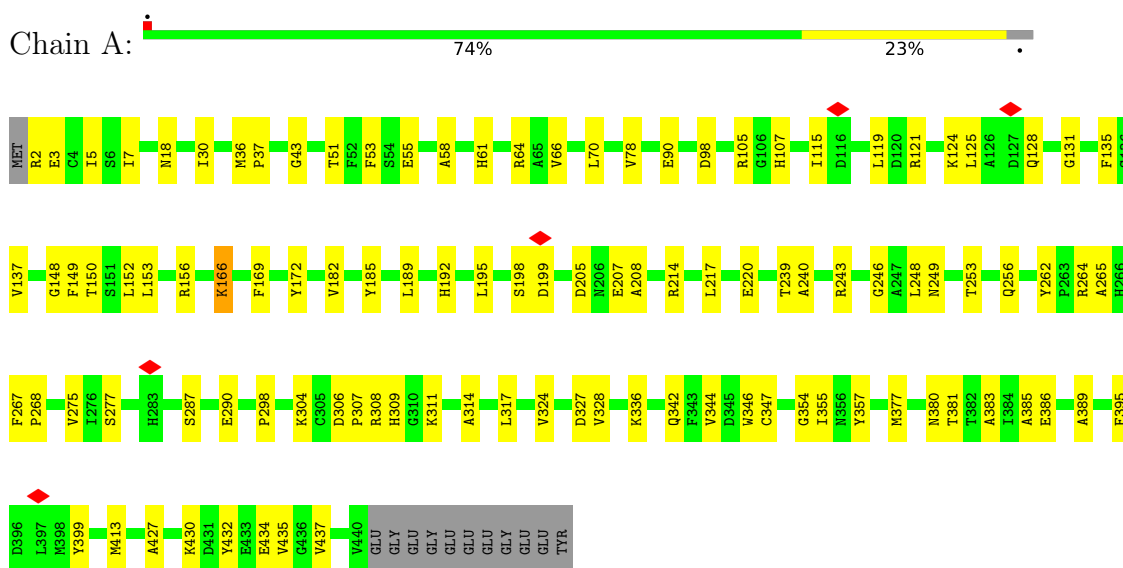
- Molecule 3 is a protein called Protein Rev.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	55	Total	C	N	O	0	0
			472	291	103	78		
3	F	55	Total	C	N	O	0	0
			475	294	103	78		
3	G	55	Total	C	N	O	0	0
			475	294	103	78		
3	H	55	Total	C	N	O	0	0
			475	294	103	78		
3	I	55	Total	C	N	O	0	0
			475	294	103	78		
3	J	51	Total	C	N	O	0	0
			447	276	99	72		

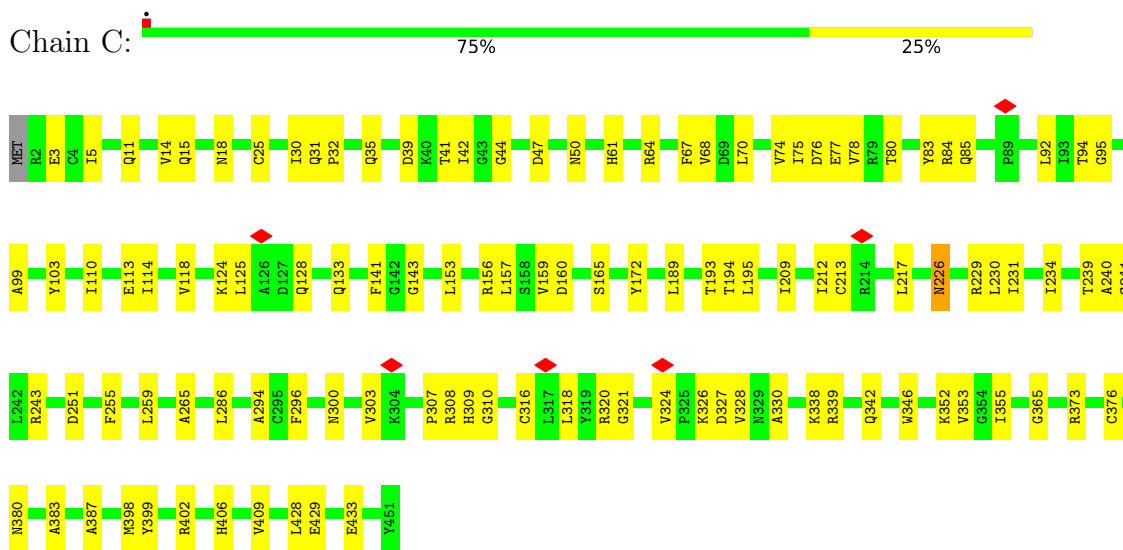
3 Residue-property plots

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.

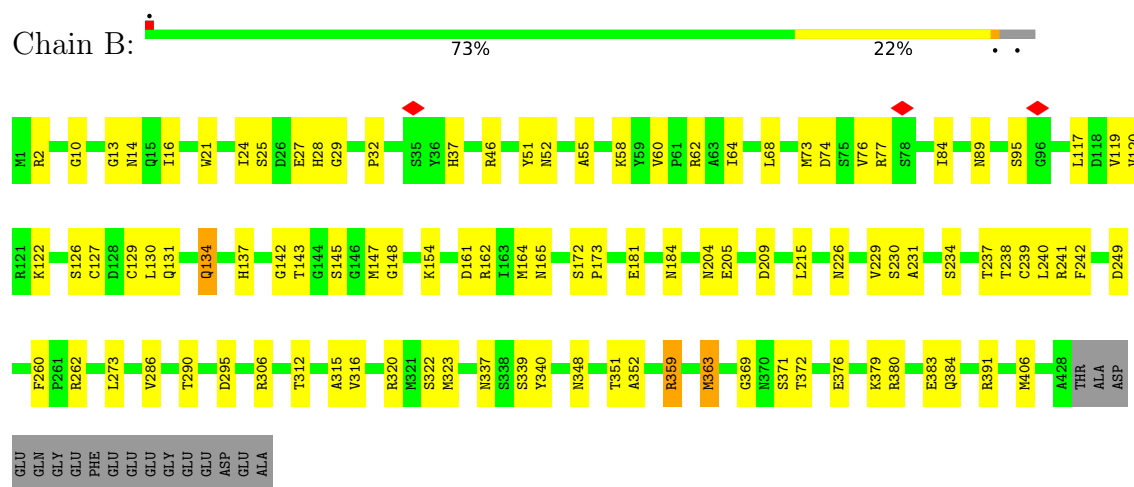
- Molecule 1: Tubulin alpha-1A chain



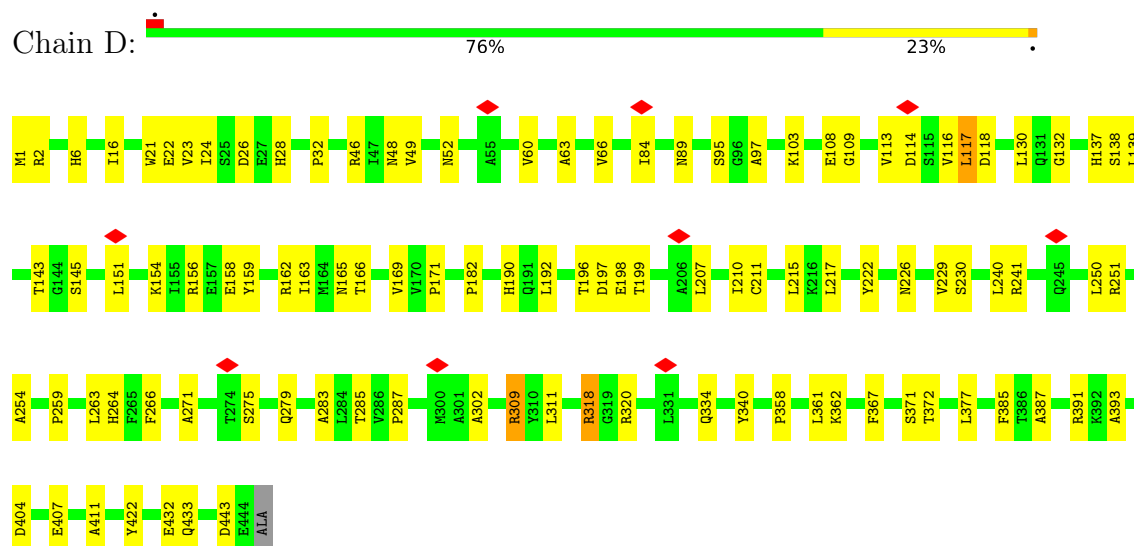
- Molecule 1: Tubulin alpha-1A chain



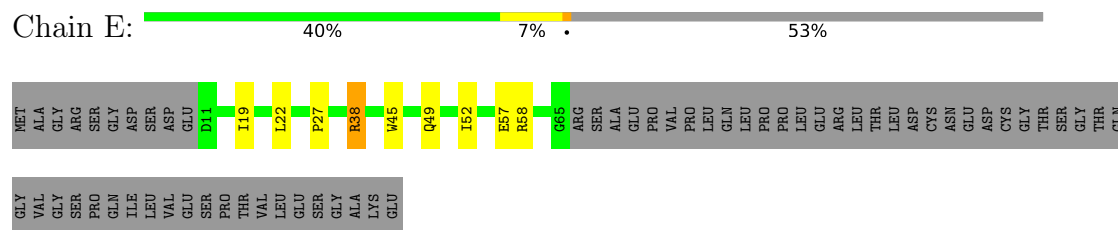
- Molecule 2: Tubulin beta chain



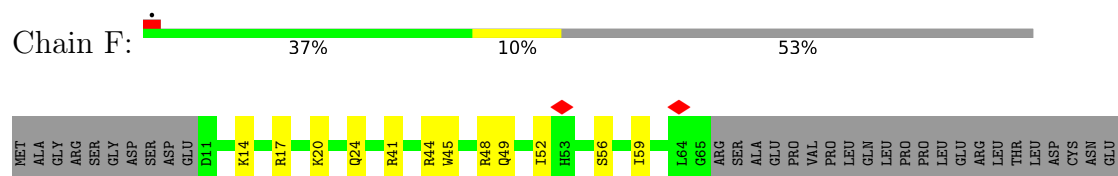
• Molecule 2: Tubulin beta chain



• Molecule 3: Protein Rev




• Molecule 3: Protein Rev



CYS
GLY
THR
SER
GLY
THR
THR
GLN
GLY
VAL
GLY
SER
SER
PRO
GLN
ILE
LEU
VAL
GLU
SER
SER
PRO
THR
VAL
LEU
GLU
SER
GLY
ALA
LYS
GLU

● Molecule 3: Protein Rev

Chain G:  34% 13% 53%

MET
ALA
GLY
ASP
ARG
SER
GLY
THR
ASP
SER
SER
GLY
D11
K14
A15
Y16
R17
L18
R17
K20
F21
L22
Y23
N30
M40
R41
R42
R43
R44
R45
R46
E47
R48
Q49
R50
H53
G65
ARG
SER
SER
ALA
GLU
PRO
VAL
PRO
LEU
GLN
LEU
PRO
PRO
LEU
GLU
ARG
LEU
THR
LEU
ASP
CYS

ASN
GLU
ASP
CYS
GLY
THR
SER
GLY
THR
GLN
VAL
GLY
SER
PRO
GLN
ILE
LEU
VAL
GLU
SER
THR
VAL
LEU
GLU
SER
GLY
ALA
LYS
GLU


● Molecule 3: Protein Rev

Chain H:  28% 19% 53%

MET
ALA
GLY
ARG
SER
GLY
ASP
SER
SER
ASP
GLY
D11
L12
L13
K14
A15
V16
R17
L18
I19
K20
F21
L22
P31
R38
R41
R42
R43
R44
R45
R46
E47
R48
Q51
I52
I55
S56
S57
R58
I59
G65
ARG
SER
SER
ALA
GLU
VAL
PRO
PRO
LEU
GLN
LEU
PRO
PRO
LEU
LEU
GLU

ARG
LEU
THR
LEU
ASP
CYS
ASN
GLU
ASP
ASP
CYS
GLY
THR
SER
GLY
THR
GLN
VAL
GLY
SER
PRO
GLN
ILE
LEU
VAL
GLU
SER
PRO
THR
VAL
VAL
GLU
SER
GLY
ALA
LYS
GLU


● Molecule 3: Protein Rev

Chain I:  29% 18% 53%

MET
ALA
GLY
SER
SER
GLY
ASP
SER
ASP
GLY
D11
L12
L13
K14
A15
V16
R17
L18
I19
L22
N26
P29
T34
R35
R38
R41
R45
Q48
Q49
R50
Q51
I52
H53
L60
S61
T62
Y63
L64
G65
ARG
SER
SER
ALA
GLU
PRO
VAL
PRO
LEU
GLN
LEU
PRO
PRO
LEU
LEU
GLU

LEU
GLU
ARG
LEU
THR
SER
CYS
ASN
GLU
ASP
ASP
CYS
GLY
THR
SER
GLY
THR
GLN
GLY
VAL
GLY
SER
PRO
GLN
ILE
LEU
VAL
GLU
SER
PRO
SER
PRO
THR
VAL
GLY
SER
GLY
ALA
LYS
GLU

● Molecule 3: Protein Rev

Chain J:  34% 10% 56%

MET
ALA
GLY
ARG
SER
GLY
ASP
SER
SER
GLN
GLY
VAL
GLY
LEU
L13
K20
F21
L22
P29
E32
R35
R38
R41
R42
R48
I52
R58
T62
Y63
LEU
GLY
ARG
SER
SER
ALA
GLU
PRO
VAL
PRO
LEU
GLN
LEU
PRO
PRO
PRO
GLU
ARG
THR
THR
LEU
ASP
CYS
ASN

GLU
ASP
CYS
GLY
THR
SER
GLY
THR
GLN
GLY
VAL
GLY
SER
PRO
GLN
ILE
LEU
VAL
VAL
GLU
SER
PRO
THR
VAL
VAL
GLU
SER
GLY
ALA
LYS
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C15	Depositor
Number of particles used	34534	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 ($e^-/\text{\AA}^2$)	73	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	45.739	Depositor
Minimum map value	-28.933	Depositor
Average map value	0.101	Depositor
Map value standard deviation	1.211	Depositor
Recommended contour level	2.7	Depositor
Map size (Å)	556.5, 556.5, 556.5	wwPDB
Map dimensions	525, 525, 525	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.27	0/3497	0.57	0/4750
1	C	0.26	0/3579	0.56	0/4860
2	B	0.27	0/3422	0.59	0/4636
2	D	0.27	0/3558	0.57	0/4821
3	E	0.24	0/481	0.66	0/645
3	F	0.29	0/484	0.82	0/649
3	G	0.28	0/484	0.70	0/649
3	H	0.28	0/484	0.78	0/649
3	I	0.28	0/484	0.71	0/649
3	J	0.28	0/456	0.74	0/611
All	All	0.27	0/16929	0.60	0/22919

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3419	0	3312	70	0
1	C	3500	0	3361	71	0
2	B	3349	0	3220	63	0
2	D	3482	0	3308	63	0
3	E	472	0	485	7	0
3	F	475	0	494	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	475	0	494	18	0
3	H	475	0	494	26	0
3	I	475	0	494	14	0
3	J	447	0	465	8	0
All	All	16569	0	16127	327	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 10.

The worst 5 of 327 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)
3:G:17:ARG:HB3	3:H:18:LEU:HD21	1.43	0.98
3:G:21:PHE:CE2	3:H:18:LEU:HD22	2.23	0.74
2:B:172:SER:HB2	2:B:204:ASN:HB3	1.71	0.73
2:D:114:ASP:HA	2:D:117:LEU:HD23	1.73	0.71
3:G:21:PHE:HE2	3:H:18:LEU:HD22	1.56	0.70

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	437/451 (97%)	391 (90%)	46 (10%)	0	100	100
1	C	448/451 (99%)	405 (90%)	43 (10%)	0	100	100
2	B	426/445 (96%)	380 (89%)	46 (11%)	0	100	100
2	D	442/445 (99%)	398 (90%)	44 (10%)	0	100	100
3	E	53/116 (46%)	51 (96%)	2 (4%)	0	100	100
3	F	53/116 (46%)	47 (89%)	6 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	53/116 (46%)	49 (92%)	4 (8%)	0	100	100
3	H	53/116 (46%)	50 (94%)	3 (6%)	0	100	100
3	I	53/116 (46%)	49 (92%)	4 (8%)	0	100	100
3	J	49/116 (42%)	47 (96%)	2 (4%)	0	100	100
All	All	2067/2488 (83%)	1867 (90%)	200 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	367/377 (97%)	366 (100%)	1 (0%)	92	98
1	C	374/377 (99%)	373 (100%)	1 (0%)	92	98
2	B	365/381 (96%)	361 (99%)	4 (1%)	73	88
2	D	378/381 (99%)	373 (99%)	5 (1%)	69	87
3	E	50/102 (49%)	49 (98%)	1 (2%)	55	79
3	F	51/102 (50%)	51 (100%)	0	100	100
3	G	51/102 (50%)	51 (100%)	0	100	100
3	H	51/102 (50%)	49 (96%)	2 (4%)	32	65
3	I	51/102 (50%)	51 (100%)	0	100	100
3	J	48/102 (47%)	47 (98%)	1 (2%)	53	79
All	All	1786/2128 (84%)	1771 (99%)	15 (1%)	82	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	117	LEU
3	H	51	GLN
2	D	309	ARG
3	J	35	ARG

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Mol	Chain	Res	Type
3	E	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	11	GLN
1	C	18	ASN
3	G	49	GLN
3	H	51	GLN
3	I	51	GLN

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 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.

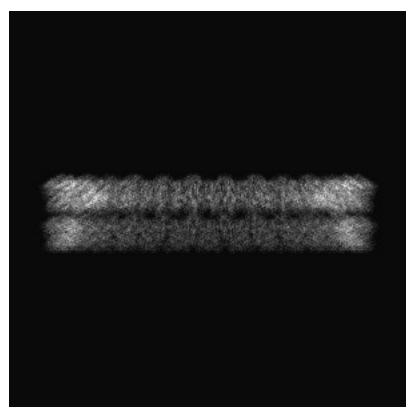
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26257. These allow visual inspection of the internal detail of the map and identification of artifacts.

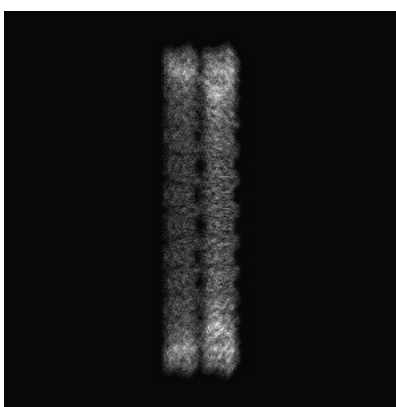
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

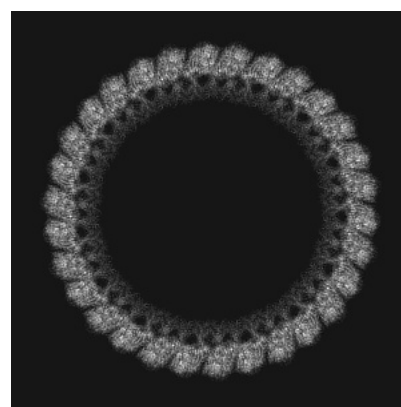
6.1.1 Primary map



X



Y

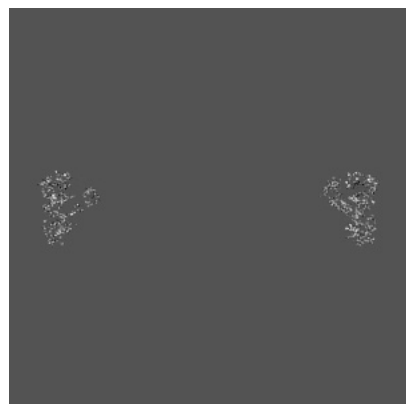


Z

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

6.2 Central slices [i](#)

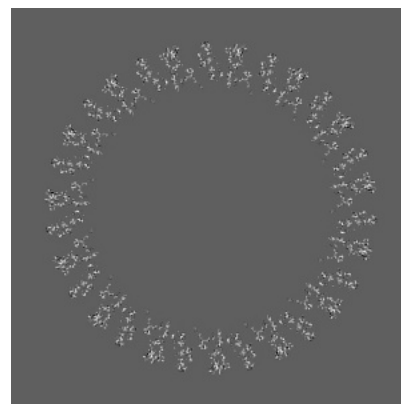
6.2.1 Primary map



X Index: 262



Y Index: 262



Z Index: 262

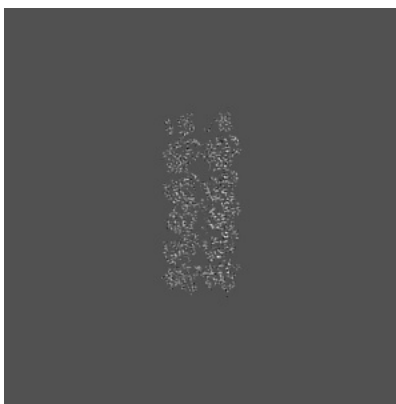
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

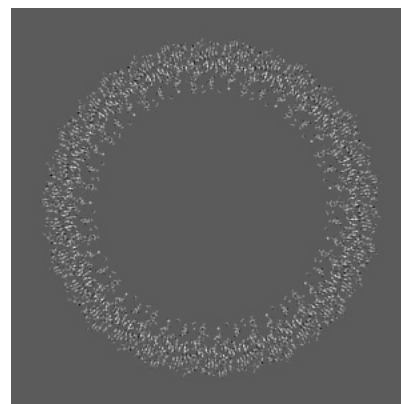
6.3.1 Primary map



X Index: 81



Y Index: 446

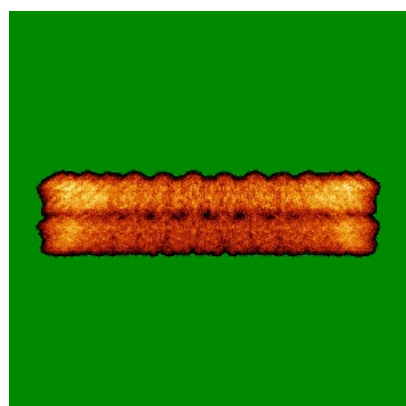


Z Index: 291

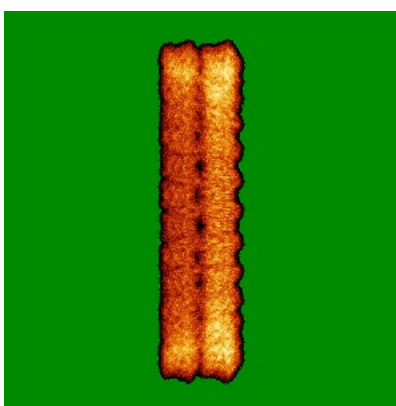
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

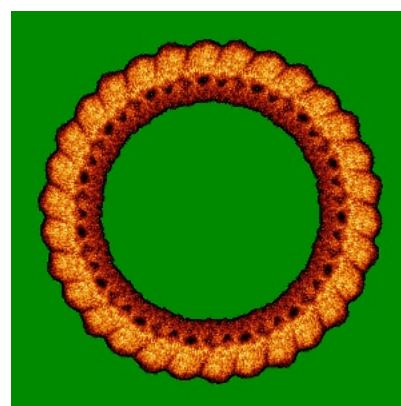
6.4.1 Primary map



X



Y

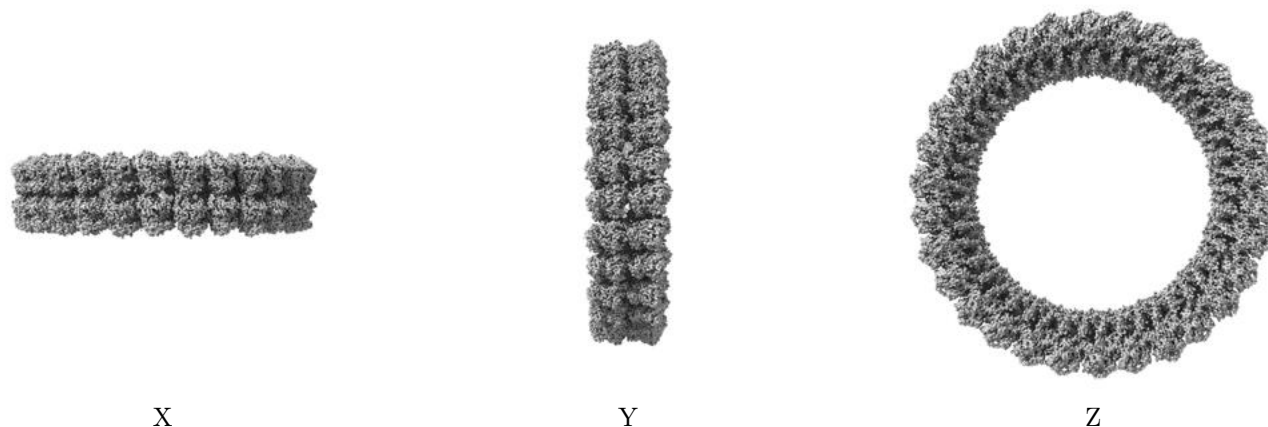


Z

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



The images above show the 3D surface view of the map at the recommended contour level 2.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

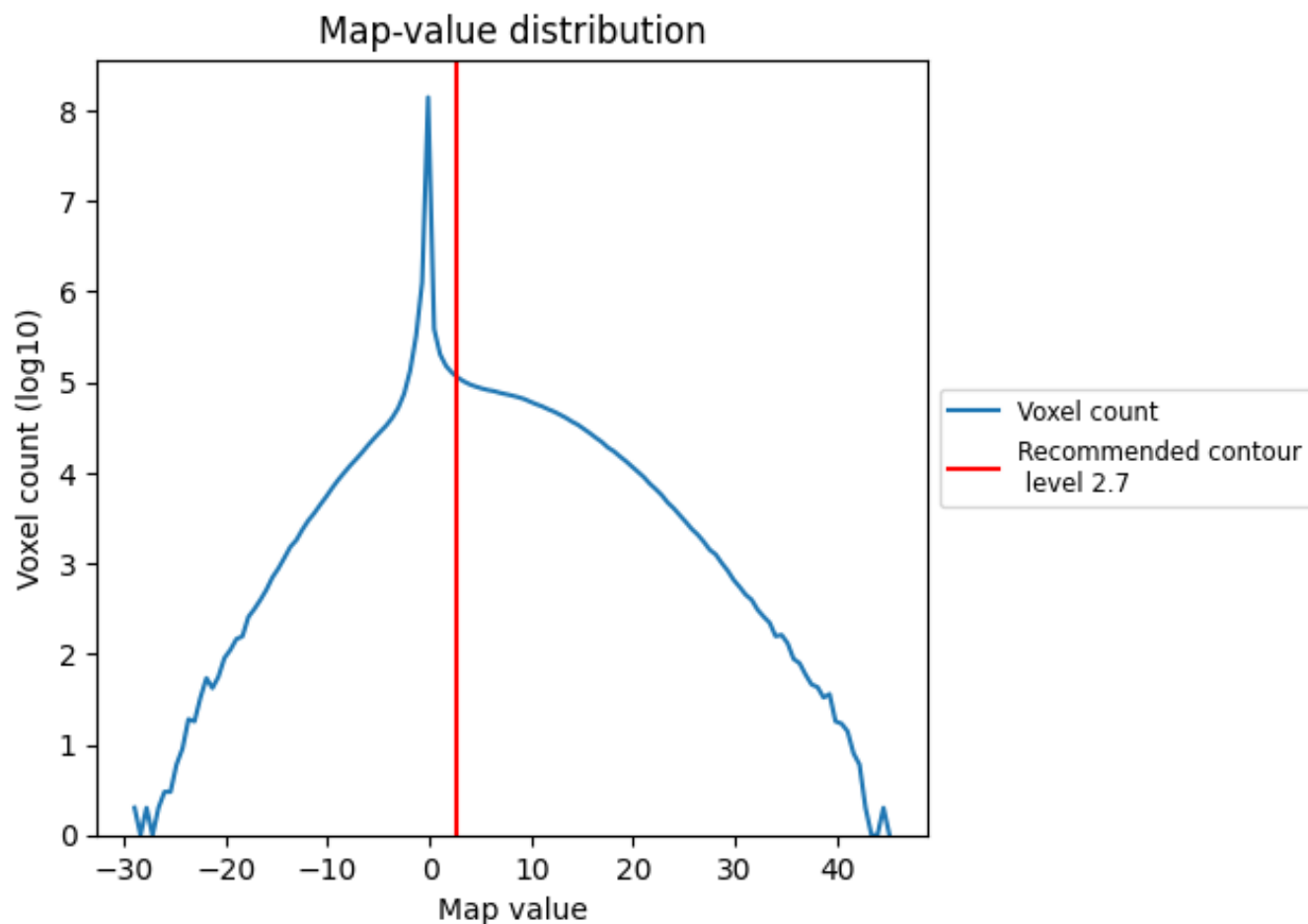
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

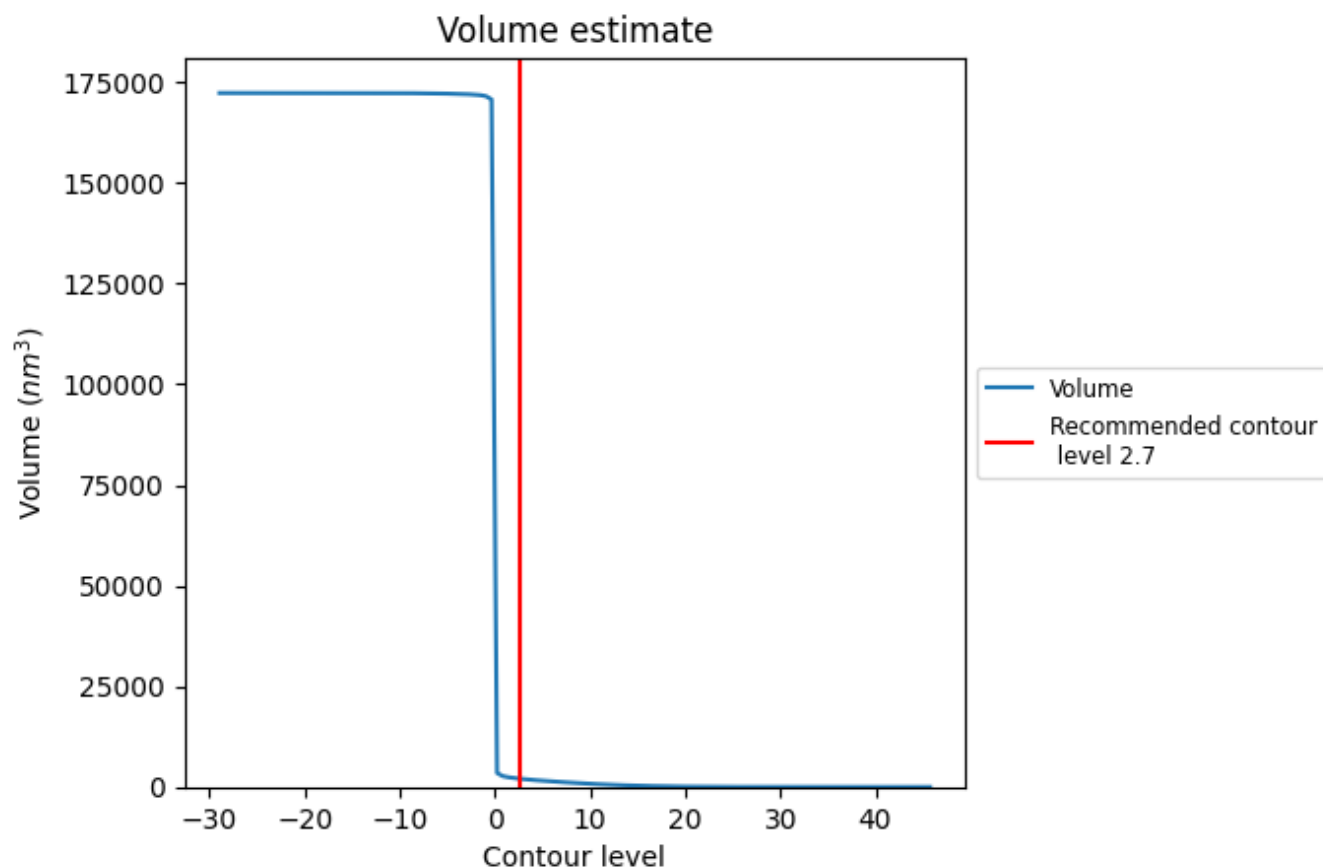
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

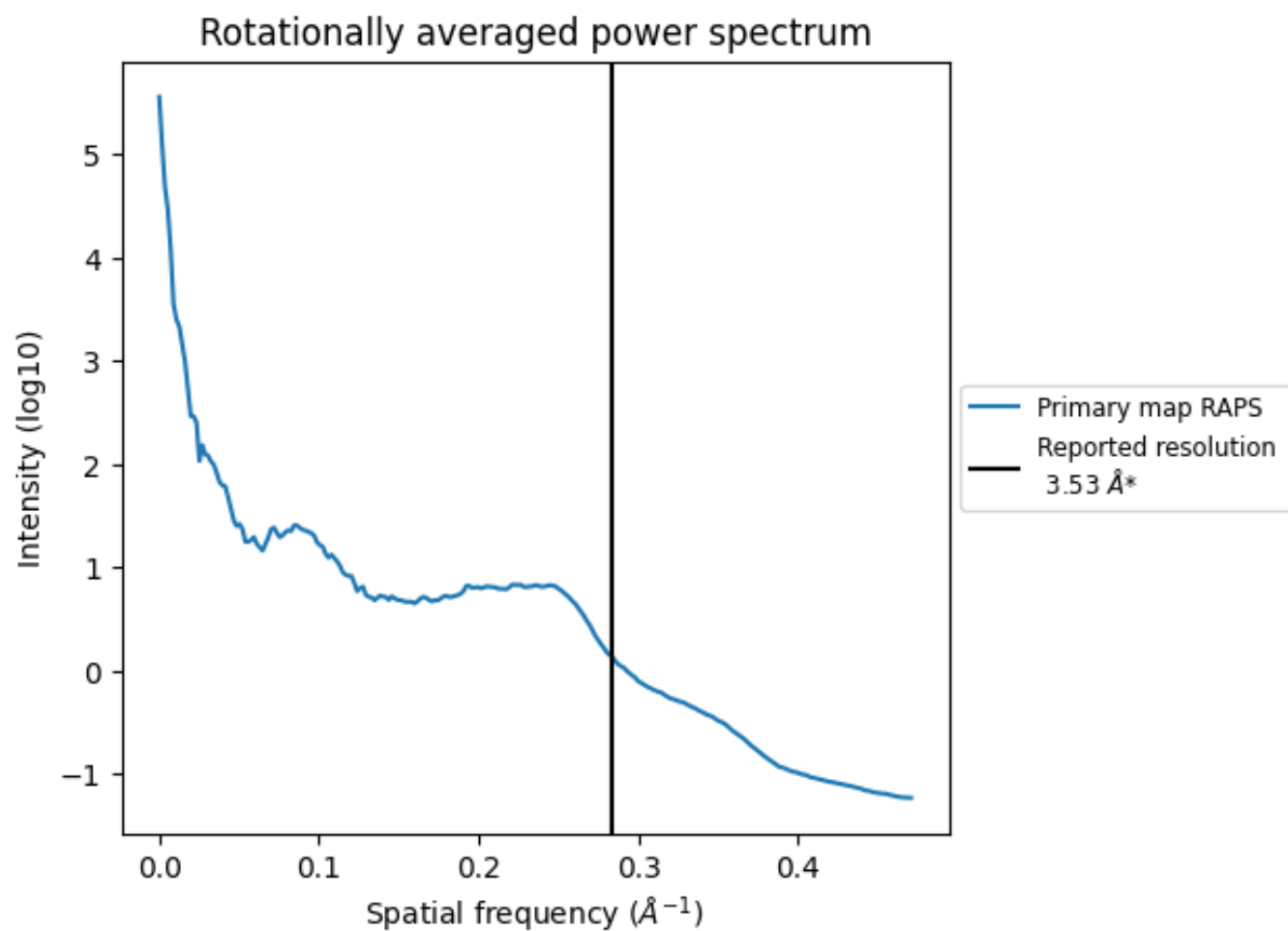
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2024 nm^3 ; this corresponds to an approximate mass of 1828 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 ⓘ

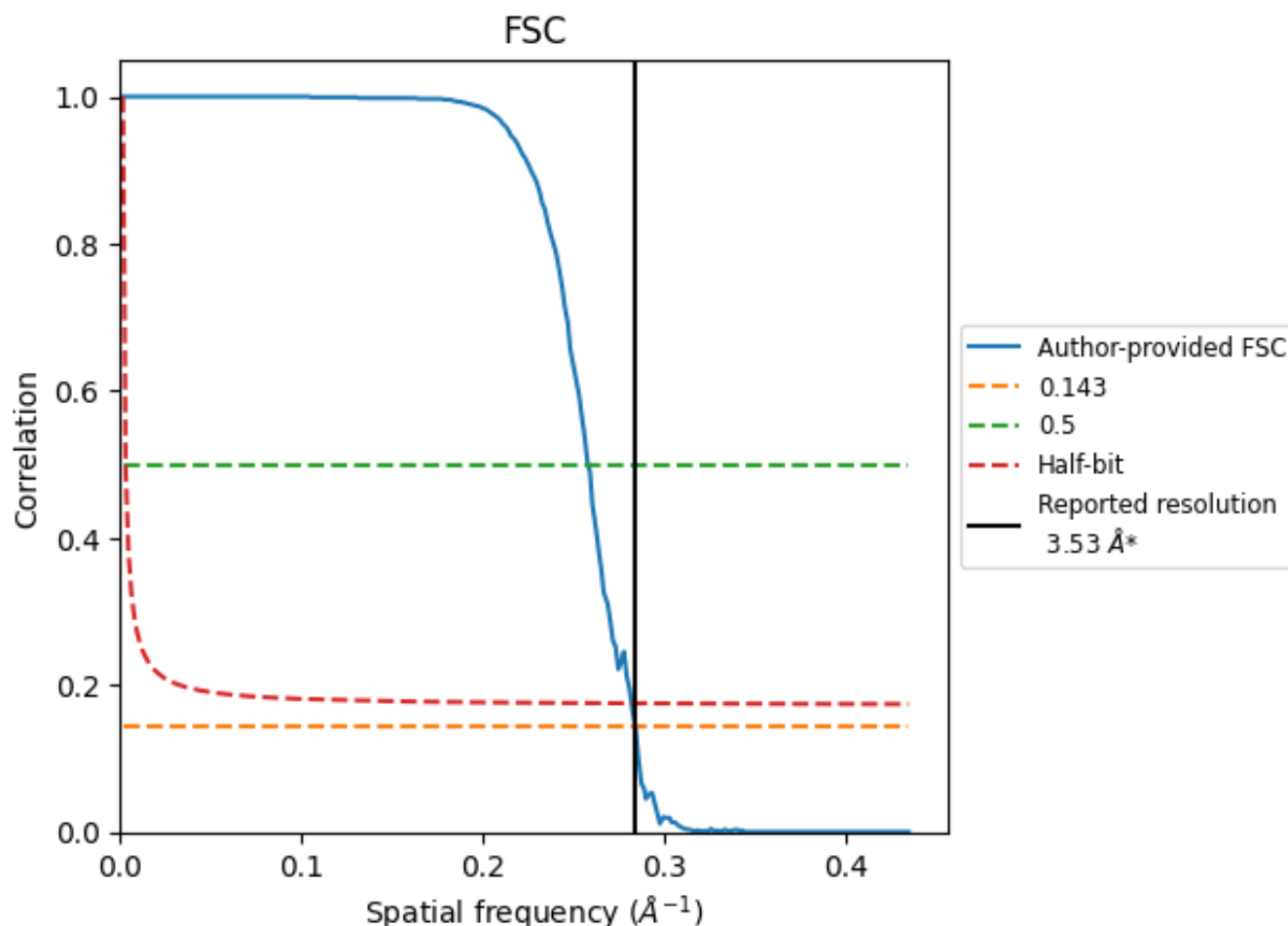


*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.283 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.52	3.88	3.55
Unmasked-calculated*	-	-	-

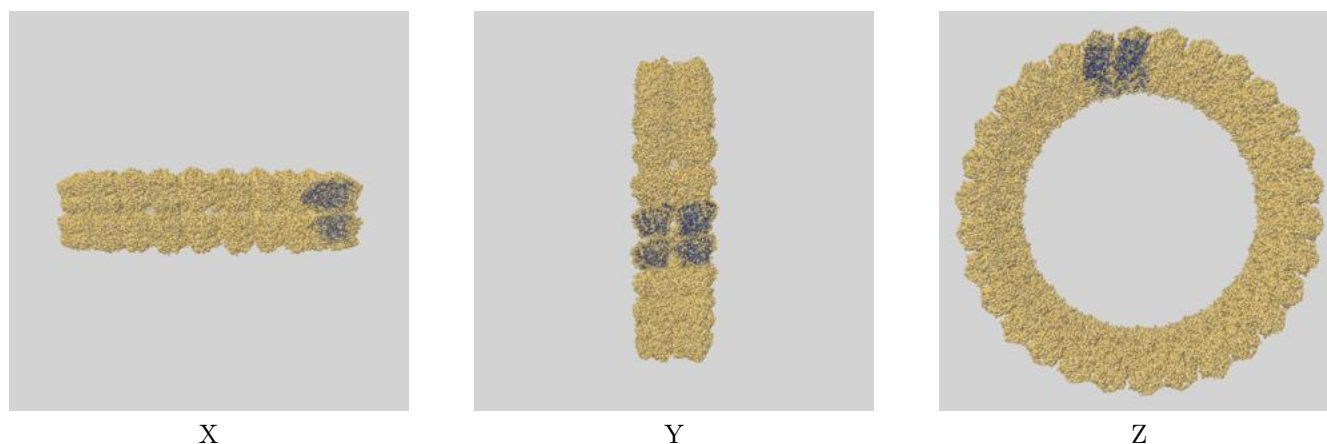
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

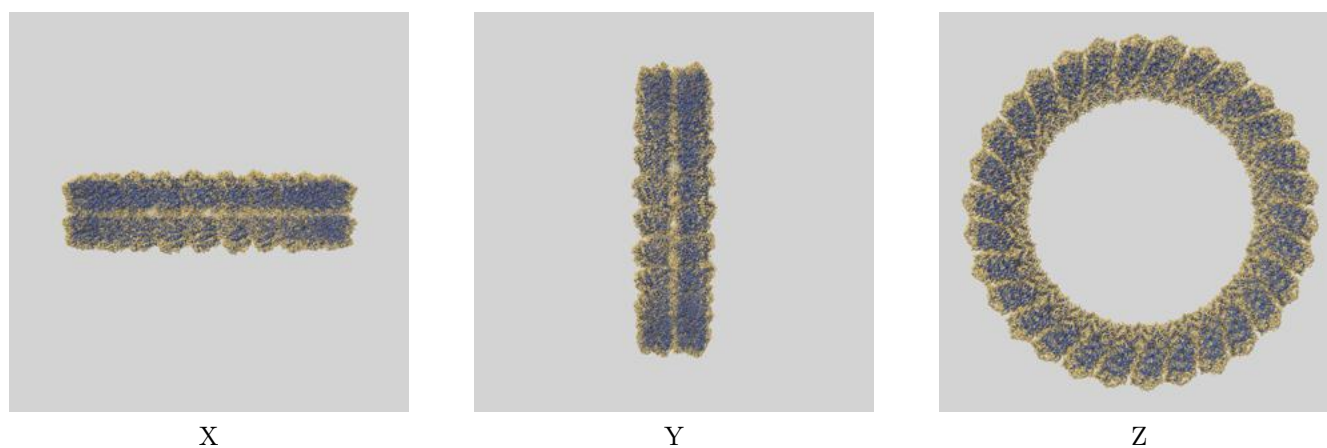
This section contains information regarding the fit between EMDB map EMD-26257 and PDB model 7U0F. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

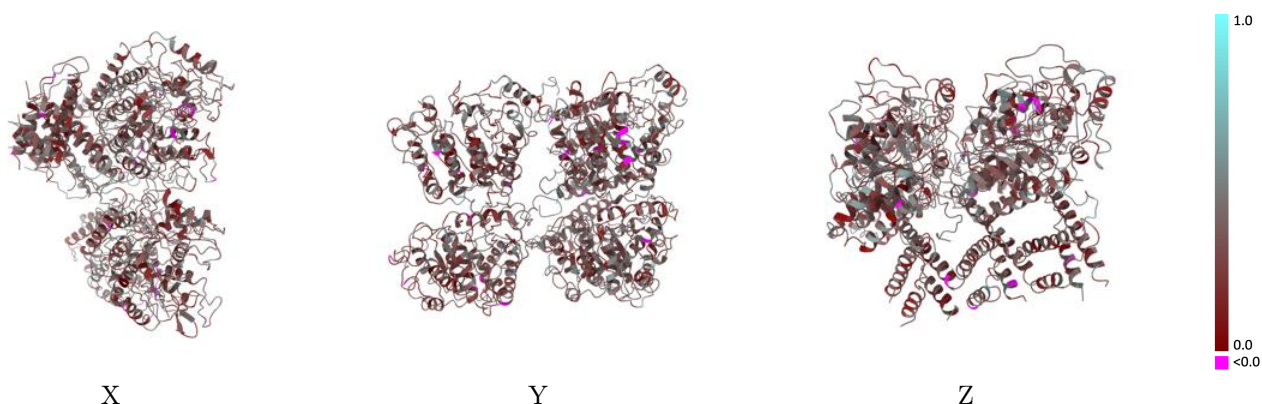


9.1.2 Map-model assembly overlay [i](#)



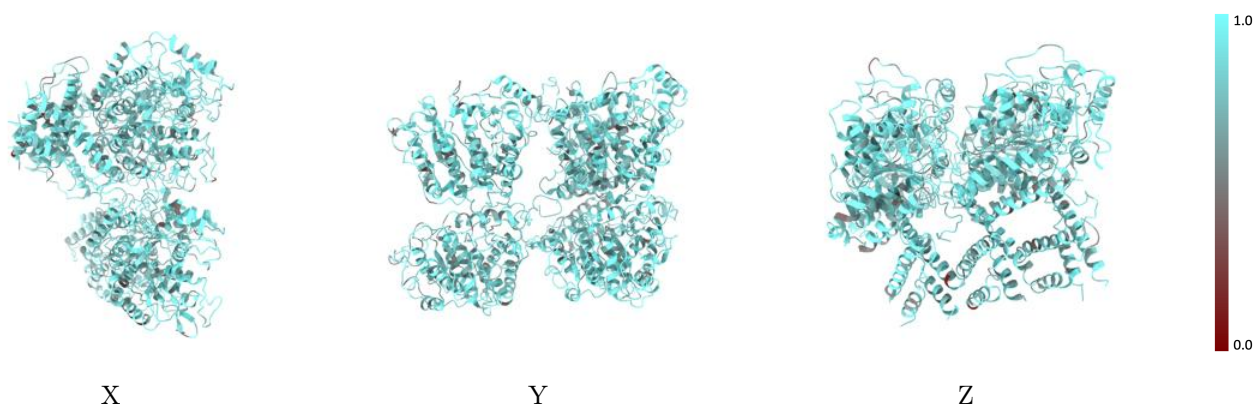
The images above show the 3D surface view of the map at the recommended contour level 2.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



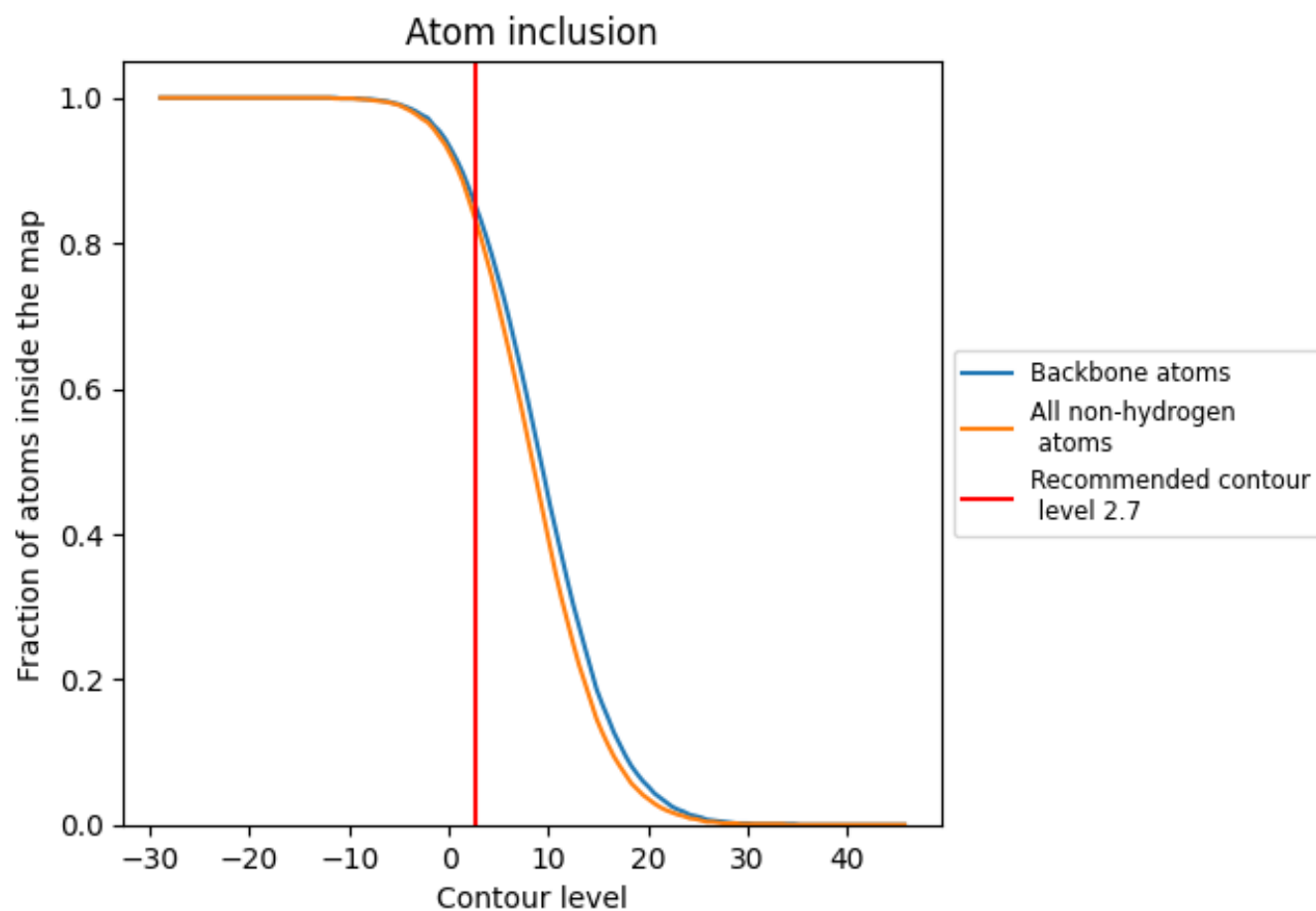
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (2.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (2.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8310</div>	<div><div></div>0.3440</div>
A	<div><div></div>0.8420</div>	<div><div></div>0.3540</div>
B	<div><div></div>0.8450</div>	<div><div></div>0.3530</div>
C	<div><div></div>0.8170</div>	<div><div></div>0.3340</div>
D	<div><div></div>0.8380</div>	<div><div></div>0.3470</div>
E	<div><div></div>0.8290</div>	<div><div></div>0.3320</div>
F	<div><div></div>0.7340</div>	<div><div></div>0.3020</div>
G	<div><div></div>0.8570</div>	<div><div></div>0.3580</div>
H	<div><div></div>0.7860</div>	<div><div></div>0.3350</div>
I	<div><div></div>0.8370</div>	<div><div></div>0.3350</div>
J	<div><div></div>0.8170</div>	<div><div></div>0.3230</div>

1.0

0.0

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