



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2024 – 01:12 PM JST

PDB ID : 7EYQ
EMDB ID : EMD-31384
Title : Cryo-EM (SPA) structure of human Nup155 Longer N-terminus (19-1069) at 5.4 Angstrom resolution
Authors : Niranjan, S.
Deposited on : 2021-05-31
Resolution : 5.40 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

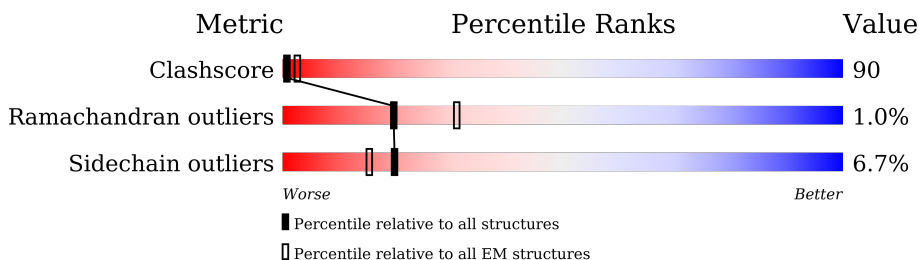
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 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	1642	<div> <div>18%</div> <div>12%</div> <div>36%</div> <div>•</div> <div>49%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6577 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 G protein/GFP fusion protein,Nuclear pore complex protein Nup155.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	833	Total	C	N	O	S	0	0
			6577	4181	1128	1229	39		

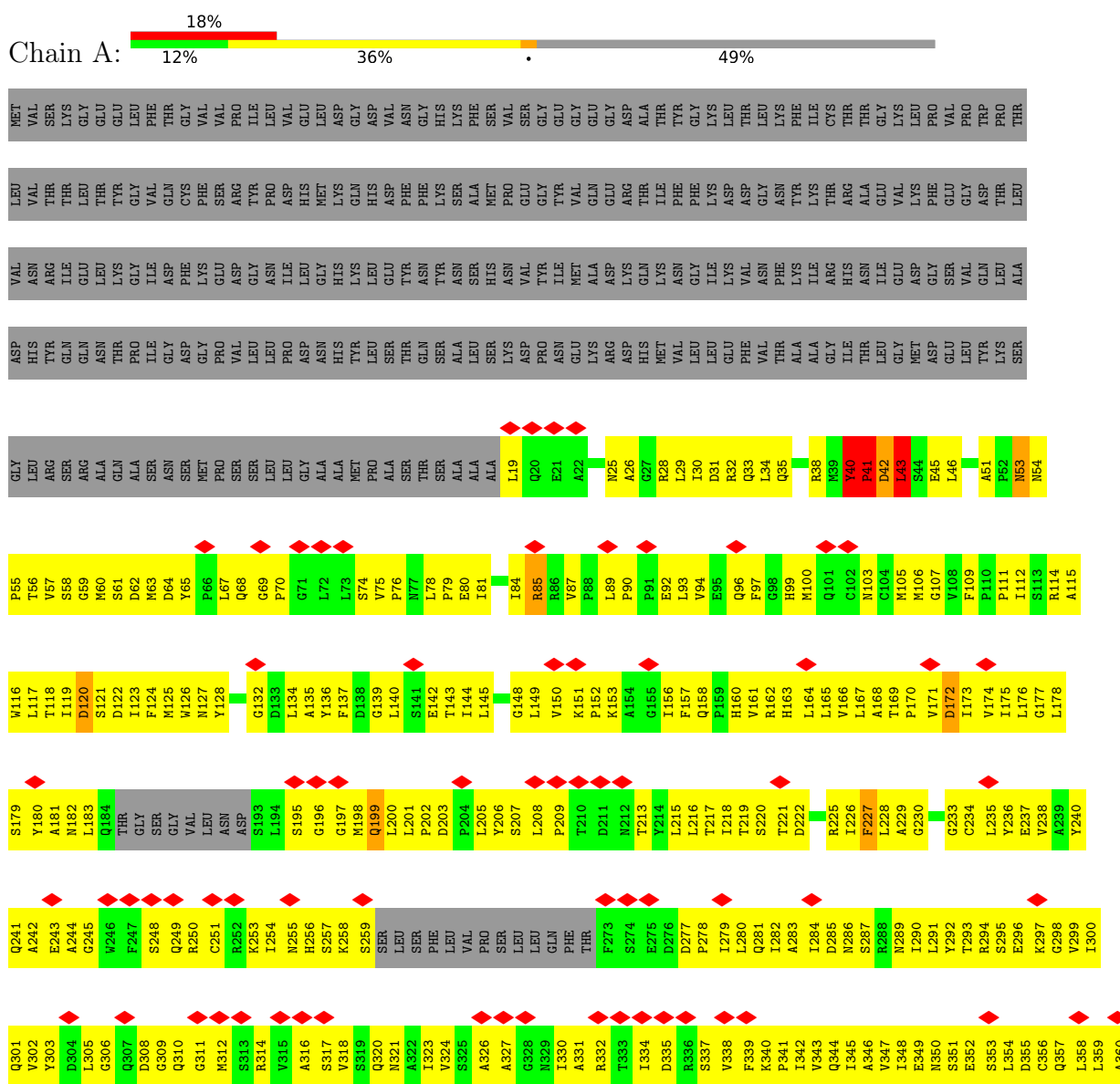
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	SER	-	linker	UNP B7UCZ6
A	-10	GLY	-	linker	UNP B7UCZ6
A	-9	LEU	-	linker	UNP B7UCZ6
A	-8	ARG	-	linker	UNP B7UCZ6
A	-7	SER	-	linker	UNP B7UCZ6
A	-6	ARG	-	linker	UNP B7UCZ6
A	-5	ALA	-	linker	UNP B7UCZ6
A	-4	GLN	-	linker	UNP B7UCZ6
A	-3	ALA	-	linker	UNP B7UCZ6
A	-2	SER	-	linker	UNP B7UCZ6
A	-1	ASN	-	linker	UNP B7UCZ6
A	0	SER	-	linker	UNP B7UCZ6

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: G protein/GFP fusion protein,Nuclear pore complex protein Nup155





CYS	VAL	HIS	GLU
ALA	GLN	VAL	ARG
GLY	PHE	LEU	LEU
TYR	LEU	LEU	HIS
SER	ILE	ILE	
ASP	GLN	ARG	
PRO	GLN	TYR	
ILE	VAL	VAL	
LEU	CYS	GLU	
VAL	THR	ASN	
GLN	LEU	PRO	
THR	ASN	SER	
LEU	TRP	GLN	
TRP	ASP	VAL	
GLN	VAL	LEU	
ASP	GLY	ASN	
ILE	PHE	CYS	
ILE	VAL	GLU	
GLU	ILE	ARG	
LYS	GLN	ARG	
GLU	THR	ARG	
LEU	MET	PHE	
SER	ASN	THR	
ASP	GLU	ASN	
SER	ILE	LEU	
VAL	GLY	CYS	
THR	VAL	LEU	
LEU	PRO	ASP	
SER	LEU	ALA	
SER	PRO	VAL	
ASP	ARG	CYS	
ASP	LEU	GLY	
ARG	LEU	TYR	
MET	GLU	LEU	
HIS	VAL	VAL	
ALA	TYR	GLU	
LEU	ASP	LEU	
SER	GLN	GLN	
LEU	PHE	SER	
LYS	LYS	MET	
ILE	SER	SER	
VAL	VAL	SER	
LEU	ARG	SER	
LEU	ASP	VAL	
GLY	PRO	ALA	
LYS	PHE	VAL	
ILE	TRP	GLN	
TYR	ASN	ALA	
ALA	TYR	ILE	
GLY	MET	THR	
THR	LYS	GLY	
PRO	PRO	ASN	
ARG	ARG	PHE	
PHE	LEU	LYS	
PHE	HIS	SER	
PRO	LEU	LEU	
LEU	PRO	GLN	
ASP	LEU	ALA	
PHE	CYS	LYS	
ILE	ILE	LEU	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37100	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 ($e^-/\text{\AA}^2$)	1.15	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	2.577	Depositor
Minimum map value	-1.262	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.26	Depositor
Map size (\AA)	230.44, 230.44, 230.44	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.823, 0.823, 0.823	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	0.34	0/6702	0.59	6/9069 (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	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	TYR	C-N-CD	-10.72	97.01	120.60
1	A	40	TYR	C-N-CA	7.65	154.13	122.00
1	A	838	ILE	CB-CA-C	-5.94	99.72	111.60
1	A	43	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	42	ASP	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	TYR	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	6577	0	6592	1188	0
All	All	6577	0	6592	1188	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 90.

The worst 5 of 1188 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:HIS:HB3	1:A:841:LEU:CB	1.33	1.57
1:A:880:LEU:HA	1:A:883:ARG:CG	1.45	1.43
1:A:801:HIS:ND1	1:A:841:LEU:HD13	1.34	1.40
1:A:843:ASN:ND2	1:A:879:GLU:HA	1.44	1.33
1:A:879:GLU:CG	1:A:905:GLN:HE21	1.45	1.29

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	811/1642 (49%)	697 (86%)	106 (13%)	8 (1%)	15 54

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	528	VAL
1	A	678	TRP
1	A	704	CYS
1	A	807	VAL

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	733/1440 (51%)	684 (93%)	49 (7%)	16 43

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	824	LYS
1	A	886	GLN
1	A	825	ASP
1	A	841	LEU
1	A	892	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	542	HIS
1	A	782	GLN
1	A	889	ASN
1	A	801	HIS
1	A	676	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

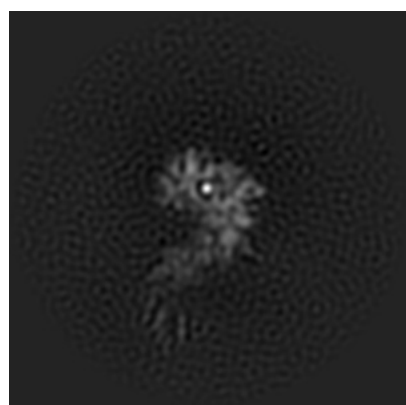
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31384. These allow visual inspection of the internal detail of the map and identification of artifacts.

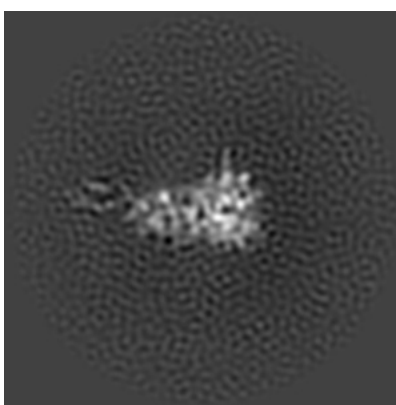
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

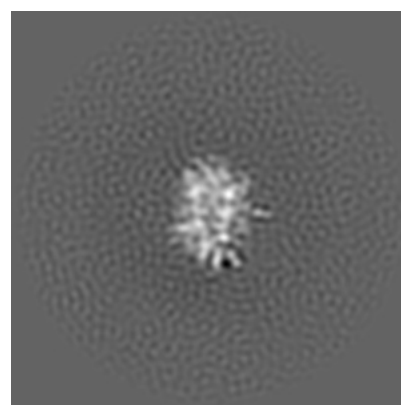
6.1.1 Primary map



X



Y

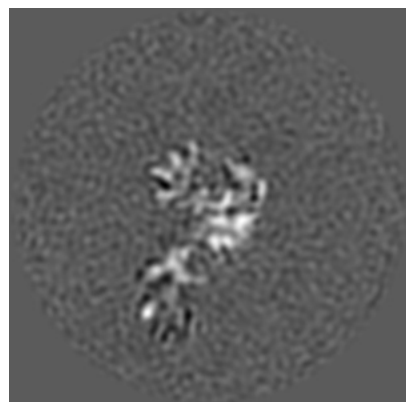


Z

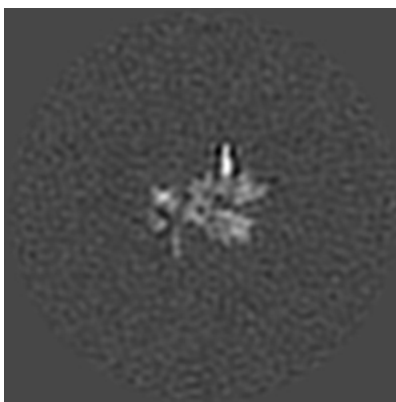
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

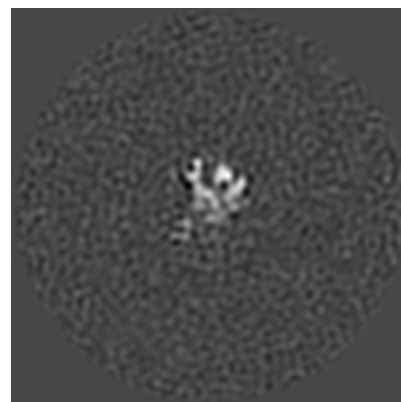
6.2.1 Primary map



X Index: 140



Y Index: 140

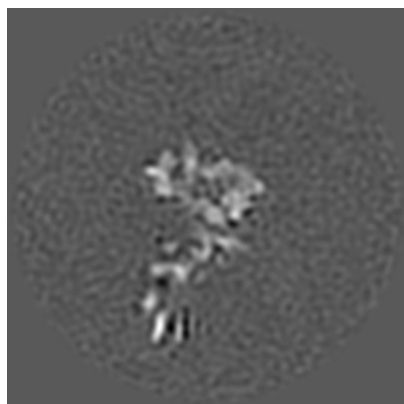


Z Index: 140

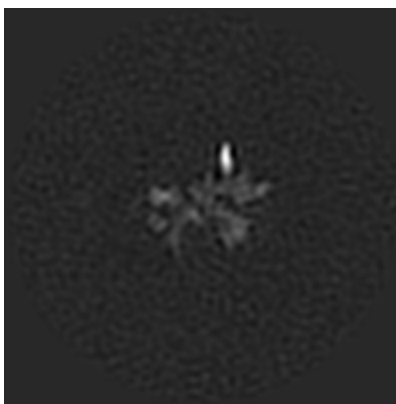
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

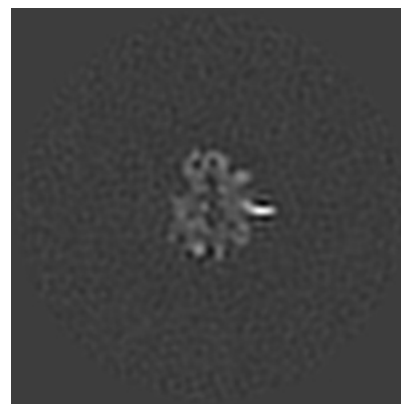
6.3.1 Primary map



X Index: 144



Y Index: 138

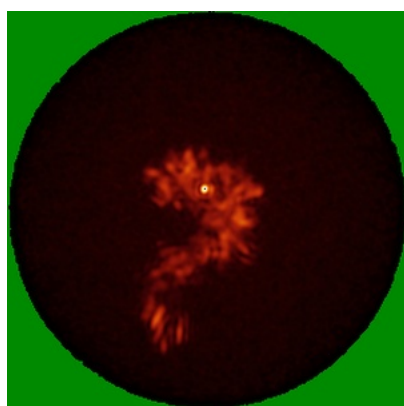


Z Index: 155

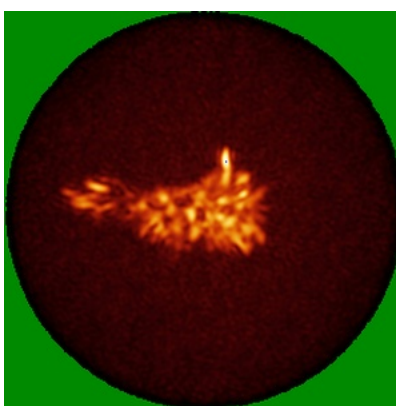
The images above show the largest variance slices of the map in three orthogonal directions.

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

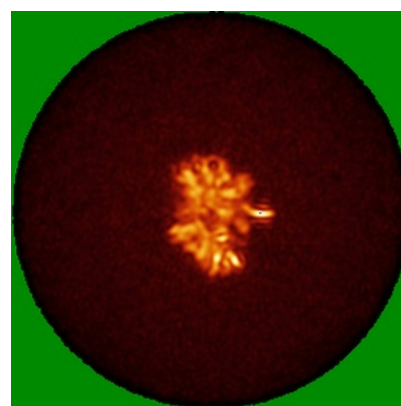
6.4.1 Primary map



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

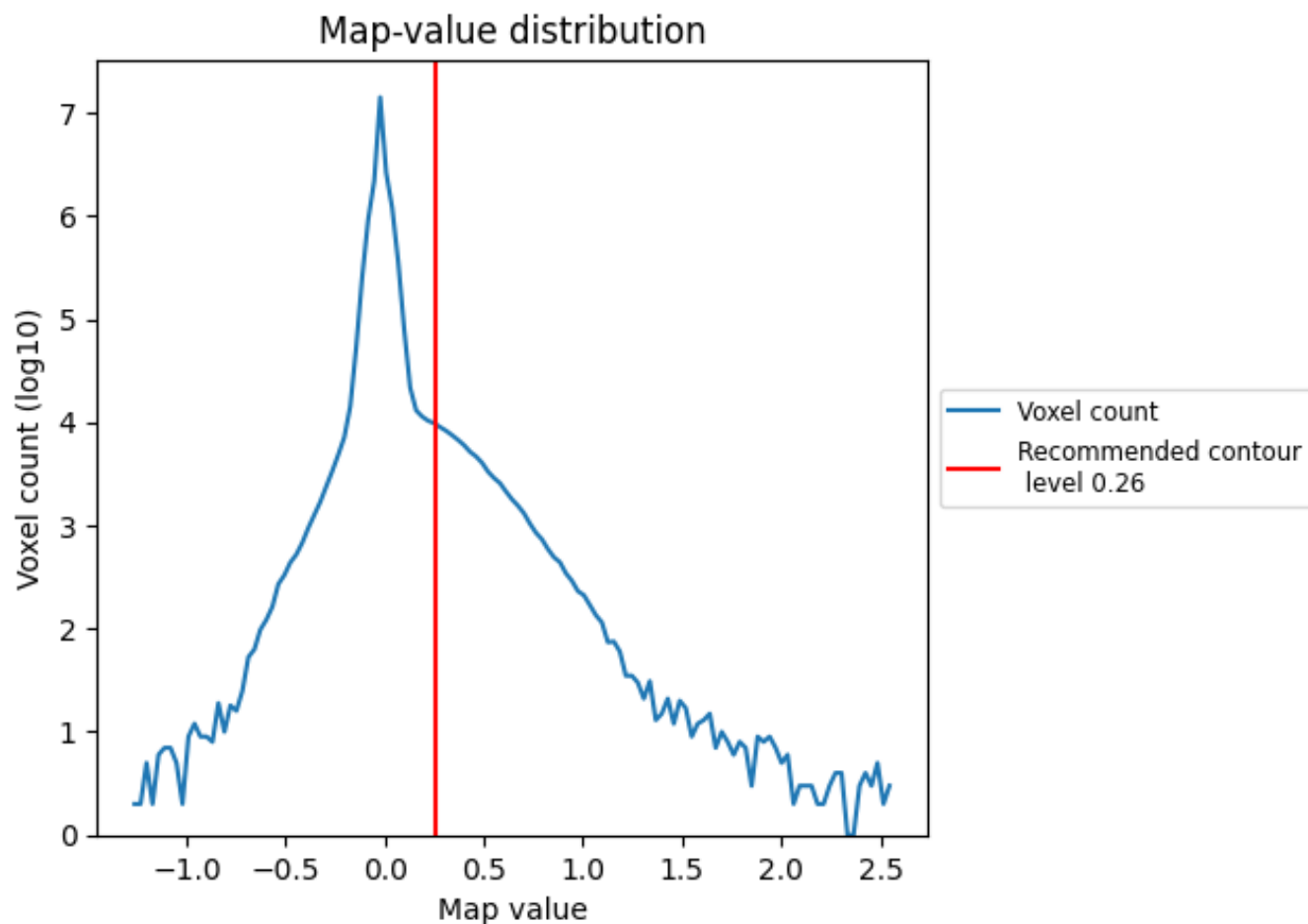
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

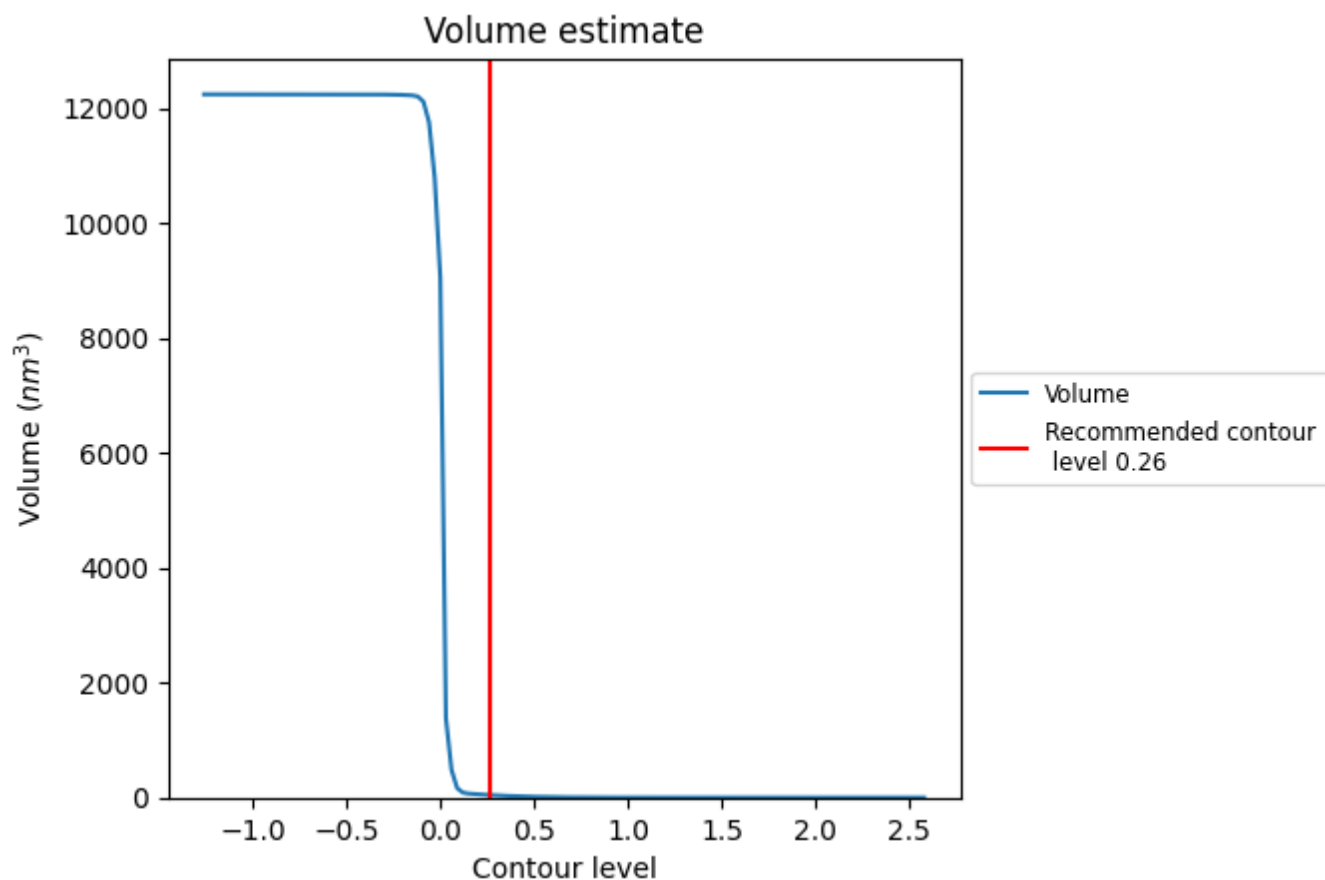
This section contains the results of statistical analysis of the map.

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.

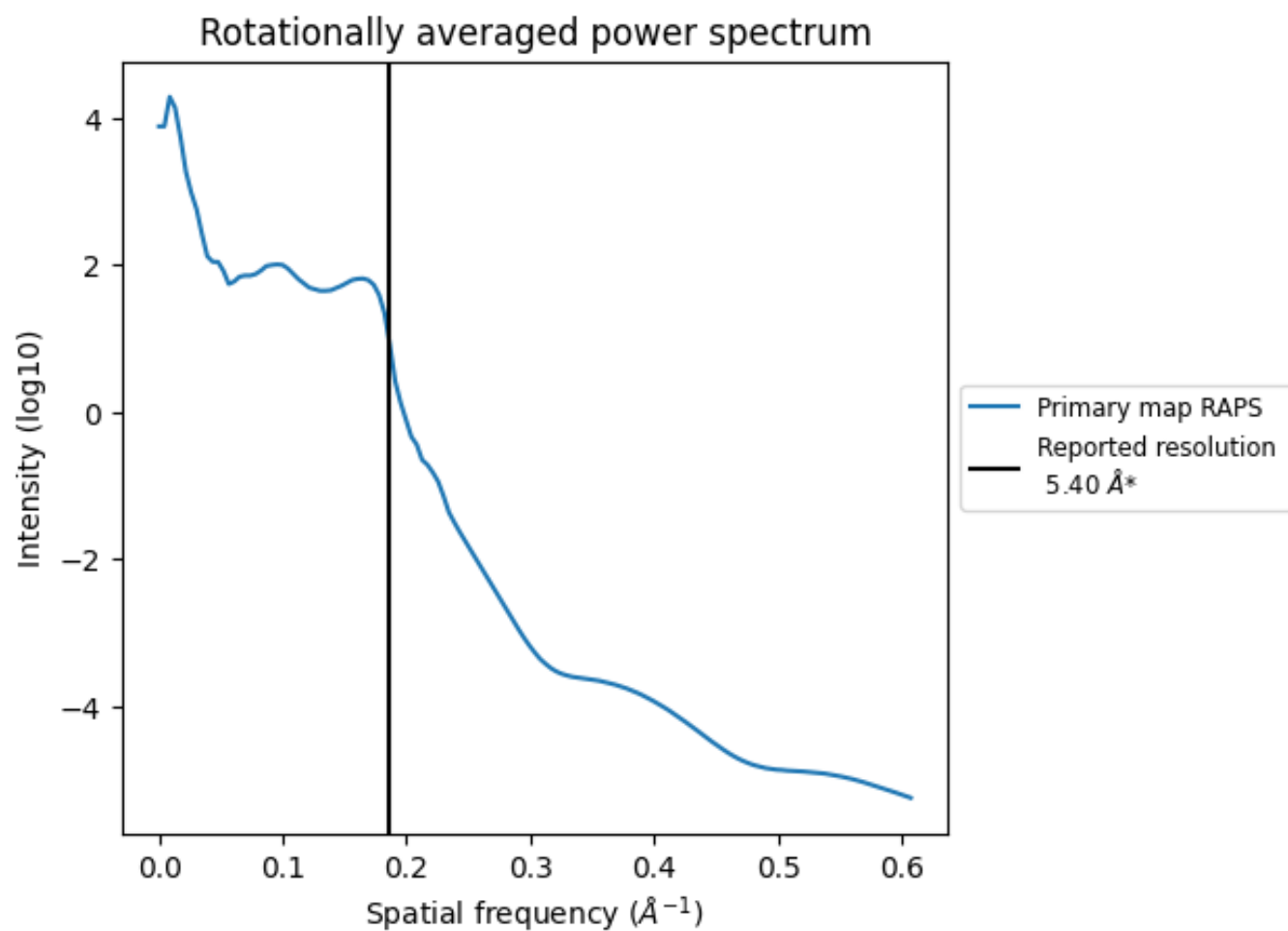
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm^3 ; this corresponds to an approximate mass of 40 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 0.185 \AA^{-1}

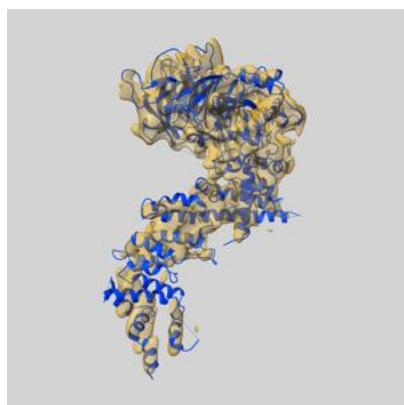
8 Fourier-Shell correlation

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

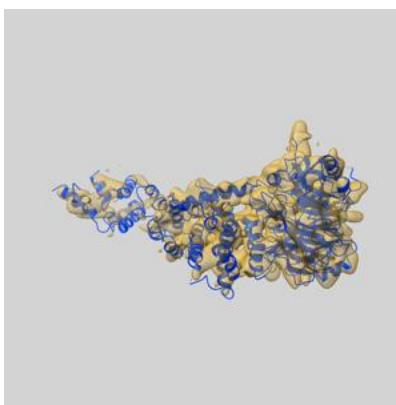
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31384 and PDB model 7EYQ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

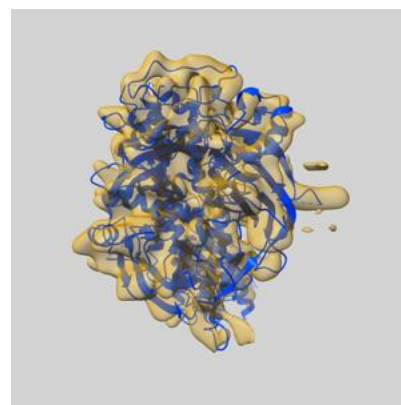
9.1 Map-model overlay [i](#)



X



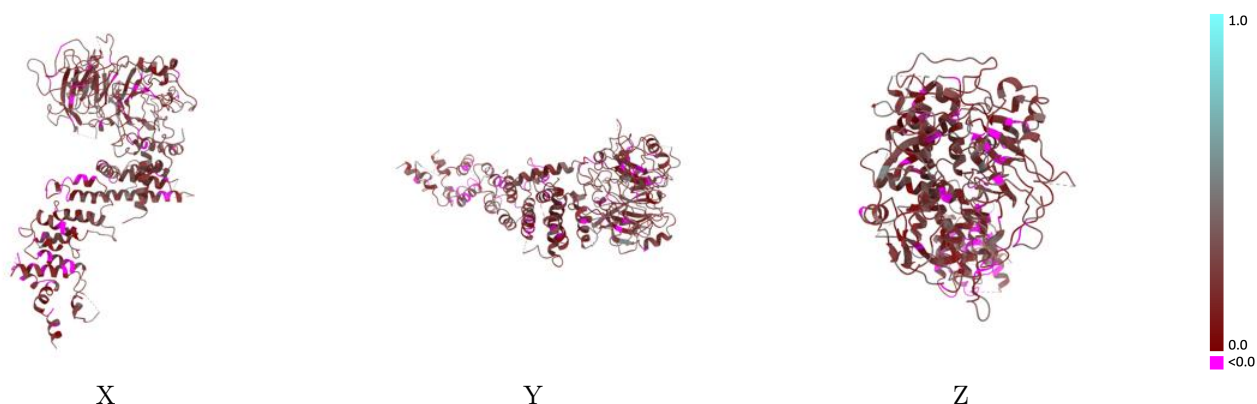
Y



Z

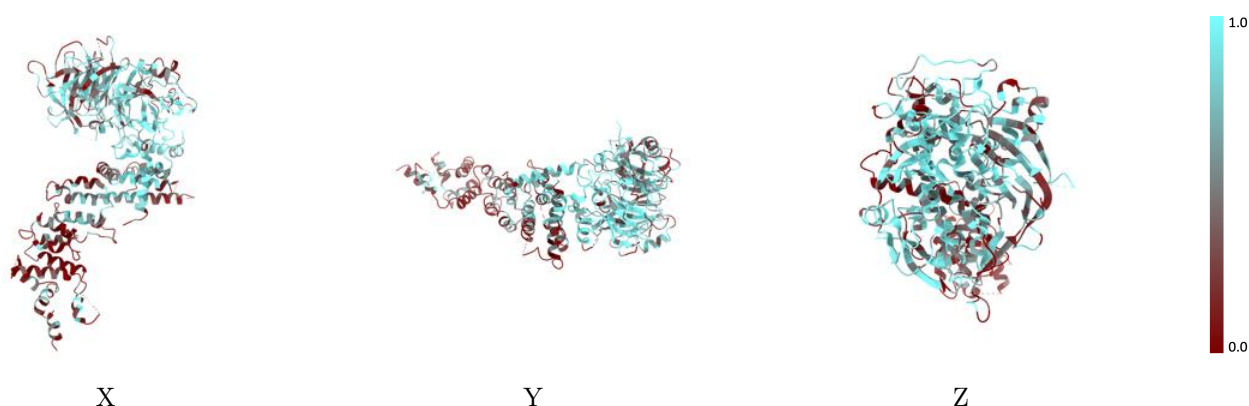
The images above show the 3D surface view of the map at the recommended contour level 0.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



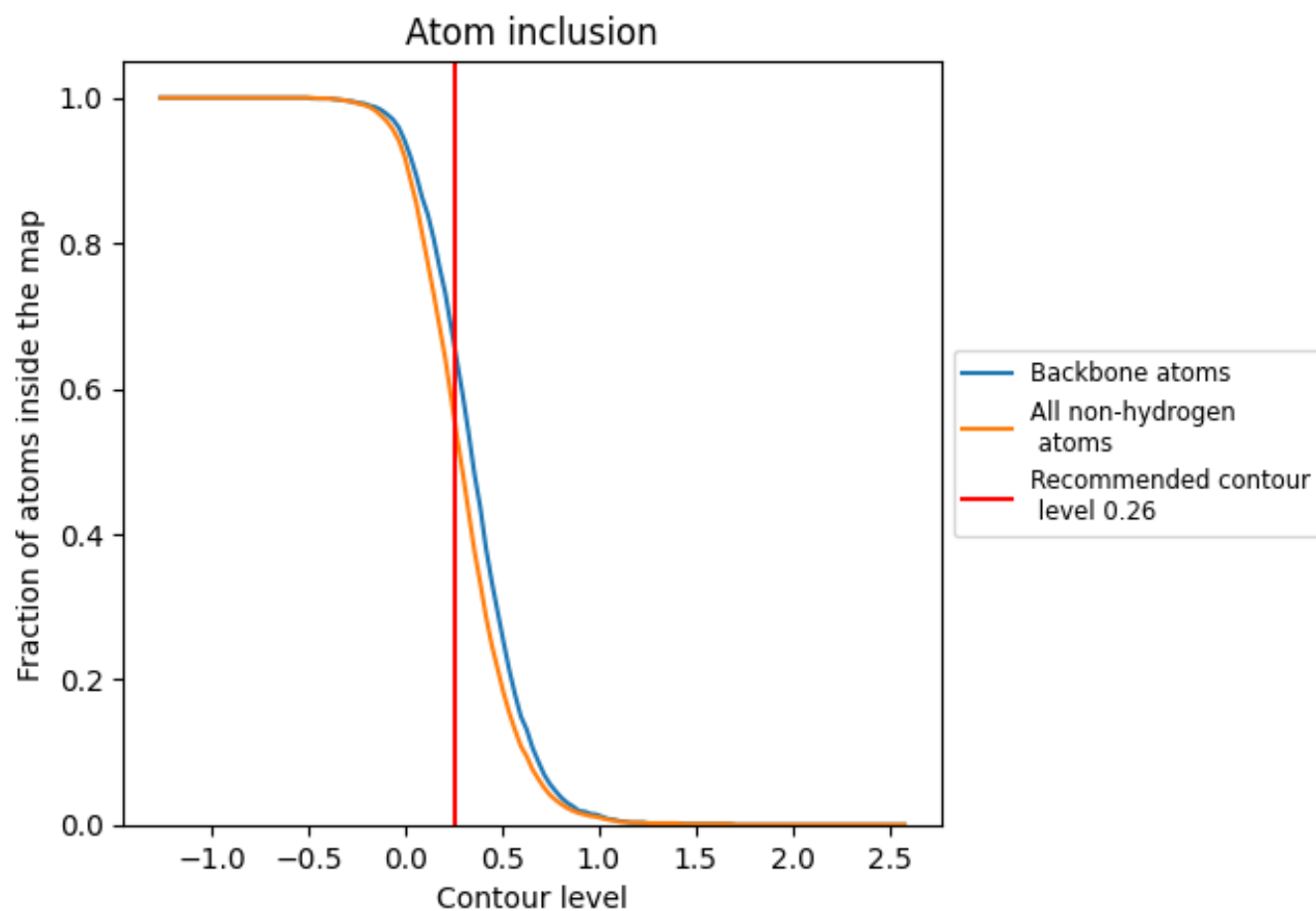
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% 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 (0.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5480	<div></div> 0.2100
A	<div></div> 0.5480	<div></div> 0.2100

