



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 04:05 PM EDT

PDB ID : 6C4H  
EMDB ID : EMD-7340  
Title : Conformation of methylated GGQ in the peptidyl transferase center during translation termination (PTC region)  
Authors : Zeng, F.; Jin, H.  
Deposited on : 2018-01-12  
Resolution : 3.10 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

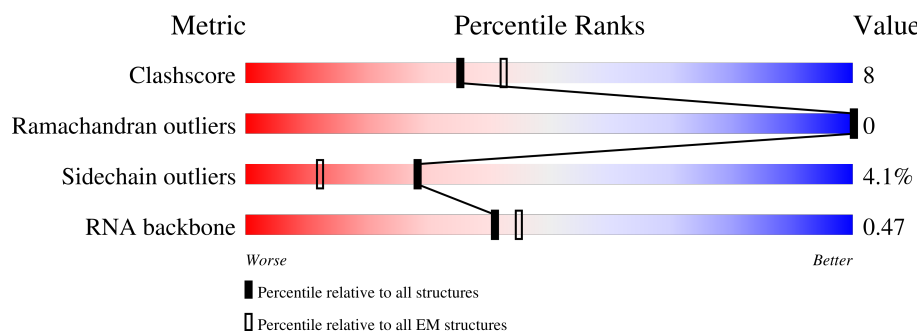
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	2904	
2	C	273	
3	D	209	
4	N	136	
5	X	85	
6	x	77	
7	v	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	A	2069	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15326 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	636	Total	C	N	O	P	0	0
			13622	6086	2470	4430	636		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 687670942

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	47	Total	C	N	O	S	0	0
			361	224	77	59	1		

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	47	Total	C	N	O	S	0	0
			361	224	73	63	1		

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	17	Total	C	N	O	S	0	0
			125	77	24	23	1		

- Molecule 5 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	X	10	Total	C	N	O	0	0
			75	40	17	18		

- Molecule 6 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	x	12	Total	C	N	O	P	0	0
			252	114	48	79	11		

- Molecule 7 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	v	63	Total	C	N	O	S	0	0
			496	301	99	93	3		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-18	ALA	-	expression tag	UNP P07012
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	A	34	Total	Mg	0
			34	34	



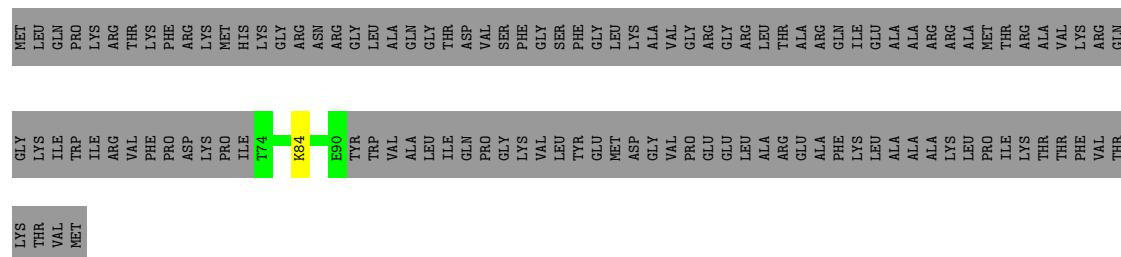






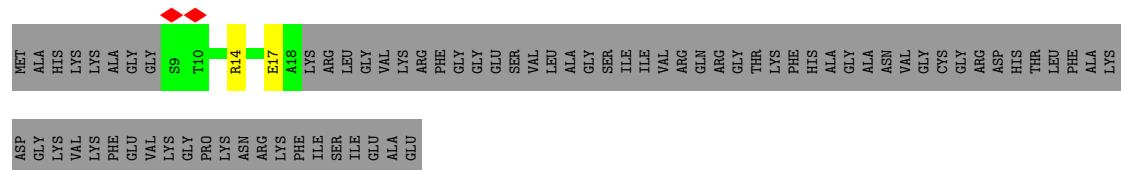
- Molecule 4: 50S ribosomal protein L16

Chain N:  12% : 88%



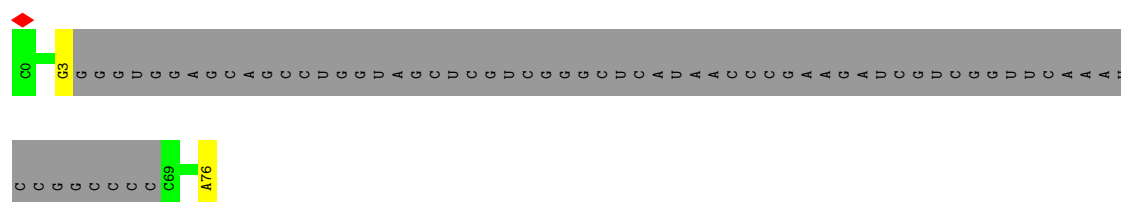
- Molecule 5: 50S ribosomal protein L27

Chain X:  9% 88%



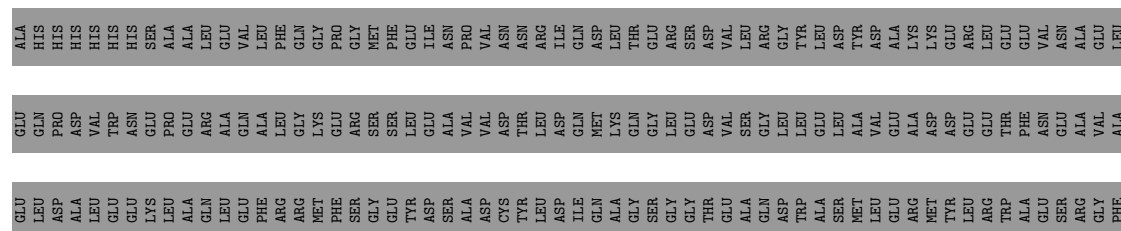
- Molecule 6: P-site tRNA fMet

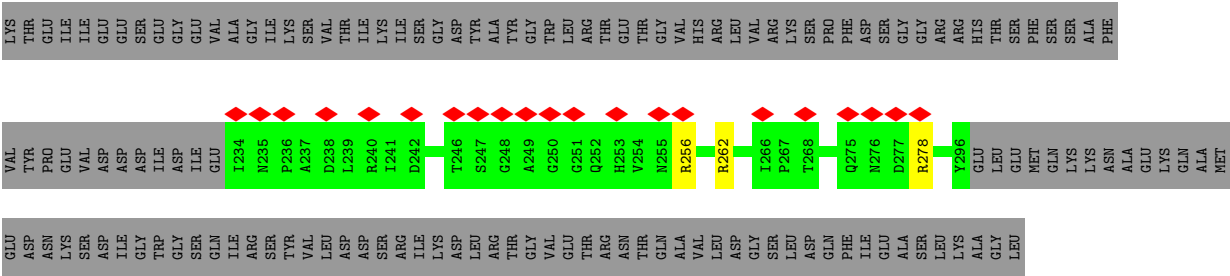
Chain x:  13% 84%



- Molecule 7: Peptide chain release factor RF2

Chain v:  5% 16% 84%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.392	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MC, G7M, 1MG, PSU, MEQ, 2MG, OMU, 2MA, 5MU, OMC, OMG

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	0.25	0/14827	0.65	0/23099
2	C	0.37	0/373	0.68	0/504
3	D	0.38	0/369	0.61	0/493
4	N	0.43	0/125	0.78	0/164
5	X	0.45	0/74	0.76	0/97
6	x	0.21	0/280	0.64	0/432
7	v	0.37	0/491	0.64	0/658
All	All	0.26	0/16539	0.65	0/25447

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	13622	0	6888	159	0
2	C	361	0	357	11	0
3	D	361	0	359	12	0
4	N	125	0	135	0	0
5	X	75	0	66	0	0
6	x	252	0	135	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	v	496	0	501	0	0
8	A	34	0	0	0	0
All	All	15326	0	8441	167	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 8.

The worst 5 of 167 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:2074:U:H2'	1:A:2075:U:C6	1.88	1.08
1:A:742:A:H2'	1:A:743:A:C8	1.97	1.00
1:A:2244:U:H2'	1:A:2245:U:C6	1.97	0.99
1:A:754:U:H2'	1:A:755:U:C6	2.05	0.92
1:A:2069:G7M:O6	1:A:2070:A:N6	2.13	0.81

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	C	45/273 (16%)	44 (98%)	1 (2%)	0	100	100
3	D	45/209 (22%)	40 (89%)	5 (11%)	0	100	100
4	N	15/136 (11%)	13 (87%)	2 (13%)	0	100	100
5	X	8/85 (9%)	7 (88%)	1 (12%)	0	100	100
7	v	60/384 (16%)	60 (100%)	0	0	100	100
All	All	173/1087 (16%)	164 (95%)	9 (5%)	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	C	36/218 (16%)	36 (100%)	0	100	100
3	D	37/164 (23%)	37 (100%)	0	100	100
4	N	13/109 (12%)	12 (92%)	1 (8%)	10	35
5	X	8/63 (13%)	6 (75%)	2 (25%)	0	1
7	v	53/324 (16%)	50 (94%)	3 (6%)	17	46
All	All	147/878 (17%)	141 (96%)	6 (4%)	28	57

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	v	256	ARG
7	v	262	ARG
7	v	278	ARG
5	X	14	ARG
4	N	84	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	v	290	GLN
7	v	286	GLN
7	v	273	GLN
7	v	253	HIS
7	v	283	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	625/2904 (21%)	128 (20%)	11 (1%)
6	x	10/77 (12%)	2 (20%)	0
All	All	635/2981 (21%)	130 (20%)	11 (1%)

5 of 130 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	738	G
1	A	747	5MU
1	A	748	G
1	A	749	A
1	A	752	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1900	A
1	A	2468	A
1	A	2581	G
1	A	2529	G
1	A	791	C

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PSU	A	2457	1	18,21,22	1.51	2 (11%)	21,30,33	2.06	3 (14%)
1	5MU	A	1939	1	19,22,23	1.49	5 (26%)	27,32,35	2.16	7 (25%)
1	OMC	A	2498	1,8	19,22,23	0.81	0	25,31,34	1.13	3 (12%)
1	PSU	A	2504	1	18,21,22	1.50	3 (16%)	21,30,33	2.08	5 (23%)
1	OMG	A	2251	6,1	19,26,27	0.98	2 (10%)	21,38,41	1.18	2 (9%)
1	2MA	A	2503	1	17,25,26	1.15	3 (17%)	16,37,40	1.48	4 (25%)
1	PSU	A	2605	1	18,21,22	1.44	2 (11%)	21,30,33	2.03	4 (19%)
1	5MC	A	1962	1	19,22,23	1.86	2 (10%)	26,32,35	1.35	4 (15%)
1	OMU	A	2552	1,8	19,22,23	1.25	2 (10%)	25,31,34	1.88	5 (20%)
1	5MU	A	747	1	19,22,23	1.55	5 (26%)	27,32,35	2.16	8 (29%)
1	2MG	A	2445	1	18,26,27	0.96	1 (5%)	16,38,41	1.60	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MEQ	v	252	7	8,9,10	0.42	0	5,10,12	0.63	0
1	1MG	A	745	1	19,26,27	1.13	2 (10%)	18,39,42	1.62	4 (22%)
1	PSU	A	955	1	18,21,22	1.46	2 (11%)	21,30,33	2.21	4 (19%)
1	G7M	A	2069	1	20,26,27	1.04	1 (5%)	16,39,42	3.40	5 (31%)
1	2MG	A	1835	1	18,26,27	0.98	2 (11%)	16,38,41	1.21	2 (12%)
1	PSU	A	2580	1	18,21,22	1.45	2 (11%)	21,30,33	2.16	4 (19%)
1	PSU	A	746	1	18,21,22	1.38	2 (11%)	21,30,33	1.86	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
1	OMC	A	2498	1,8	-	2/9/27/28	0/2/2/2
1	PSU	A	2504	1	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	6,1	-	1/5/27/28	0/3/3/3
1	2MA	A	2503	1	-	2/3/25/26	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1,8	-	0/9/27/28	0/2/2/2
1	5MU	A	747	1	-	1/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
7	MEQ	v	252	7	-	2/8/9/11	-
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	G7M	A	2069	1	-	2/3/25/26	0/3/3/3
1	2MG	A	1835	1	-	2/5/27/28	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1	-	3/7/25/26	0/2/2/2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1962	5MC	C5-C4	7.01	1.49	1.44
1	A	2504	PSU	C6-C5	4.76	1.40	1.35
1	A	746	PSU	C6-C5	4.34	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2457	PSU	C6-C5	4.31	1.40	1.35
1	A	2605	PSU	C6-C5	4.25	1.40	1.35

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2069	G7M	C4'-O4'-C1'	-11.23	99.64	109.92
1	A	955	PSU	N1-C2-N3	6.82	122.37	115.17
1	A	2504	PSU	N1-C2-N3	6.55	122.08	115.17
1	A	2457	PSU	N1-C2-N3	6.36	121.88	115.17
1	A	2580	PSU	N1-C2-N3	6.33	121.85	115.17

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2251	OMG	C1'-C2'-O2'-CM2
7	v	252	MEQ	N-CA-CB-CG
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2498	OMC	O4'-C4'-C5'-O5'
1	A	1939	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1939	5MU	1	0
1	A	2503	2MA	1	0
1	A	2605	PSU	1	0
1	A	747	5MU	1	0
1	A	2445	2MG	1	0
1	A	2069	G7M	12	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 34 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

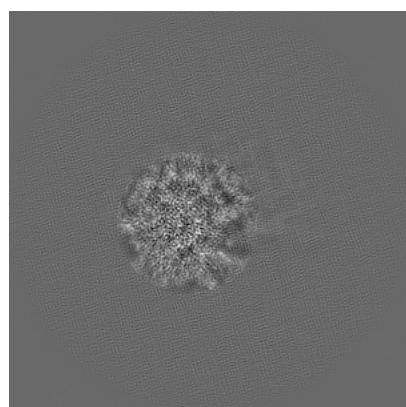
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7340. These allow visual inspection of the internal detail of the map and identification of artifacts.

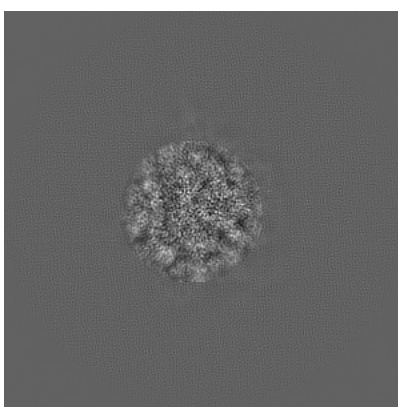
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

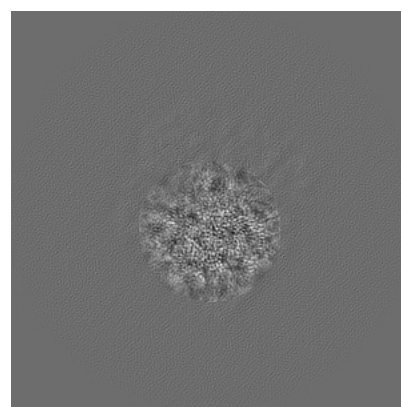
#### 6.1.1 Primary map



X



Y

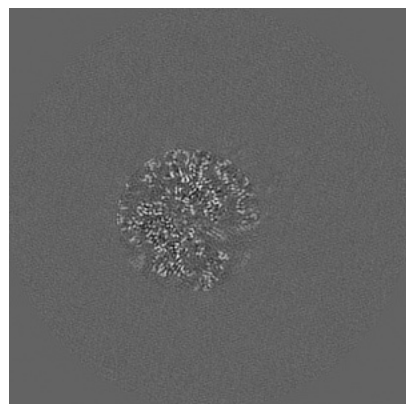


Z

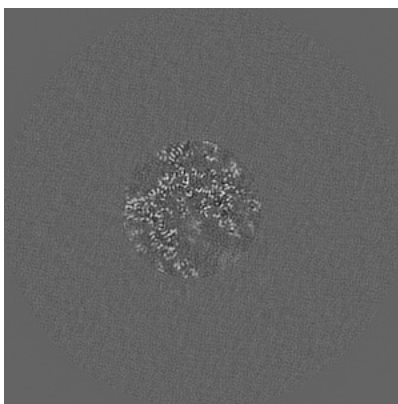
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

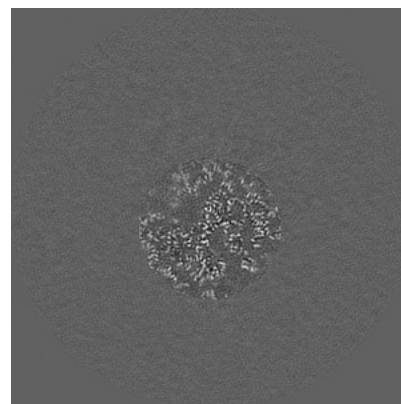
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

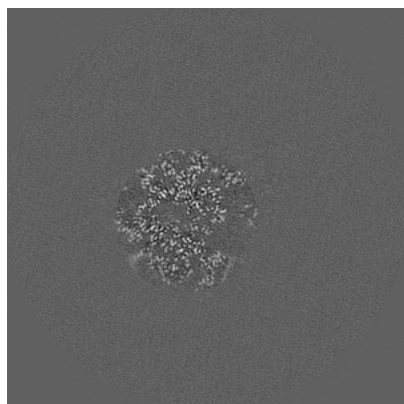


Z Index: 192

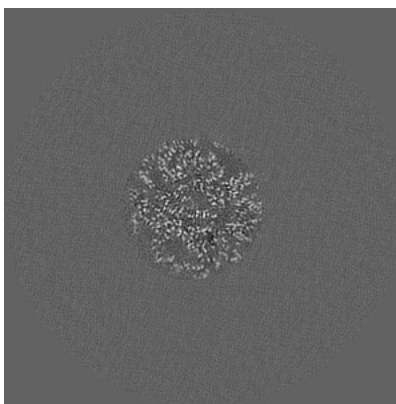
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

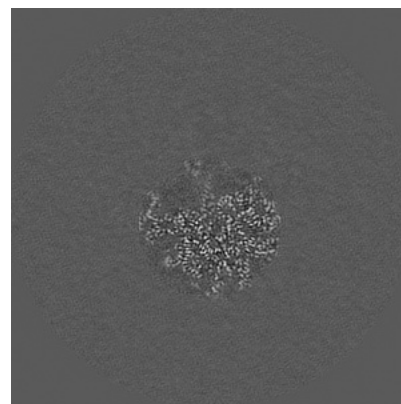
### 6.3.1 Primary map



X Index: 198



Y Index: 159

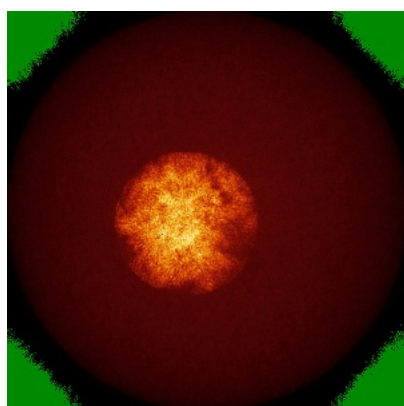


Z Index: 169

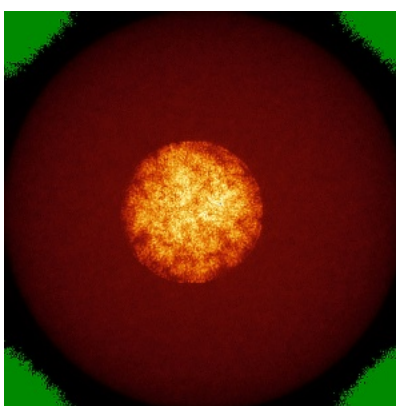
The images above show the largest variance slices of the map in three orthogonal directions.

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

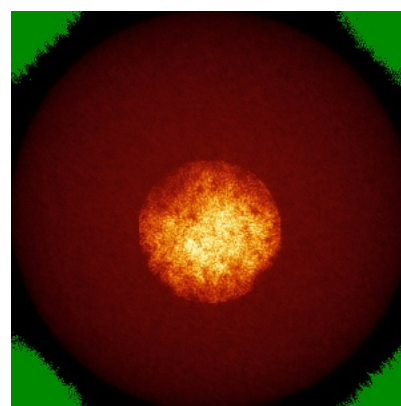
### 6.4.1 Primary map



X



Y

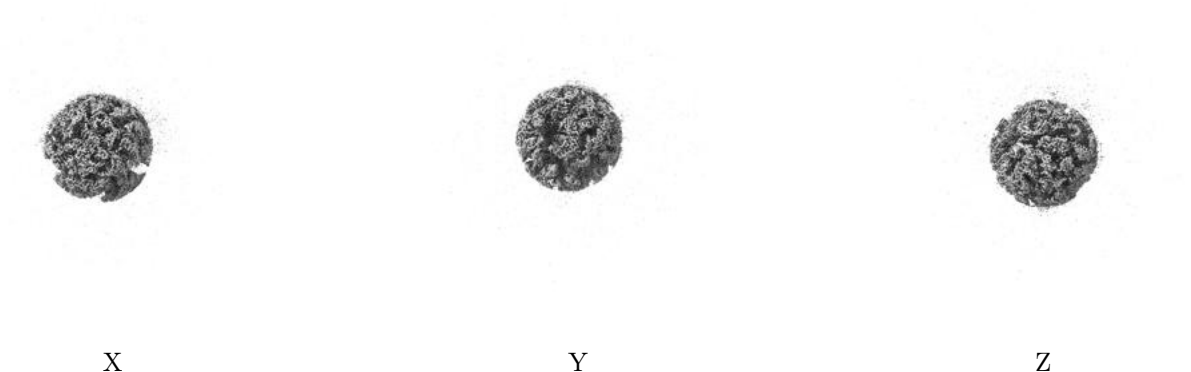


Z

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

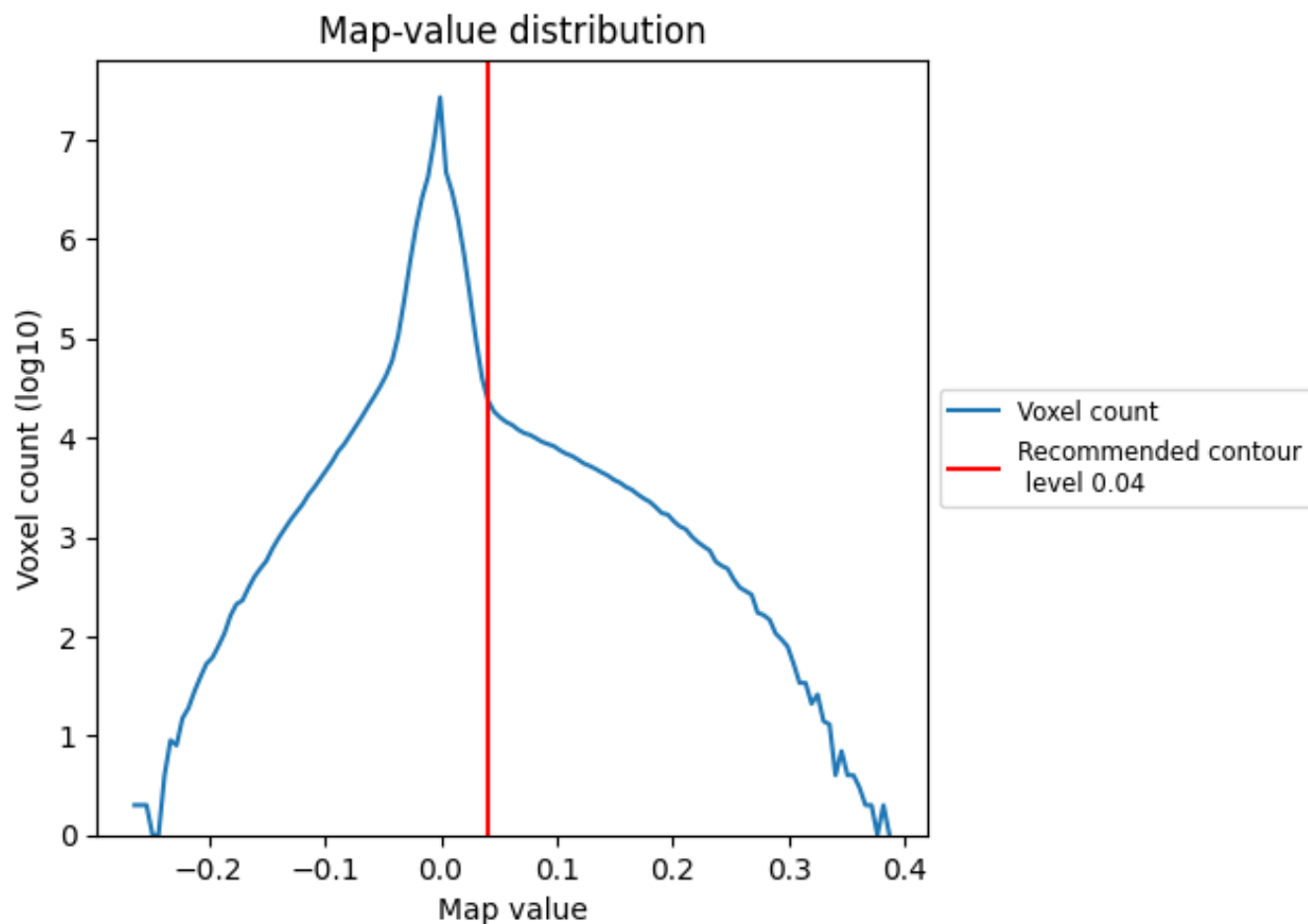
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

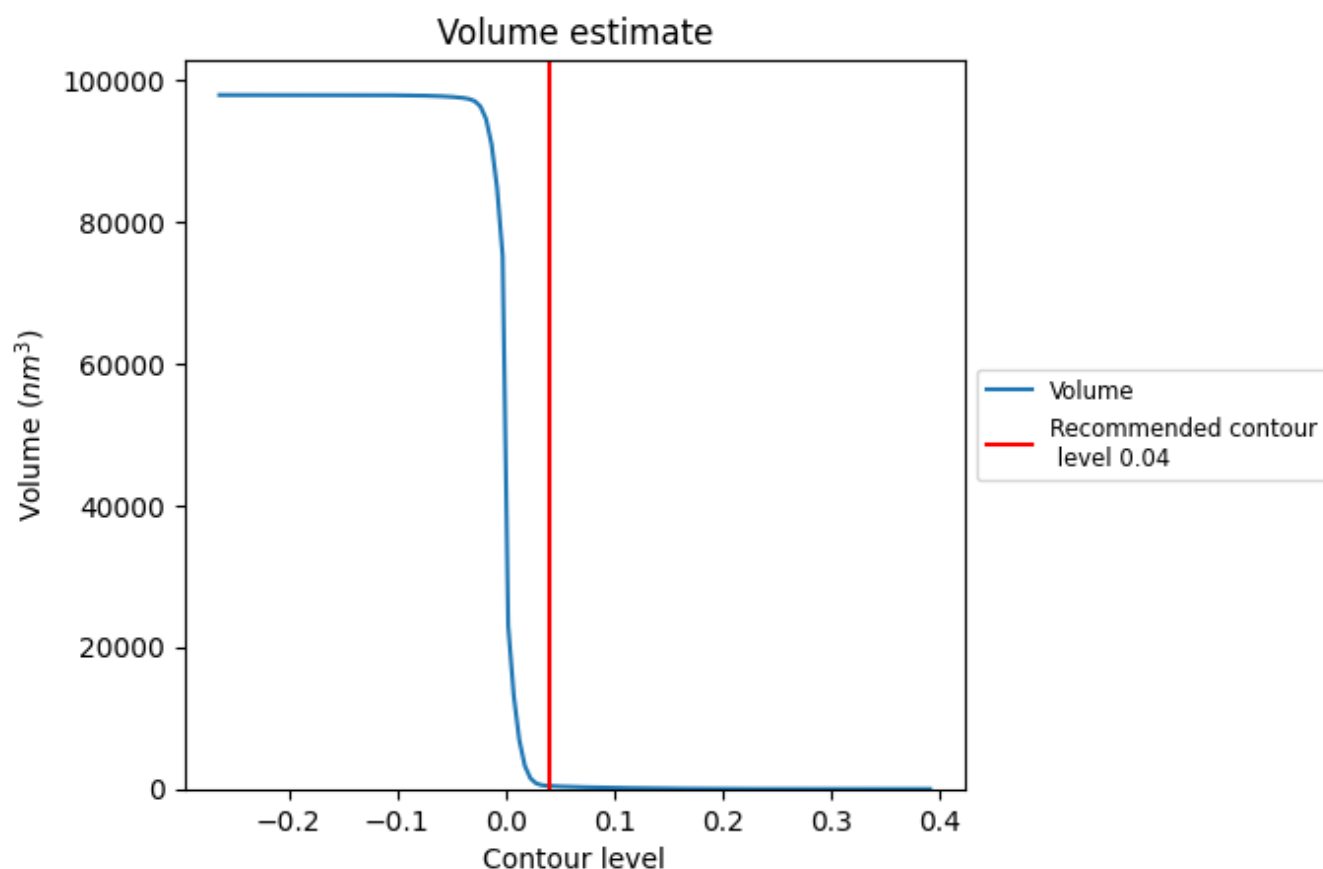
This section contains the results of statistical analysis of the map.

### 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.

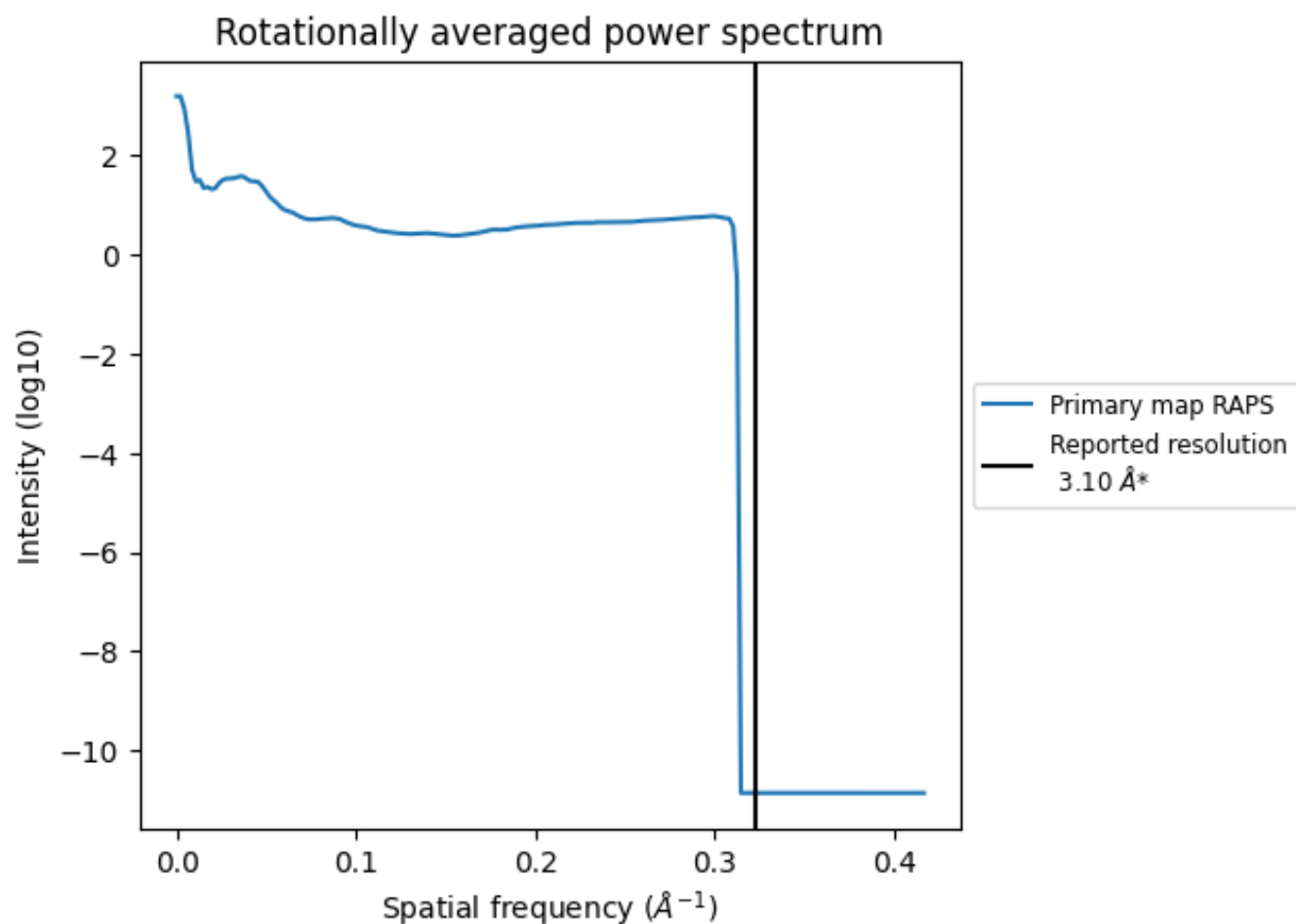
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 432  $\text{nm}^3$ ; this corresponds to an approximate mass of 390 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 ⓘ



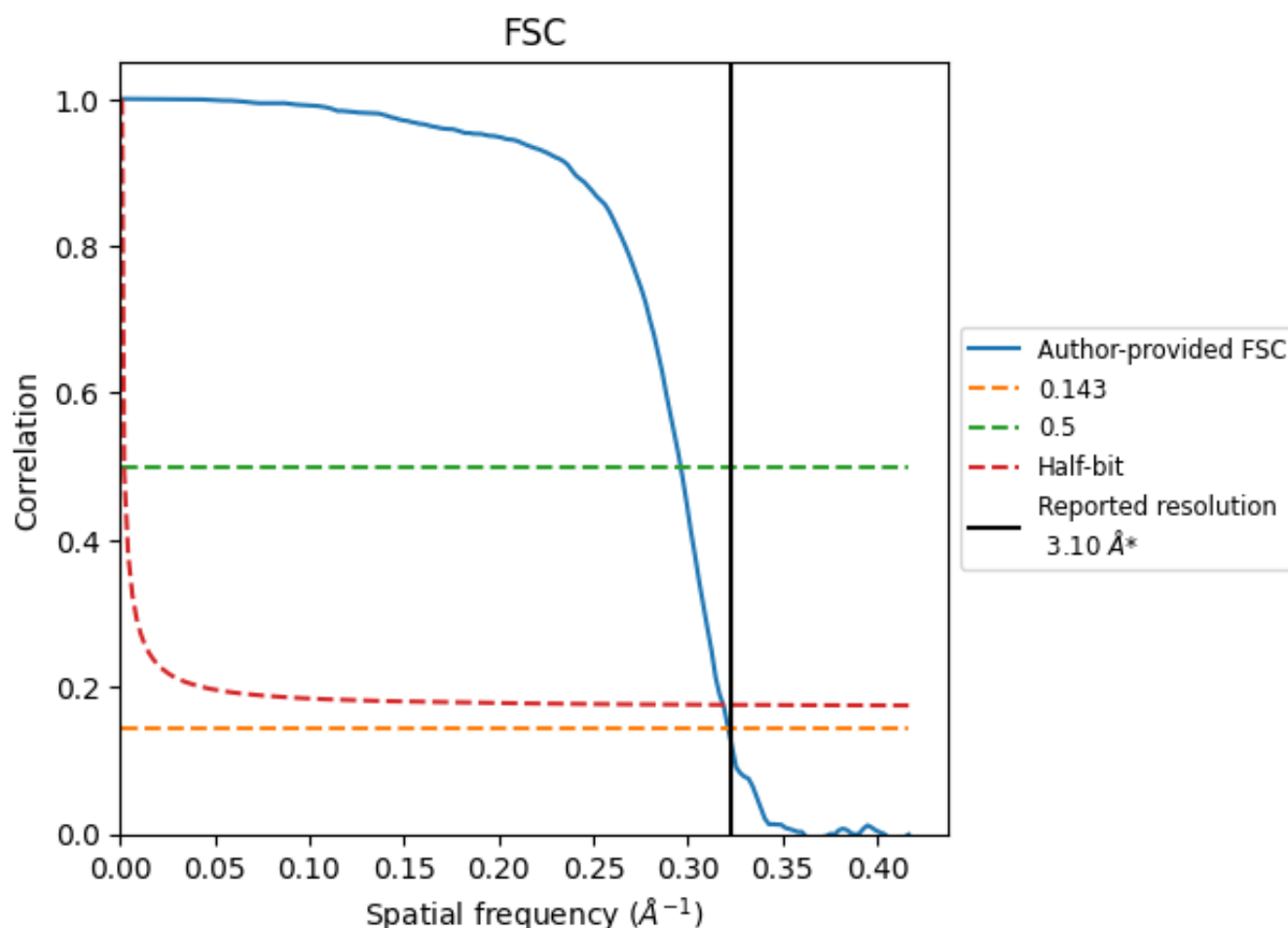
\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$



## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

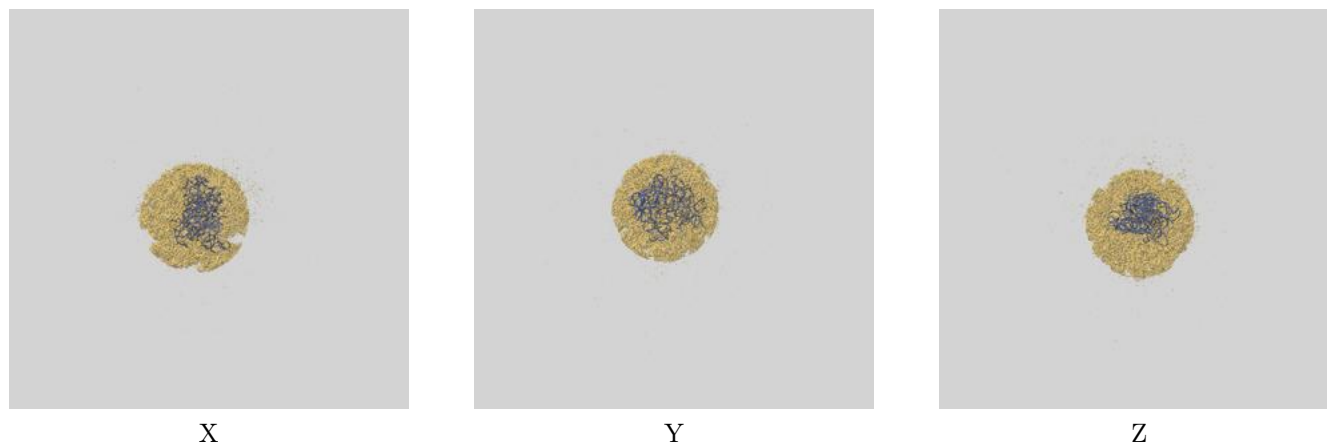
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.38	3.14
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

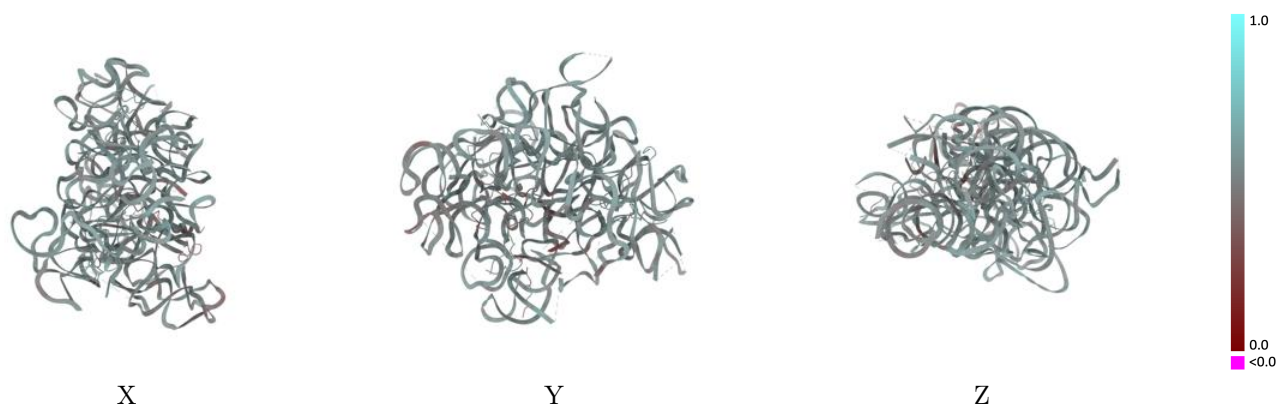
This section contains information regarding the fit between EMDB map EMD-7340 and PDB model 6C4H. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



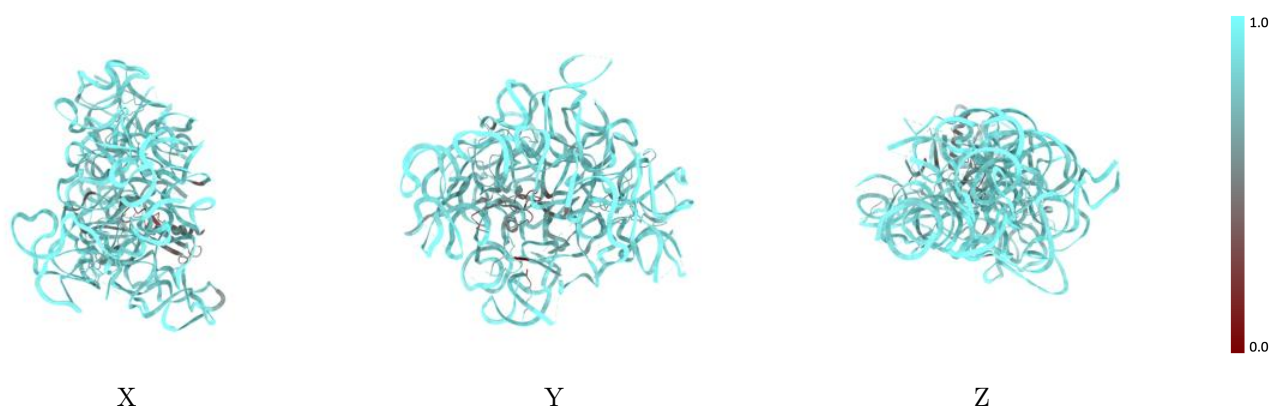
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



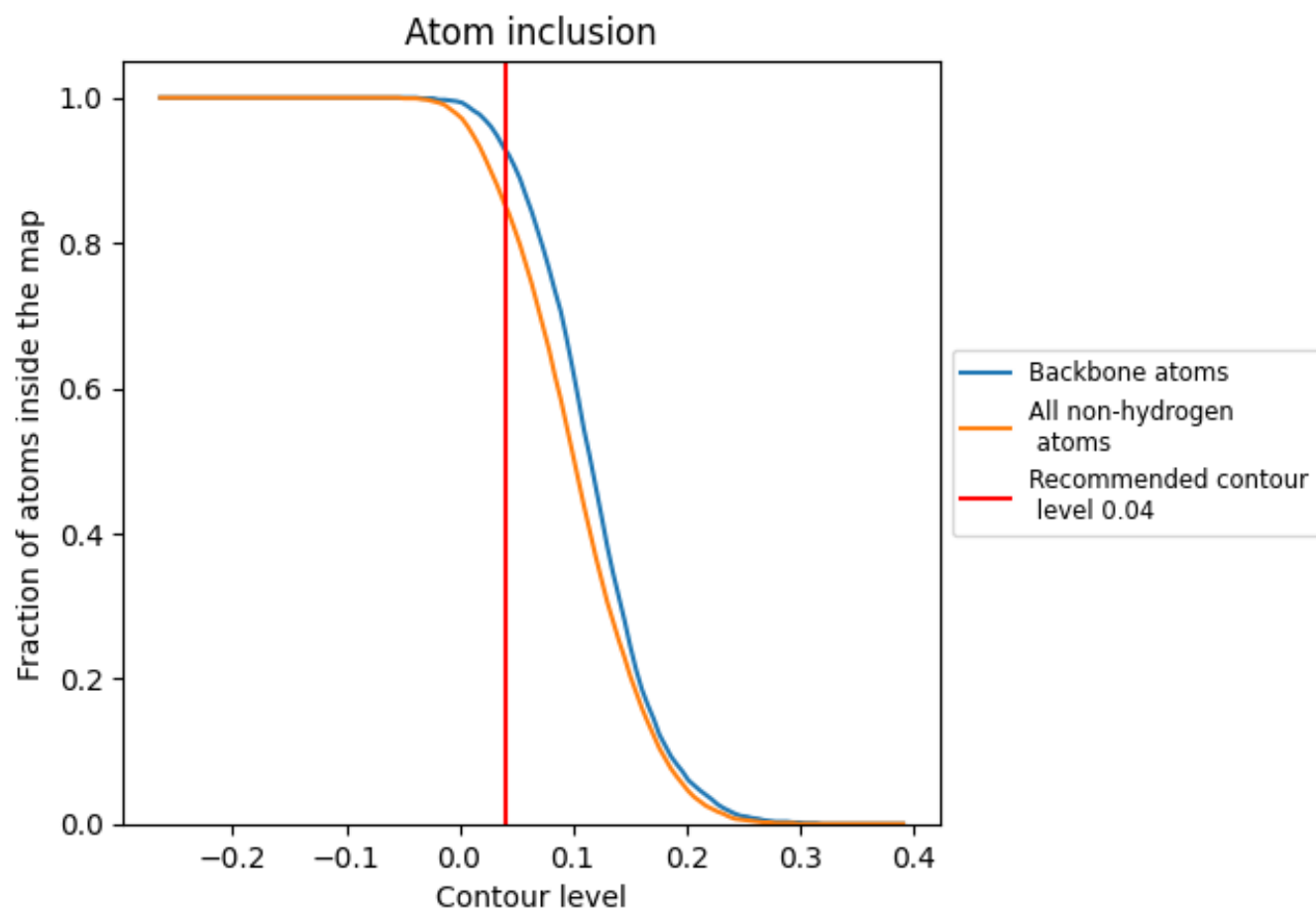
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 85% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8530	<div><div></div></div> 0.5290
A	<div><div></div></div> 0.8750	<div><div></div></div> 0.5320
C	<div><div></div></div> 0.8200	<div><div></div></div> 0.5550
D	<div><div></div></div> 0.8140	<div><div></div></div> 0.5670
N	<div><div></div></div> 0.7560	<div><div></div></div> 0.5410
X	<div><div></div></div> 0.5920	<div><div></div></div> 0.4630
v	<div><div></div></div> 0.4900	<div><div></div></div> 0.4570
x	<div><div></div></div> 0.6270	<div><div></div></div> 0.4170

1.0

0.0

<0.0