



# wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 01:22 AM EDT

PDB ID : 8E82 / pdb\_00008e82  
EMDB ID : EMD-27942  
Title : Mycobacterium tuberculosis RNAP elongation complex with NusG transcription factor  
Authors : Delbeau, M.; Darst, S.A.; Campbell, E.A.  
Deposited on : 2022-08-25  
Resolution : 3.03 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.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

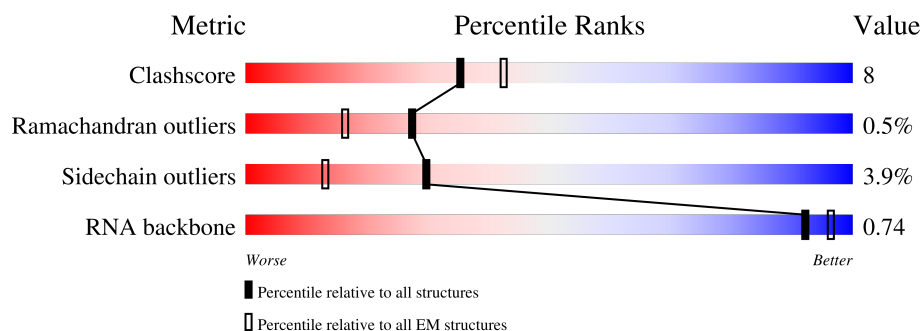
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.03 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	347	
1	B	347	
2	C	1172	
3	D	1318	
4	E	110	
5	Z	238	
6	P	54	

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Mol	Chain	Length	Quality of chain
7	Q	54	<div><div><div></div><div></div><div></div></div><div>17%43%54%</div></div>
8	R	20	<div><div><div></div><div></div><div></div></div><div>5%30%20%50%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24900 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1769	1117	301	348	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1095	Total	C	N	O	S	0	0
			8485	5310	1490	1646	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1269	Total	C	N	O	S	0	0
			9916	6212	1802	1860	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A0A045J9E2
D	0	ALA	-	expression tag	UNP A0A045J9E2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	82	Total	C	N	O	0	0
			645	412	107	126		

- Molecule 5 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	122	Total	C	N	O	S	0	0
			957	607	168	181	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	VAL	-	expression tag	UNP A0A045HU92

- Molecule 6 is a DNA chain called DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	33	Total	C	N	O	P	0	0
			666	316	116	201	33		

- Molecule 7 is a DNA chain called DNA (54-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	25	Total	C	N	O	P	0	0
			514	242	97	150	25		

- Molecule 8 is a RNA chain called RNA (5'-R(P\*CP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*UP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	10	Total	C	N	O	P	0	0
			221	98	45	68	10		

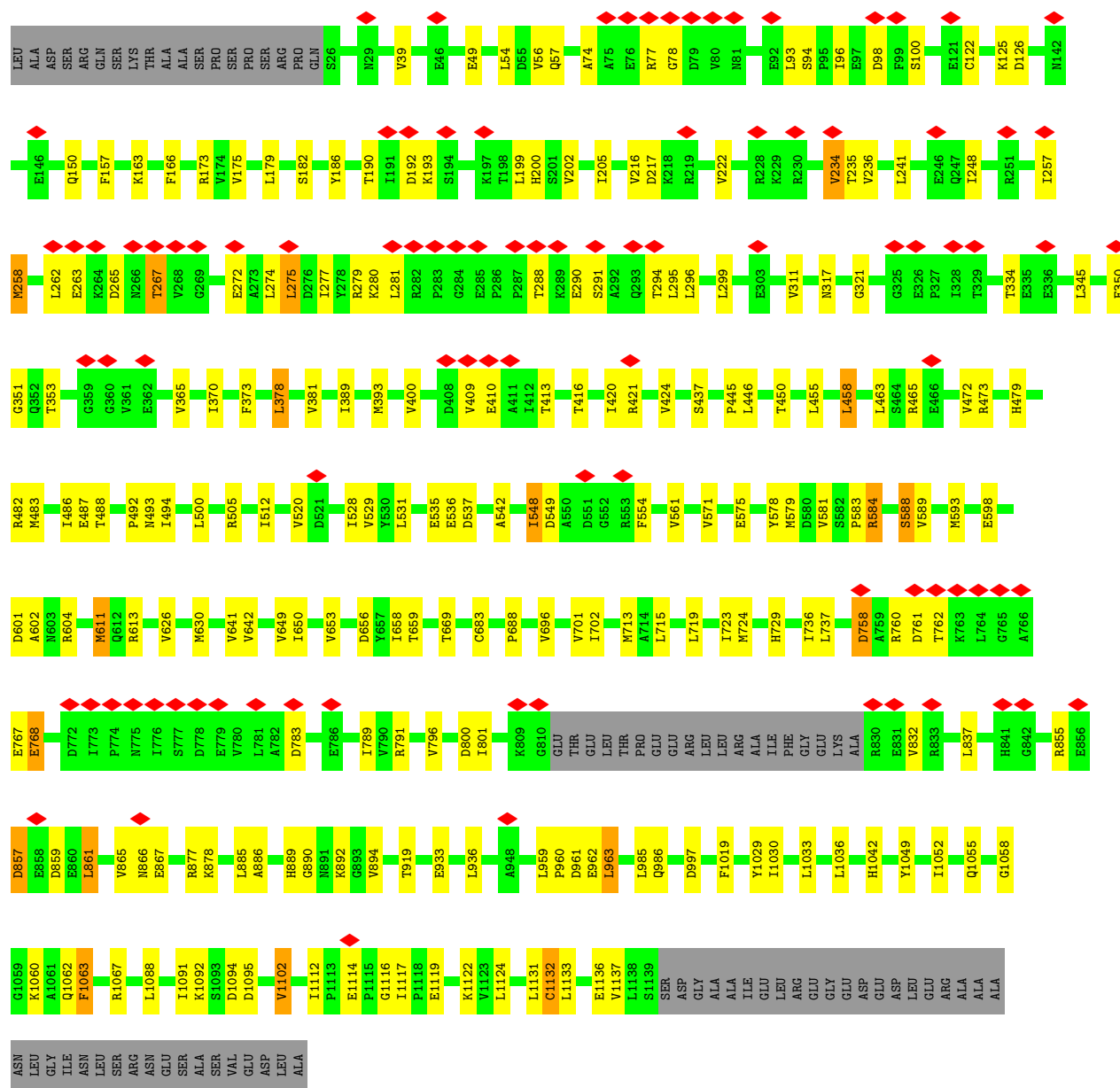
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

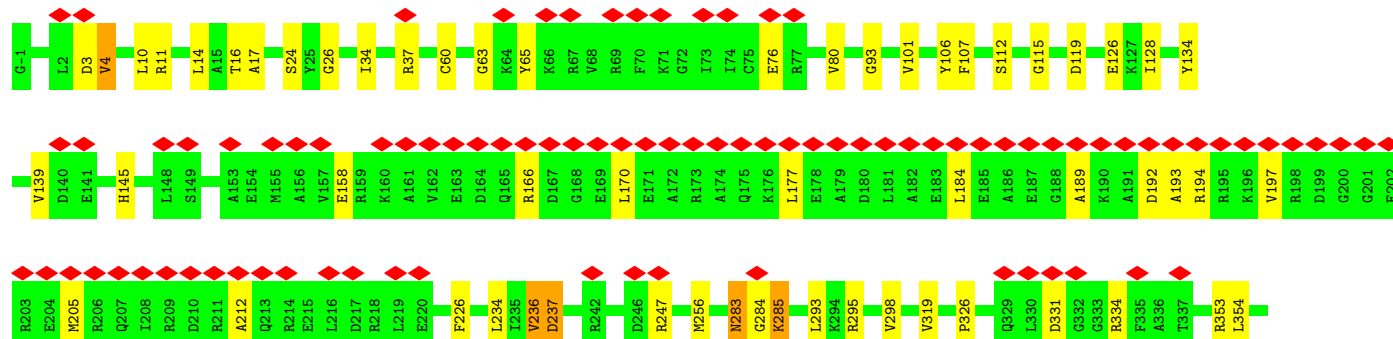
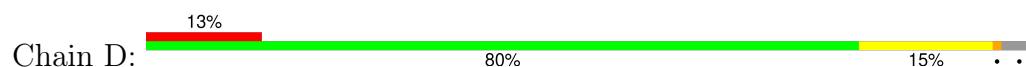
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

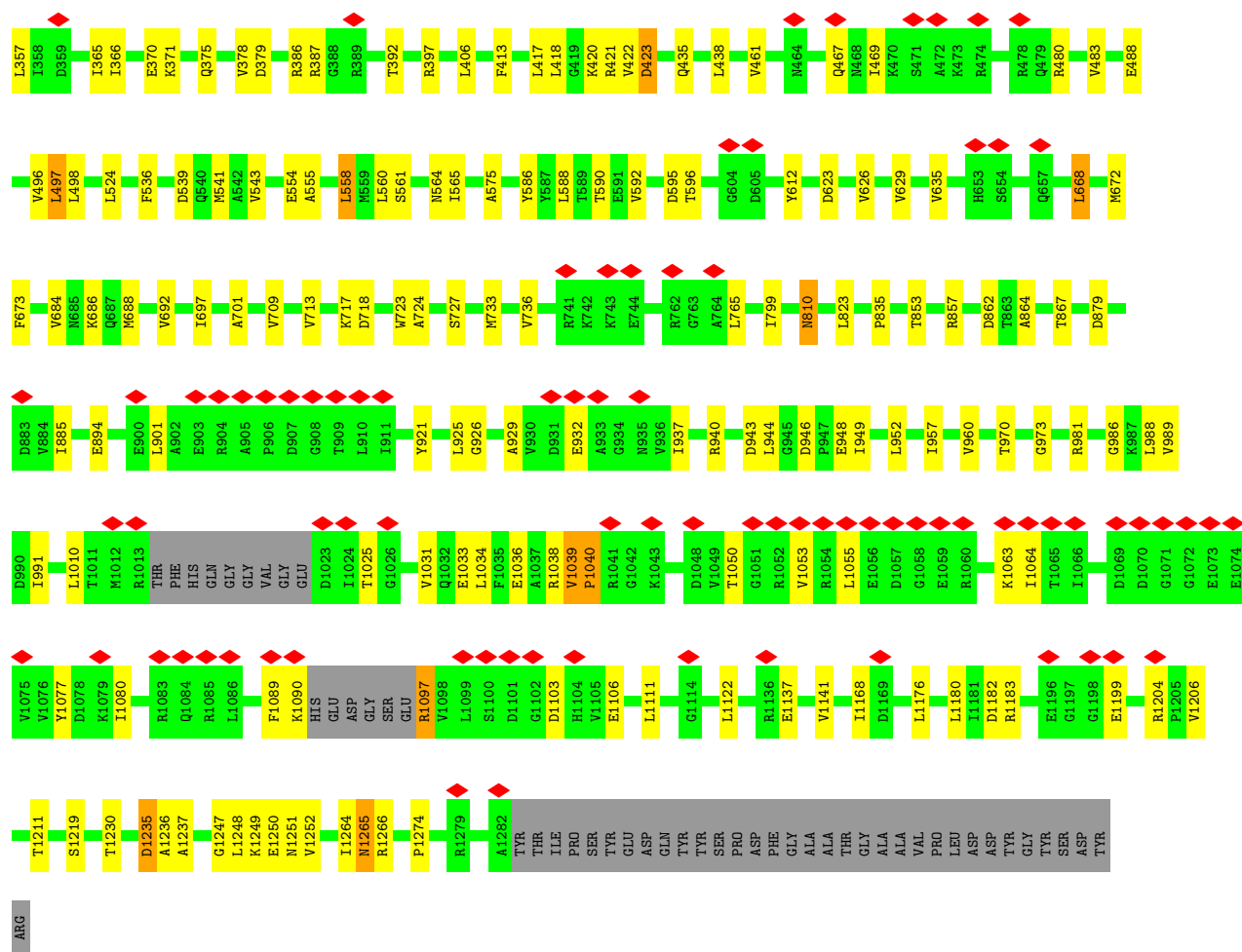
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	



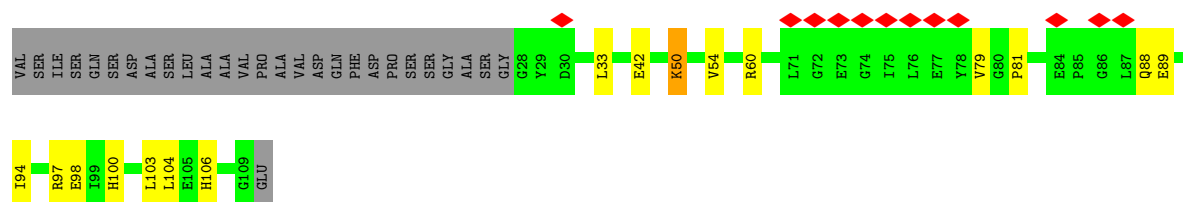


• Molecule 3: DNA-directed RNA polymerase subunit beta'

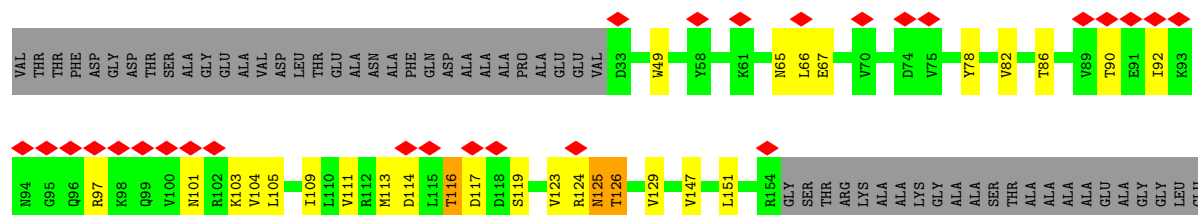




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: Transcription termination/antitermination protein NusG





ARG	PRO	VAL	VAL	GLU	ASP	TYR	GLU	VAL	GLY	GLU	SER	VAL	THR	VAL	MET	ASP	GLY	PRO	PHE	ALA	THR	LEU	PRO	ALA	THR	ILE	SER	GLU	VAL	ASN	ALA	GLU	GLN	GLN	LYS	LEU	LYS	VAL	LEU	VAL	SER	ILE	PHE	GLY	ARG	GLU	THR	PRO	VAL	GLU	THR	PHE	GLY	GLN	VAL	SER	LYS
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• Molecule 6: DNA (54-MER)



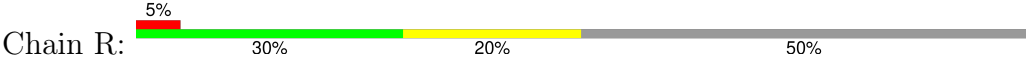
DC	DC	DG	DT	DC	DG	DA	DT	DG	DA	G110	A111	G112	G113	G114	T115	A116	T117	T118	A127	G128	C129	A136	G137	C138	C139	C140	G141	C142	DA	DA	DG	DT	DA	DT	DC	DC	DA	DA	DC	DG
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• Molecule 7: DNA (54-MER)



DC	DG	DC	DC	DG	DA	DT	DA	DC	DT	G13	C14	G15	G16	G17	A20	DG	DC	DC	DT	DT	DT	T29	C41	C42	C43	T44	C45	DT	DC	DA	DT	DG	DC	DC	DG	DG
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• Molecule 8: RNA (5'-R(P\*CP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*UP\*A)-3')



G	C	A	U	U	C	A	A	G	C11	G12	G17	A20
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132324	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 ( $e^-/\text{\AA}^2$ )	64.78	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.742	Depositor
Minimum map value	-2.378	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	322.8, 322.8, 322.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.15	0/1750	0.34	0/2380
1	B	0.19	0/1796	0.40	0/2447
2	C	0.17	0/8641	0.38	0/11716
3	D	0.15	0/10080	0.35	0/13625
4	E	0.14	0/658	0.38	0/896
5	Z	0.17	0/976	0.43	0/1328
6	P	0.31	0/743	0.60	2/1142 (0.2%)
7	Q	0.18	0/575	0.38	0/883
8	R	0.13	0/248	0.27	0/386
All	All	0.17	0/25467	0.38	2/34803 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	111	DA	P-O3'-C3'	-6.54	110.39	120.20
6	P	112	DG	P-O3'-C3'	-5.89	111.37	120.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1724	0	1768	31	0
1	B	1769	0	1798	35	0
2	C	8485	0	8415	166	0
3	D	9916	0	10006	141	0
4	E	645	0	642	10	0
5	Z	957	0	961	18	0
6	P	666	0	371	14	0
7	Q	514	0	281	3	0
8	R	221	0	109	3	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	24900	0	24351	378	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 378 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:LEU:HD13	2:C:295:LEU:HD22	1.49	0.95
2:C:277:ILE:HG22	2:C:281:LEU:HD11	1.57	0.87
5:Z:103:LYS:O	5:Z:105:LEU:N	2.07	0.87
5:Z:65:ASN:OD1	5:Z:126:THR:OG1	1.94	0.84
2:C:1124:LEU:HD22	3:D:417:LEU:HD11	1.60	0.84

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	224/347 (65%)	209 (93%)	15 (7%)	0	100	100
1	B	235/347 (68%)	213 (91%)	18 (8%)	4 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1091/1172 (93%)	1005 (92%)	79 (7%)	7 (1%)	22	54
3	D	1263/1318 (96%)	1201 (95%)	59 (5%)	3 (0%)	44	74
4	E	80/110 (73%)	76 (95%)	4 (5%)	0	100	100
5	Z	120/238 (50%)	108 (90%)	11 (9%)	1 (1%)	16	47
All	All	3013/3532 (85%)	2812 (93%)	186 (6%)	15 (0%)	27	58

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	ILE
1	B	25	PRO
2	C	77	ARG
2	C	126	ASP
2	C	584	ARG

### 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	195/297 (66%)	191 (98%)	4 (2%)	48	74
1	B	196/297 (66%)	185 (94%)	11 (6%)	17	46
2	C	928/993 (94%)	883 (95%)	45 (5%)	21	52
3	D	1050/1095 (96%)	1021 (97%)	29 (3%)	38	67
4	E	69/90 (77%)	66 (96%)	3 (4%)	25	55
5	Z	103/189 (54%)	95 (92%)	8 (8%)	10	34
All	All	2541/2961 (86%)	2441 (96%)	100 (4%)	30	59

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1062	GLN
3	D	353	ARG

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Mol	Chain	Res	Type
5	Z	126	THR
2	C	1117	ILE
3	D	205	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1066	GLN
3	D	510	GLN
3	D	1239	ASN
3	D	767	HIS
3	D	1125	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	R	9/20 (45%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

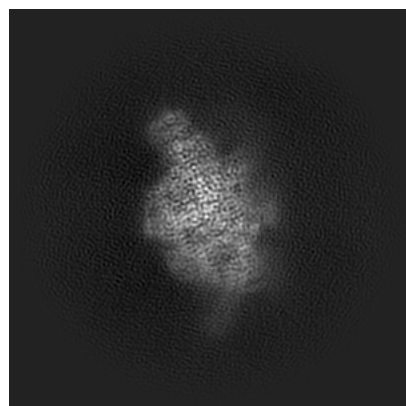
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27942. These allow visual inspection of the internal detail of the map and identification of artifacts.

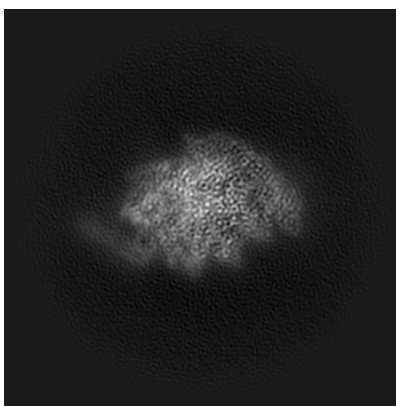
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

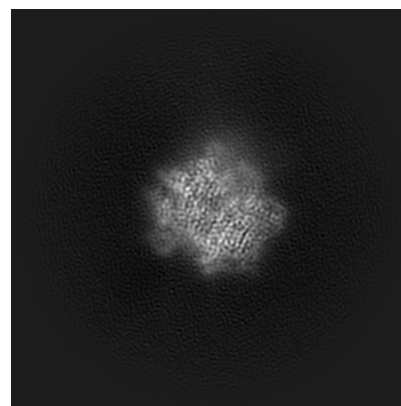
#### 6.1.1 Primary map



X

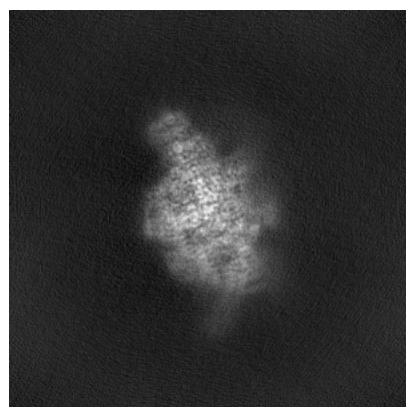


Y

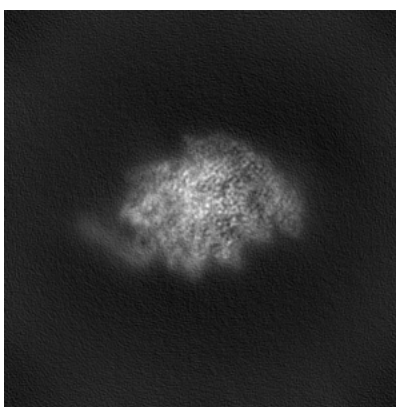


Z

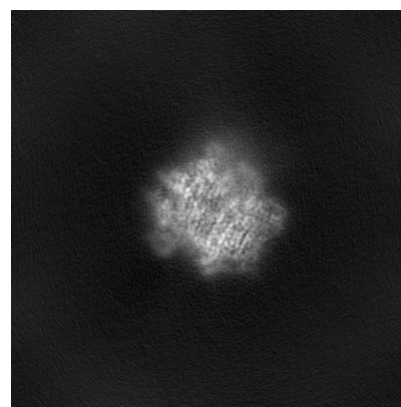
#### 6.1.2 Raw map



X



Y



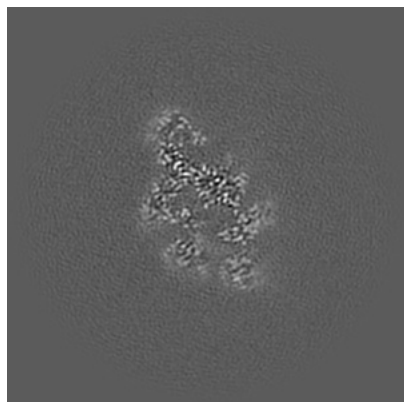
Z

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

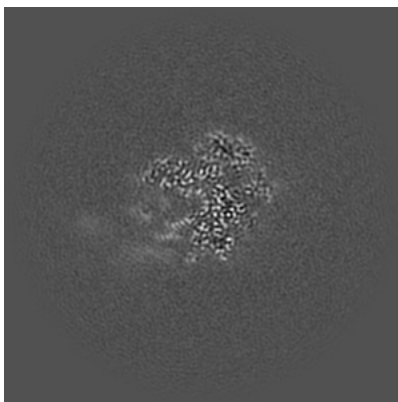


## 6.2 Central slices [i](#)

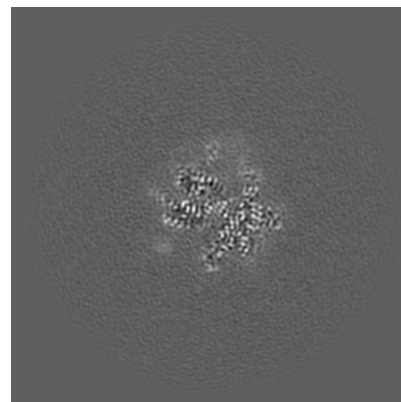
### 6.2.1 Primary map



X Index: 150

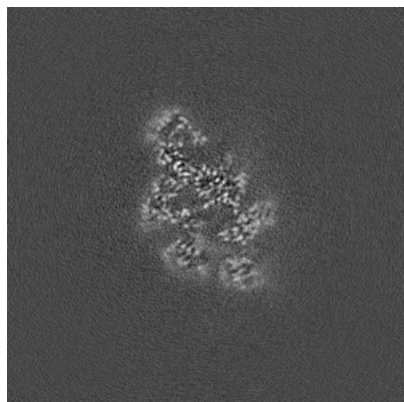


Y Index: 150

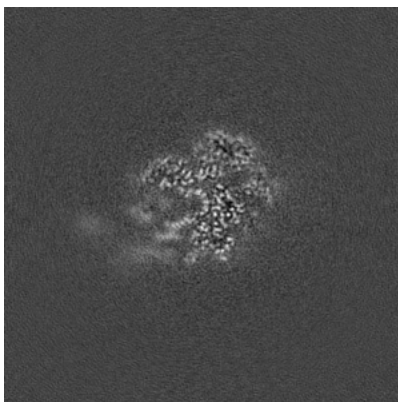


Z Index: 150

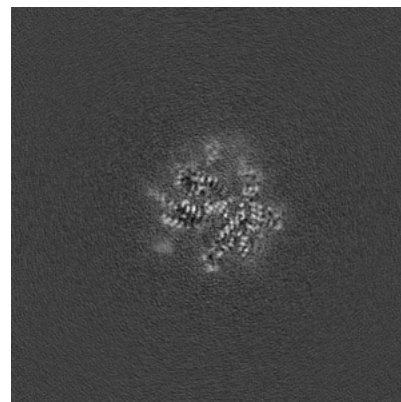
### 6.2.2 Raw map



X Index: 150



Y Index: 150

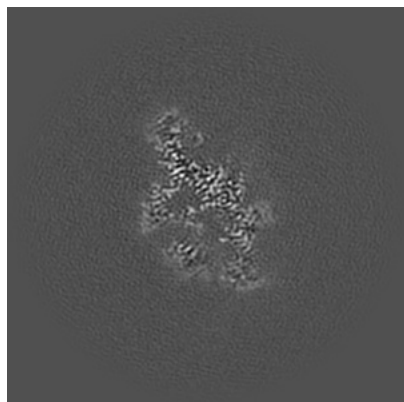


Z Index: 150

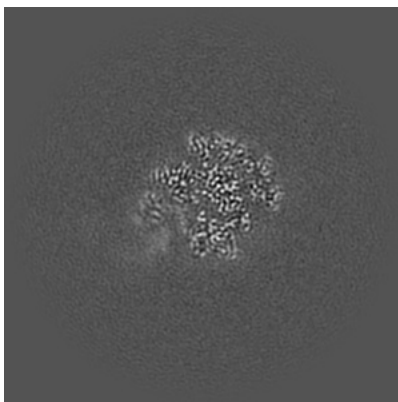
The images above show central slices of the map in three orthogonal directions.

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

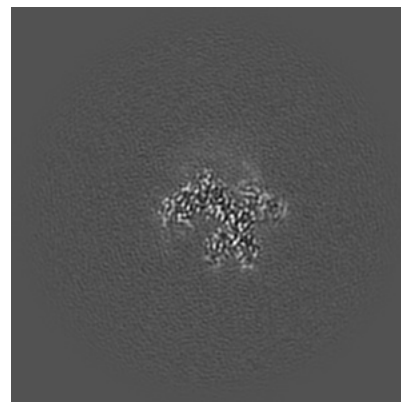
### 6.3.1 Primary map



X Index: 148

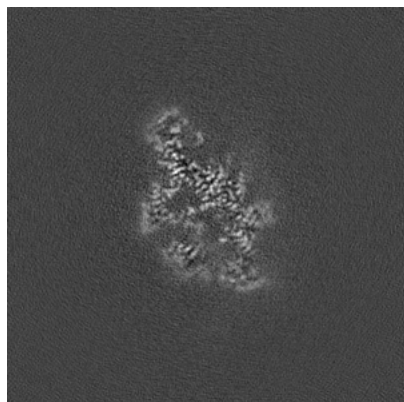


Y Index: 143

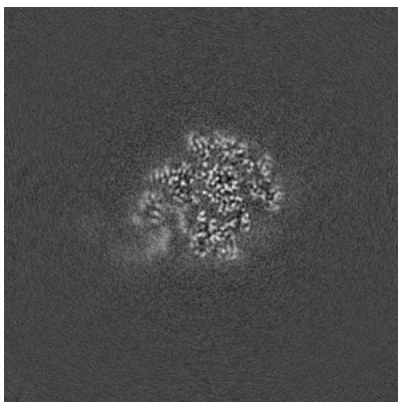


Z Index: 160

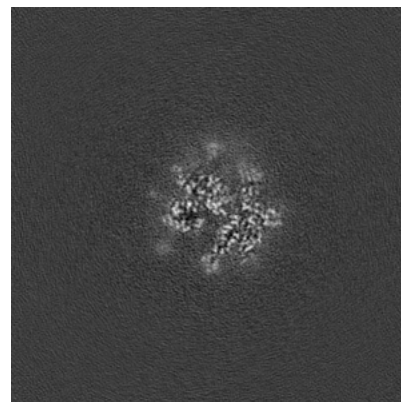
### 6.3.2 Raw map



X Index: 148



Y Index: 143

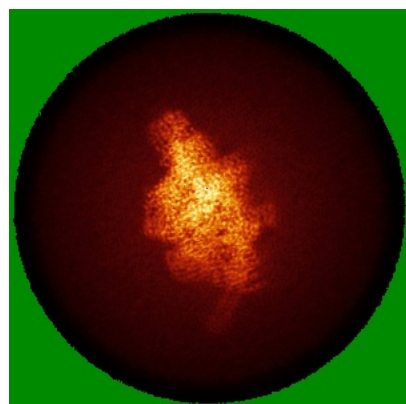


Z Index: 152

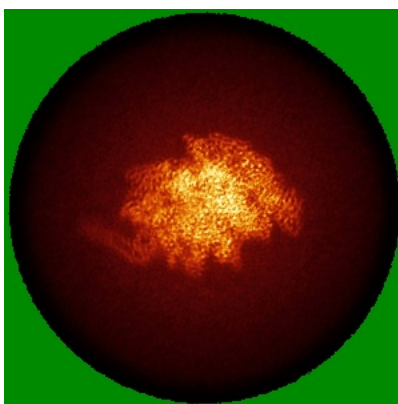
The images above show the largest variance slices of the map in three orthogonal directions.

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

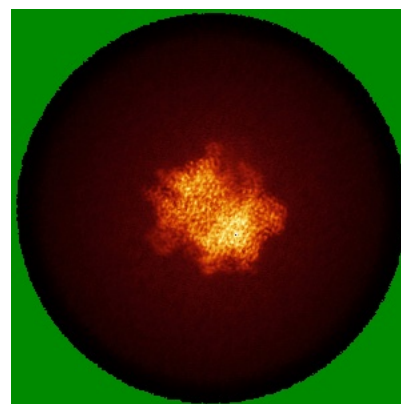
### 6.4.1 Primary map



X

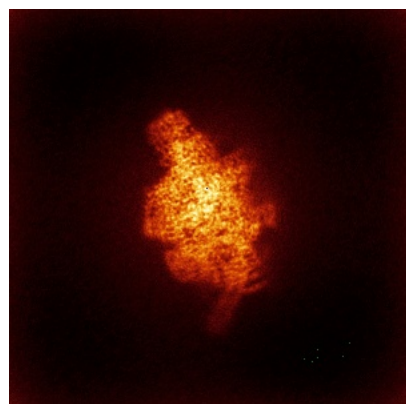


Y

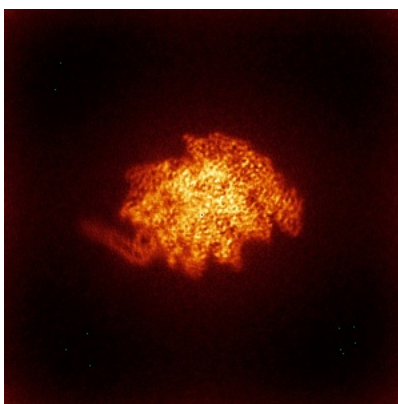


Z

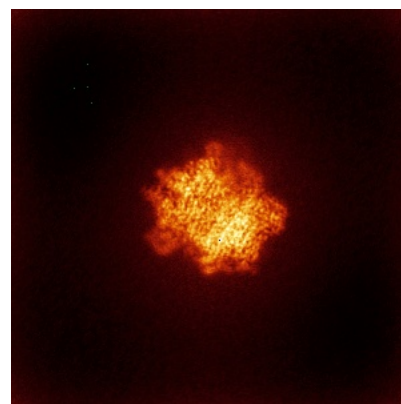
### 6.4.2 Raw map



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.

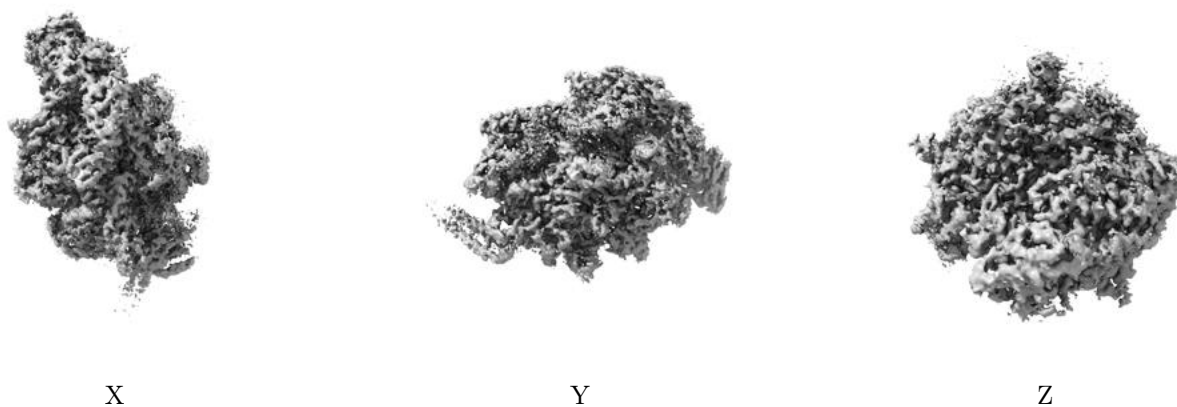
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

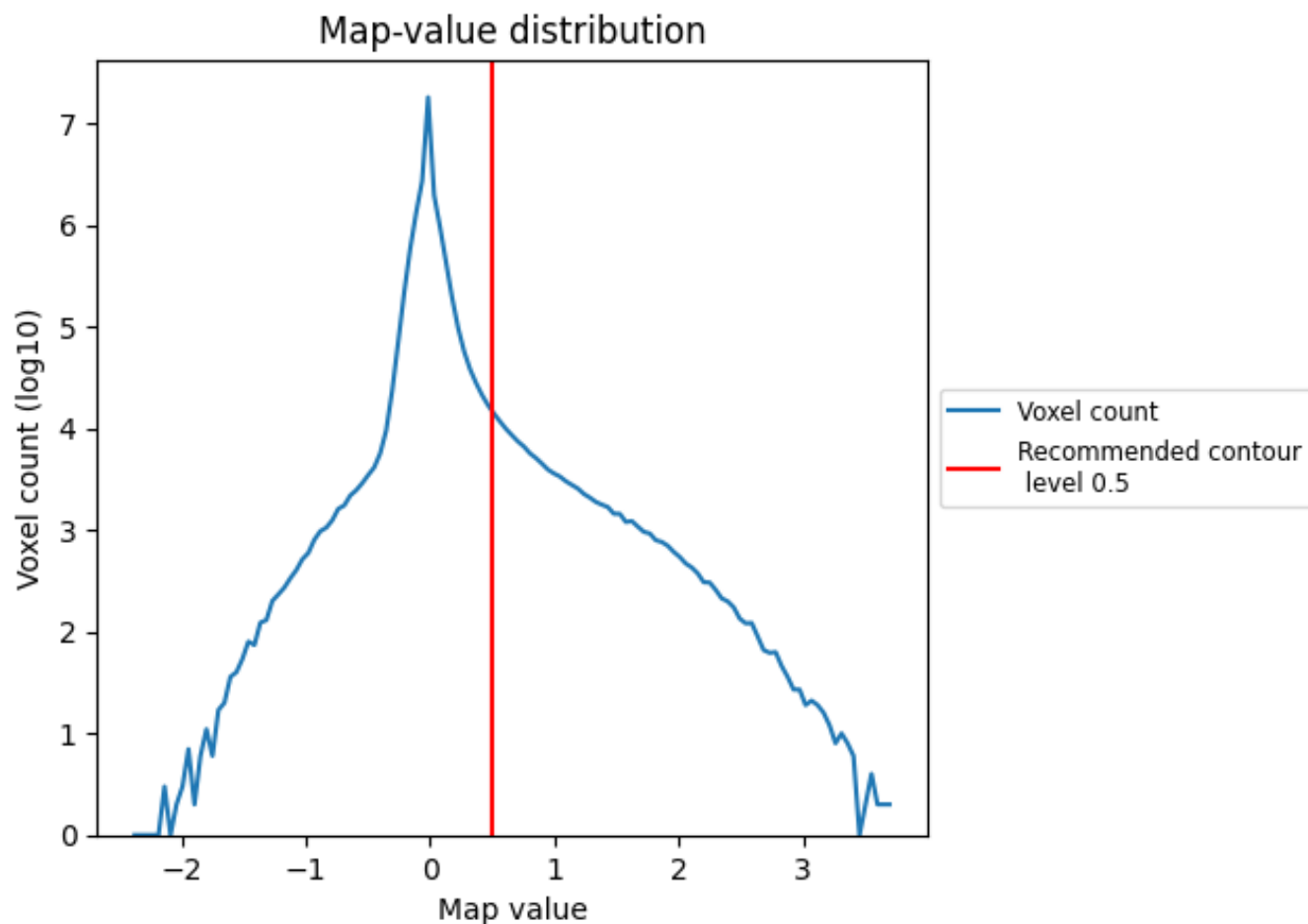
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

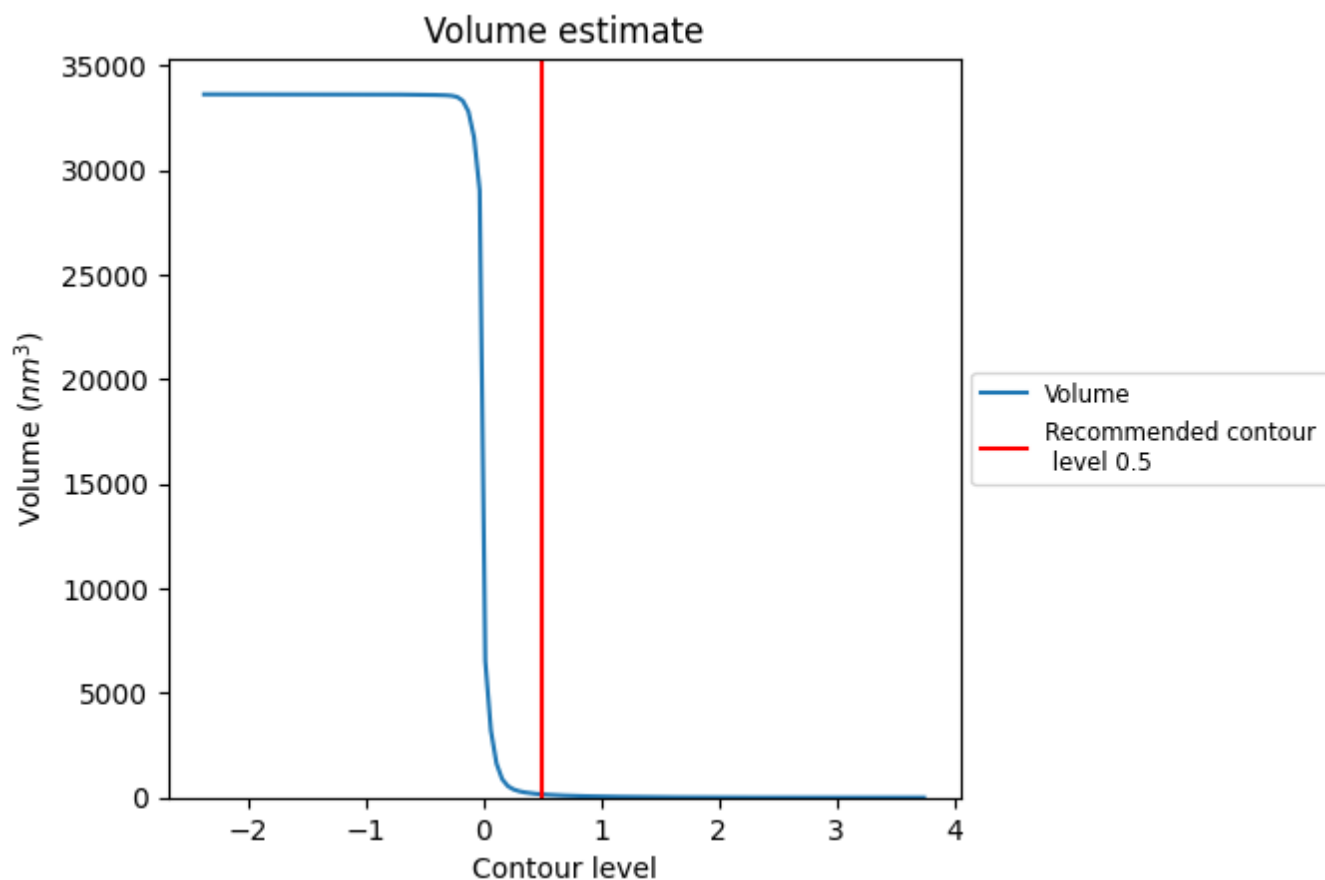
This section contains the results of statistical analysis of the map.

### 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.

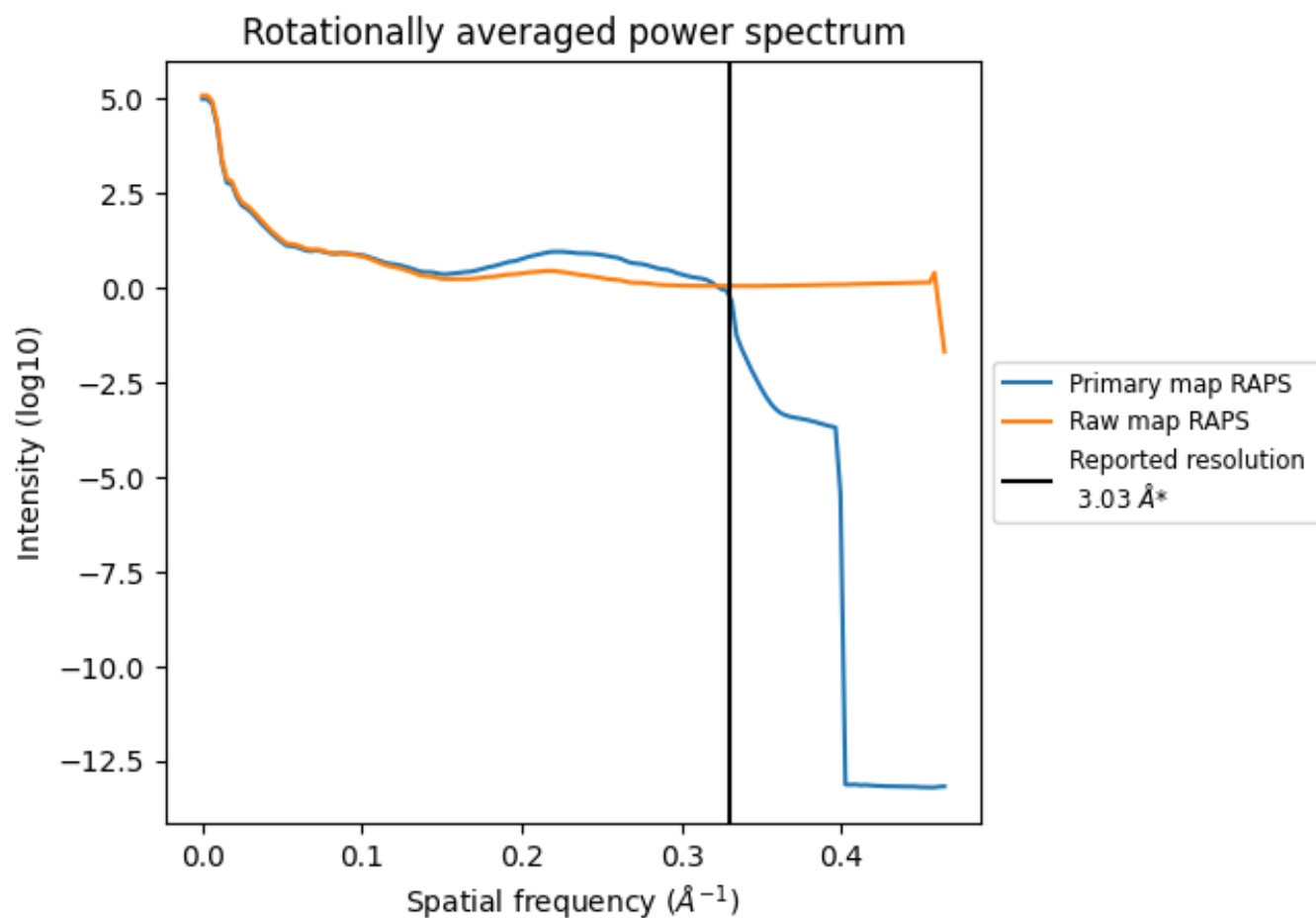
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm<sup>3</sup>; this corresponds to an approximate mass of 138 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 ⓘ



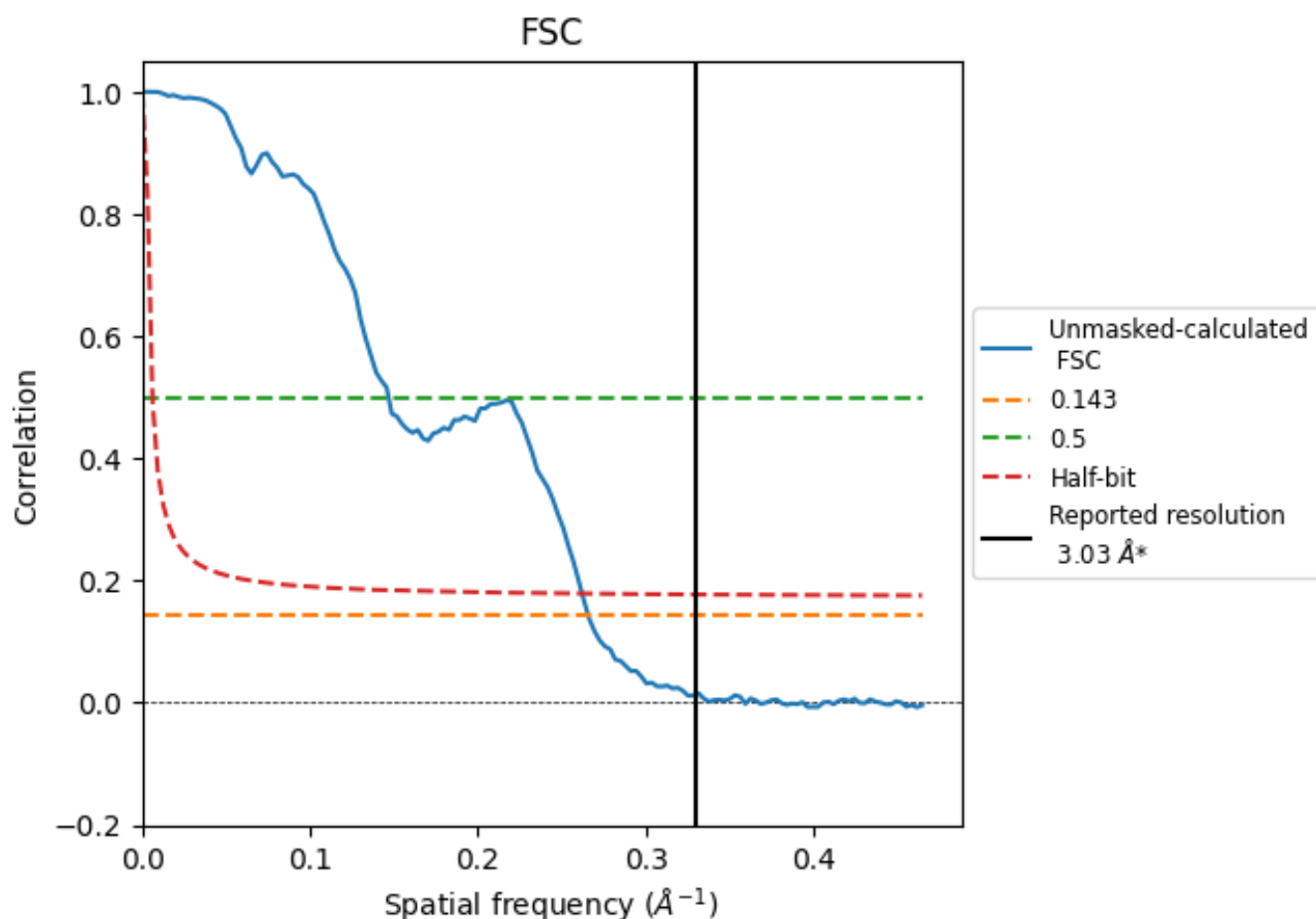
\*Reported resolution corresponds to spatial frequency of 0.330 Å<sup>-1</sup>



## 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 0.330 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

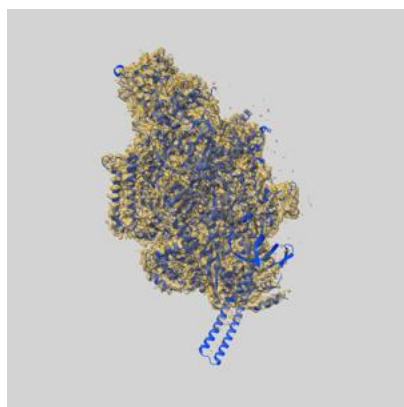
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	6.81	3.82

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.03 by more than 10 %

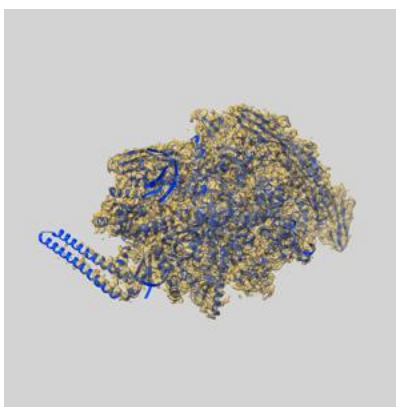
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27942 and PDB model 8E82. Per-residue inclusion information can be found in section 3 on page 6.

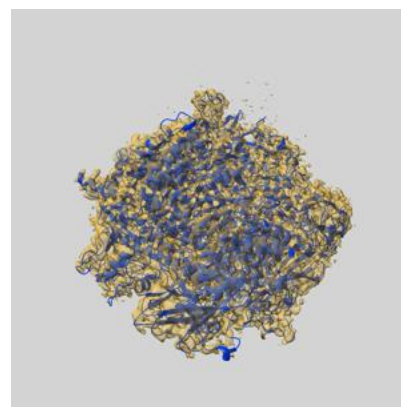
### 9.1 Map-model overlay [i](#)



X



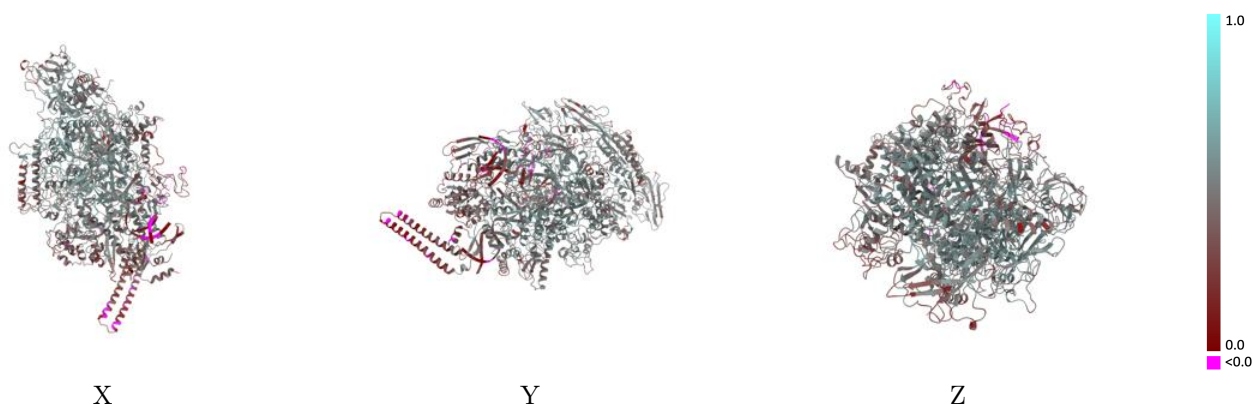
Y



Z

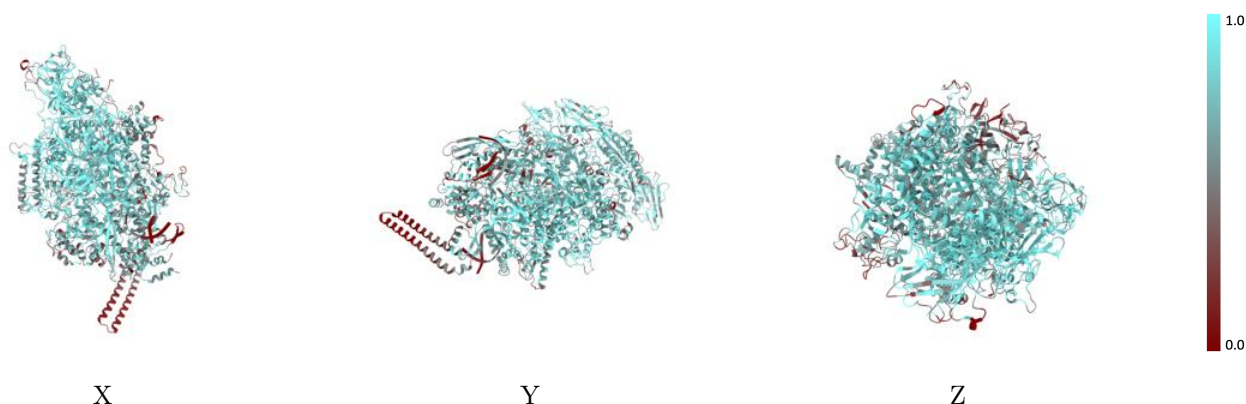
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



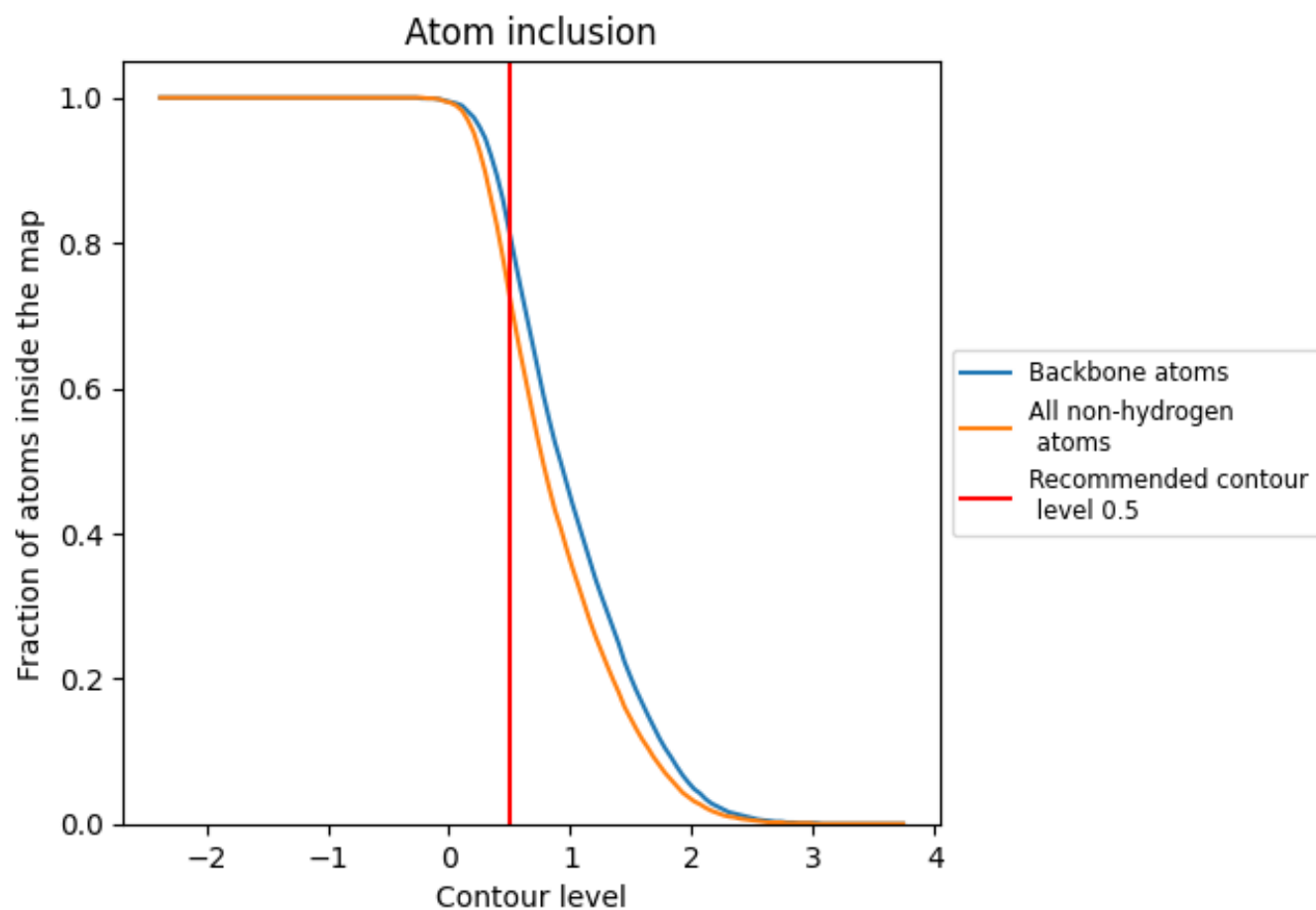
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7270	<div></div> 0.4470
A	<div></div> 0.7780	<div></div> 0.4770
B	<div></div> 0.7240	<div></div> 0.4510
C	<div></div> 0.7650	<div></div> 0.4710
D	<div></div> 0.7190	<div></div> 0.4430
E	<div></div> 0.6690	<div></div> 0.4730
P	<div></div> 0.6260	<div></div> 0.3200
Q	<div></div> 0.5160	<div></div> 0.2740
R	<div></div> 0.8820	<div></div> 0.5090
Z	<div></div> 0.5850	<div></div> 0.3620

1.0

0.0

<0.0