



# wwPDB EM Validation Summary Report ⓘ

Feb 11, 2023 – 12:28 PM EST

PDB ID : 8E3F  
EMDB ID : EMD-27864  
Title : Escherichia coli Rho-dependent transcription pre-termination complex containing 18 nt long RNA spacer, Mg-ADP-BeF<sub>3</sub>, and NusG; TEC part  
Authors : Molodtsov, V.; Wang, C.  
Deposited on : 2022-08-17  
Resolution : 6.50 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:

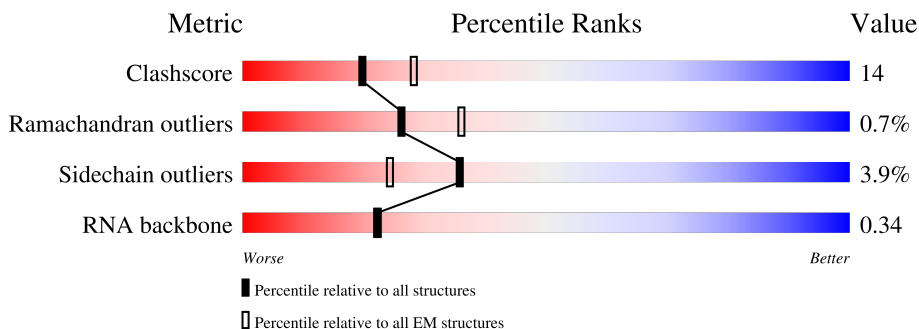
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.50 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
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	5	60	18% (green), 28% (yellow), 8% (orange), 45% (grey)
2	6	60	23% (green), 33% (yellow), 5% (orange), 38% (grey)
3	7	35	6% (red), 31% (green), 17% (yellow), 51% (grey)
4	A	1342	81% (green), 18% (yellow), 1% (orange)
5	B	1407	67% (green), 24% (yellow), 5% (orange)
6	C	329	61% (green), 5% (yellow), 33% (grey)
6	D	329	54% (green), 12% (yellow), 34% (grey)

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Mol	Chain	Length	Quality of chain
7	E	91	
8	F	181	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 39229 atoms, of which 11229 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 DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	5	33	913	322	237	125	196	33	0	0

- Molecule 2 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	6	37	1031	357	283	126	228	37	0	0

- Molecule 3 is a RNA chain called RNA with 18 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
3	7	17	464	163	97	64	123	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1340	10567	6631	1841	2052	43	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	B	1335	21000	6526	10612	1854	1958	50	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	221	1698	1060	299	333	6	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	218	1677	1048	297	326	6	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	75	600	365	114	120	1	0	0

- Molecule 8 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	161	1276	813	221	235	7	0	0

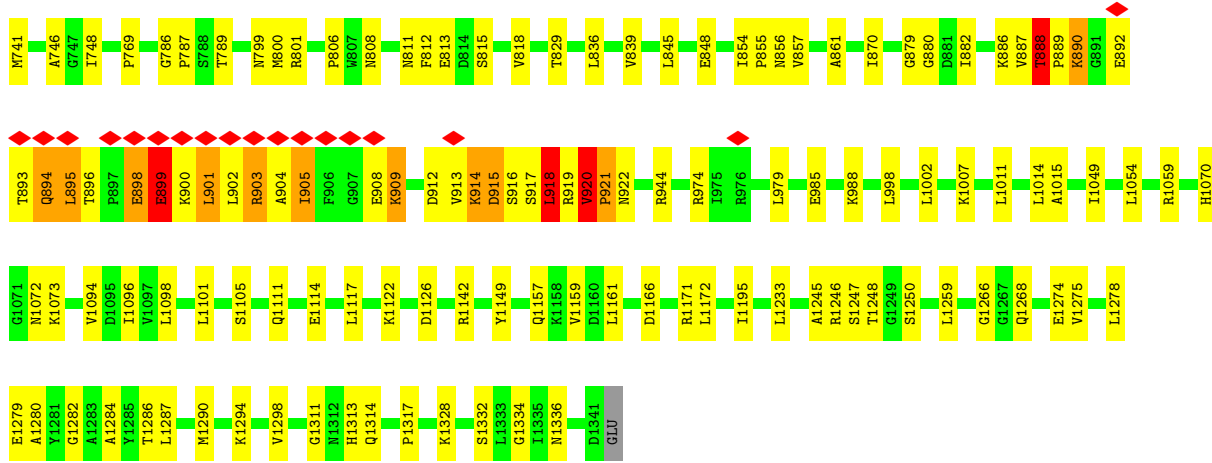
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	B	1	1	1	0

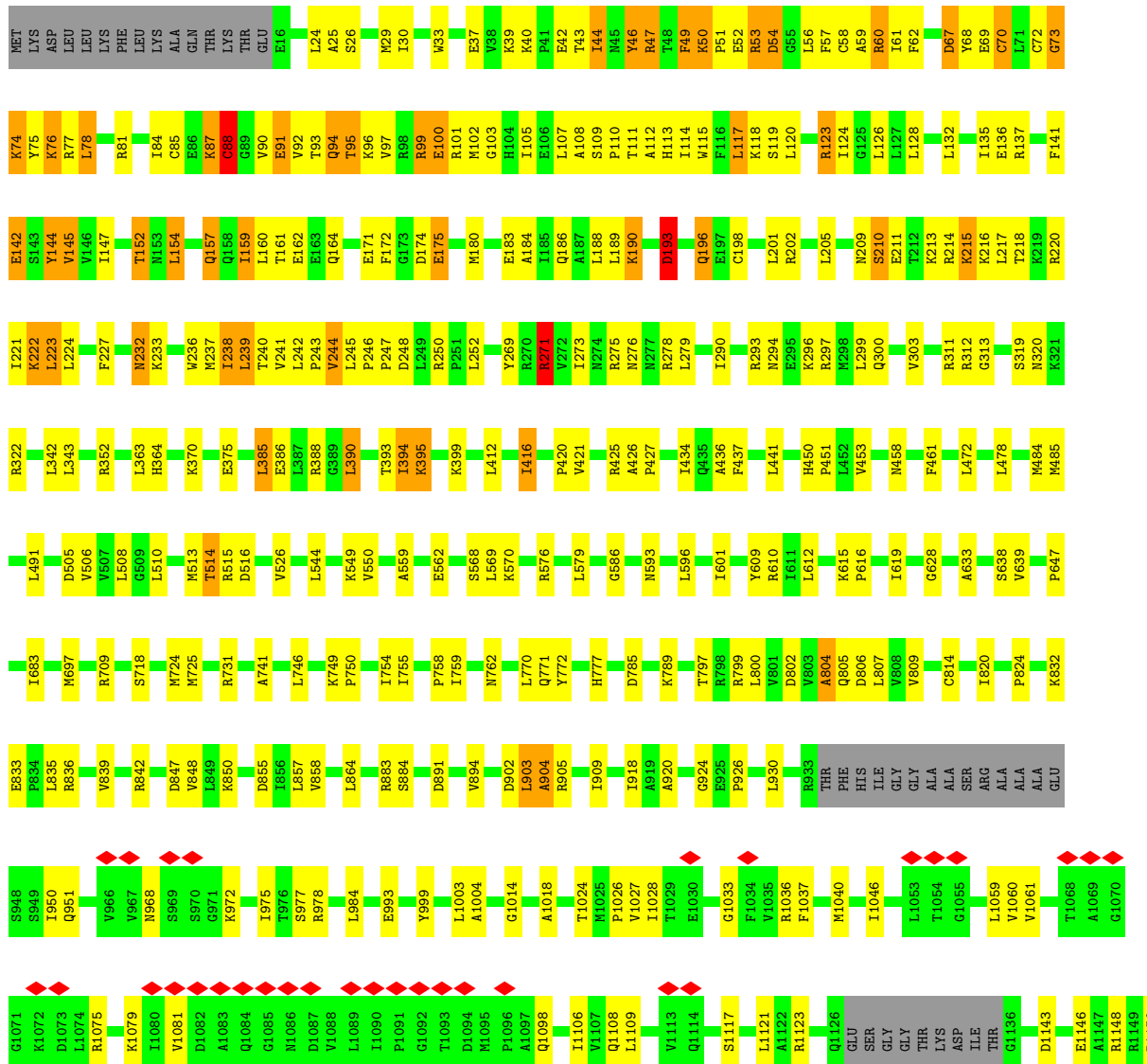
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

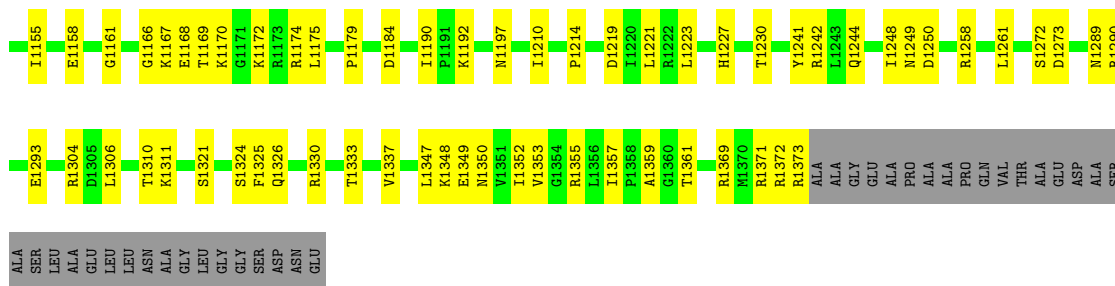
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	B	2	2	2	0



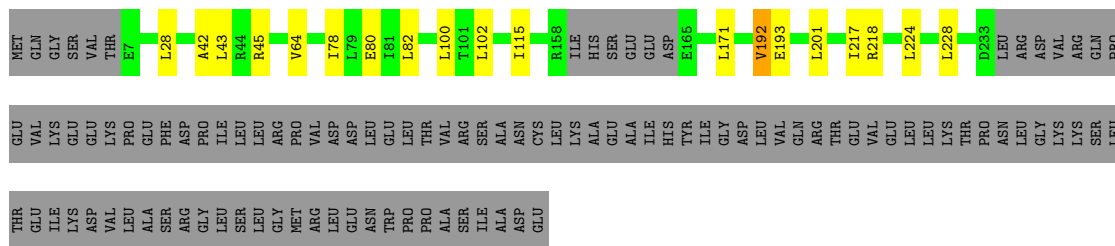


• Molecule 5: DNA-directed RNA polymerase subunit beta'

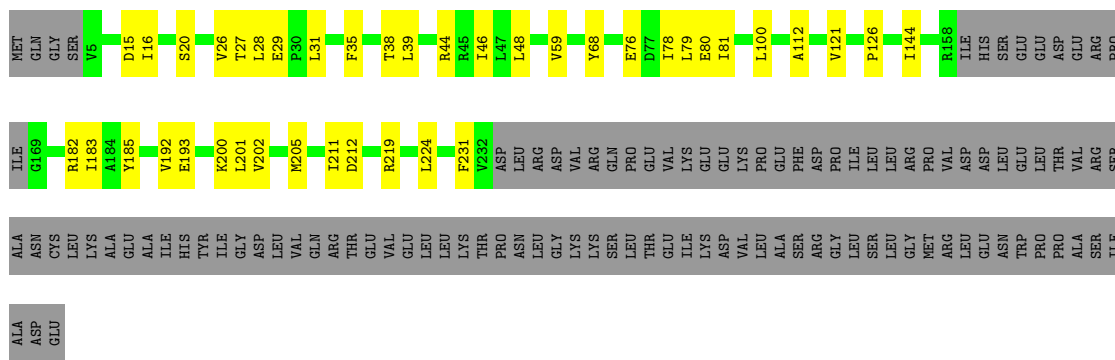




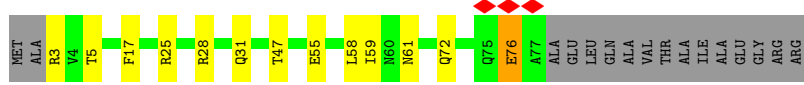
• Molecule 6: DNA-directed RNA polymerase subunit alpha



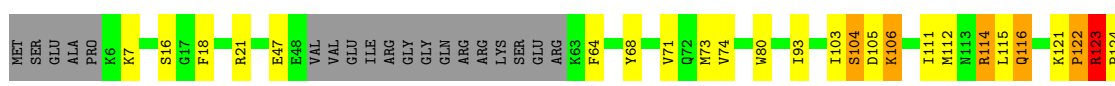
• Molecule 6: DNA-directed RNA polymerase subunit alpha



• Molecule 7: DNA-directed RNA polymerase subunit omega



• Molecule 8: Transcription termination/antitermination protein NusG







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15936	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	398.59198, 398.59198, 398.59198	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.038, 1.038, 1.038	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: ZN, MG

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	5	1.12	8/757 (1.1%)	0.95	1/1163 (0.1%)
2	6	1.11	5/834 (0.6%)	1.44	7/1283 (0.5%)
3	7	0.63	1/410 (0.2%)	0.80	0/638
4	A	0.43	1/10736 (0.0%)	0.61	2/14487 (0.0%)
5	B	0.52	3/10545 (0.0%)	0.66	5/14236 (0.0%)
6	C	0.41	0/1718	0.62	0/2328
6	D	0.36	0/1696	0.62	0/2298
7	E	0.34	0/602	0.58	0/810
8	F	0.36	0/1304	0.54	1/1759 (0.1%)
All	All	0.52	18/28602 (0.1%)	0.68	16/39002 (0.0%)

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
5	B	0	5
6	C	0	1
6	D	0	1
All	All	0	7

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	88	CYS	CB-SG	-10.12	1.65	1.82
1	5	109	DT	O3'-P	8.75	1.71	1.61
4	A	920	VAL	C-N	8.39	1.50	1.34
2	6	10	DG	C1'-N9	-8.08	1.35	1.47
1	5	121	DG	C1'-N9	-7.27	1.37	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	27	DG	O3'-P-O5'	23.15	147.99	104.00
2	6	27	DG	OP1-P-O3'	-20.71	59.64	105.20
2	6	28	DA	P-O3'-C3'	13.79	136.25	119.70
2	6	28	DA	O3'-P-O5'	11.59	126.02	104.00
5	B	271	ARG	NE-CZ-NH2	-9.51	115.55	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	1184	ASP	Peptide
5	B	1326	GLN	Peptide
5	B	313	GLY	Peptide
5	B	416	ILE	Peptide
5	B	804	ALA	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	5	676	237	372	41	0
2	6	748	283	419	37	0
3	7	367	97	180	46	0
4	A	10567	0	10584	242	0
5	B	10388	10612	10611	370	0
6	C	1698	0	1718	11	0
6	D	1677	0	1713	24	0
7	E	600	0	607	11	0
8	F	1276	0	1247	98	0
9	B	1	0	0	0	0
10	B	2	0	0	0	0
All	All	28000	11229	27451	764	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 14.

The worst 5 of 764 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)
8:F:129:GLU:HB3	8:F:130:PRO:CD	1.35	1.44
4:A:920:VAL:HG22	4:A:921:PRO:CD	1.51	1.38
4:A:854:ILE:CG2	4:A:917:SER:HB3	1.52	1.36
4:A:857:VAL:CG1	4:A:919:ARG:HH21	1.39	1.35
8:F:123:ARG:CG	8:F:124:PRO:HD2	1.57	1.34

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	
4	A	1338/1342 (100%)	1207 (90%)	125 (9%)	6 (0%)	34	72
5	B	1329/1407 (94%)	1199 (90%)	121 (9%)	9 (1%)	22	63
6	C	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	17	57
6	D	214/329 (65%)	198 (92%)	16 (8%)	0	100	100
7	E	73/91 (80%)	70 (96%)	3 (4%)	0	100	100
8	F	157/181 (87%)	137 (87%)	14 (9%)	6 (4%)	3	24
All	All	3328/3679 (90%)	3014 (91%)	291 (9%)	23 (1%)	26	63

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	888	THR
8	F	122	PRO
8	F	123	ARG
8	F	129	GLU
4	A	918	LEU

### 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	
4	A	1155/1157 (100%)	1136 (98%)	19 (2%)	62	79
5	B	1120/1168 (96%)	1051 (94%)	69 (6%)	18	43
6	C	186/286 (65%)	186 (100%)	0	100	100
6	D	185/286 (65%)	185 (100%)	0	100	100
7	E	65/75 (87%)	64 (98%)	1 (2%)	65	80
8	F	138/158 (87%)	117 (85%)	21 (15%)	3	15
All	All	2849/3130 (91%)	2739 (96%)	110 (4%)	36	56

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	159	ILE
5	B	237	MET
8	F	176	SER
8	F	143	ASP
5	B	180	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	227	GLN
8	F	116	GLN
4	A	688	GLN
4	A	894	GLN
4	A	1268	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	7	16/35 (45%)	8 (50%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	7	20	U
3	7	21	U
3	7	22	G
3	7	23	A
3	7	25	U

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 monosaccharides 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

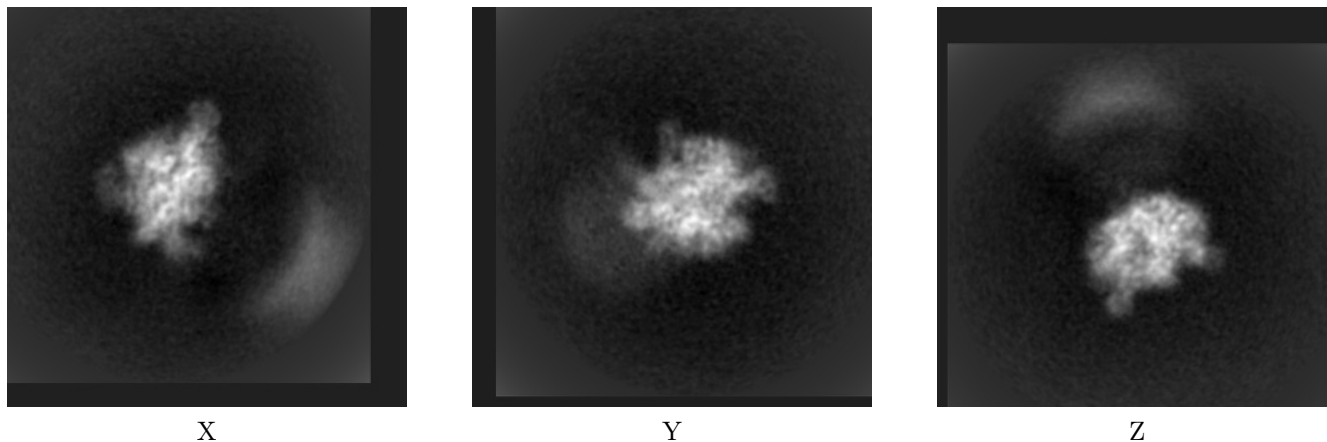
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27864. These allow visual inspection of the internal detail of the map and identification of artifacts.

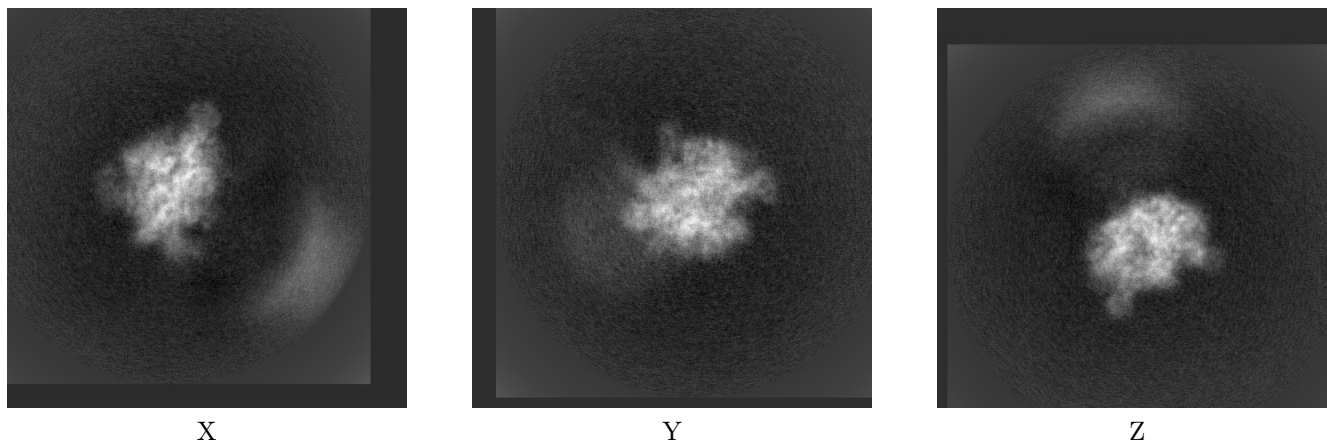
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



#### 6.1.2 Raw map

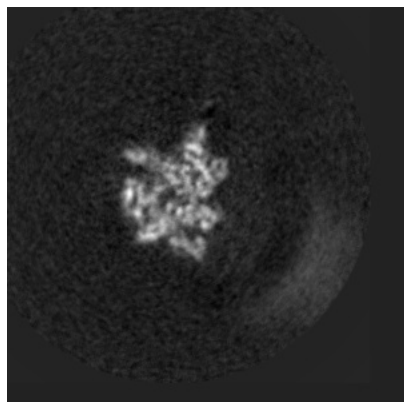


The images above show the map projected in three orthogonal directions.

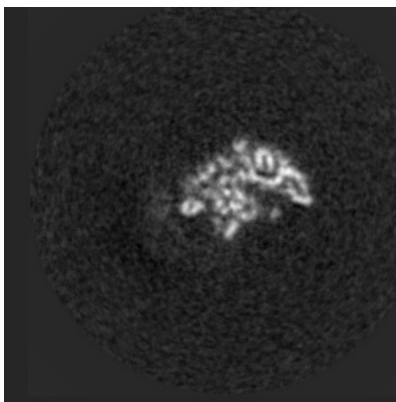


## 6.2 Central slices [i](#)

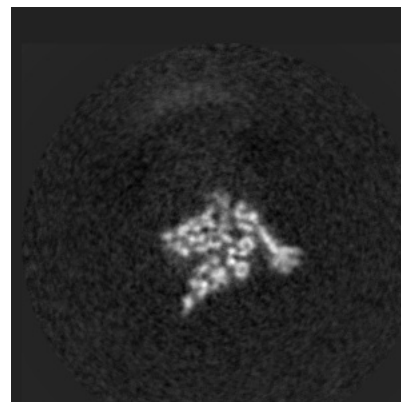
### 6.2.1 Primary map



X Index: 192

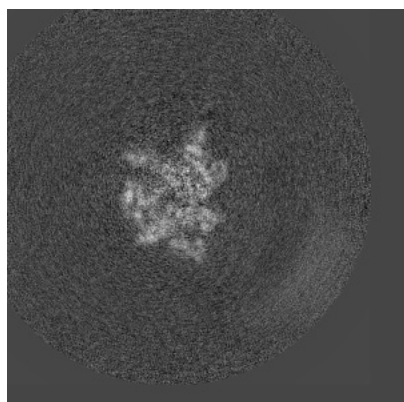


Y Index: 192

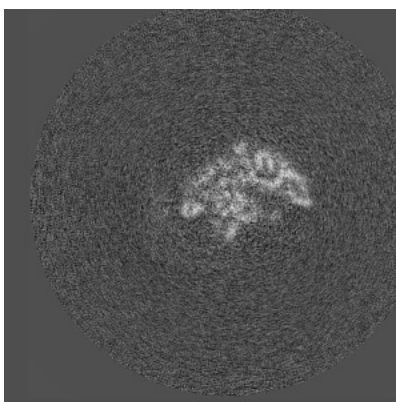


Z Index: 192

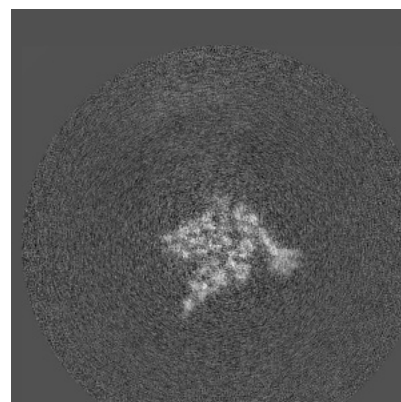
### 6.2.2 Raw map



X Index: 192



Y Index: 192

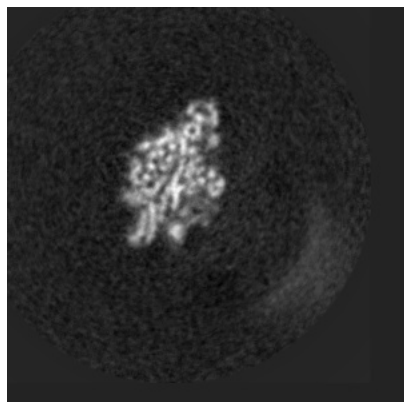


Z Index: 192

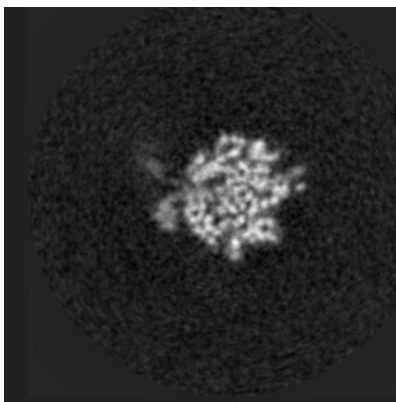
The images above show central slices of the map in three orthogonal directions.

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

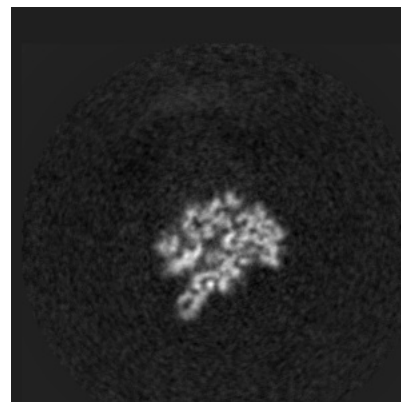
### 6.3.1 Primary map



X Index: 209

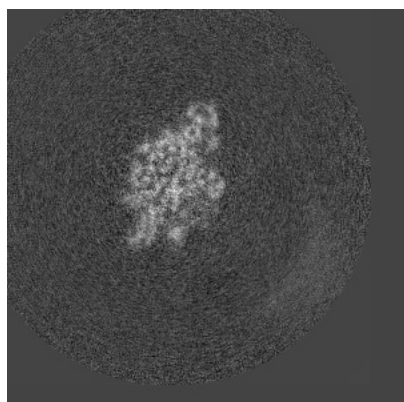


Y Index: 173

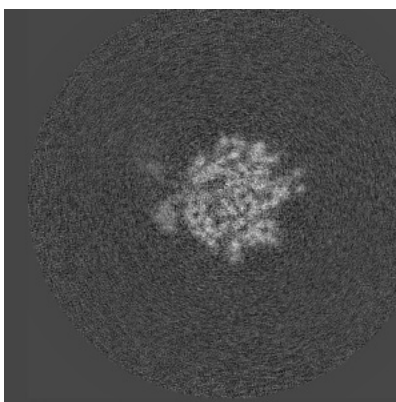


Z Index: 206

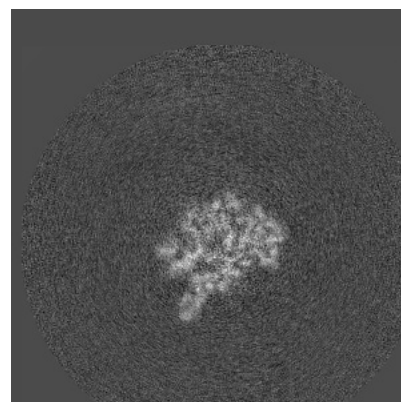
### 6.3.2 Raw map



X Index: 209



Y Index: 173

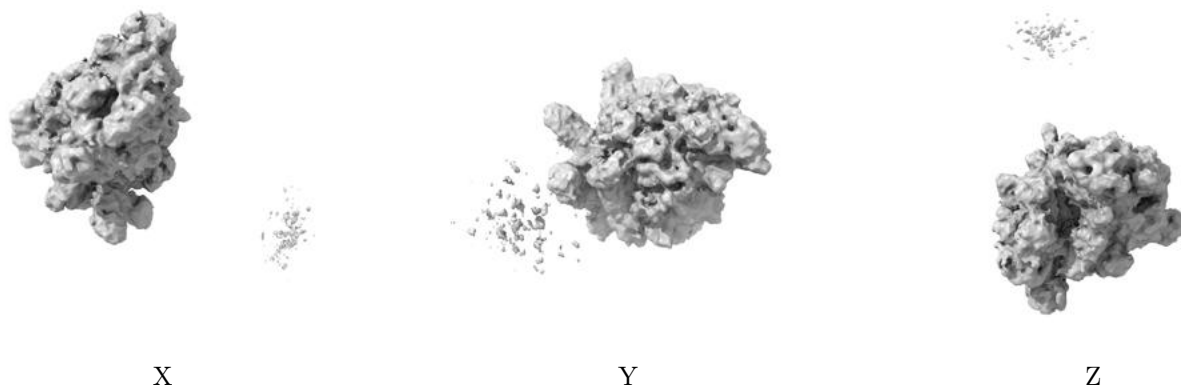


Z Index: 208

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

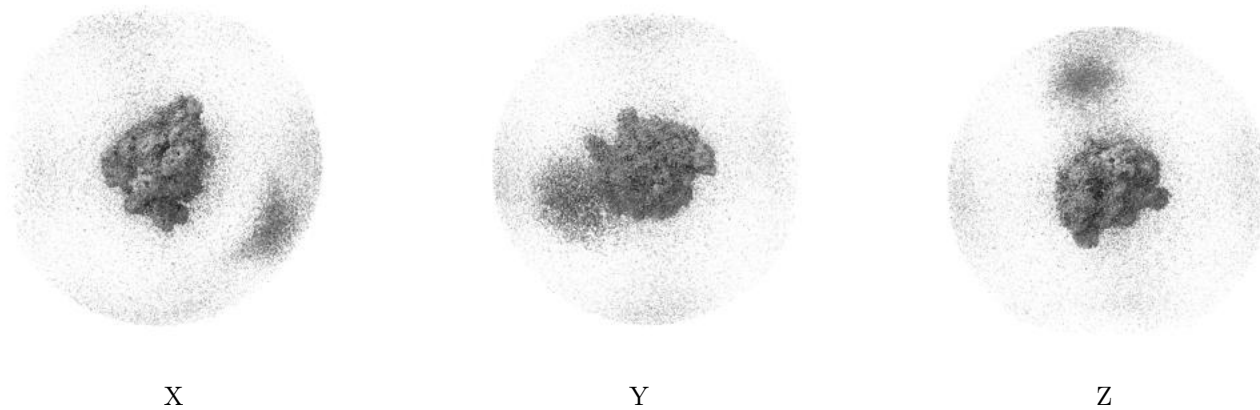
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

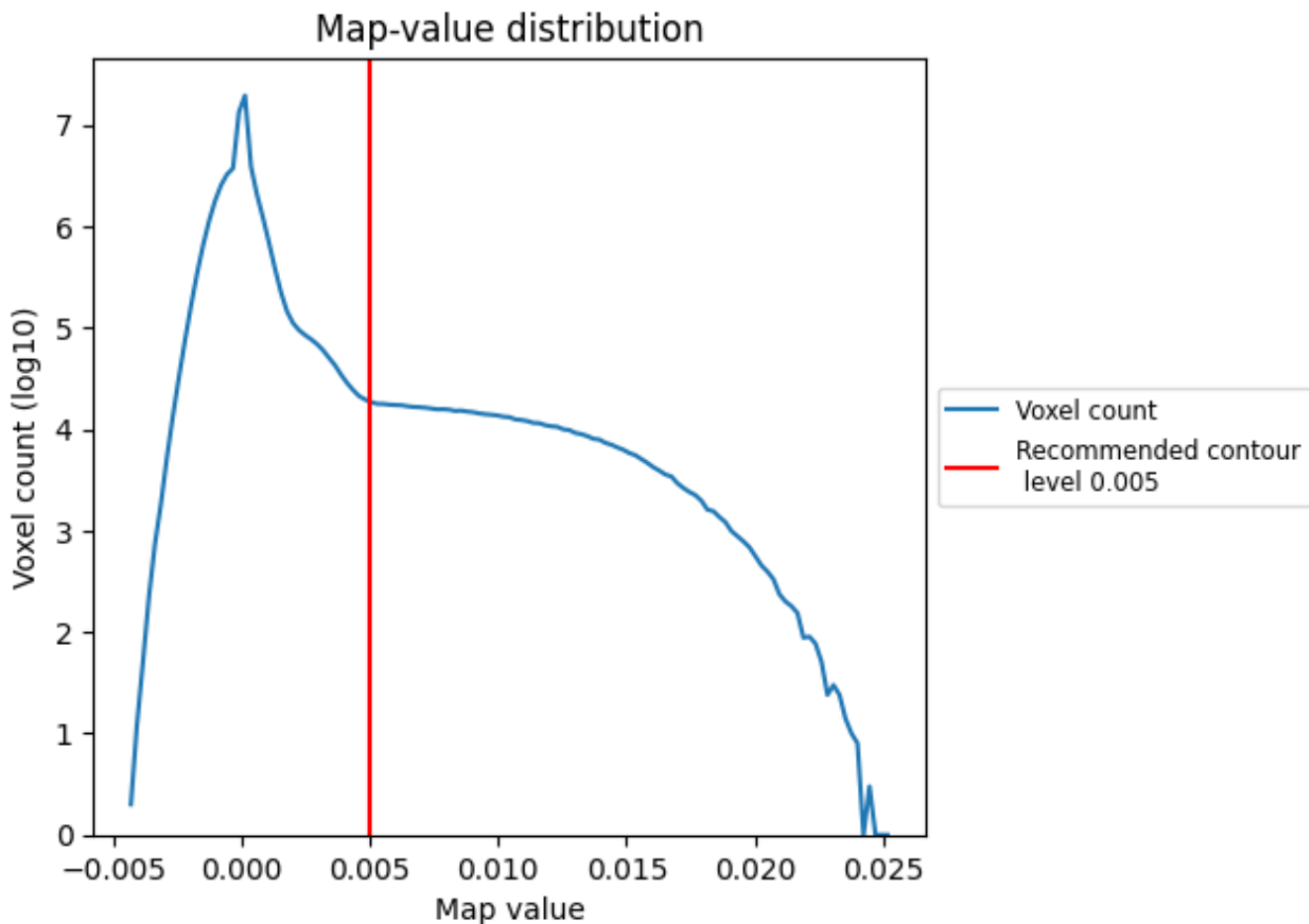
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

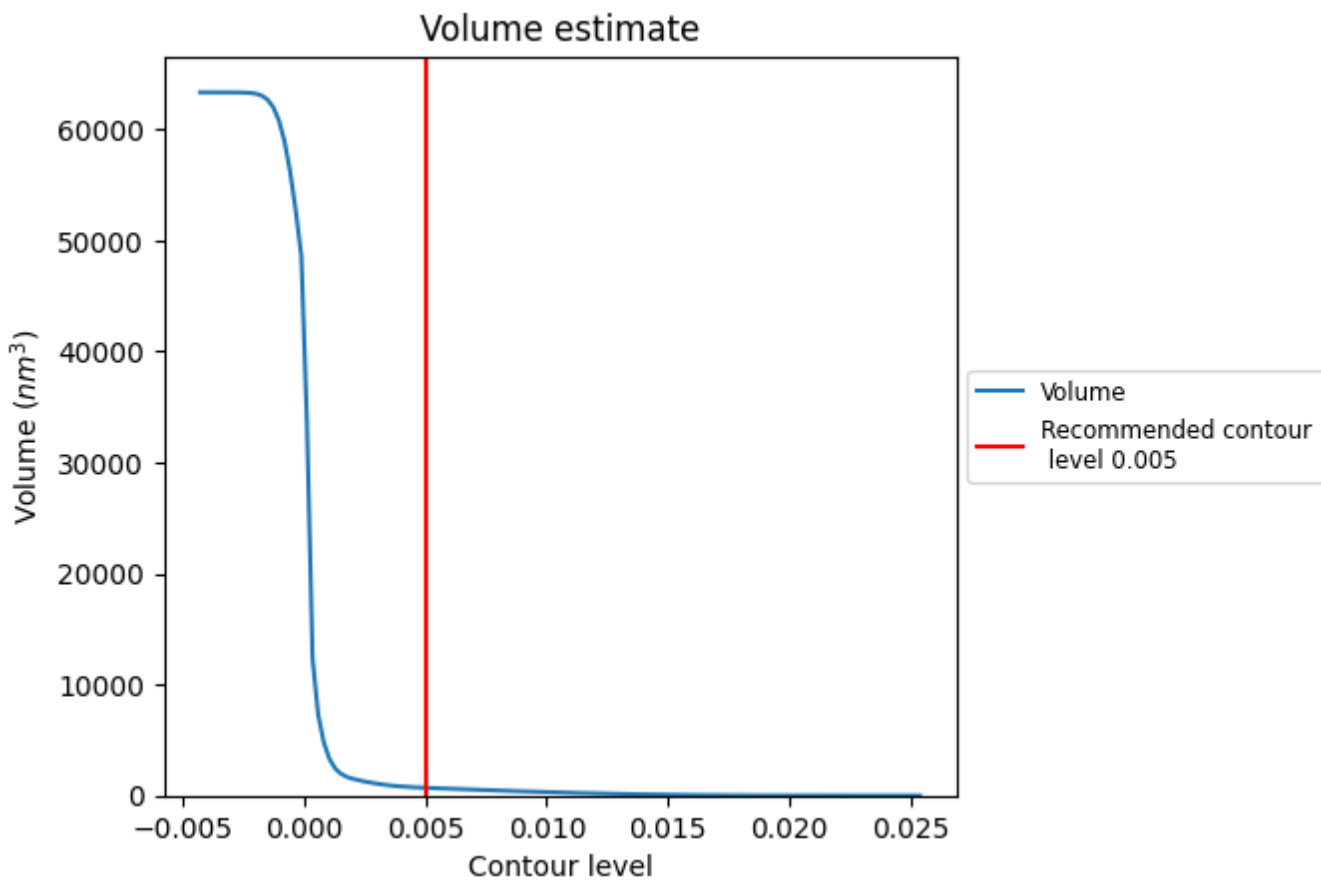
This section contains the results of statistical analysis of the map.

### 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.

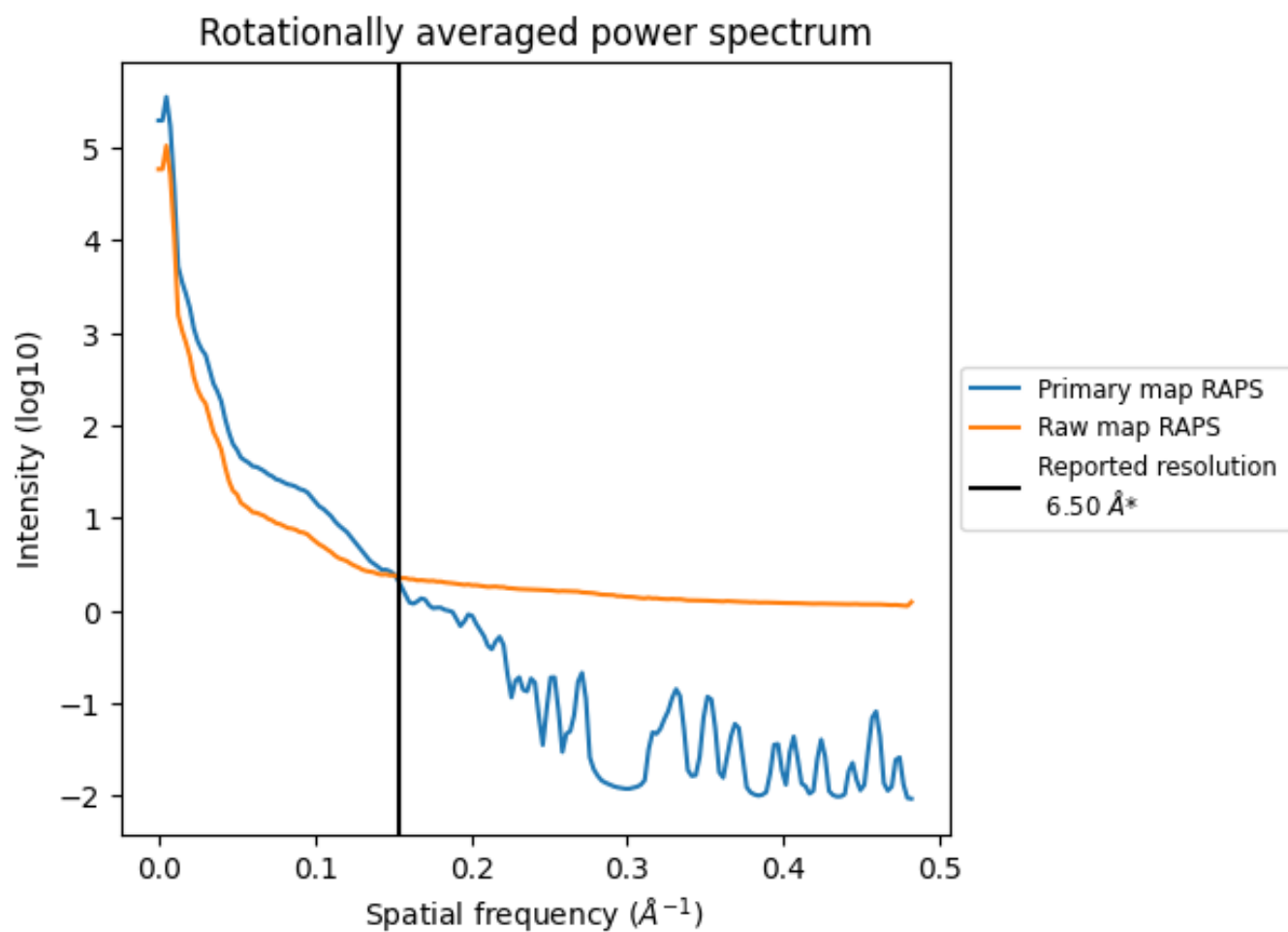
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 699 nm<sup>3</sup>; this corresponds to an approximate mass of 631 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

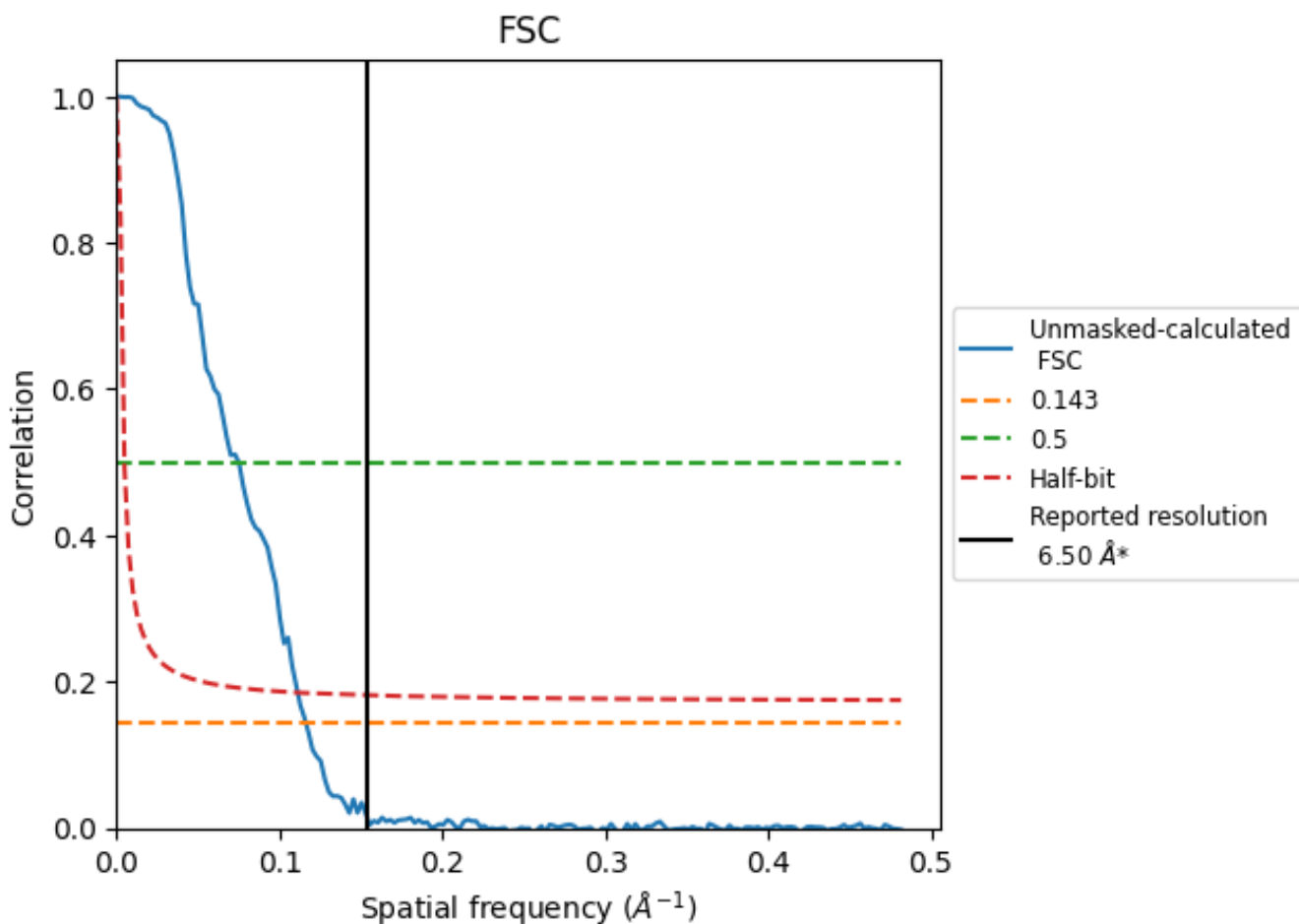


\*Reported resolution corresponds to spatial frequency of 0.154 Å<sup>-1</sup>

## 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 0.154 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	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.60	13.33	8.98

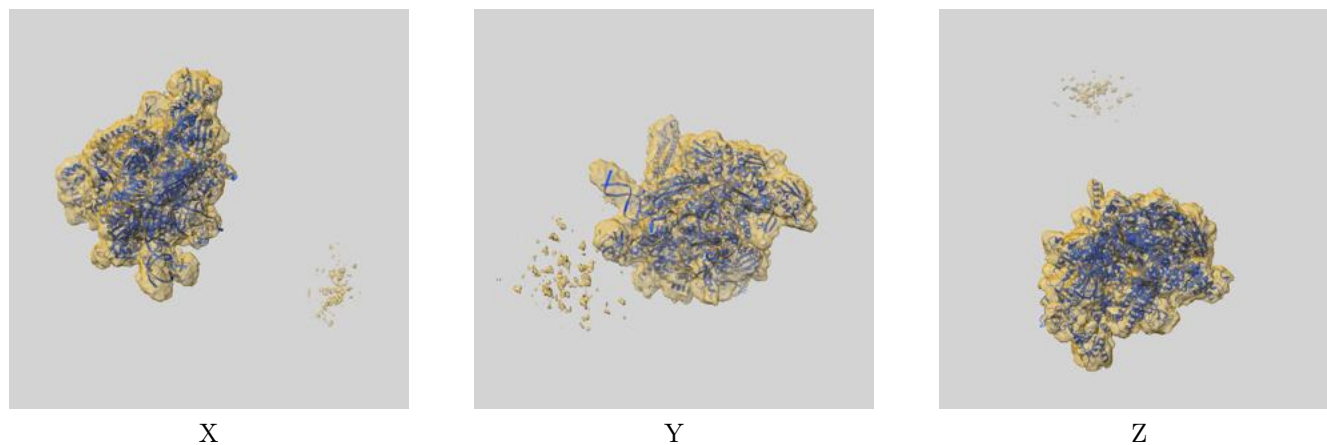
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.60 differs from the reported value 6.5 by more than 10 %



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

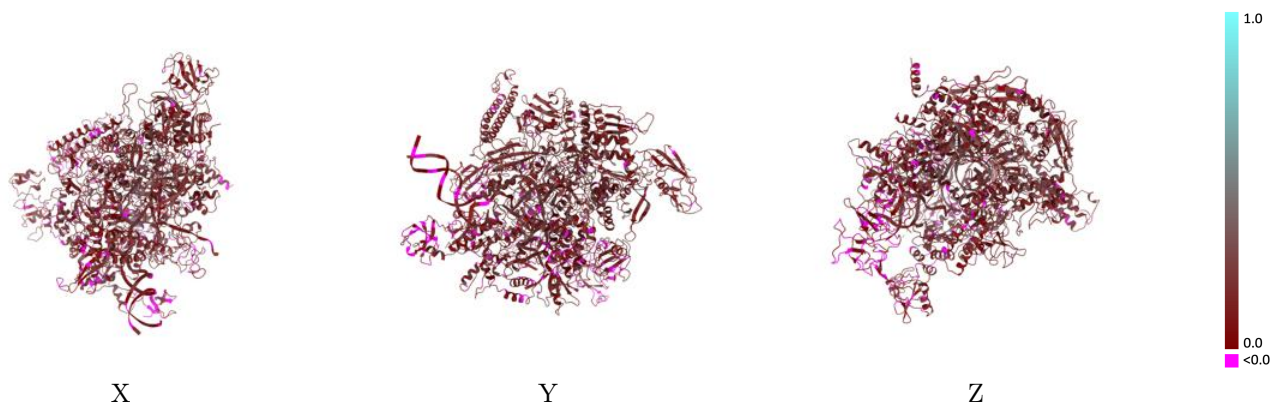
This section contains information regarding the fit between EMDB map EMD-27864 and PDB model 8E3F. Per-residue inclusion information can be found in section 3 on page 6.

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



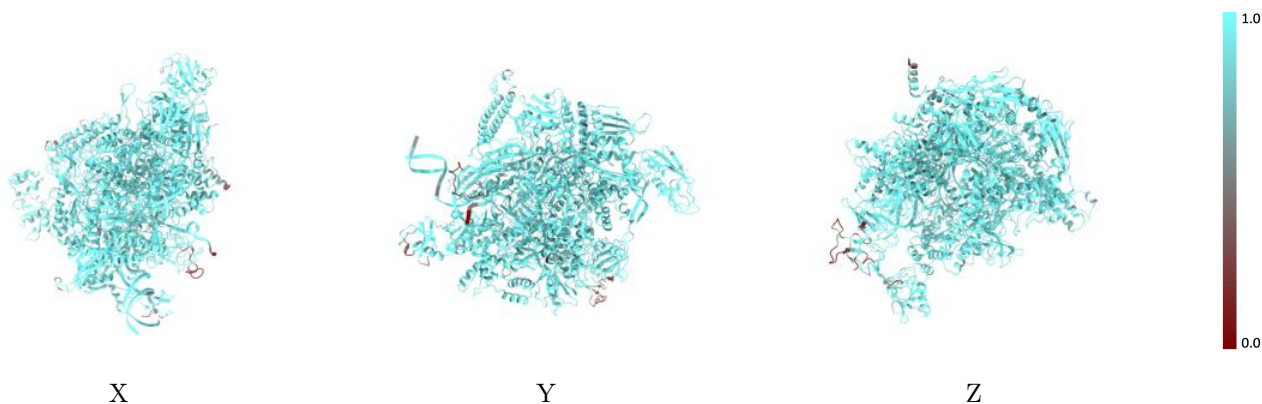
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



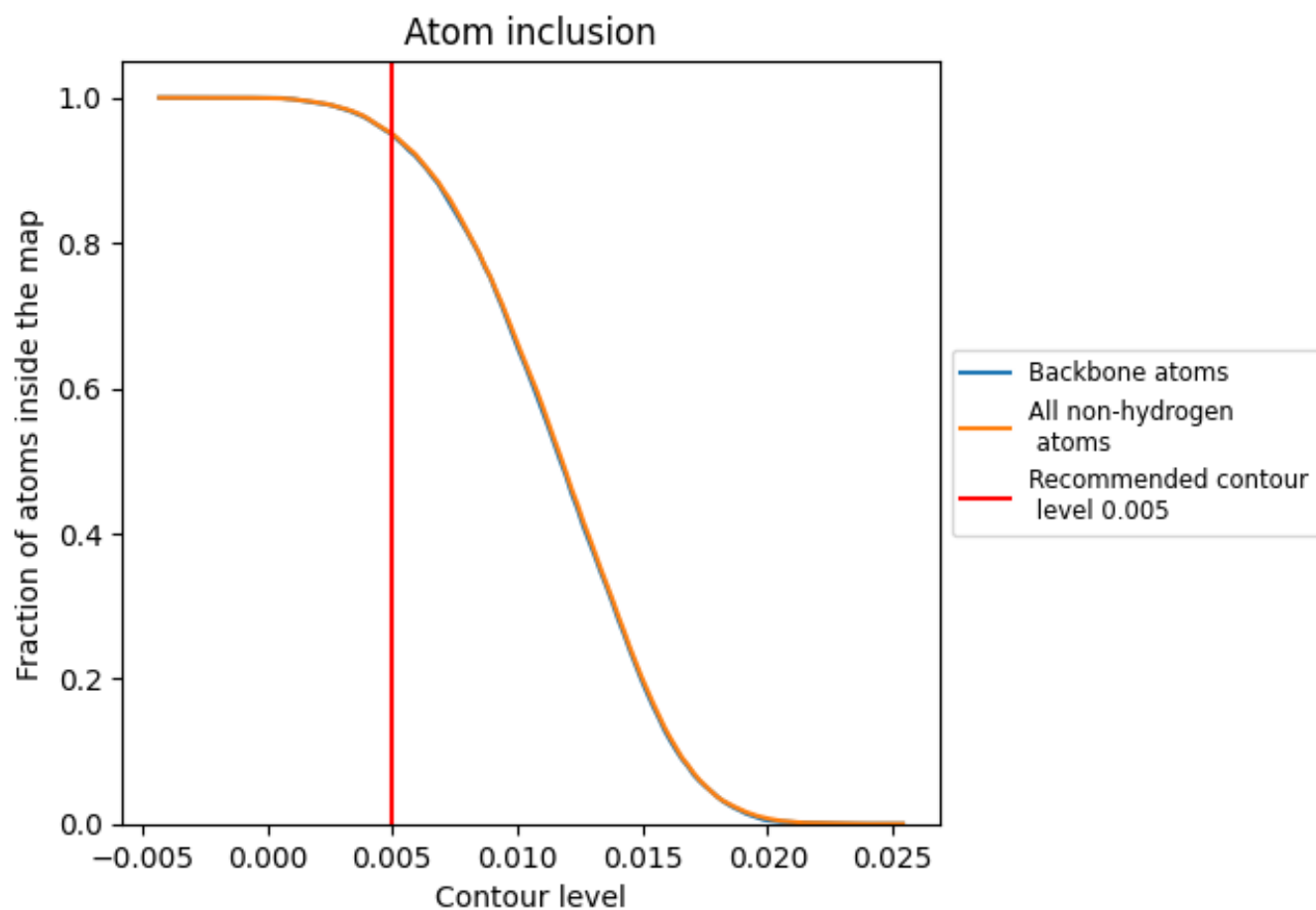
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).





















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9502	 0.1580
5	 0.9645	 0.1270
6	 0.9626	 0.1790
7	 0.8801	 0.1980
A	 0.9570	 0.1660
B	 0.9504	 0.1490
C	 0.9700	 0.1870
D	 0.9568	 0.1830
E	 0.8425	 0.1560
F	 0.9159	 0.0910

