



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 10:01 am GMT

PDB ID : 7P3Z  
EMDB ID : EMD-13189  
Title : Homology model of the full-length AP-3 complex in a stretched open conformation  
Authors : Schubert, E.; Raunser, S.  
Deposited on : 2021-07-09  
Resolution : 10.50 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.dev113  
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

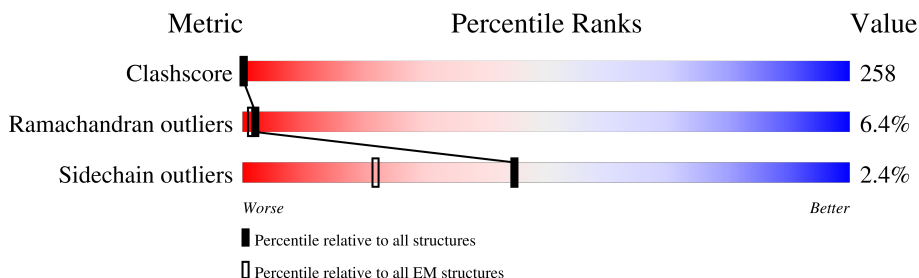
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	964	
2	B	809	
3	M	483	
4	S	194	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14041 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 AP-3 complex subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	576	Total	C	N	O	S	0	0
			4625	2978	738	881	28		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	933	ARG	-	expression tag	UNP A0A7I9C4X2
A	934	THR	-	expression tag	UNP A0A7I9C4X2
A	935	LEU	-	expression tag	UNP A0A7I9C4X2
A	936	GLN	-	expression tag	UNP A0A7I9C4X2
A	937	VAL	-	expression tag	UNP A0A7I9C4X2
A	938	ASP	-	expression tag	UNP A0A7I9C4X2
A	939	GLY	-	expression tag	UNP A0A7I9C4X2
A	940	SER	-	expression tag	UNP A0A7I9C4X2
A	941	ASP	-	expression tag	UNP A0A7I9C4X2
A	942	TYR	-	expression tag	UNP A0A7I9C4X2
A	943	LYS	-	expression tag	UNP A0A7I9C4X2
A	944	ASP	-	expression tag	UNP A0A7I9C4X2
A	945	ASP	-	expression tag	UNP A0A7I9C4X2
A	946	ASP	-	expression tag	UNP A0A7I9C4X2
A	947	ASP	-	expression tag	UNP A0A7I9C4X2
A	948	LYS	-	expression tag	UNP A0A7I9C4X2
A	949	ASP	-	expression tag	UNP A0A7I9C4X2
A	950	TYR	-	expression tag	UNP A0A7I9C4X2
A	951	LYS	-	expression tag	UNP A0A7I9C4X2
A	952	ASP	-	expression tag	UNP A0A7I9C4X2
A	953	ASP	-	expression tag	UNP A0A7I9C4X2
A	954	ASP	-	expression tag	UNP A0A7I9C4X2
A	955	ASP	-	expression tag	UNP A0A7I9C4X2
A	956	LYS	-	expression tag	UNP A0A7I9C4X2
A	957	ASP	-	expression tag	UNP A0A7I9C4X2
A	958	TYR	-	expression tag	UNP A0A7I9C4X2
A	959	LYS	-	expression tag	UNP A0A7I9C4X2
A	960	ASP	-	expression tag	UNP A0A7I9C4X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	961	ASP	-	expression tag	UNP A0A7I9C4X2
A	962	ASP	-	expression tag	UNP A0A7I9C4X2
A	963	ASP	-	expression tag	UNP A0A7I9C4X2
A	964	LYS	-	expression tag	UNP A0A7I9C4X2

- Molecule 2 is a protein called Y55\_G0035830.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	621	Total	C	N	O	S	0	0
			4954	3160	830	936	28		

- Molecule 3 is a protein called AP-3 complex subunit mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	391	Total	C	N	O	S	0	0
			3106	1986	509	599	12		

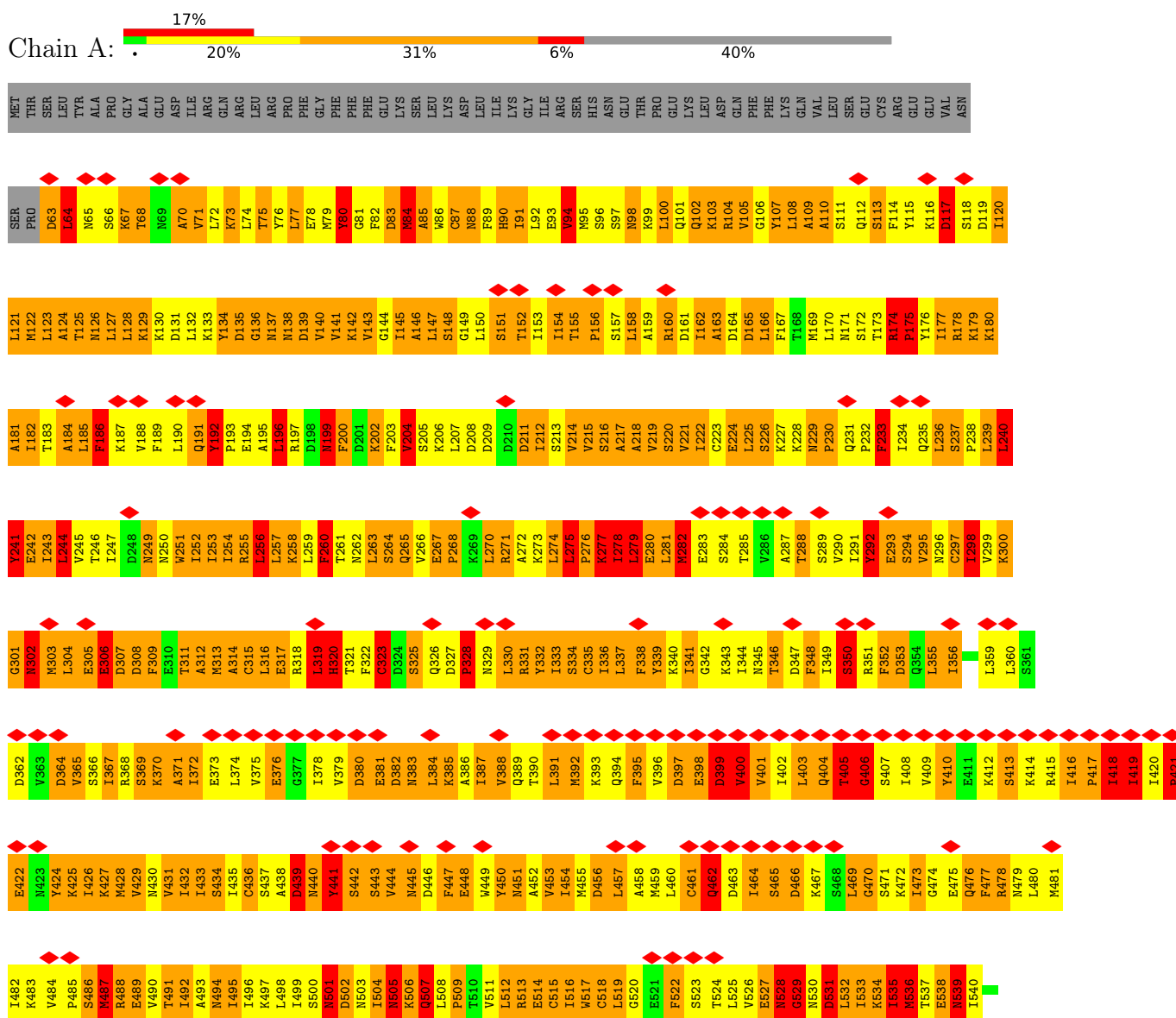
- Molecule 4 is a protein called AP complex subunit sigma.

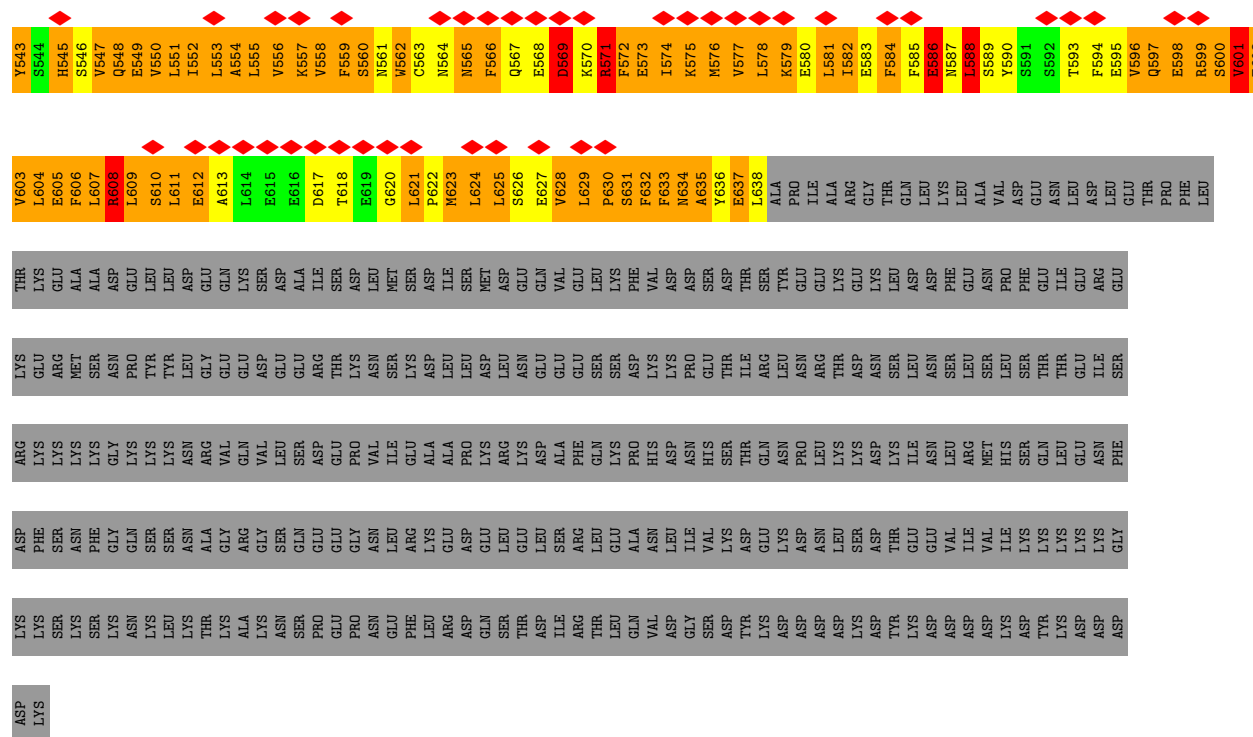
Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	168	Total	C	N	O	S	0	0
			1356	867	215	270	4		

### 3 Residue-property plots

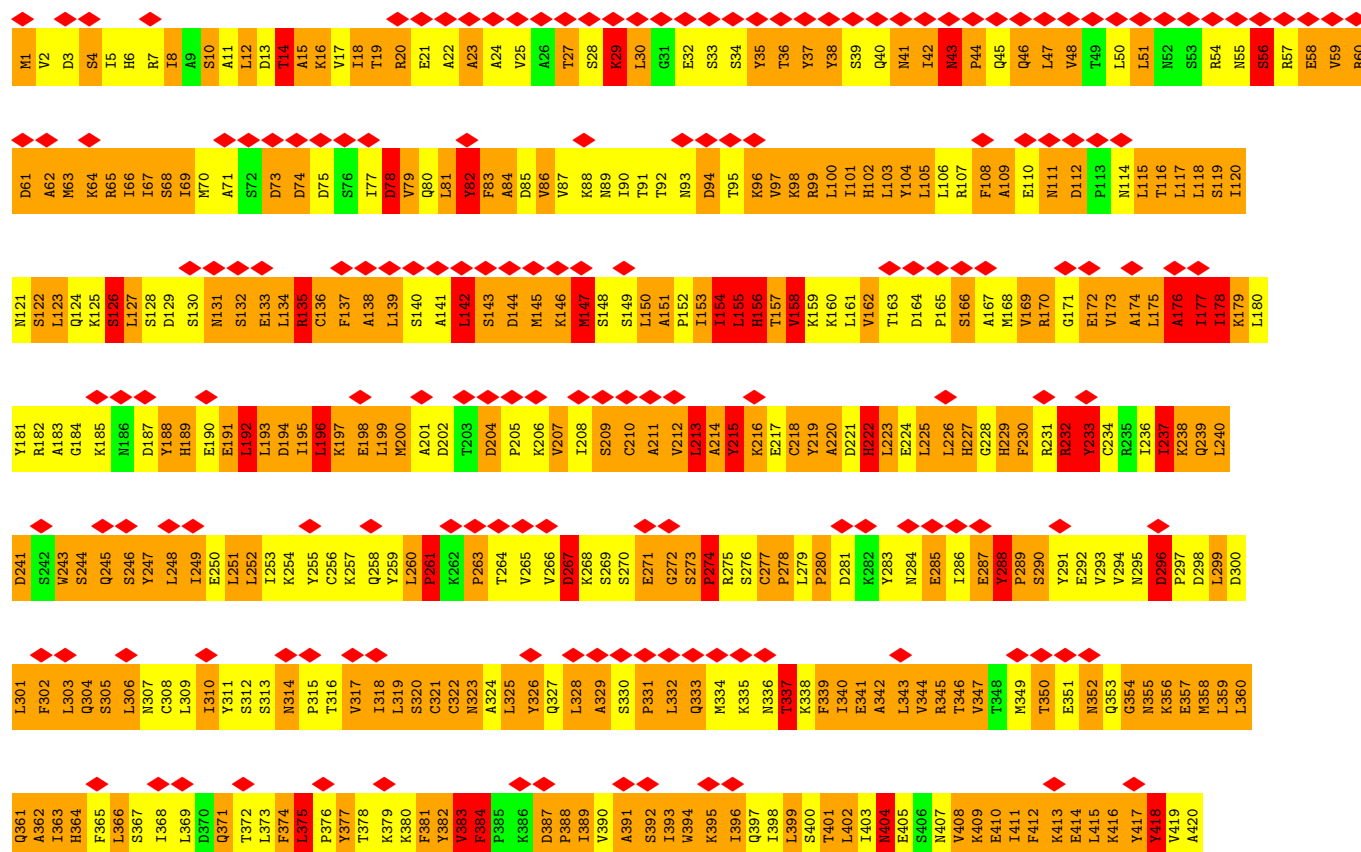
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

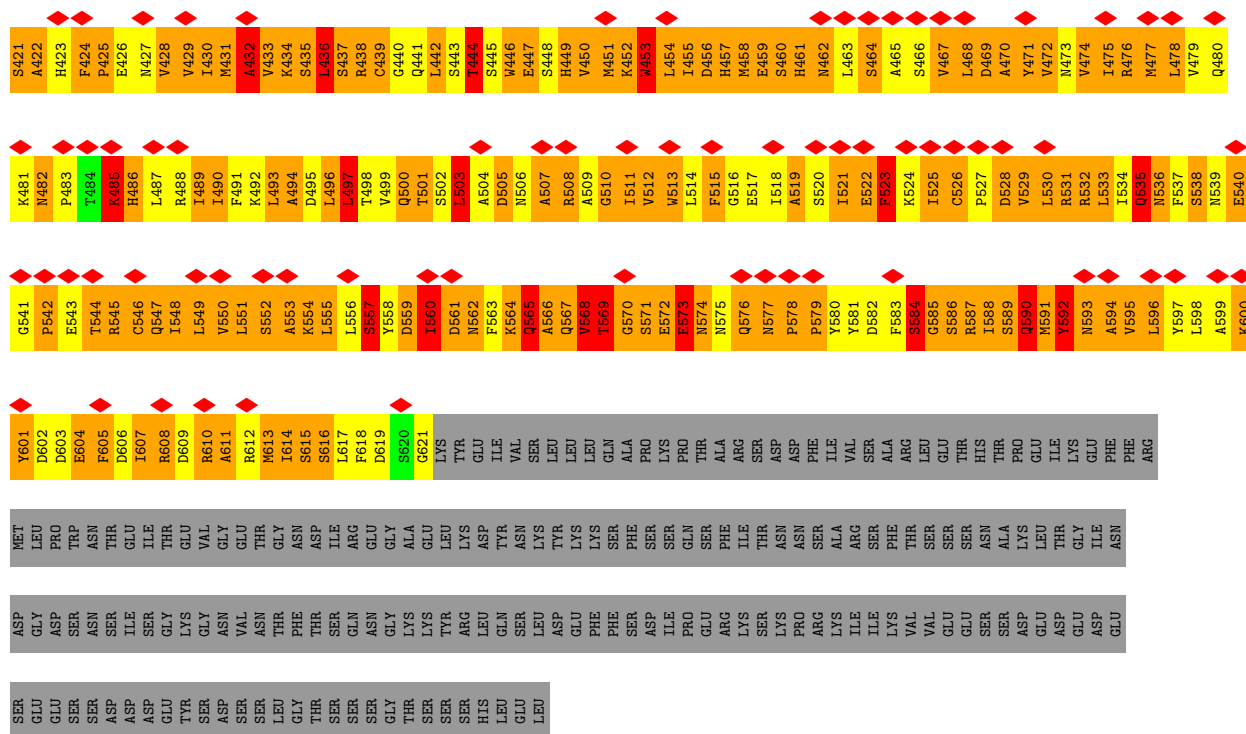
#### • Molecule 1: AP-3 complex subunit delta



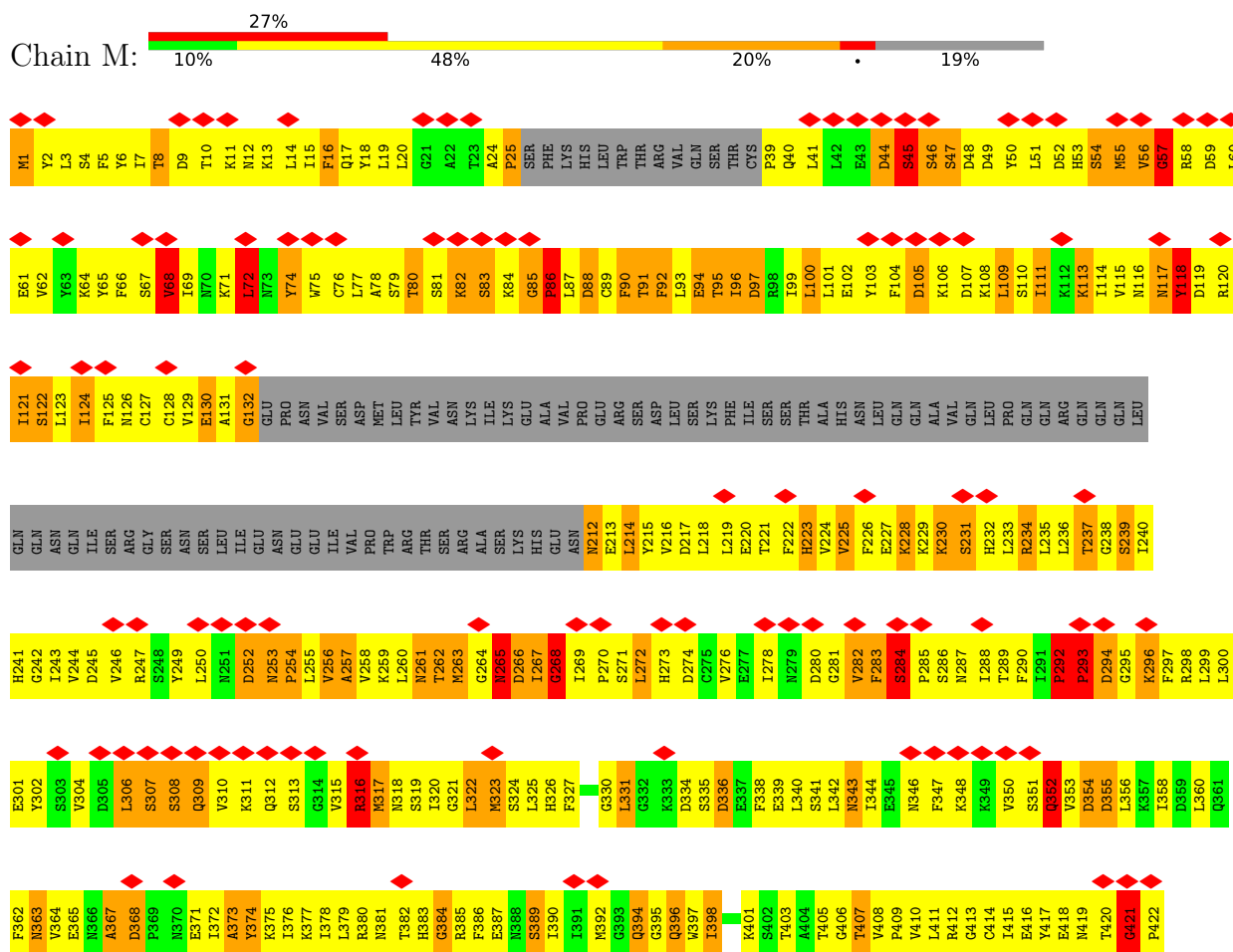


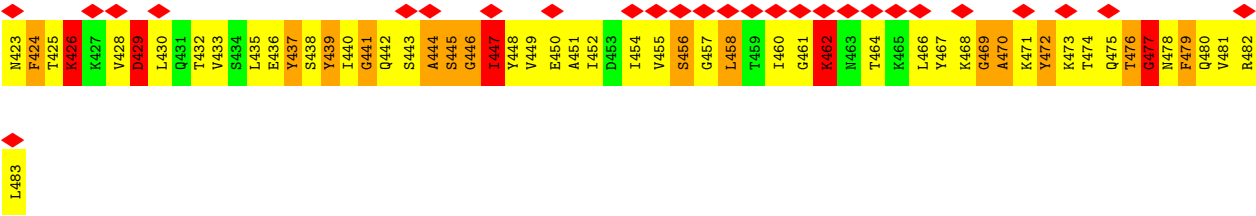
• Molecule 2: Y55\_G0035830.mRNA.1.CDS.1



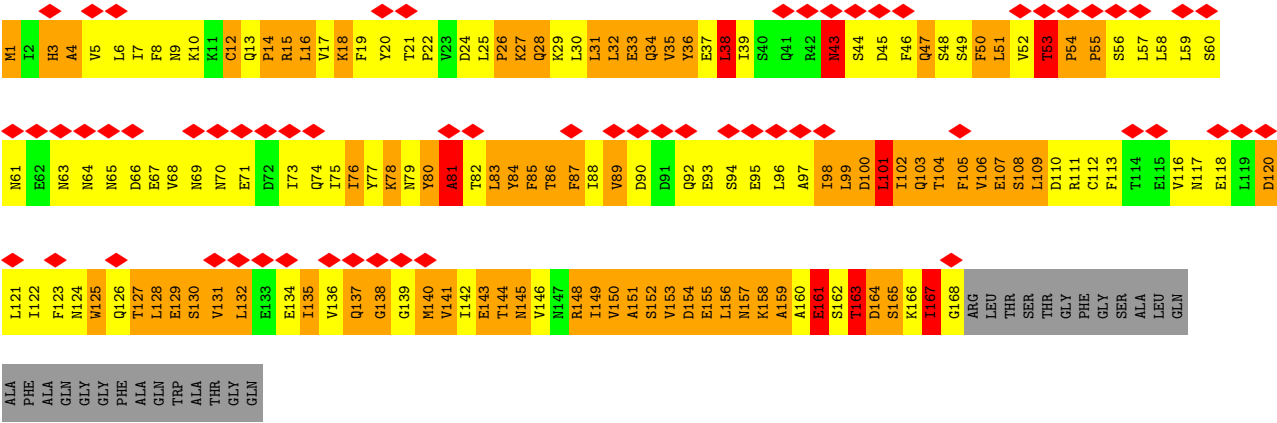


• Molecule 3: AP-3 complex subunit mu





• Molecule 4: AP complex subunit sigma



ALA
PHE
ALA
GLN
GLY
GLY
PHE
ALA
ALA
TRP
ALA
THR
GLY
GLN



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20312	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	81	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0155	Depositor
Map size ( $\text{\AA}$ )	282.48, 282.48, 282.48	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.07, 1.07, 1.07	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	1.68	70/4699 (1.5%)	2.61	607/6358 (9.5%)
2	B	1.52	52/5047 (1.0%)	2.32	540/6841 (7.9%)
3	M	1.59	61/3163 (1.9%)	1.85	139/4271 (3.3%)
4	S	1.84	33/1377 (2.4%)	2.17	116/1872 (6.2%)
All	All	1.62	216/14286 (1.5%)	2.31	1402/19342 (7.2%)

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	49
2	B	0	28
3	M	0	14
4	S	0	8
All	All	0	99

The worst 5 of 216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	132	GLY	CA-C	-17.19	1.24	1.51
4	S	53	THR	N-CA	-14.56	1.17	1.46
3	M	132	GLY	N-CA	-14.40	1.24	1.46
1	A	406	GLY	CA-C	13.34	1.73	1.51
3	M	293	PRO	N-CD	12.51	1.65	1.47

The worst 5 of 1402 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	GLU	C-N-CA	22.76	178.60	121.70
1	A	265	GLN	N-CA-C	-19.23	59.09	111.00
1	A	80	TYR	N-CA-C	-18.37	61.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	45	SER	C-N-CA	-17.46	78.06	121.70
1	A	277	LYS	C-N-CA	17.23	164.78	121.70

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ASP	Mainchain
1	A	64	LEU	Mainchain
1	A	80	TYR	Mainchain
1	A	84	MET	Mainchain
1	A	94	VAL	Mainchain

## 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	4625	0	4688	2296	0
2	B	4954	0	4969	3353	0
3	M	3106	0	3081	1519	0
4	S	1356	0	1329	910	0
All	All	14041	0	14067	7266	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 258.

The worst 5 of 7266 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)
4:S:8:PHE:CE1	4:S:84:TYR:HB2	1.15	1.68
2:B:171:GLY:CA	2:B:207:VAL:HG13	1.22	1.64
1:A:140:VAL:HA	1:A:177:ILE:CG1	1.17	1.64
1:A:102:GLN:CG	4:S:166:LYS:H	1.11	1.63
1:A:633:PHE:CE1	2:B:513:TRP:CE3	1.74	1.63

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	574/964 (60%)	511 (89%)	39 (7%)	24 (4%)	2	17
2	B	619/809 (76%)	474 (77%)	79 (13%)	66 (11%)	0	6
3	M	385/483 (80%)	315 (82%)	52 (14%)	18 (5%)	2	16
4	S	166/194 (86%)	150 (90%)	12 (7%)	4 (2%)	5	27
All	All	1744/2450 (71%)	1450 (83%)	182 (10%)	112 (6%)	2	13

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	GLU
1	A	278	ILE
1	A	279	LEU
1	A	305	GLU
1	A	401	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	536/898 (60%)	527 (98%)	9 (2%)	56	72
2	B	564/738 (76%)	548 (97%)	16 (3%)	38	57
3	M	353/441 (80%)	342 (97%)	11 (3%)	35	54
4	S	157/175 (90%)	155 (99%)	2 (1%)	65	77
All	All	1610/2252 (72%)	1572 (98%)	38 (2%)	45	62

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	214	LEU
3	M	479	PHE
3	M	293	PRO
3	M	437	TYR
4	S	47	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	486	HIS
2	B	574	ASN
4	S	47	GLN
2	B	567	GLN
3	M	17	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

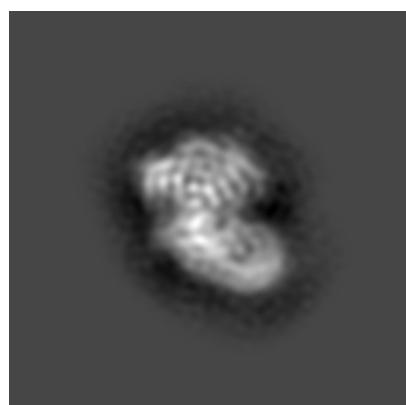
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13189. 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](#)

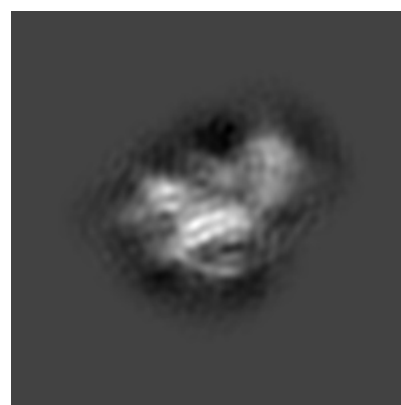
#### 6.1.1 Primary map



X



Y

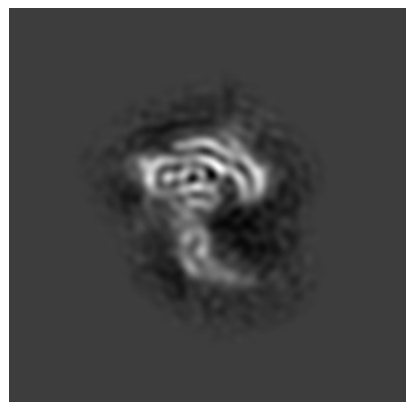


Z

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

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

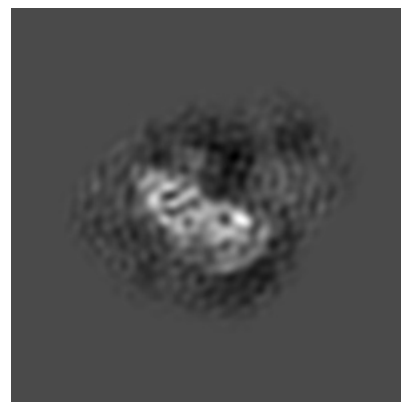
#### 6.2.1 Primary map



X Index: 132



Y Index: 132



Z Index: 132

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

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

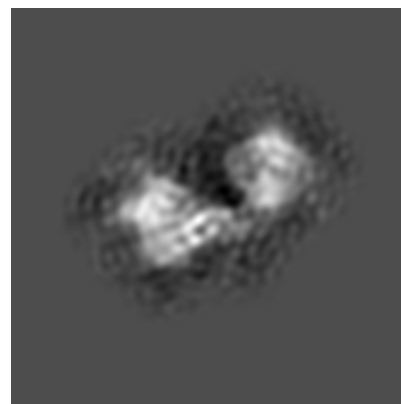
### 6.3.1 Primary map



X Index: 134



Y Index: 123



Z Index: 112

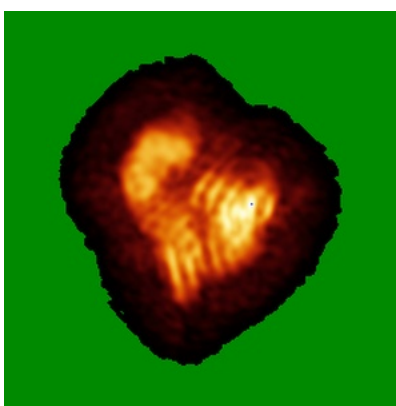
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y



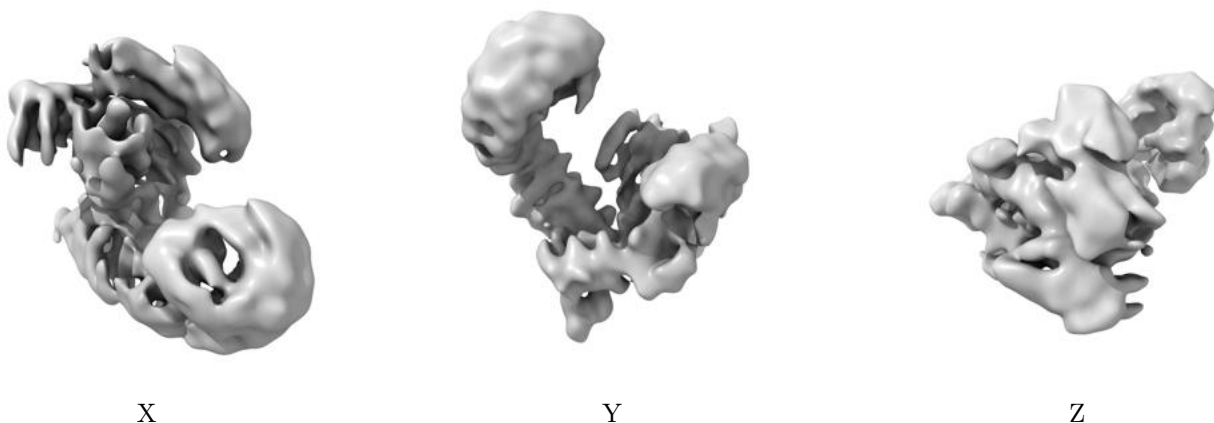
Z

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 0.0155. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

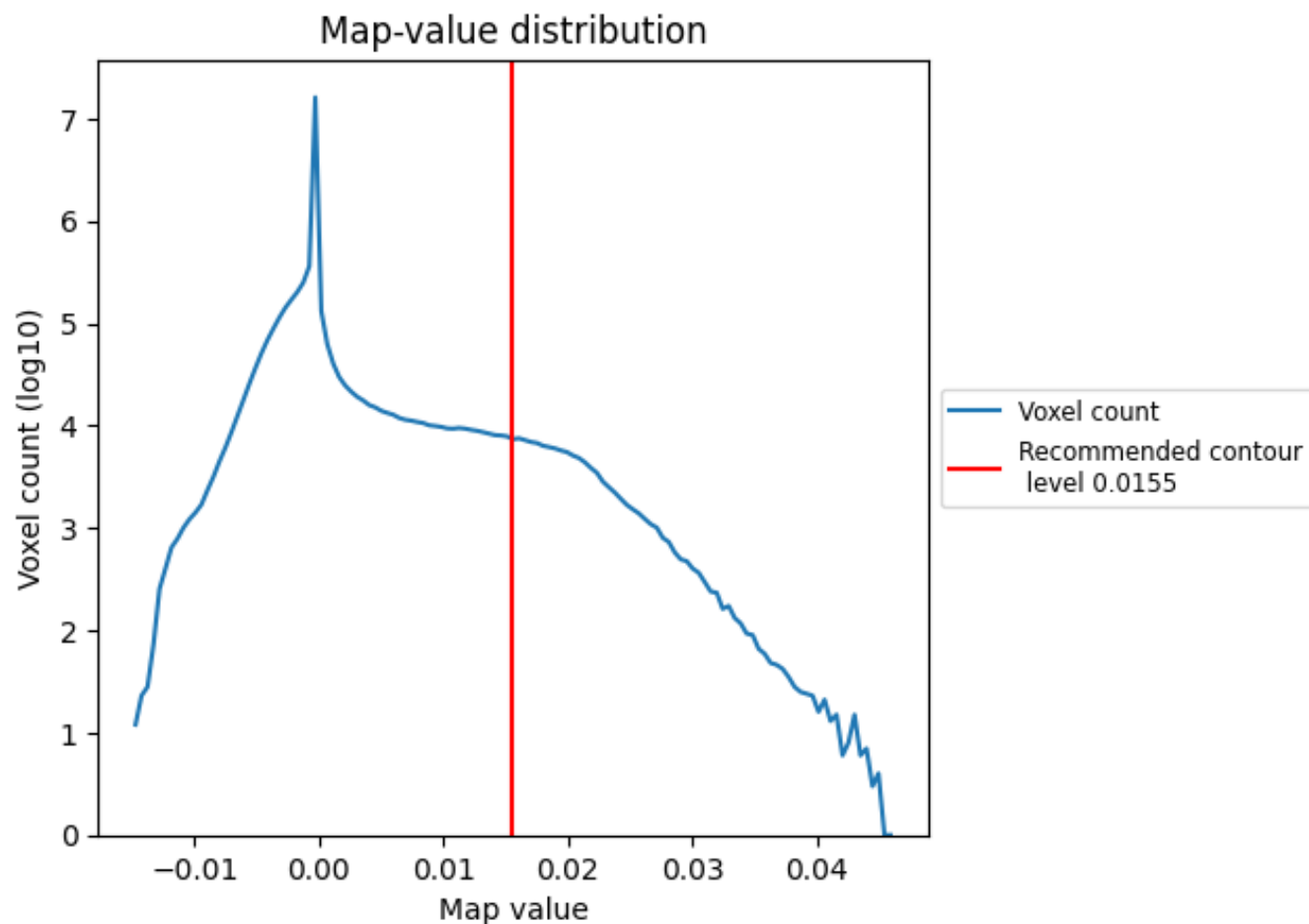
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

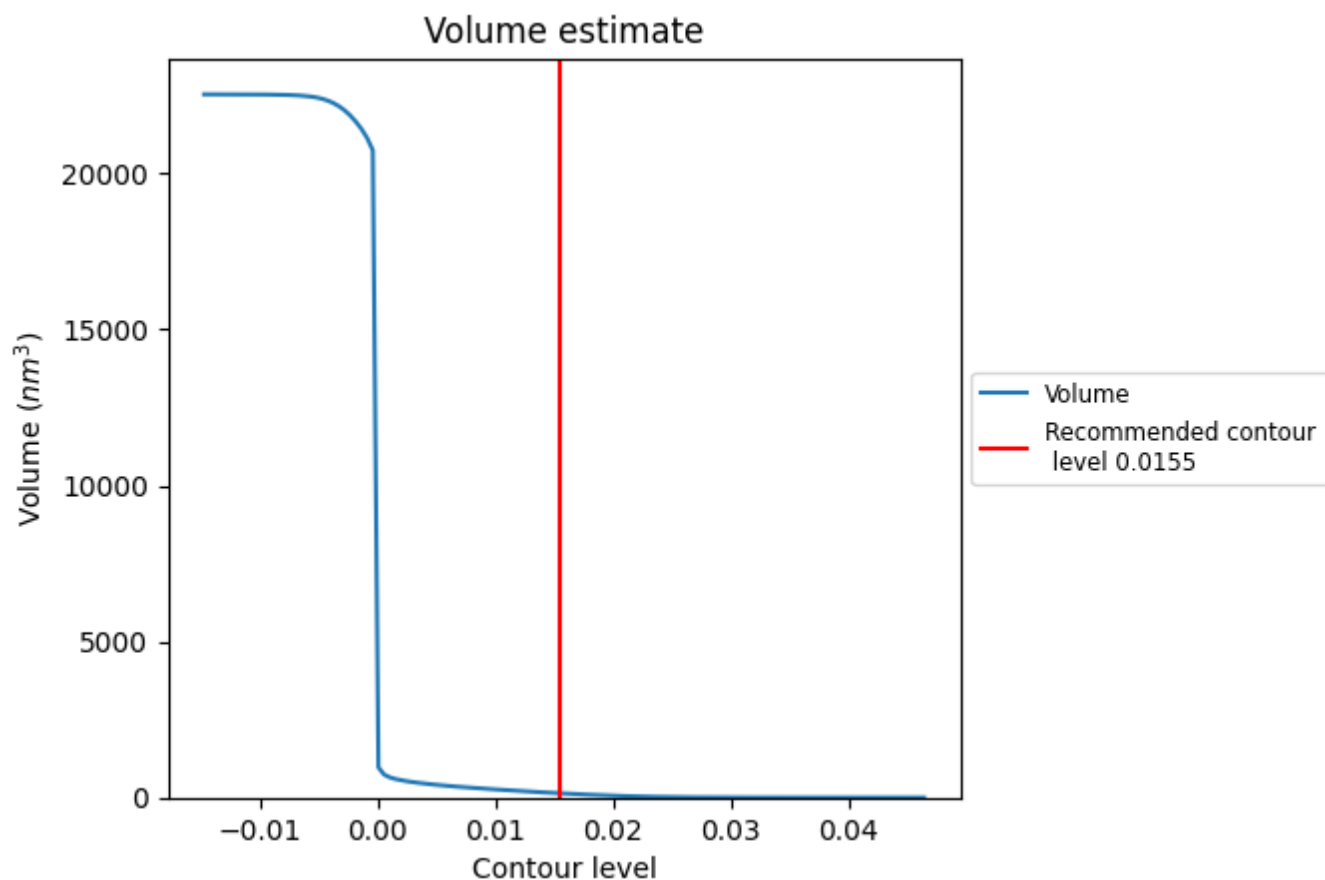
This section contains the results of statistical analysis of the map.

### 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.

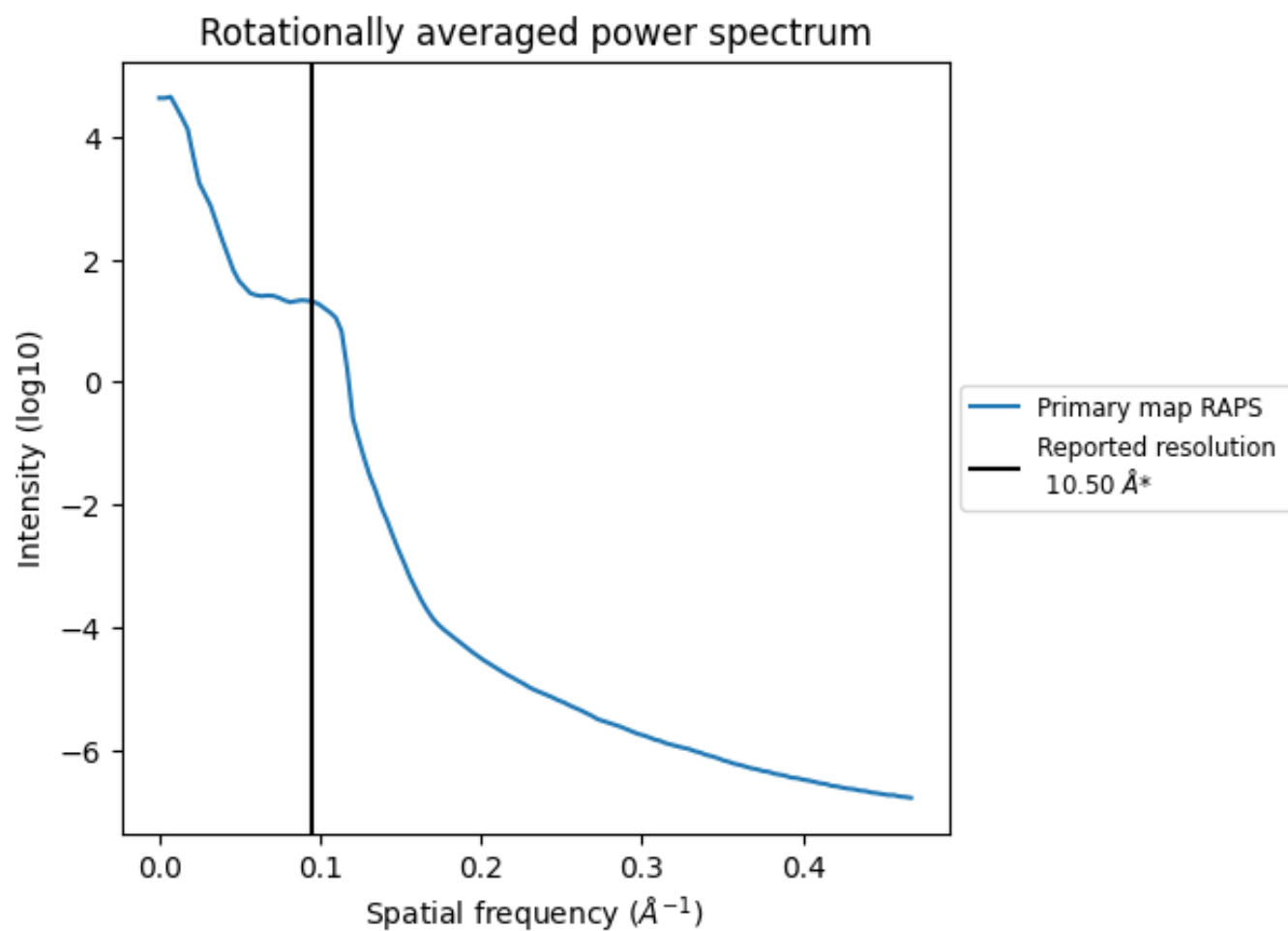
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm<sup>3</sup>; this corresponds to an approximate mass of 124 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 0.095 Å<sup>-1</sup>

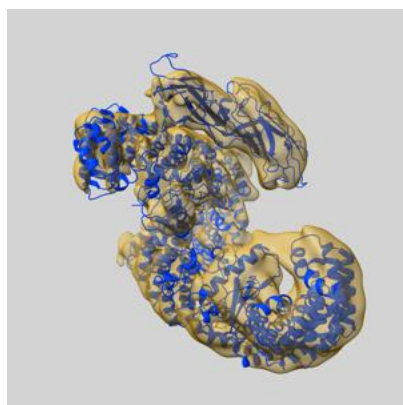
## 8 Fourier-Shell correlation

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

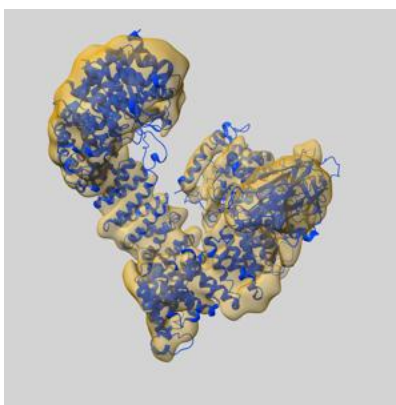
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13189 and PDB model 7P3Z. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

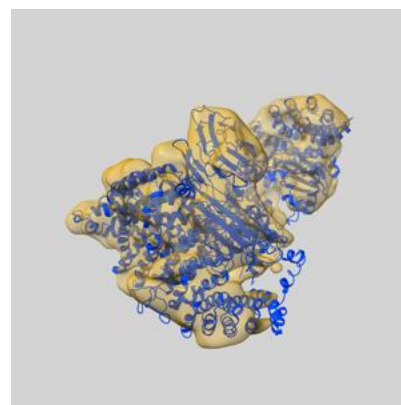
### 9.1 Map-model overlay [i](#)



X



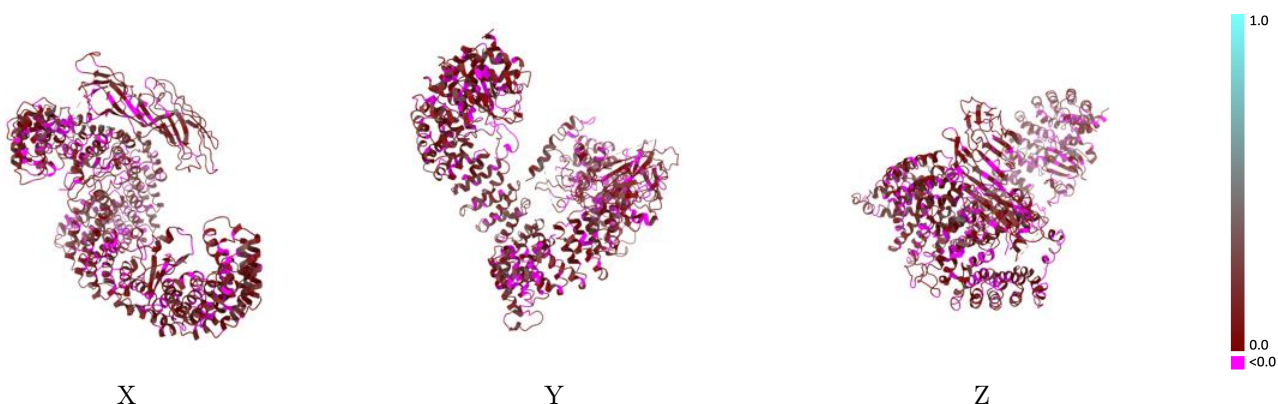
Y



Z

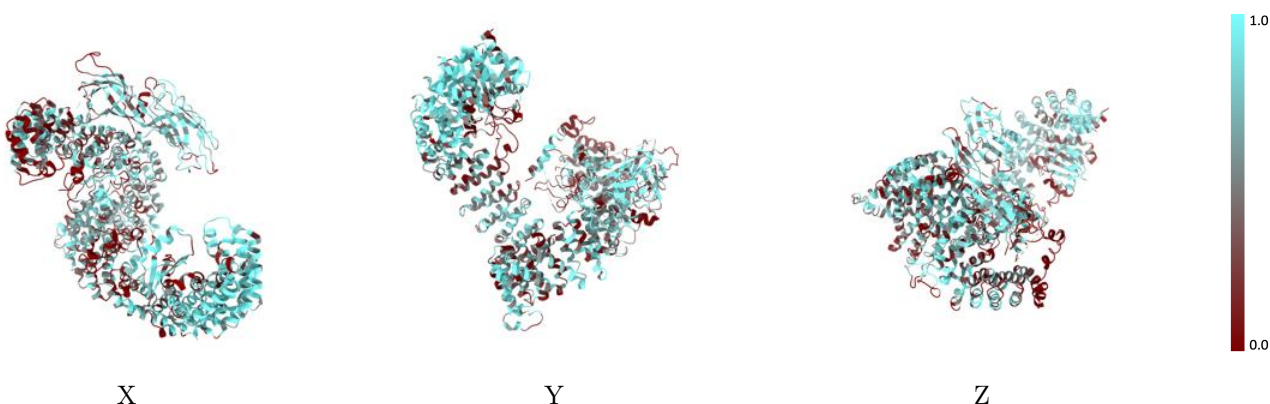
The images above show the 3D surface view of the map at the recommended contour level 0.0155 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



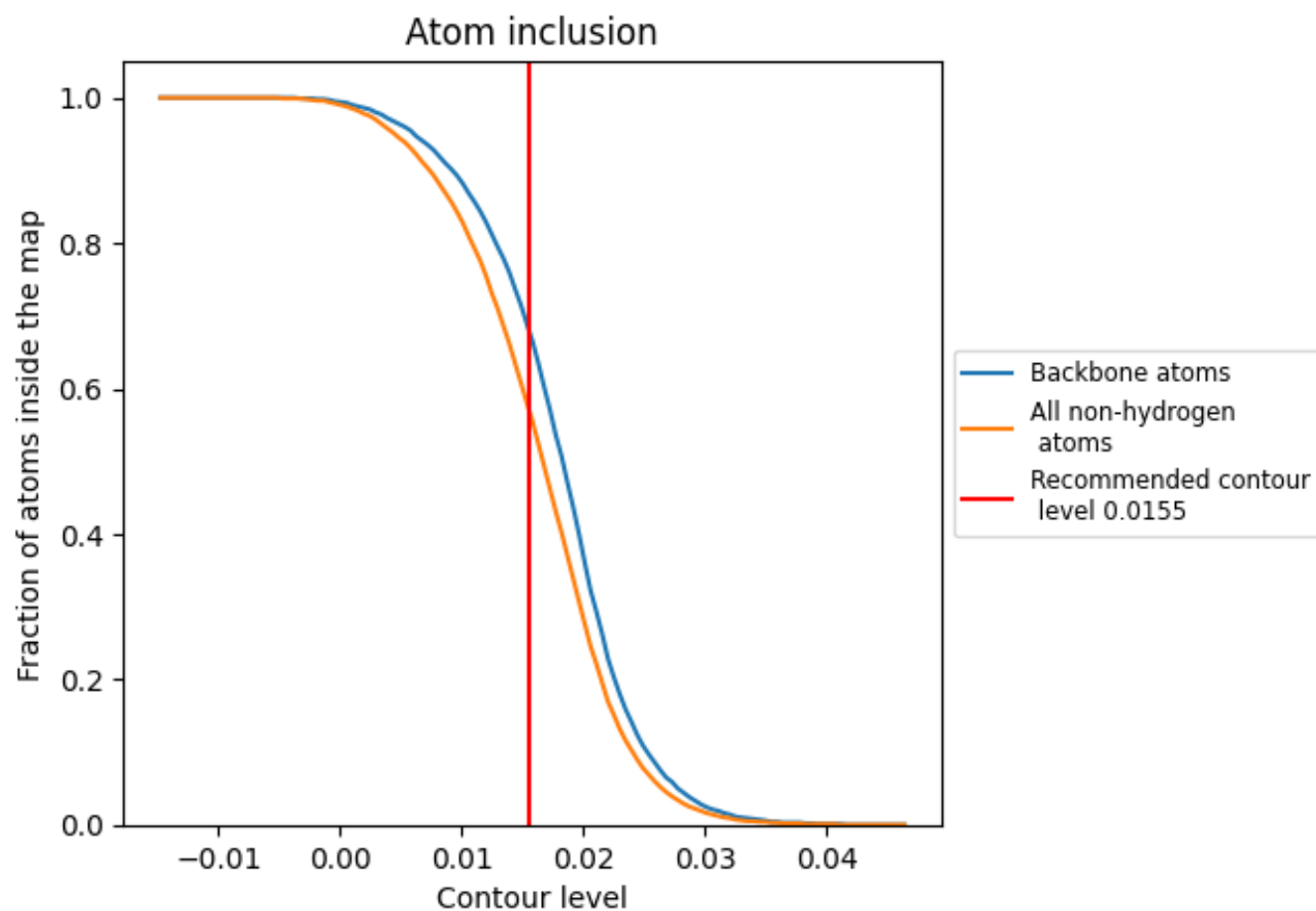
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0155).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 57% 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 (0.0155) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5720	<div></div> 0.0890
A	<div></div> 0.6260	<div></div> 0.1070
B	<div></div> 0.5360	<div></div> 0.0790
M	<div></div> 0.5570	<div></div> 0.0870
S	<div></div> 0.5510	<div></div> 0.0730

