



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 01:29 PM EST

PDB ID : 6X0V
EMDB ID : EMD-21985
Title : Structure of MZT2/GCP-NHD and CDK5Rap2 at position 13 of the gamma-TuRC
Authors : Wieczorek, M.; Huang, T.-L.; Urnavicius, L.; Hsia, K.-C.; Kapoor, T.M.
Deposited on : 2020-05-17
Resolution : 4.50 Å(reported)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
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The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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) : 2.31.2

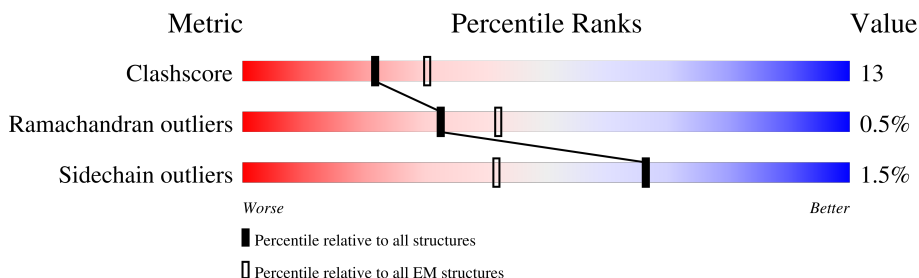
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	158	<div> <div>9%</div> <div>29%</div> <div>71%</div> </div>
2	F	930	<div> <div>10%</div> <div>90%</div> </div>
3	G	1893	<div> <div>98%</div> </div>
3	H	1893	<div> <div>98%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1384 atoms, of which 62 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 Mitotic-spindle organizing protein 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	46	Total	C	N	O	0	0
			227	135	46	46		

- Molecule 2 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	F	95	Total	C	N	O	0	0
			475	285	95	95		

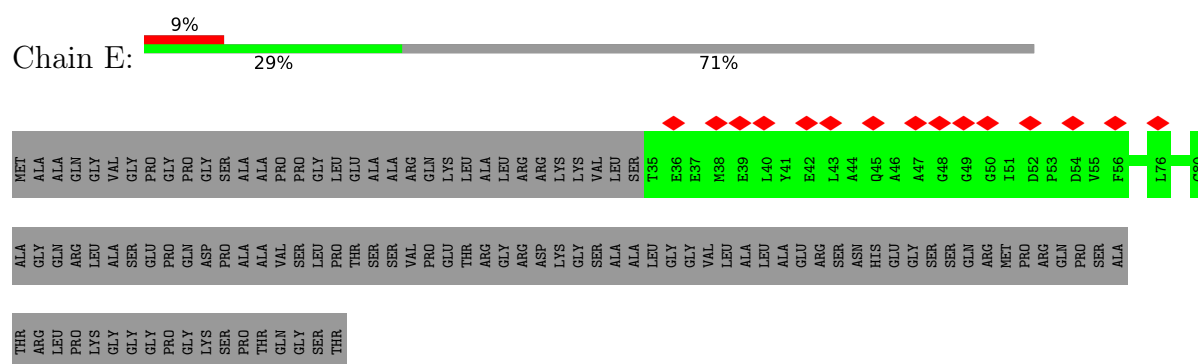
- Molecule 3 is a protein called Centrosome protein Cep215.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	35	Total	C	H	N	O	S	0	0
			333	192	30	54	55	2		
3	H	35	Total	C	H	N	O	S	0	0
			349	202	32	55	58	2		

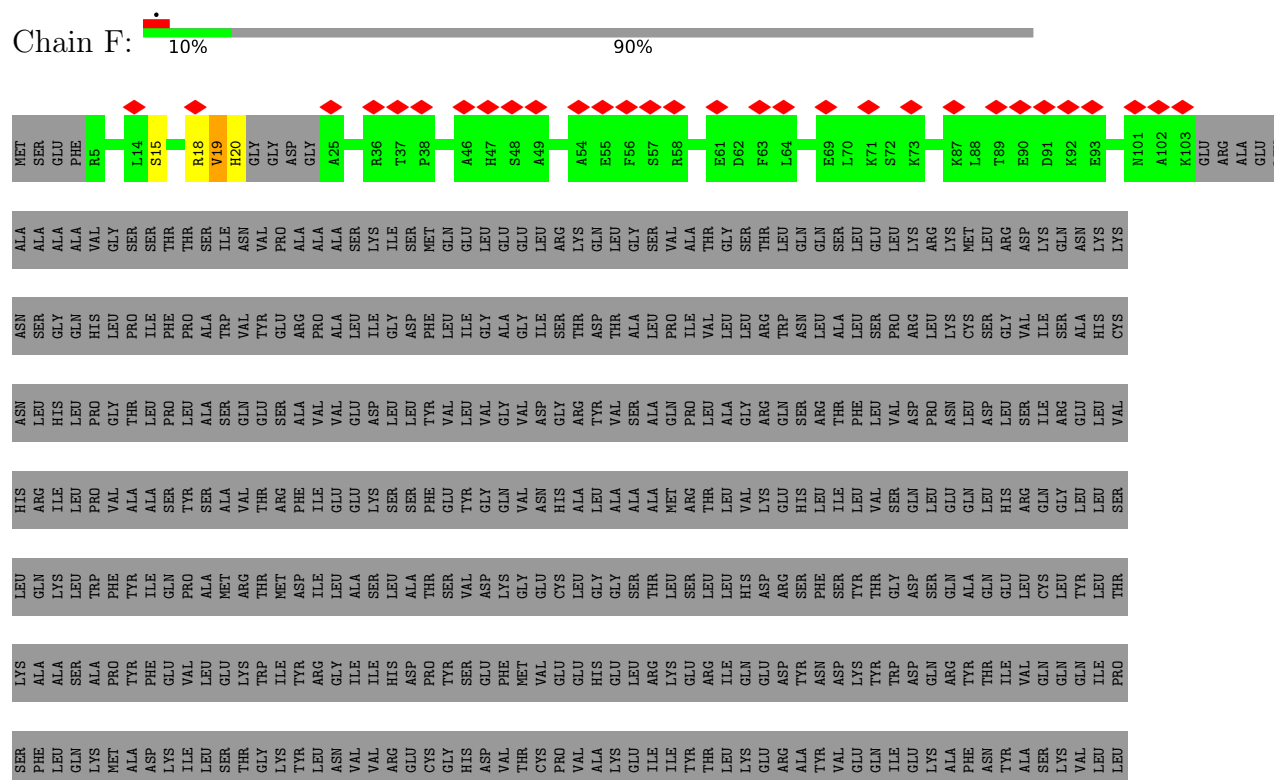
3 Residue-property plots [i](#)

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: Mitotic-spindle organizing protein 2A



• Molecule 2: Gamma-tubulin complex component 2



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

- Molecule 3: Centrosome protein Cep215

Chain G:

98%

[illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.101	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.032	Depositor
Map size (\AA)	381.24802, 381.24802, 381.24802	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.036, 1.036, 1.036	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.24	0/226	0.39	0/313
2	F	0.22	0/473	0.37	0/659
3	G	0.37	0/306	0.47	0/405
3	H	0.26	0/321	0.36	0/424
All	All	0.27	0/1326	0.40	0/1801

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	E	227	0	107	0	0
2	F	475	0	200	4	0
3	G	303	30	300	16	0
3	H	317	32	314	23	0
All	All	1322	62	921	29	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 13.

All (29) 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:F:18:ARG:O	2:F:20:HIS:N	2.29	0.67
3:H:69:GLU:OE1	3:H:70:LEU:HD22	1.99	0.62
3:G:81:ILE:HD12	3:H:81:ILE:HD12	1.80	0.61
3:G:78:LYS:CG	3:H:77:LEU:HD11	2.31	0.61
3:G:74:ASN:HD21	3:H:73:GLU:HG2	1.67	0.58
3:G:78:LYS:HG3	3:H:77:LEU:HD11	1.87	0.56
3:H:84:LEU:O	3:H:88:MET:HG2	2.07	0.55
2:F:15:SER:O	2:F:19:VAL:HA	2.08	0.52
3:G:77:LEU:HD23	3:H:77:LEU:HD22	1.90	0.52
3:H:77:LEU:HD23	3:H:77:LEU:O	2.11	0.51
3:G:78:LYS:HG2	3:H:77:LEU:HD11	1.92	0.51
3:G:74:ASN:ND2	3:H:73:GLU:HG2	2.26	0.51
3:G:84:LEU:HD22	3:H:84:LEU:HD23	1.94	0.49
3:G:60:MET:HG3	3:G:60:MET:O	2.12	0.49
3:G:81:ILE:HG13	3:H:81:ILE:HD11	1.95	0.49
3:G:84:LEU:CD2	3:H:84:LEU:HG	2.44	0.48
3:H:58:ARG:O	3:H:58:ARG:HG3	2.14	0.47
2:F:15:SER:O	2:F:19:VAL:N	2.49	0.45
3:G:67:ILE:HD13	3:G:67:ILE:HA	1.85	0.45
3:H:64:GLU:HG2	3:H:65:ASN:N	2.32	0.45
3:H:77:LEU:O	3:H:81:ILE:HG12	2.17	0.44
3:H:81:ILE:N	3:H:81:ILE:HD13	2.33	0.43
3:G:58:ARG:NH2	3:H:64:GLU:HB2	2.33	0.43
2:F:15:SER:O	2:F:19:VAL:CA	2.67	0.42
3:G:81:ILE:HG23	3:H:81:ILE:HD12	2.01	0.42
3:G:84:LEU:HD22	3:H:84:LEU:CD2	2.49	0.42
3:G:81:ILE:HG13	3:H:81:ILE:CD1	2.50	0.41
3:H:78:LYS:O	3:H:78:LYS:HG3	2.21	0.40
3:H:62:ASP:HA	3:H:65:ASN:HB3	2.04	0.40

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	E	44/158 (28%)	42 (96%)	2 (4%)	0	100	100
2	F	91/930 (10%)	88 (97%)	2 (2%)	1 (1%)	14	52
3	G	33/1893 (2%)	31 (94%)	2 (6%)	0	100	100
3	H	33/1893 (2%)	32 (97%)	1 (3%)	0	100	100
All	All	201/4874 (4%)	193 (96%)	7 (4%)	1 (0%)	32	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	19	VAL

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	
3	G	32/1704 (2%)	31 (97%)	1 (3%)	40	63
3	H	35/1704 (2%)	35 (100%)	0	100	100
All	All	67/3408 (2%)	66 (98%)	1 (2%)	66	80

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	74	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

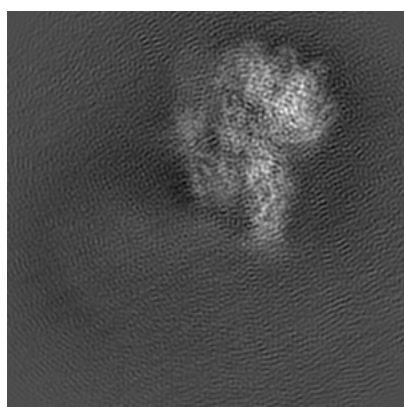
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21985. These allow visual inspection of the internal detail of the map and identification of artifacts.

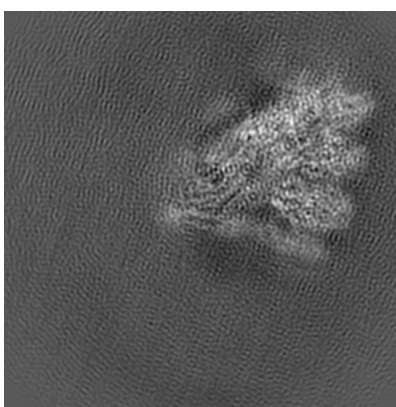
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

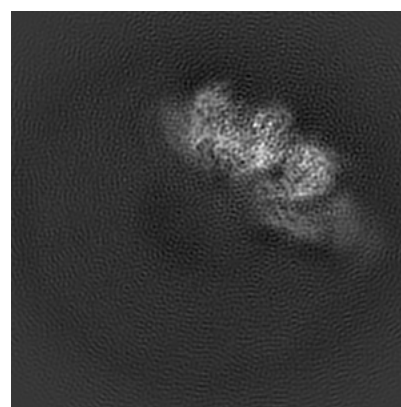
6.1.1 Primary map



X



Y

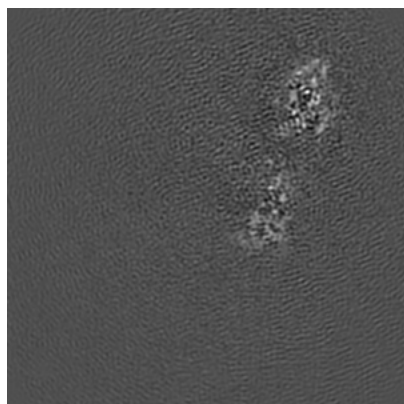


Z

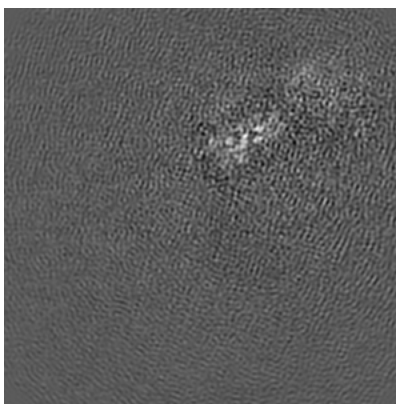
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

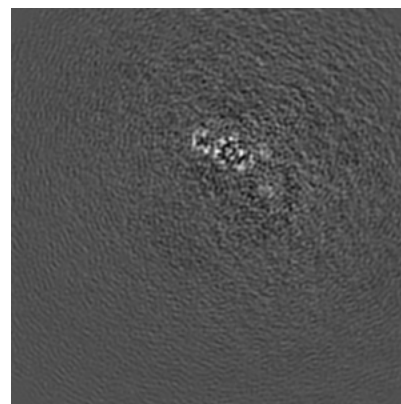
6.2.1 Primary map



X Index: 184



Y Index: 184

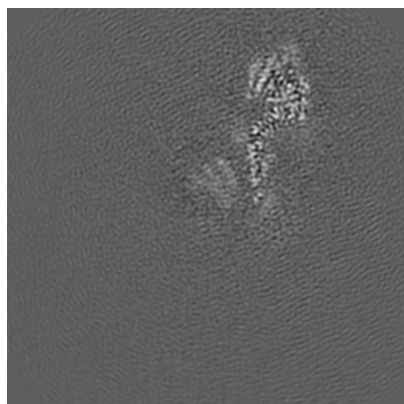


Z Index: 184

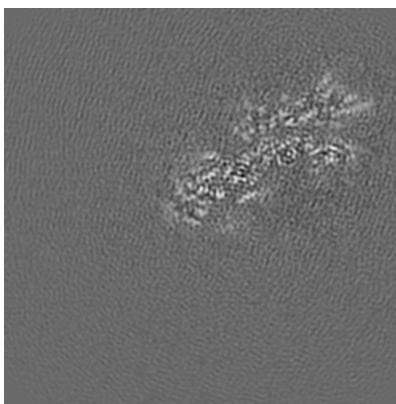
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

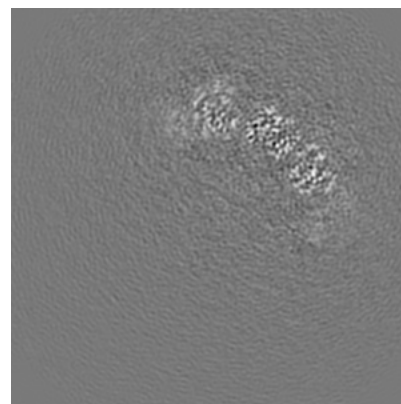
6.3.1 Primary map



X Index: 228



Y Index: 234



Z Index: 277

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

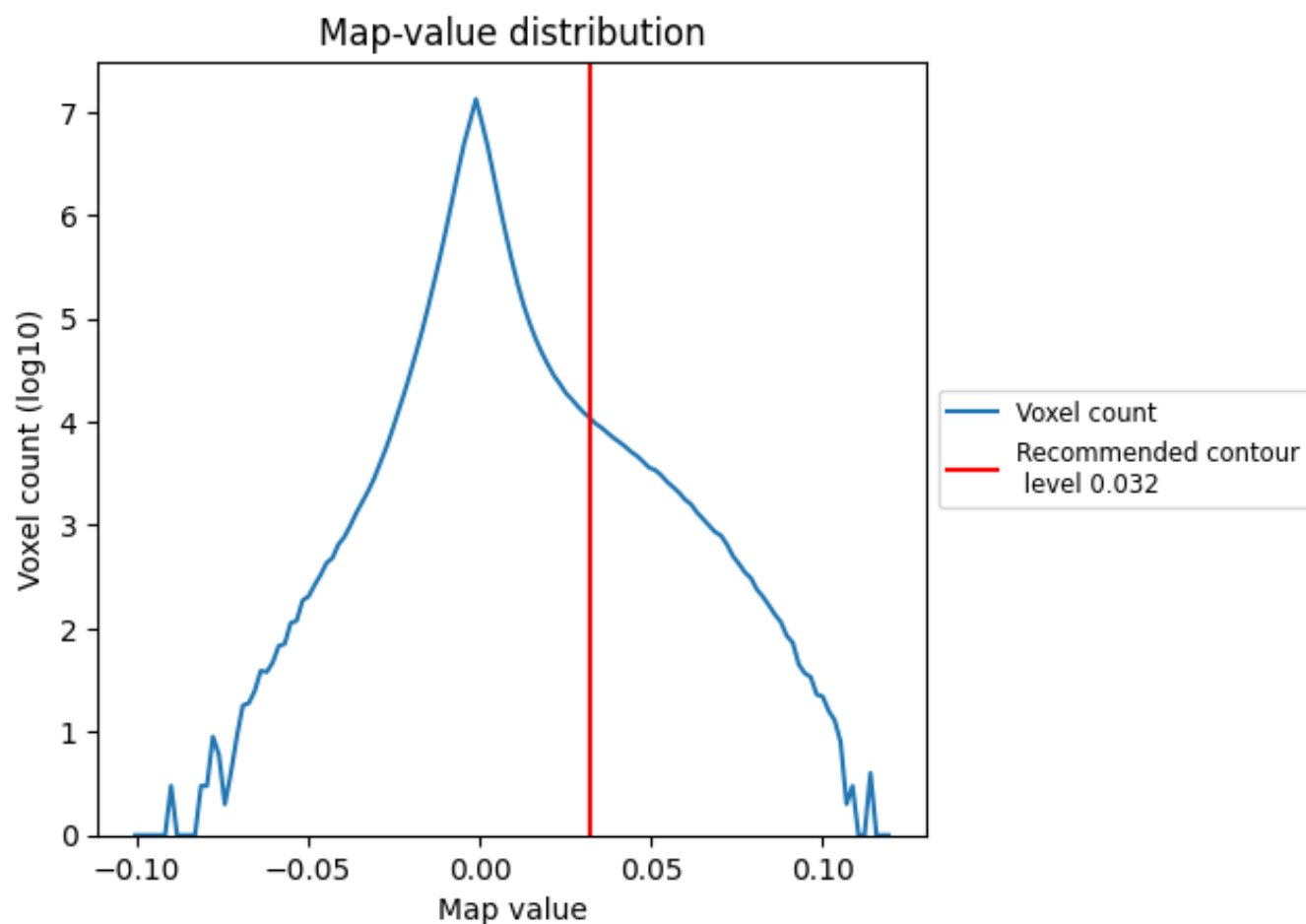
6.5 Mask visualisation

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

7 Map analysis [i](#)

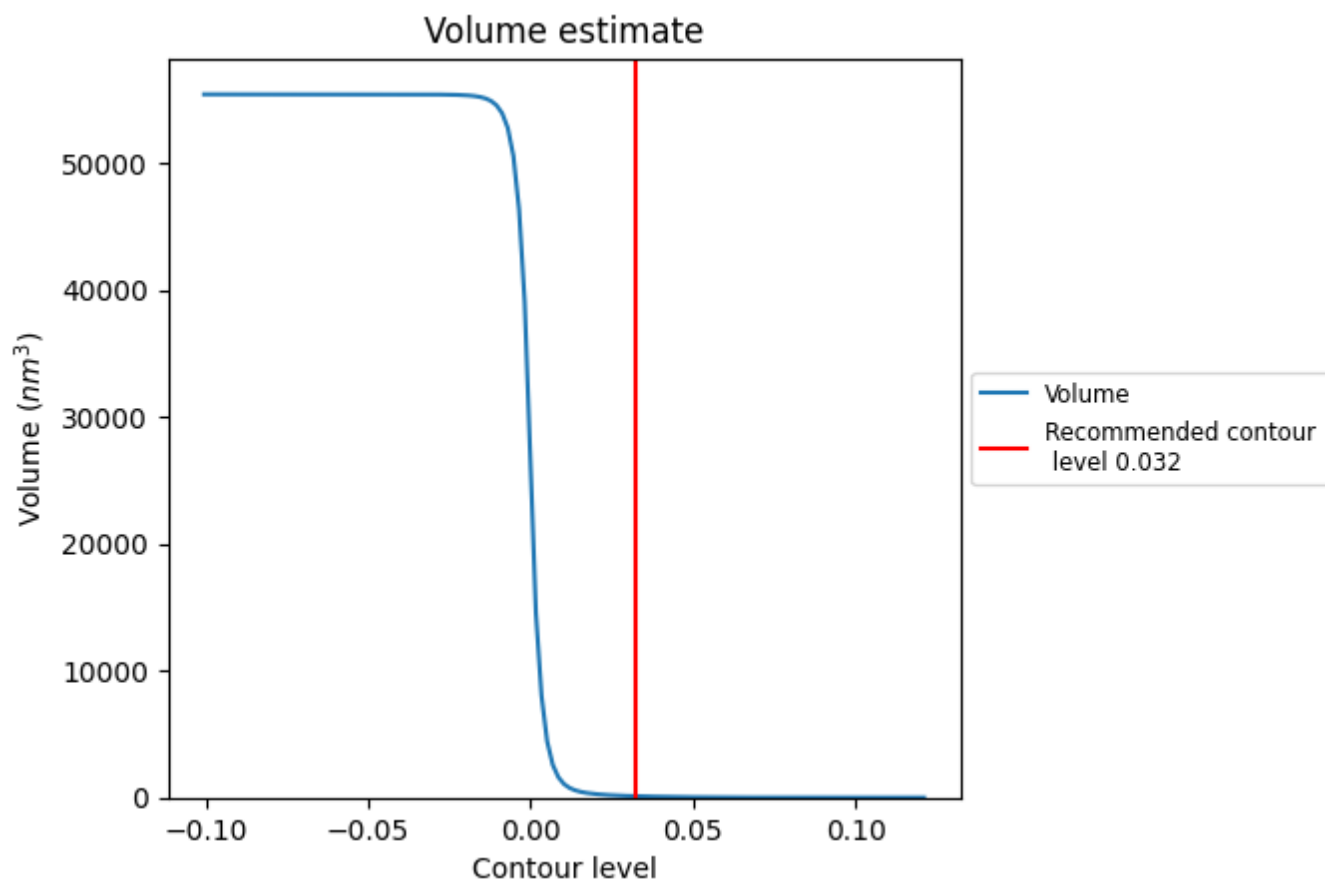
This section contains the results of statistical analysis of the map.

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.

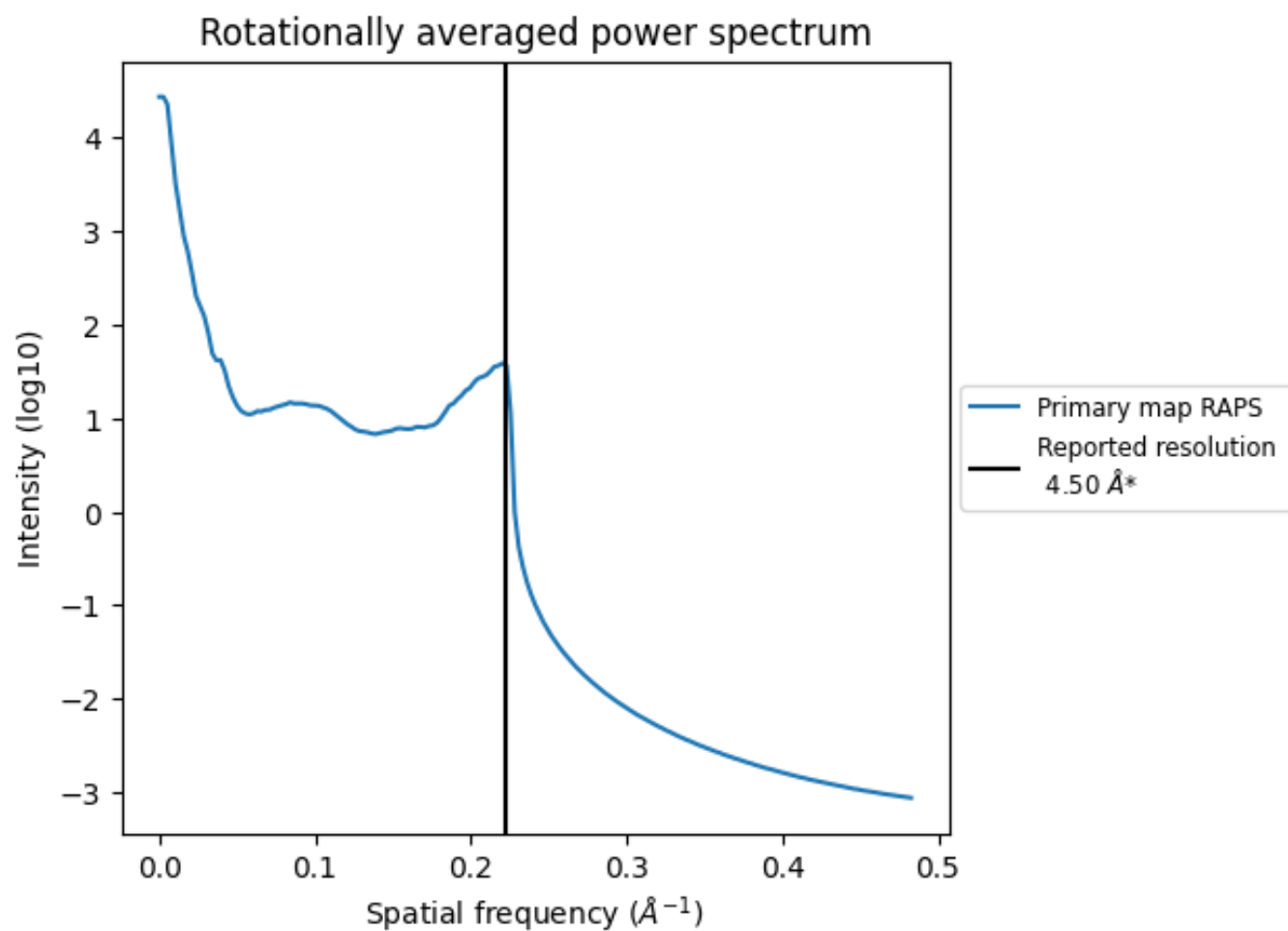
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm³; this corresponds to an approximate mass of 100 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 0.222 Å⁻¹

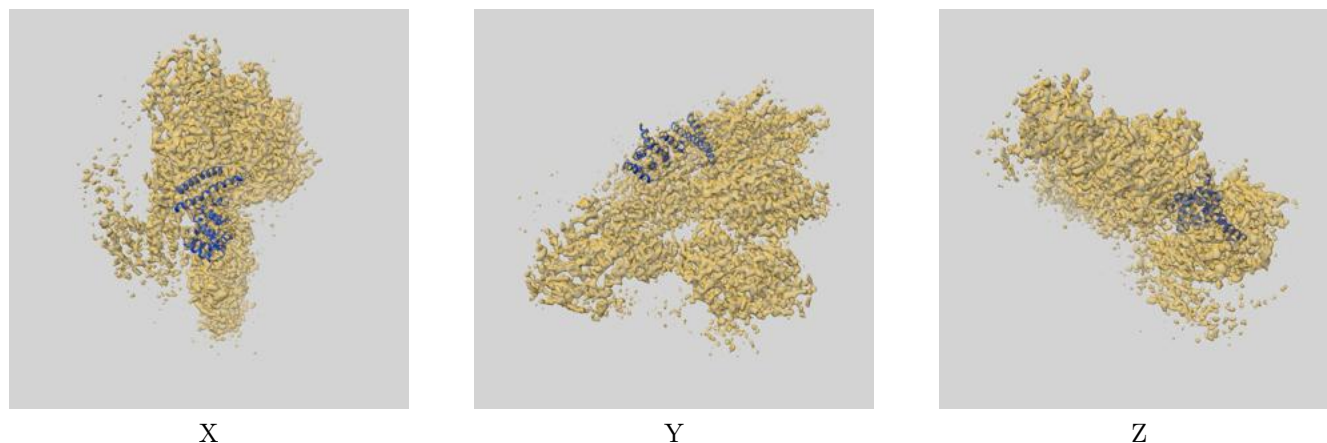
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21985 and PDB model 6X0V. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



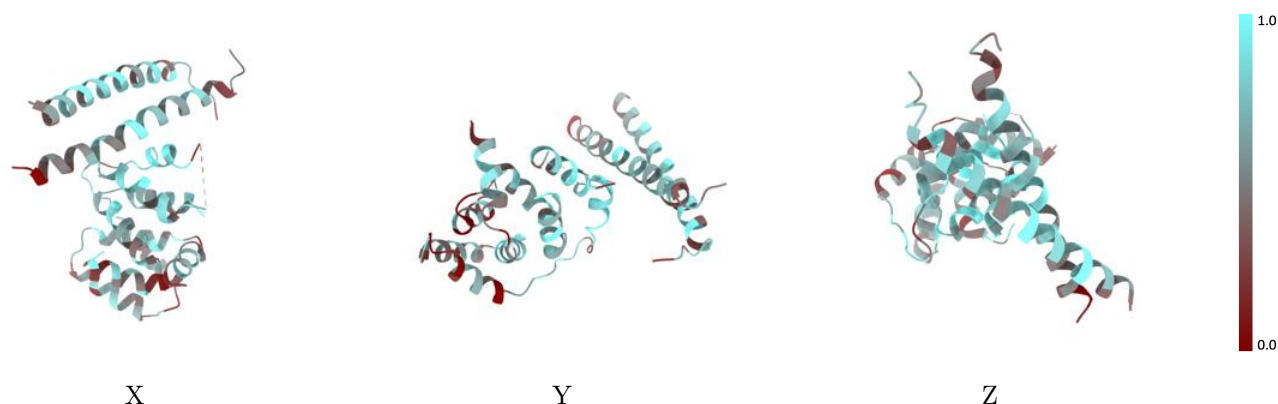
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



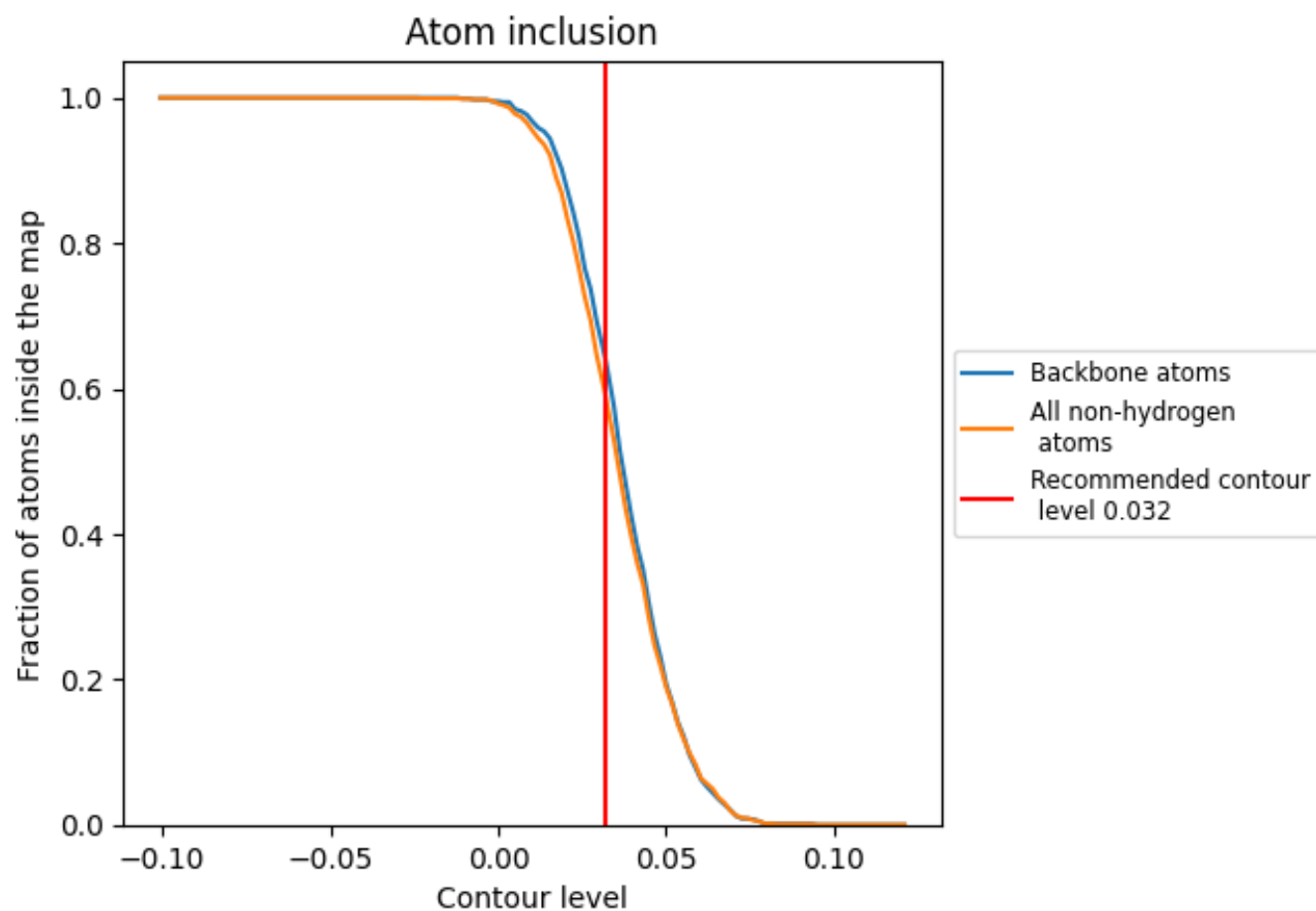
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 59% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5901	<div></div> 0.4160
E	<div></div> 0.5859	<div></div> 0.3980
F	<div></div> 0.6063	<div></div> 0.3910
G	<div></div> 0.6520	<div></div> 0.4510
H	<div></div> 0.5161	<div></div> 0.4350

