Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 10:42 pm GMT

PDB ID	:	5K1H
EMDB ID	:	EMD-8195
Title	:	eIF3b relocated to the intersubunit face to interact with eIF1 and below the eIF2 ternary-complex. from the structure of a partial yeast 48S preinitiation complex in closed conformation.
Authors	:	Simonetti, A.; Brito Querido, J.; Myasnikov, A.G.; Mancera-Martinez, E.; Renaud, A.; Kuhn, L.; Hashem, Y.
Deposited on	:	2016-05-18
Resolution	:	4.90 Å(reported)
Based on initial model	:	5A5U

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

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 (i)) were used in the production of this report:

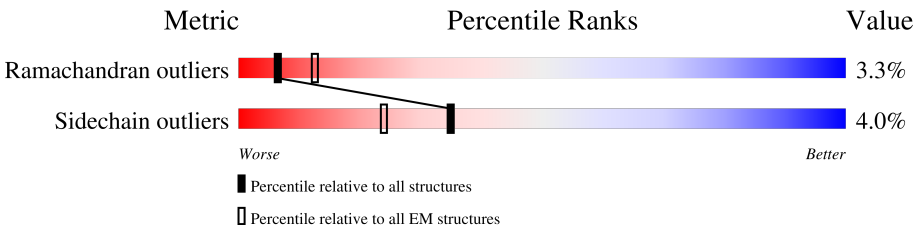
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.90 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)
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 <=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	B	576	34% 84% 10%
2	A	54	100%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4760 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 Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	554	4545	2919	779	829	18	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	403	SER	THR	conflict	UNP P55884
B	499	SER	ASN	conflict	UNP P55884
B	506	SER	ILE	conflict	UNP P55884

- Molecule 2 is a protein called eIF3a C-terminal tail.

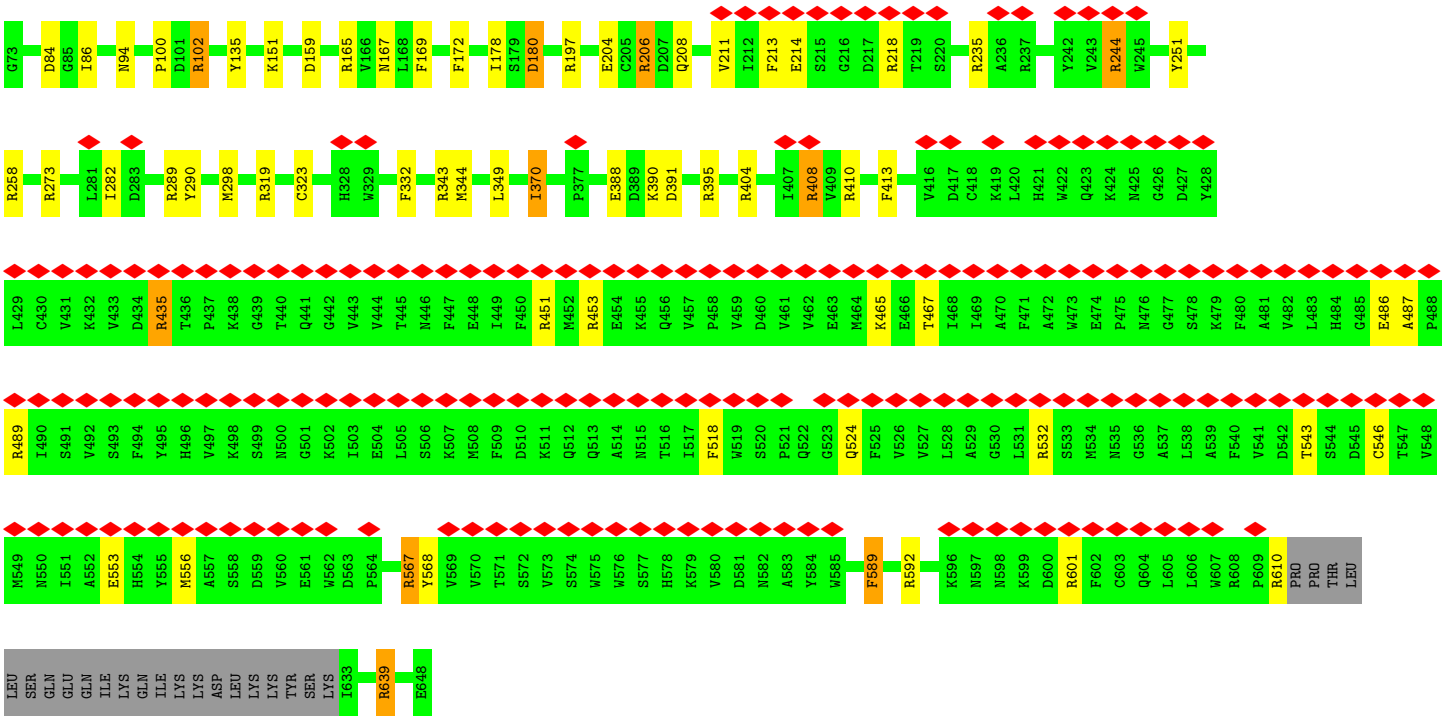
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	54	215	108	54	53	0	0

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.

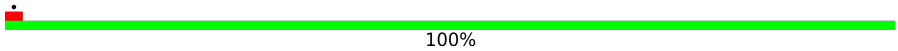
• Molecule 1: Eukaryotic translation initiation factor 3 subunit B

Chain B:



• Molecule 2: eIF3a C-terminal tail

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	254957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.0143	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.2, 2.2, 2.2	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	B	0.70	0/4672	1.16	30/6324 (0.5%)

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	B	3	18

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	258	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	B	435	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	404	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	B	453	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	610	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	197	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	B	408	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	410	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	610	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	451	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	592	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	343	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	206	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	B	532	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	489	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	451	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	235	ARG	NE-CZ-NH1	6.11	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	410	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	273	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	404	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	319	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	258	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	273	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	567	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	206	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	B	235	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	543	THR	C-N-CA	5.24	134.80	121.70
1	B	218	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	102	ARG	NE-CZ-NH1	5.08	122.84	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	211	VAL	CA
1	B	213	PHE	CA
1	B	214	GLU	CA

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	ARG	Sidechain
1	B	135	TYR	Sidechain
1	B	165	ARG	Sidechain
1	B	180	ASP	Peptide
1	B	204	GLU	Peptide
1	B	244	ARG	Sidechain
1	B	251	TYR	Sidechain
1	B	289	ARG	Sidechain
1	B	290	TYR	Sidechain
1	B	344	MET	Peptide
1	B	395	ARG	Sidechain
1	B	408	ARG	Sidechain
1	B	435	ARG	Sidechain
1	B	553	GLU	Peptide
1	B	567	ARG	Sidechain
1	B	568	TYR	Sidechain
1	B	601	ARG	Sidechain
1	B	639	ARG	Sidechain

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	B	4545	0	4434	0	0
2	A	215	0	2	0	0
All	All	4760	0	4436	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	B	550/576 (96%)	483 (88%)	49 (9%)	18 (3%)	4 29

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	ASP
1	B	211	VAL
1	B	214	GLU
1	B	546	CYS
1	B	86	ILE
1	B	208	GLN
1	B	323	CYS
1	B	467	THR
1	B	84	ASP

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Mol	Chain	Res	Type
1	B	169	PHE
1	B	178	ILE
1	B	282	ILE
1	B	589	PHE
1	B	100	PRO
1	B	206	ARG
1	B	413	PHE
1	B	487	ALA
1	B	370	ILE

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	B	495/517 (96%)	475 (96%)	20 (4%)	31 56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	ASN
1	B	151	LYS
1	B	159	ASP
1	B	167	ASN
1	B	172	PHE
1	B	213	PHE
1	B	298	MET
1	B	332	PHE
1	B	349	LEU
1	B	370	ILE
1	B	388	GLU
1	B	390	LYS
1	B	391	ASP
1	B	465	LYS
1	B	486	GLU
1	B	518	PHE
1	B	524	GLN

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Mol	Chain	Res	Type
1	B	556	MET
1	B	589	PHE
1	B	639	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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.

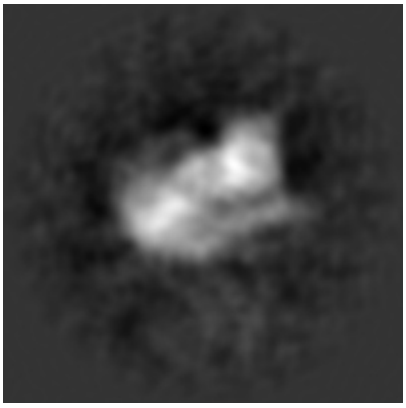
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8195. These allow visual inspection of the internal detail of the map and identification of artifacts.

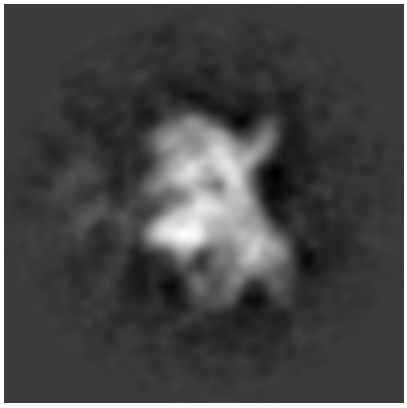
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

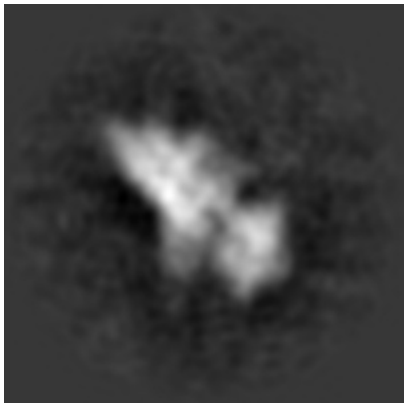
6.1.1 Primary map



X



Y

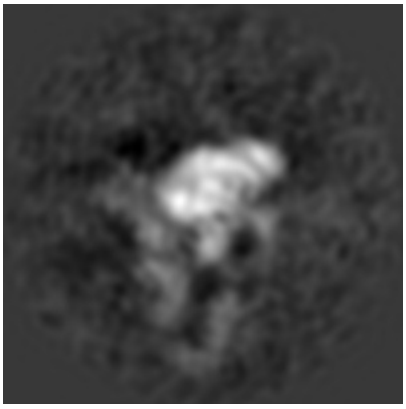


Z

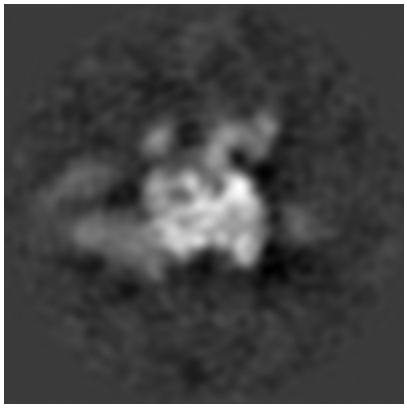
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

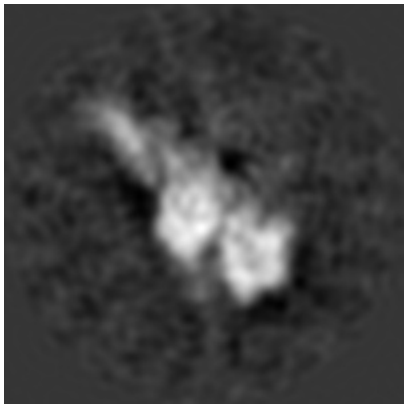
6.2.1 Primary map



X Index: 100



Y Index: 100

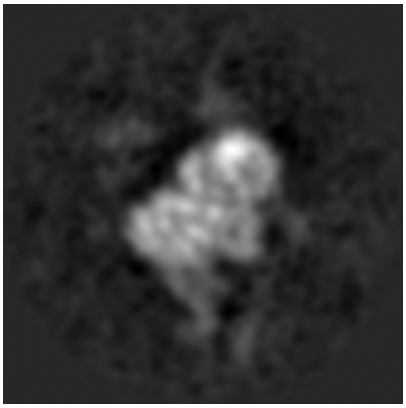


Z Index: 100

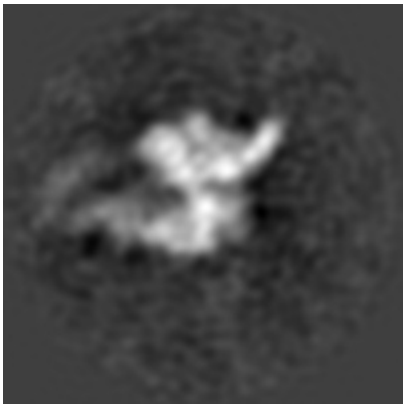
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

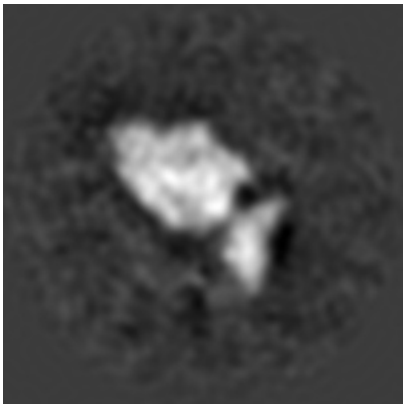
6.3.1 Primary map



X Index: 86



Y Index: 87



Z Index: 119

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 0.0143. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

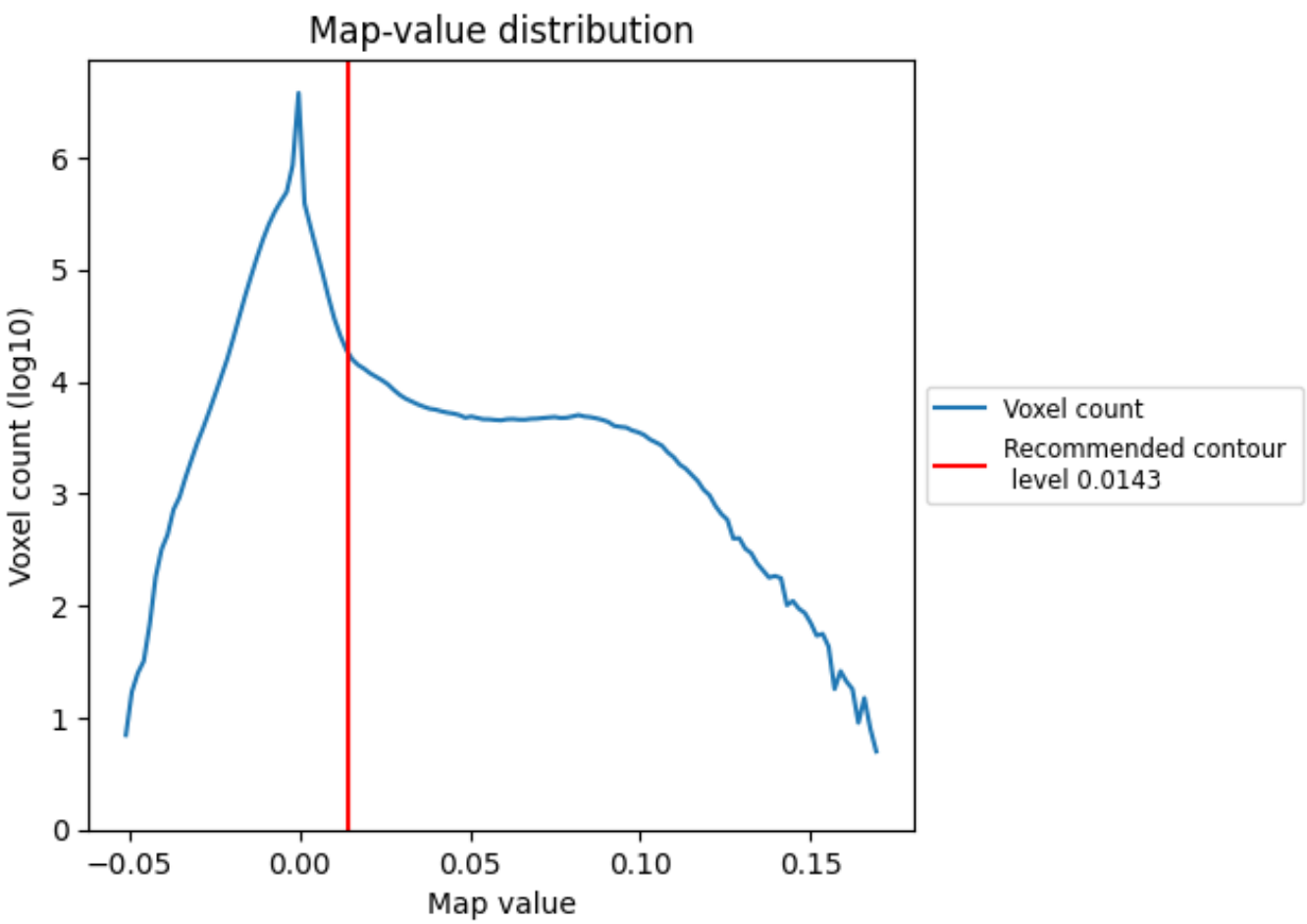
6.5 Mask visualisation (i)

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

7 Map analysis (i)

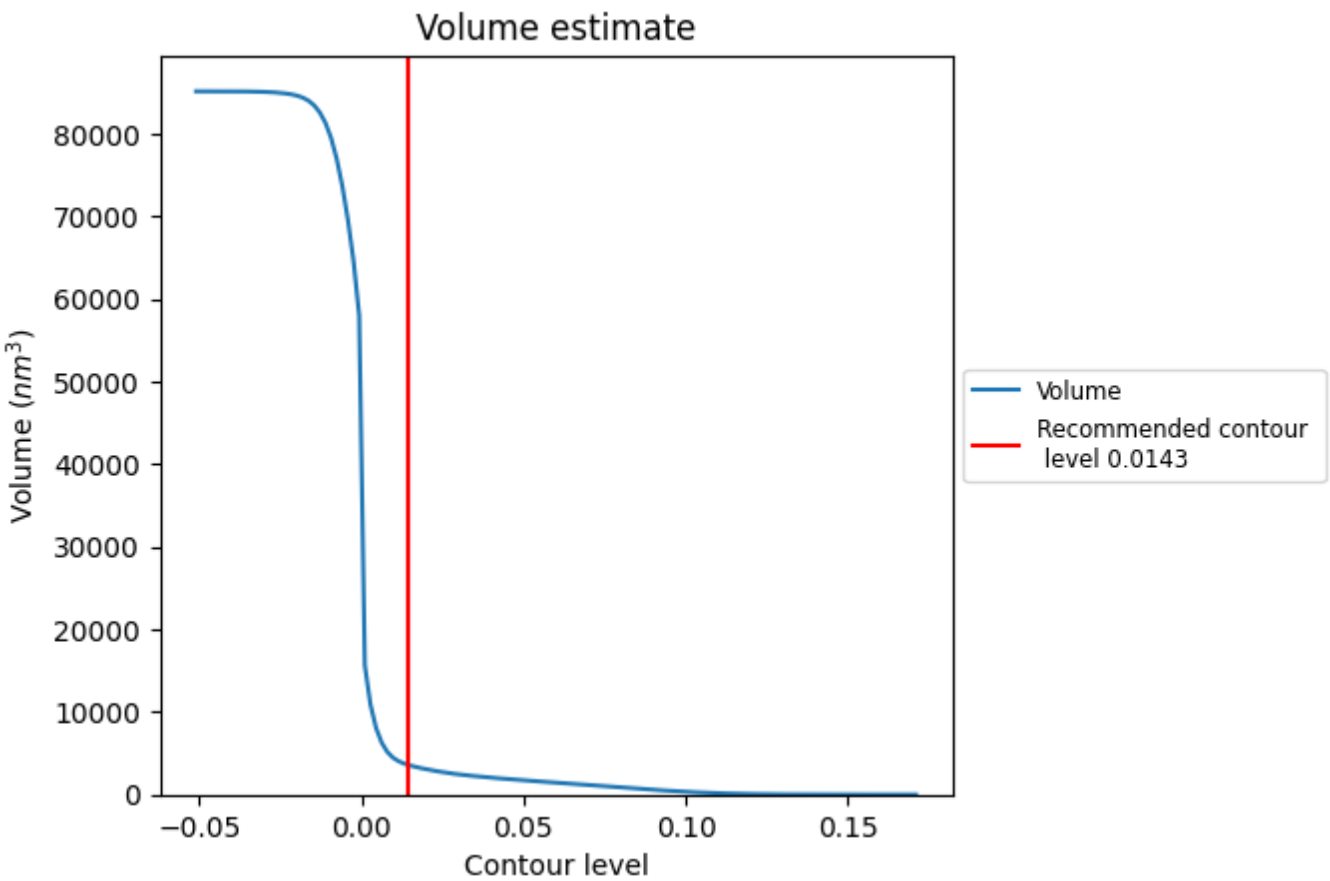
This section contains the results of statistical analysis of the map.

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.

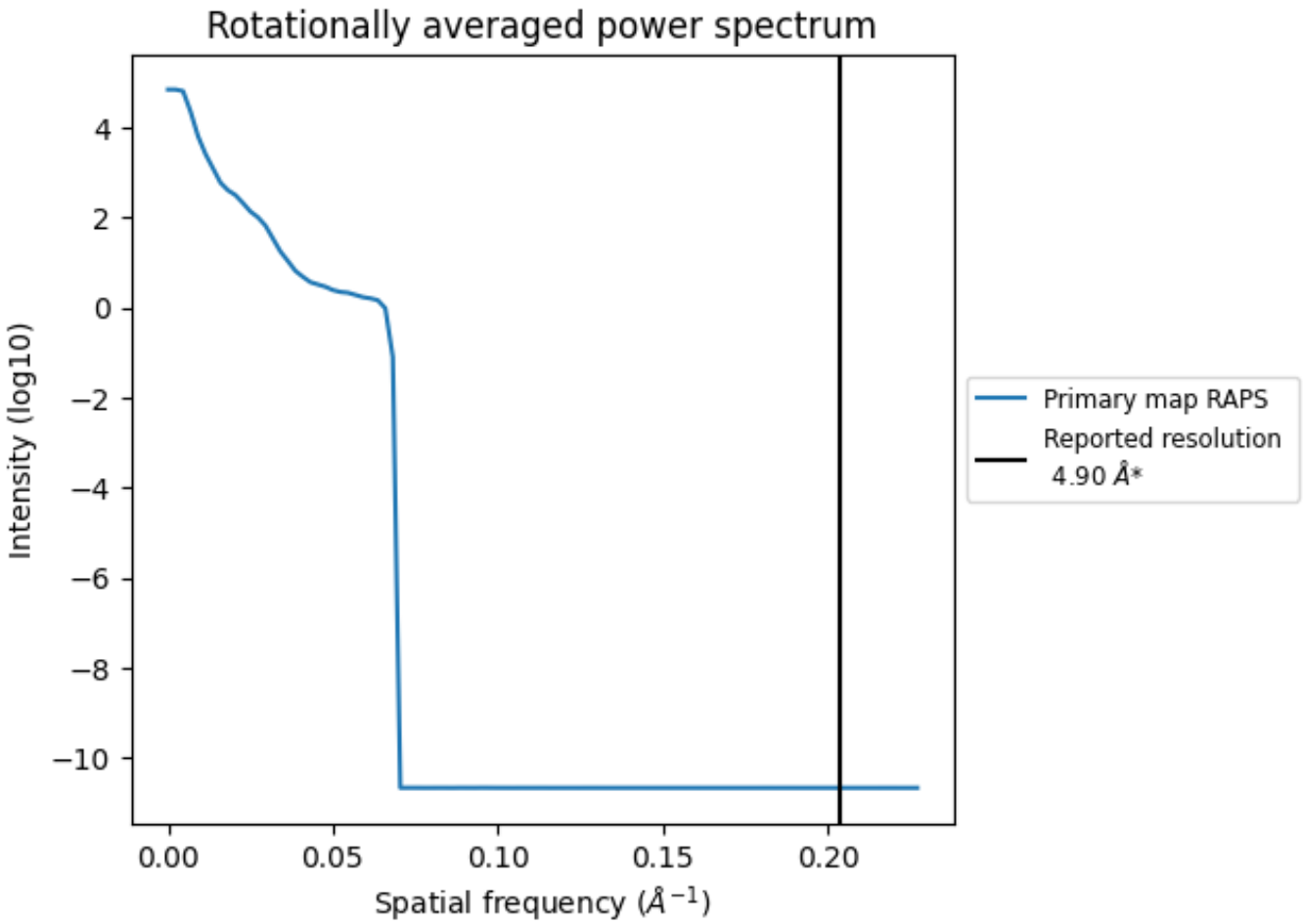
7.2 Volume estimate (i)



The volume at the recommended contour level is 3610 nm^3; this corresponds to an approximate mass of 3261 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 0.204 Å^{-1}

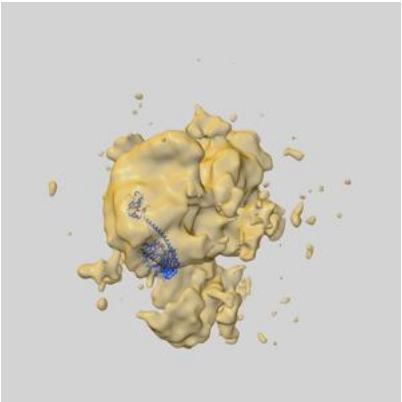
8 Fourier-Shell correlation (i)

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

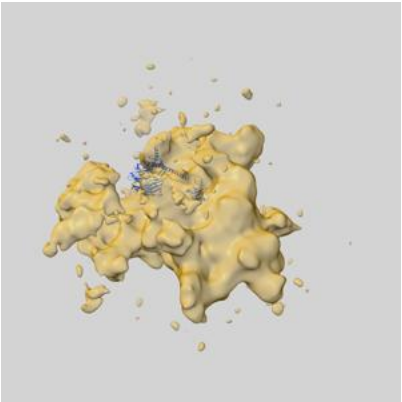
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8195 and PDB model 5K1H. Per-residue inclusion information can be found in section 3 on page 4.

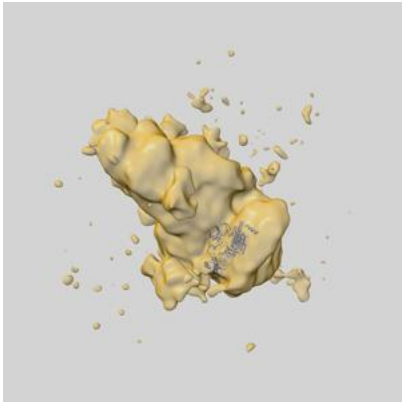
9.1 Map-model overlay (i)



X



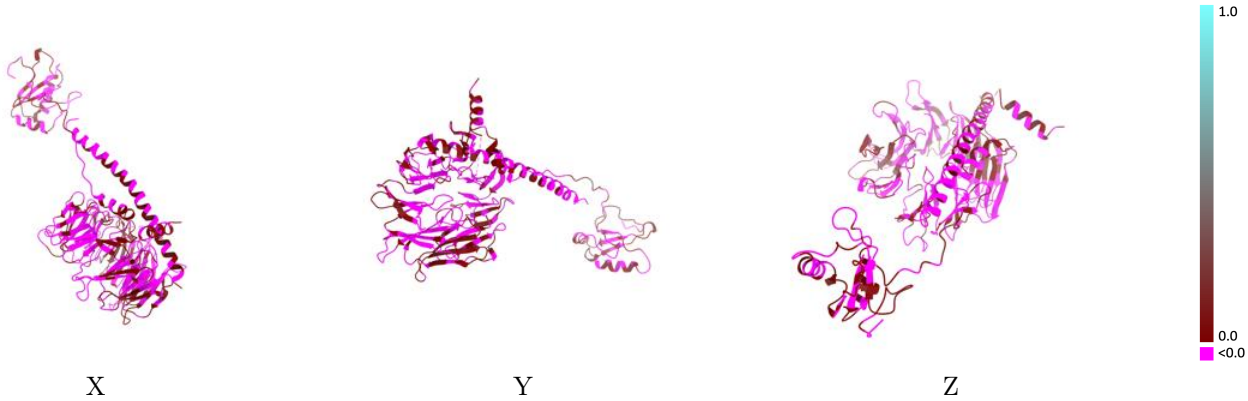
Y



Z

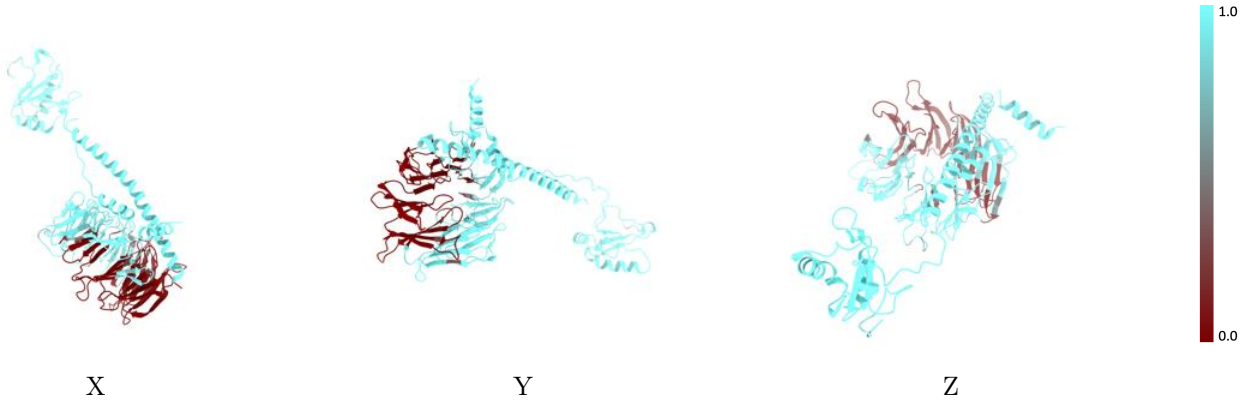
The images above show the 3D surface view of the map at the recommended contour level 0.0143 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



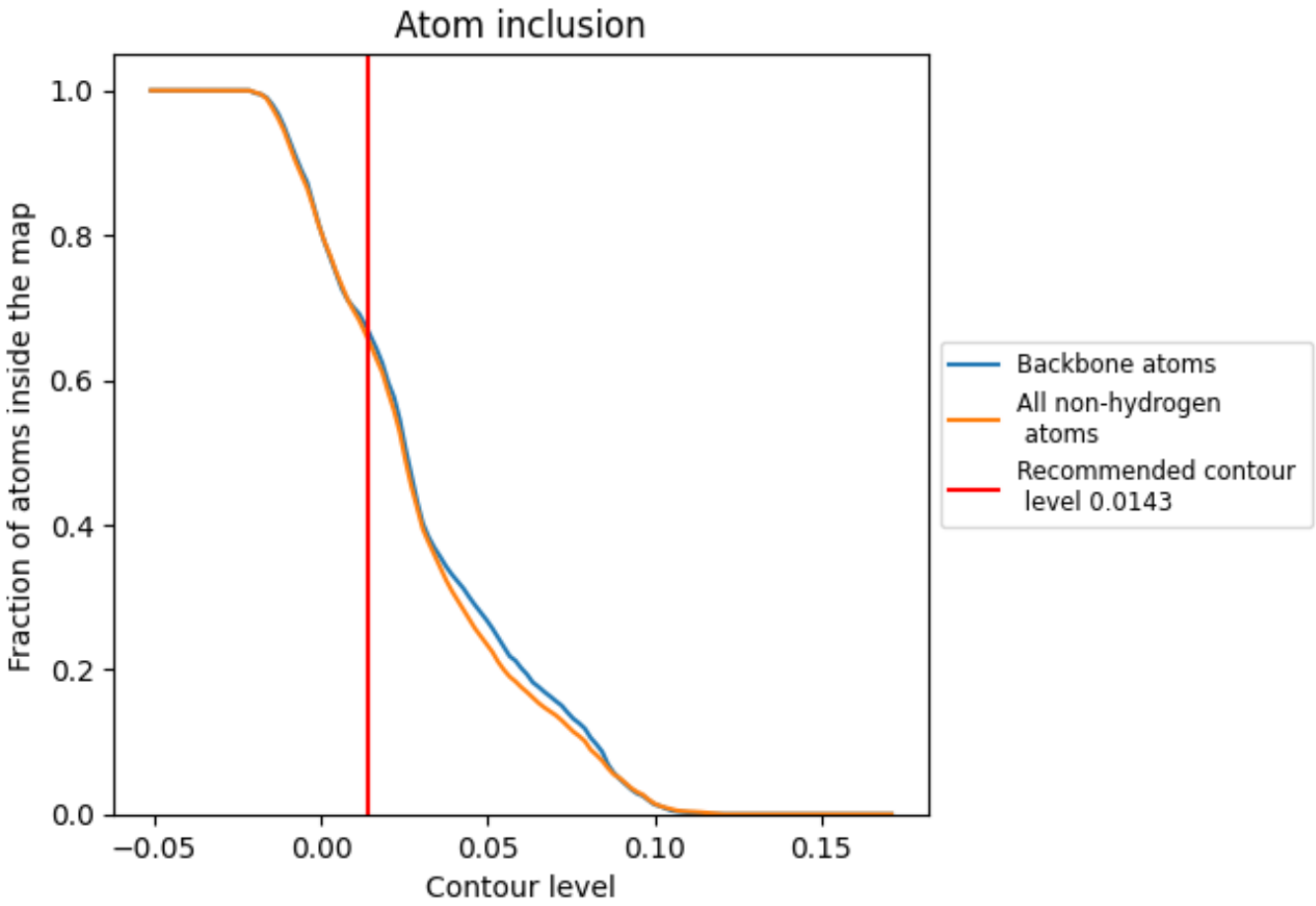
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0143).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0143) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6545	-0.0110
A	0.9767	-0.0190
B	0.6390	-0.0100