



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2024 – 02:09 PM EST

PDB ID : 8U5H
EMDB ID : EMD-41922
Title : Cryo-EM structure of human DNMT3A UDR bound to H2AK119ub1-modified nucleosome
Authors : Chen, X.; Song, J.
Deposited on : 2023-09-12
Resolution : 3.23 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

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>.

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) : 2.40

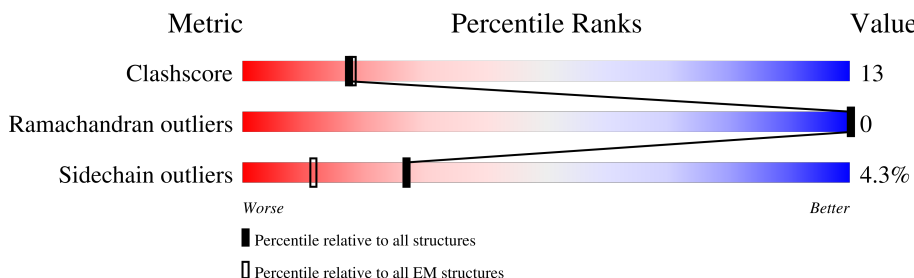
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 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 ≥ 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	98	
1	B	98	
2	C	180	
3	D	76	
4	H	180	
5	I	136	
5	O	136	
6	J	103	

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Mol	Chain	Length	Quality of chain
6	Q	103	
7	K	130	
7	R	130	
8	M	123	
8	S	123	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13436 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 (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	41	Total	C	N	O	0	0
			281	177	55	49		
1	B	23	Total	C	N	O	0	0
			163	102	34	27		

- Molecule 2 is a DNA chain called nucleosome DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	157	Total	C	N	O	P	0	0
			3200	1520	583	940	157		

- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	66	Total	C	N	O	S	0	0
			488	313	80	94	1		

- Molecule 4 is a DNA chain called nucleosome DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	157	Total	C	N	O	P	0	0
			3237	1533	603	944	157		

- Molecule 5 is a protein called Histone H3.3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	98	Total	C	N	O	S	0	0
			807	509	156	139	3		
5	O	99	Total	C	N	O	S	0	0
			816	515	158	140	3		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	84	Total	C	N	O	S	1	0
			676	427	132	116	1		
6	Q	83	Total	C	N	O	S	0	0
			647	407	125	114	1		

- Molecule 7 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	110	Total	C	N	O	S	0	0
			824	515	164	144	1		
7	R	108	Total	C	N	O	S	0	0
			825	519	161	144	1		

There are 2 discrepancies between the modelled and reference sequences:

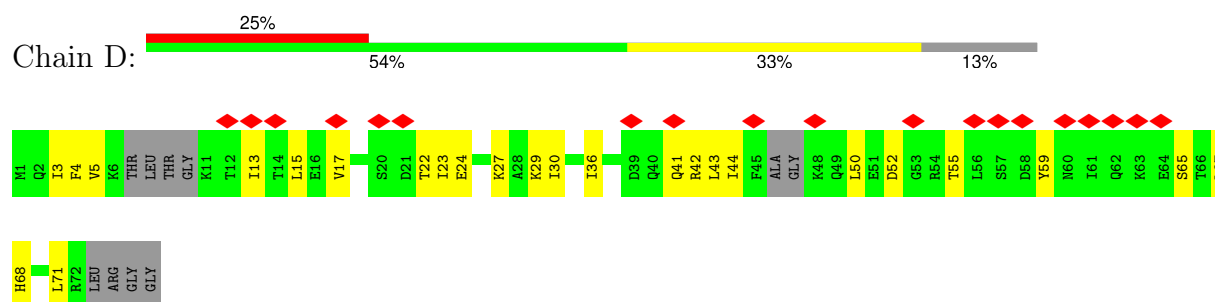
Chain	Residue	Modelled	Actual	Comment	Reference
K	119	CYS	LYS	engineered mutation	UNP Q6AZJ8
R	119	CYS	LYS	engineered mutation	UNP Q6AZJ8

- Molecule 8 is a protein called Histone H2B 1.1.

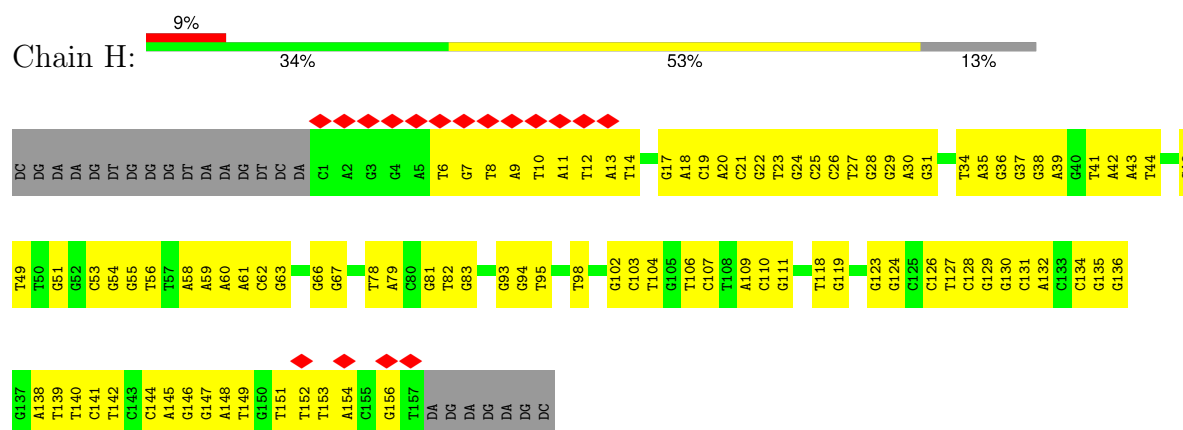
Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	95	Total	C	N	O	S	0	0
			731	460	130	139	2		
8	S	96	Total	C	N	O	S	0	0
			741	466	133	140	2		

There are 4 discrepancies between the modelled and reference sequences:

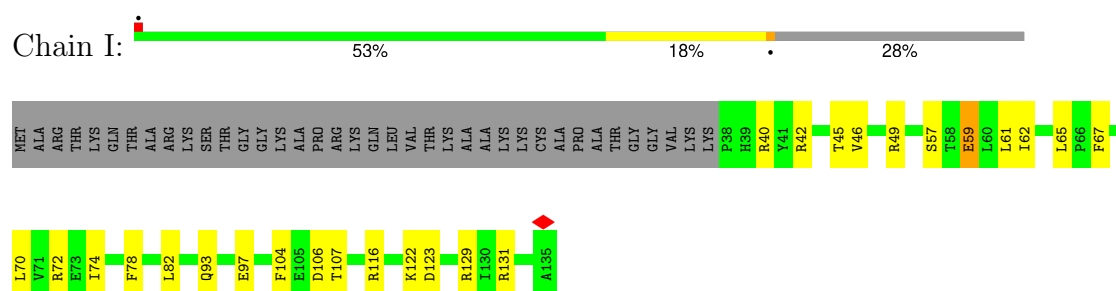
Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	initiating methionine	UNP P02281
M	29	THR	SER	engineered mutation	UNP P02281
S	0	MET	-	initiating methionine	UNP P02281
S	29	THR	SER	engineered mutation	UNP P02281



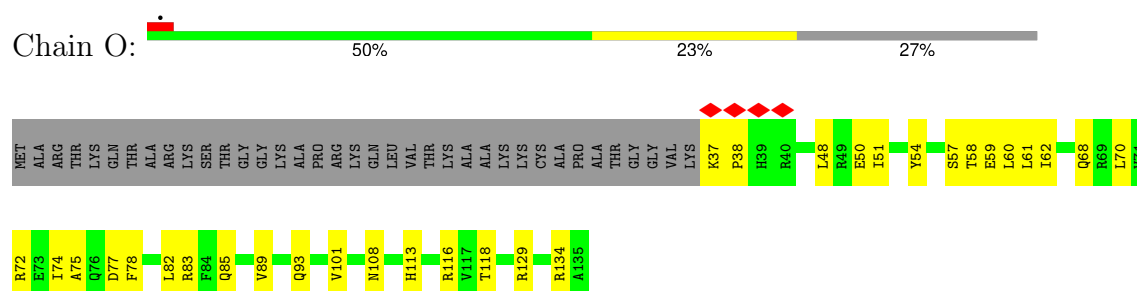
- Molecule 4: nucleosome DNA



- Molecule 5: Histone H3.3C

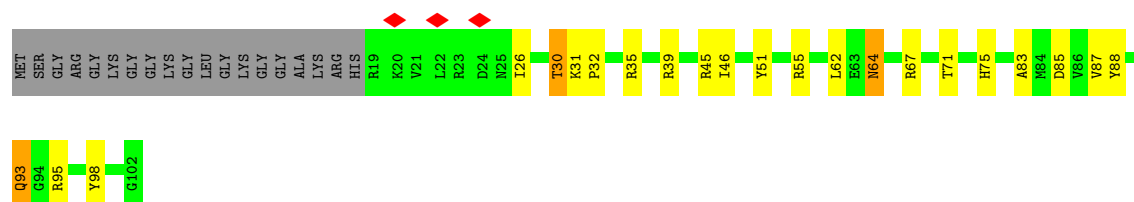


- Molecule 5: Histone H3.3C



- Molecule 6: Histone H4





• Molecule 6: Histone H4



• Molecule 7: Histone H2A



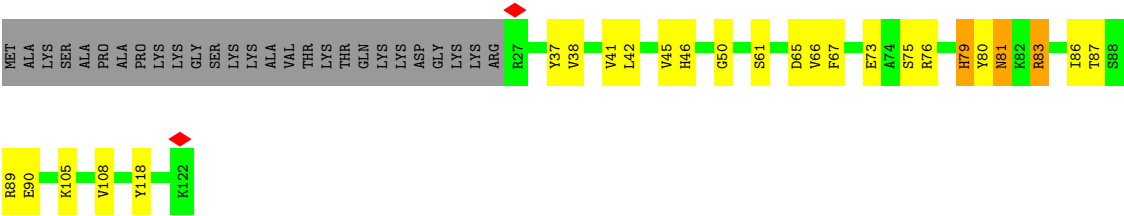
• Molecule 7: Histone H2A



• Molecule 8: Histone H2B 1.1



● Molecule 8: Histone H2B 1.1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86685	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	61.582	Depositor
Minimum map value	-36.475	Depositor
Average map value	0.004	Depositor
Map value standard deviation	2.051	Depositor
Recommended contour level	6.3	Depositor
Map size (\AA)	237.0624, 237.0624, 237.0624	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.2347, 1.2347, 1.2347	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	A	0.23	0/288	0.53	0/393
1	B	0.27	0/167	0.72	0/226
2	C	0.56	0/3586	0.95	0/5527
3	D	0.22	0/492	0.43	0/667
4	H	0.54	0/3634	0.93	0/5612
5	I	0.27	0/819	0.54	0/1098
5	O	0.27	0/828	0.56	0/1110
6	J	0.27	0/683	0.57	0/912
6	Q	0.27	0/654	0.55	0/876
7	K	0.25	0/833	0.53	0/1126
7	R	0.26	0/835	0.52	0/1128
8	M	0.27	0/741	0.48	0/999
8	S	0.29	0/752	0.55	0/1014
All	All	0.43	0/14312	0.78	0/20688

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	A	281	0	227	7	0
1	B	163	0	144	2	0
2	C	3200	0	1762	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	488	0	468	21	0
4	H	3237	0	1764	76	0
5	I	807	0	843	18	0
5	O	816	0	855	28	0
6	J	676	0	723	19	0
6	Q	647	0	671	27	0
7	K	824	0	860	29	0
7	R	825	0	876	24	0
8	M	731	0	746	28	0
8	S	741	0	753	21	0
All	All	13436	0	10692	308	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.

The worst 5 of 308 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)
5:O:60:LEU:HD13	5:O:93:GLN:HG2	1.67	0.75
7:K:39:TYR:HB3	8:M:75:SER:HB2	1.67	0.74
4:H:144:DC:H2'	4:H:145:DA:C8	2.25	0.71
2:C:300:DG:H2'	2:C:301:DA:C8	2.25	0.71
4:H:34:DT:H2'	4:H:35:DA:C8	2.26	0.70

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	39/98 (40%)	30 (77%)	9 (23%)	0	100	100
1	B	21/98 (21%)	13 (62%)	8 (38%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	60/76 (79%)	60 (100%)	0	0	100	100
5	I	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
5	O	97/136 (71%)	94 (97%)	3 (3%)	0	100	100
6	J	83/103 (81%)	78 (94%)	5 (6%)	0	100	100
6	Q	81/103 (79%)	77 (95%)	4 (5%)	0	100	100
7	K	108/130 (83%)	102 (94%)	6 (6%)	0	100	100
7	R	106/130 (82%)	106 (100%)	0	0	100	100
8	M	93/123 (76%)	93 (100%)	0	0	100	100
8	S	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
All	All	878/1256 (70%)	838 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	19/77 (25%)	17 (90%)	2 (10%)	5	23
1	B	13/77 (17%)	13 (100%)	0	100	100
3	D	50/68 (74%)	49 (98%)	1 (2%)	50	73
5	I	84/112 (75%)	82 (98%)	2 (2%)	44	68
5	O	85/112 (76%)	83 (98%)	2 (2%)	44	68
6	J	69/79 (87%)	65 (94%)	4 (6%)	17	46
6	Q	64/79 (81%)	63 (98%)	1 (2%)	58	77
7	K	81/102 (79%)	75 (93%)	6 (7%)	11	37
7	R	84/102 (82%)	80 (95%)	4 (5%)	21	52
8	M	78/103 (76%)	74 (95%)	4 (5%)	20	50
8	S	79/103 (77%)	75 (95%)	4 (5%)	20	50
All	All	706/1014 (70%)	676 (96%)	30 (4%)	27	55

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	110	ASN
8	S	79	HIS
8	M	52	SER
8	S	83	ARG
7	R	77	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
8	M	81	ASN
5	O	108	ASN
7	R	82	HIS

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 [i](#)

There are no chain breaks in this entry.

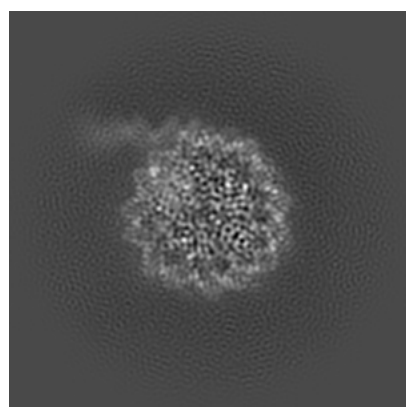
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41922. These allow visual inspection of the internal detail of the map and identification of artifacts.

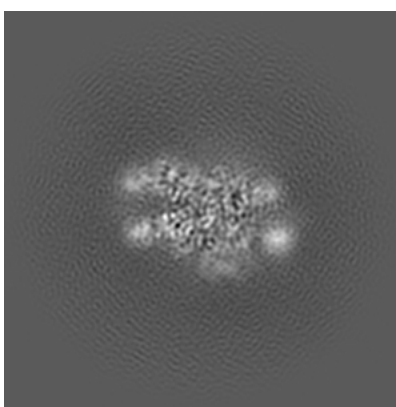
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

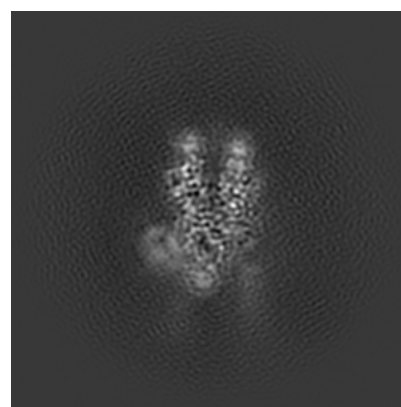
6.1.1 Primary map



X



Y

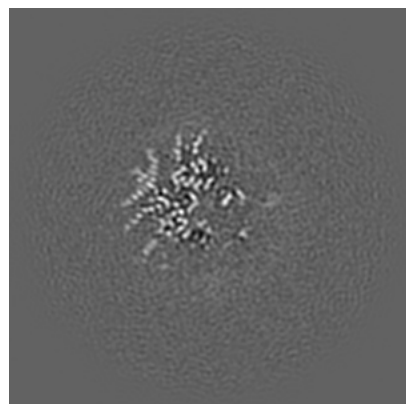


Z

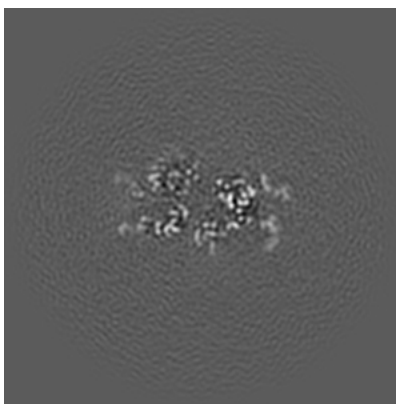
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

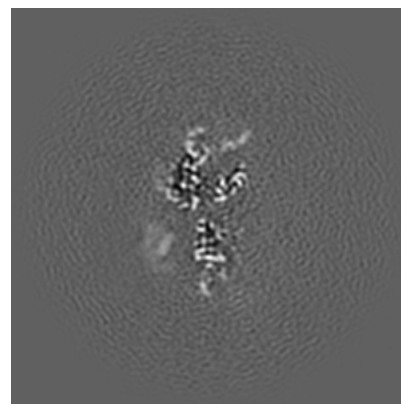
6.2.1 Primary map



X Index: 96



Y Index: 96

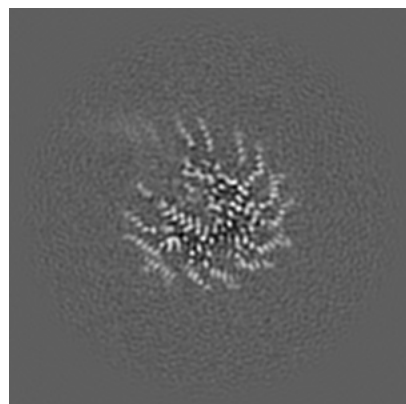


Z Index: 96

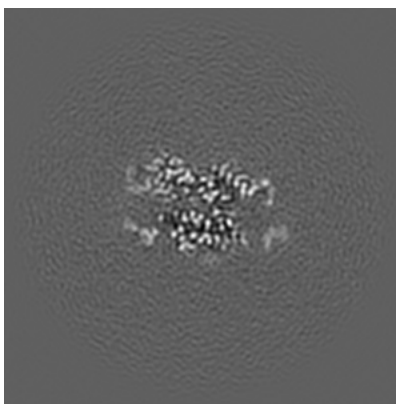
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

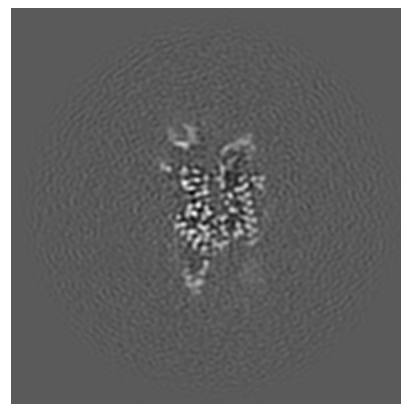
6.3.1 Primary map



X Index: 88



Y Index: 107

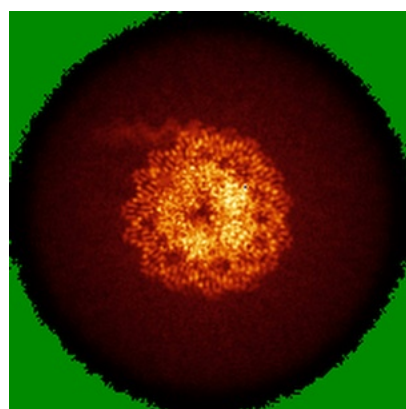


Z Index: 81

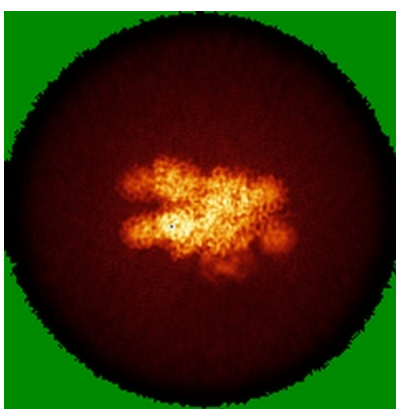
The images above show the largest variance slices of the map in three orthogonal directions.

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

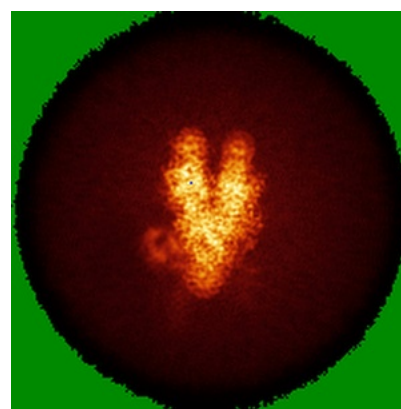
6.4.1 Primary map



X



Y

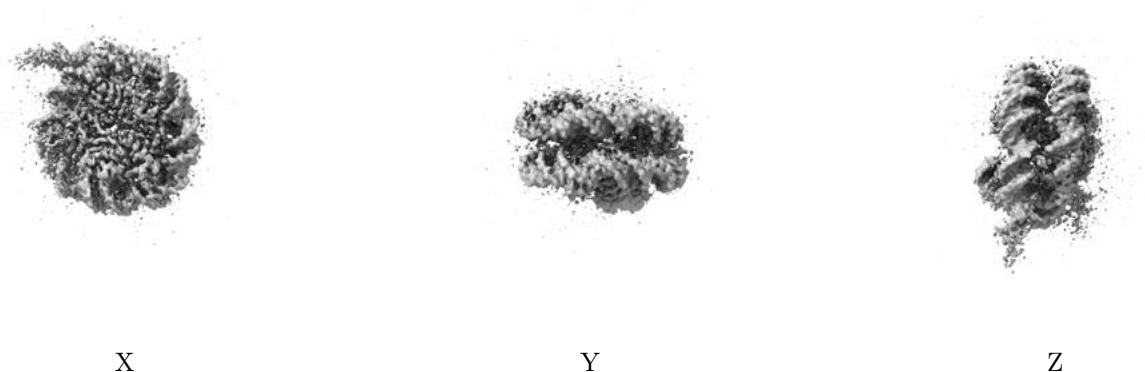


Z

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

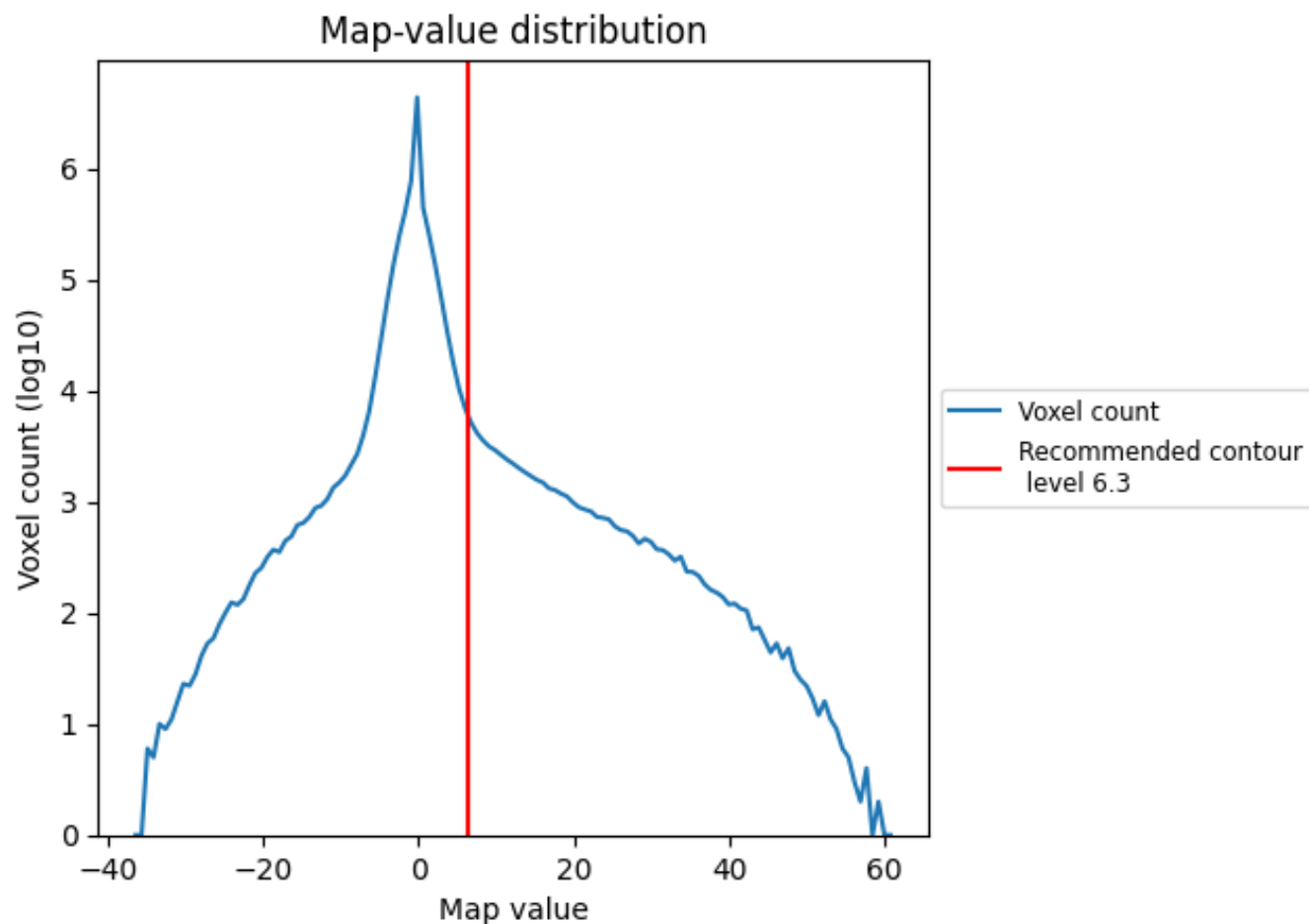
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

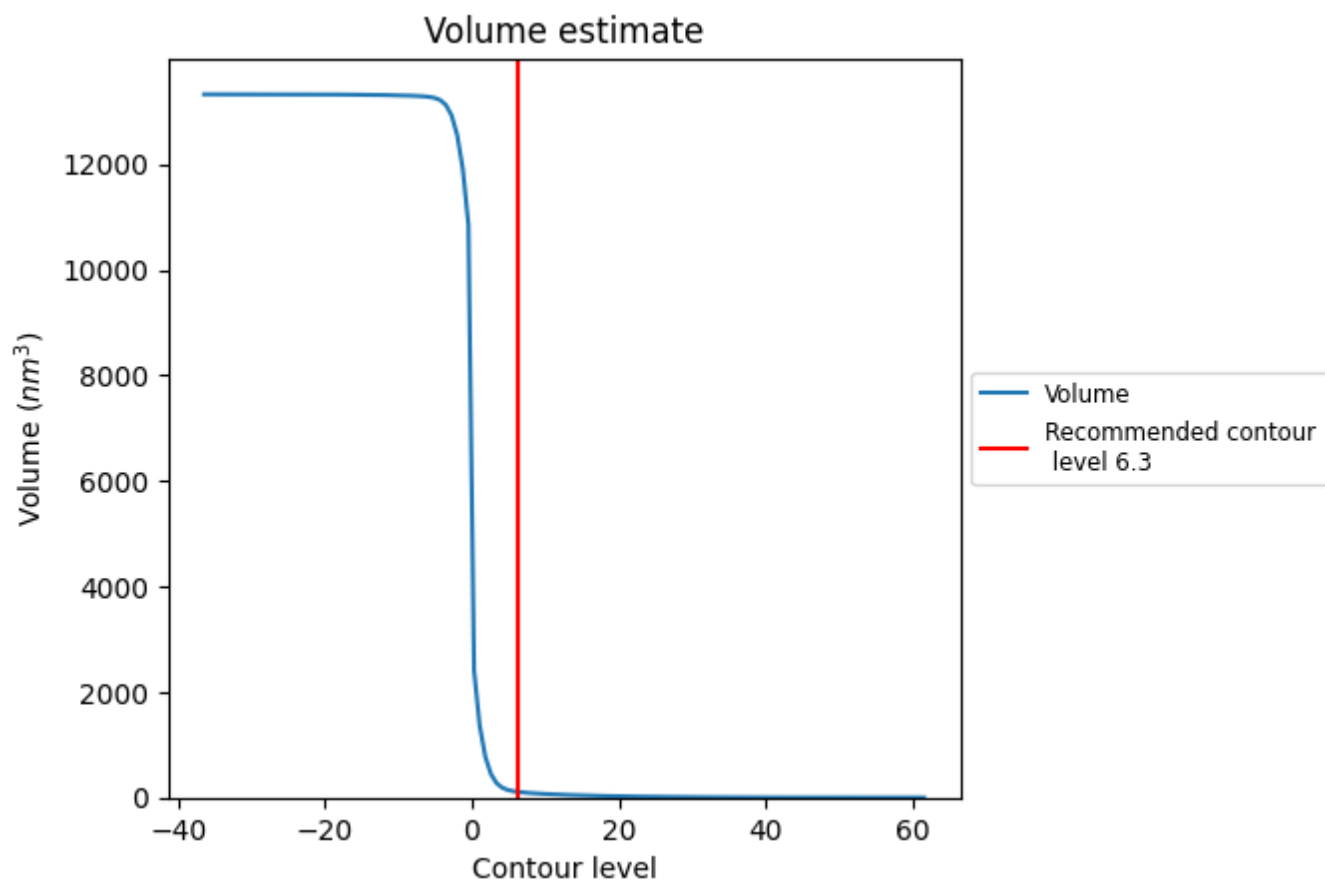
This section contains the results of statistical analysis of the map.

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.

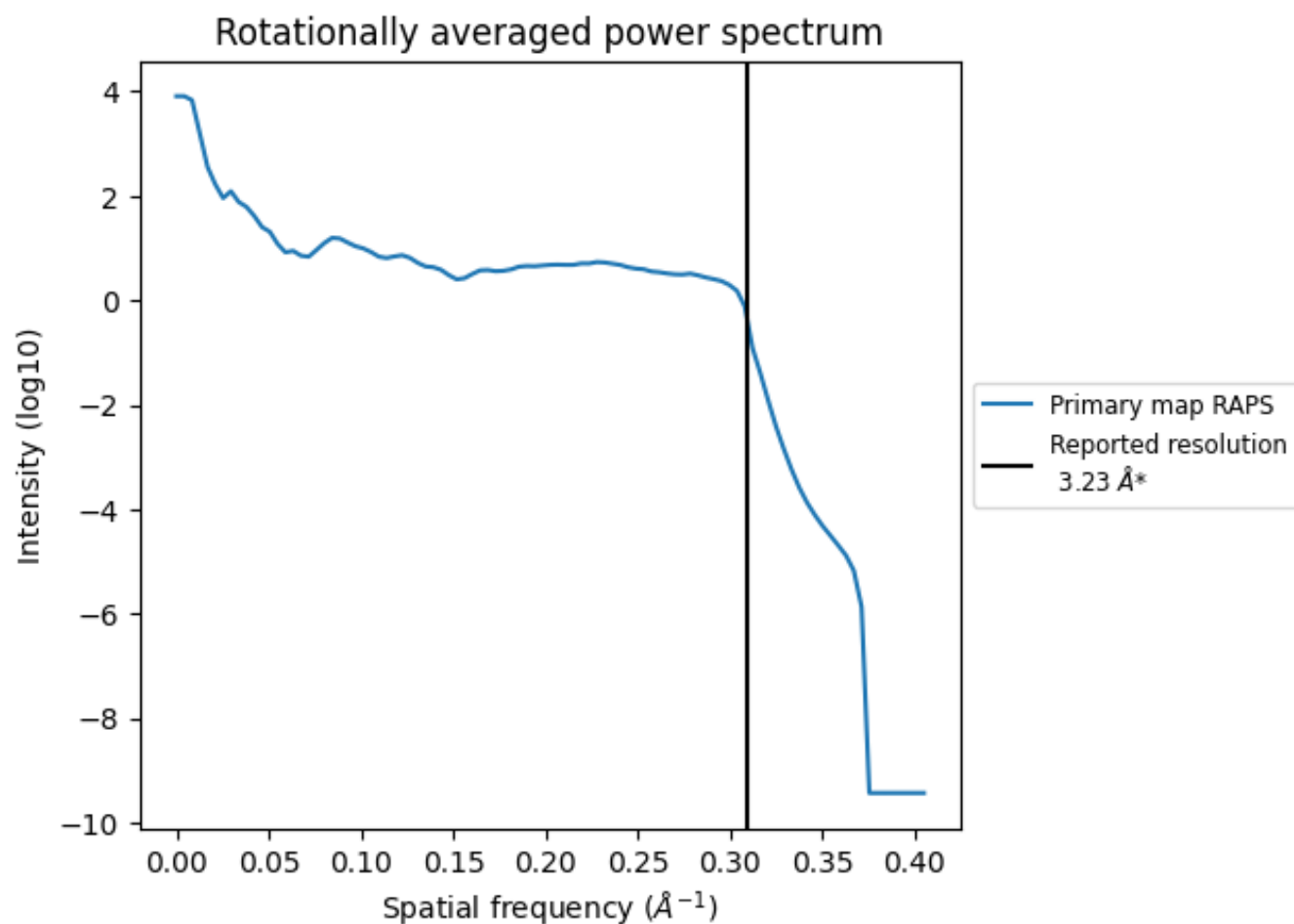
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm^3 ; this corresponds to an approximate mass of 97 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 0.310 Å⁻¹

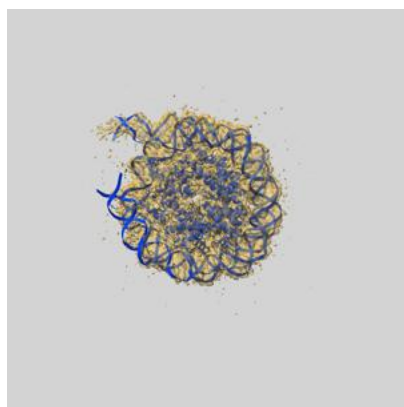
8 Fourier-Shell correlation

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

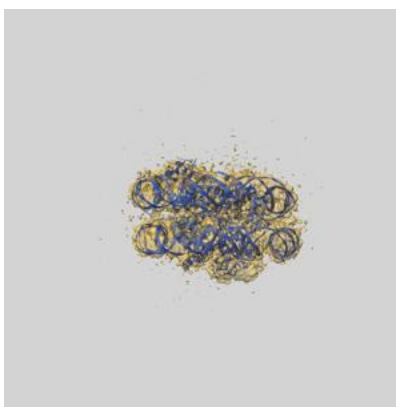
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41922 and PDB model 8U5H. Per-residue inclusion information can be found in section [3](#) on page [6](#).

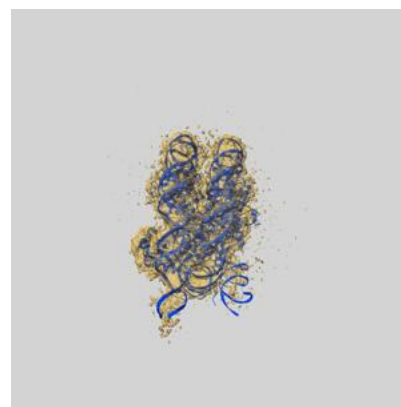
9.1 Map-model overlay [i](#)



X



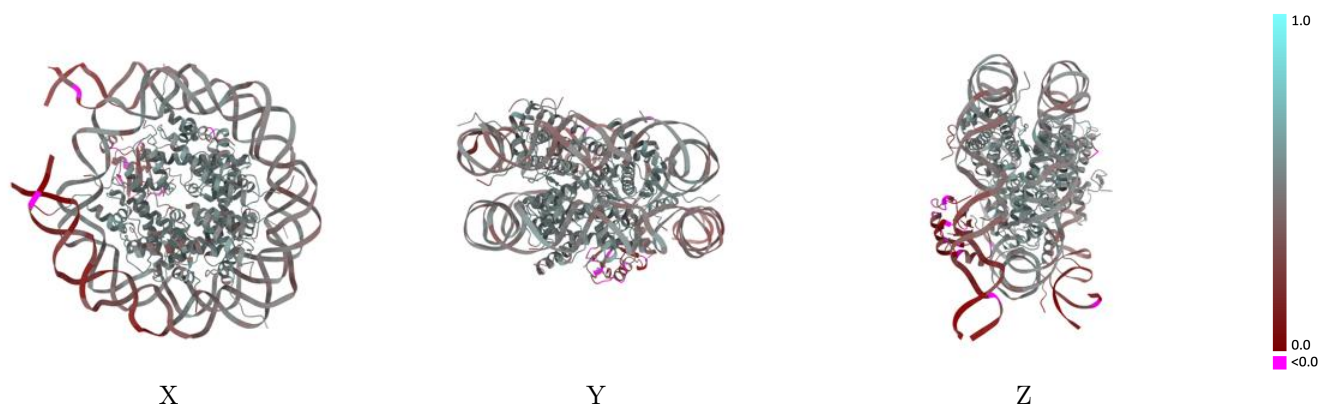
Y



Z

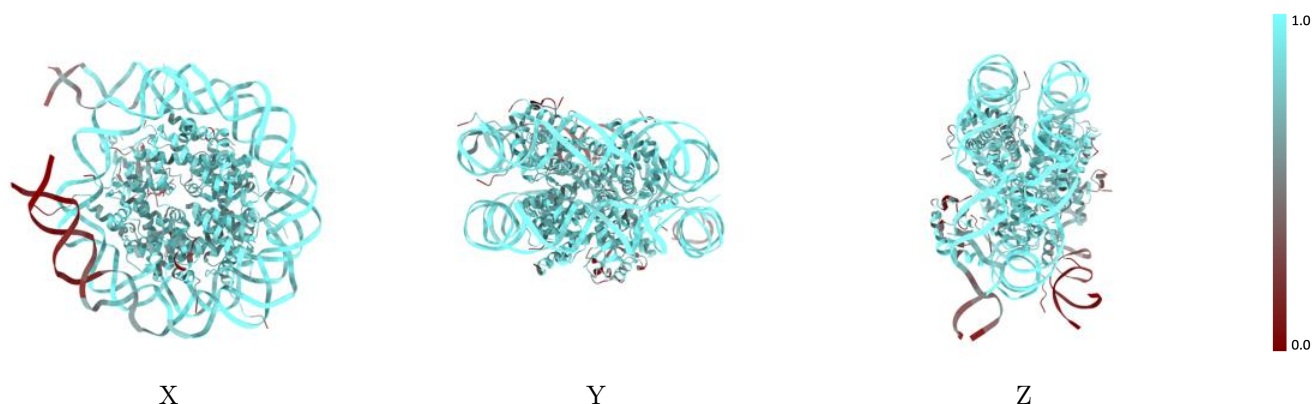
The images above show the 3D surface view of the map at the recommended contour level 6.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



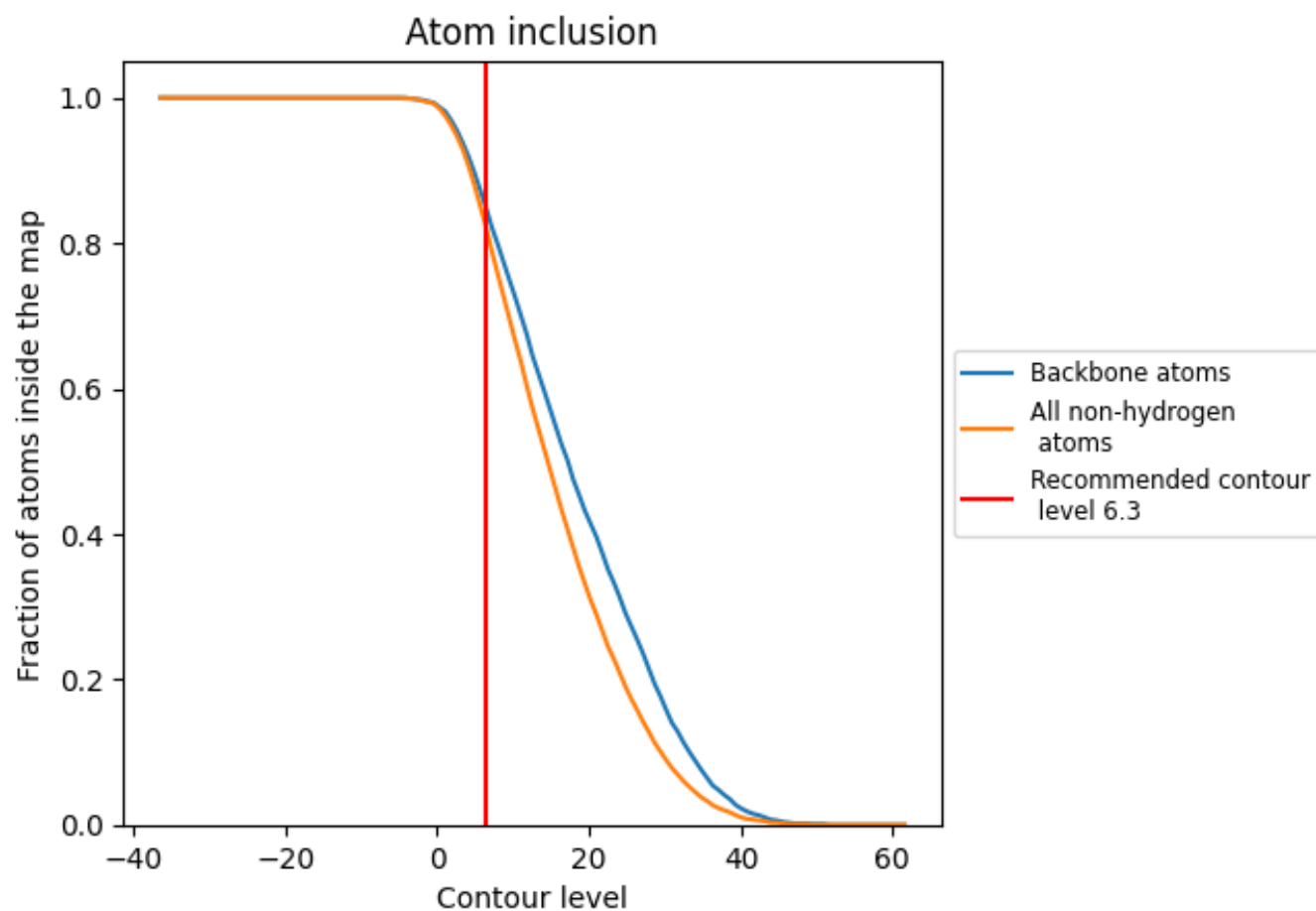
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.3).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (6.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.4430
A	 0.7740	 0.3700
B	 0.4360	 0.4180
C	 0.8070	 0.3880
D	 0.6270	 0.1050
H	 0.8230	 0.4020
I	 0.9070	 0.5480
J	 0.8810	 0.5230
K	 0.8270	 0.5160
M	 0.8500	 0.5050
O	 0.8600	 0.5300
Q	 0.8800	 0.5360
R	 0.8850	 0.5310
S	 0.8760	 0.5190

