



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 11:44 PM UTC

PDB ID : 6W5M / pdb_00006w5m
EMDB ID : EMD-21543
Title : Cryo-EM structure of MLL1 in complex with RbBP5, WDR5, SET1, and ASH2L bound to the nucleosome (Class02)
Authors : Park, S.H.; Lee, Y.T.; Ayoub, A.; Dou, Y.; Cho, U.
Deposited on : 2020-03-13
Resolution : 4.60 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

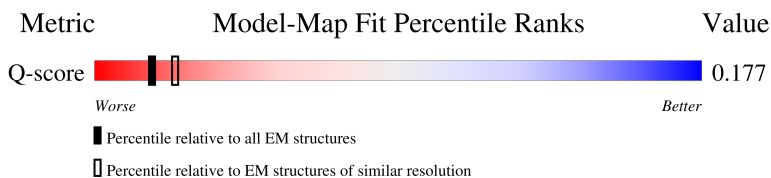
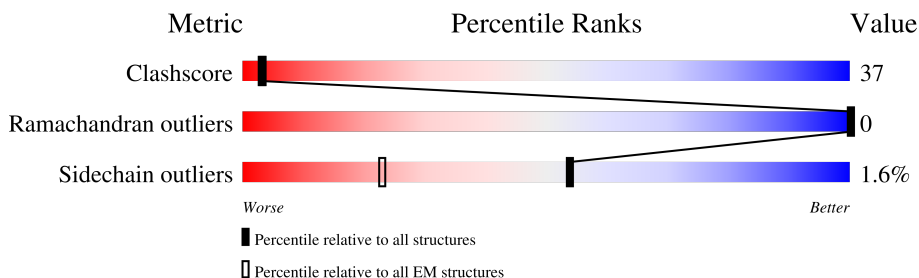
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	538	
2	B	313	
3	C	209	
4	D	534	

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Mol	Chain	Length	Quality of chain
5	G	136	
5	K	136	
6	H	103	
6	L	103	
7	I	129	
7	M	129	
8	J	123	
8	N	123	
9	O	147	
10	P	147	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19574 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 Retinoblastoma-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2381	1505	422	439	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q15291

- Molecule 2 is a protein called WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	3	0
			2302	1470	382	439	11		

- Molecule 3 is a protein called Histone-lysine N-methyltransferase 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	148	Total	C	N	O	S	0	0
			1185	751	213	208	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3761	SER	-	expression tag	UNP Q03164
C	3861	ILE	ASN	conflict	UNP Q03164
C	3867	LEU	GLN	conflict	UNP Q03164

- Molecule 4 is a protein called Set1/Ash2 histone methyltransferase complex subunit ASH2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	217	Total	C	N	O	S	0	0
			1742	1124	295	316	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP Q9UBL3

- Molecule 5 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
5	K	98	Total	C	N	O	S	0	0
			801	506	153	139	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	102	ALA	GLY	engineered mutation	UNP P84233
K	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	82	Total	C	N	O	S	0	0
			653	413	127	112	1		
6	L	82	Total	C	N	O	S	0	0
			653	413	127	112	1		

- Molecule 7 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	107	Total	C	N	O		0	0
			811	510	158	143			
7	M	107	Total	C	N	O		0	0
			815	513	159	143			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	99	ARG	GLY	engineered mutation	UNP P06897
I	123	SER	ALA	engineered mutation	UNP P06897
M	99	ARG	GLY	engineered mutation	UNP P06897
M	123	SER	ALA	engineered mutation	UNP P06897

- Molecule 8 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
8	N	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 9 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	146	Total	C	N	O	P	0	0
			2975	1413	540	876	146		

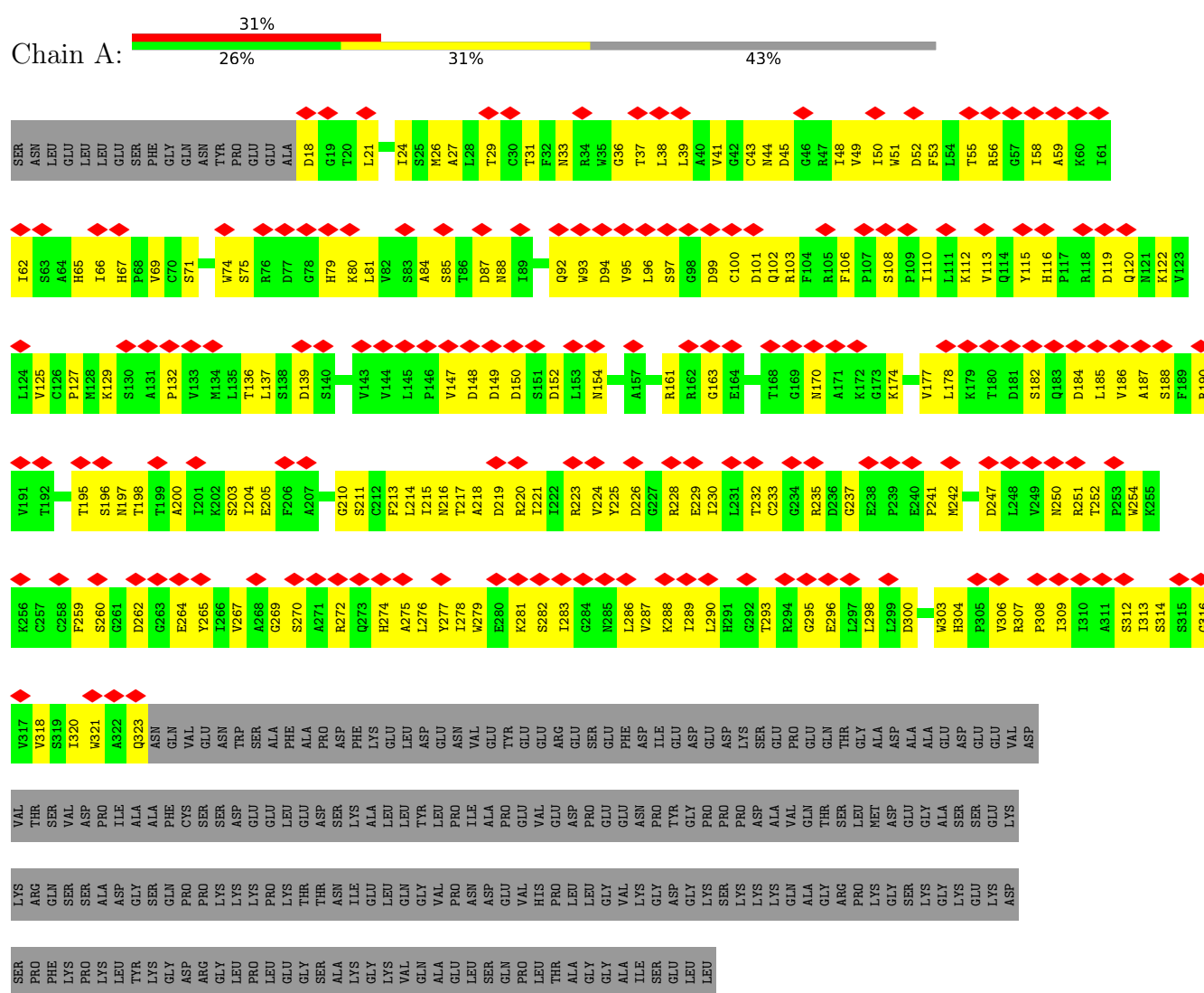
- Molecule 10 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	146	Total	C	N	O	P	0	0
			3011	1425	564	876	146		

3 Residue-property plots

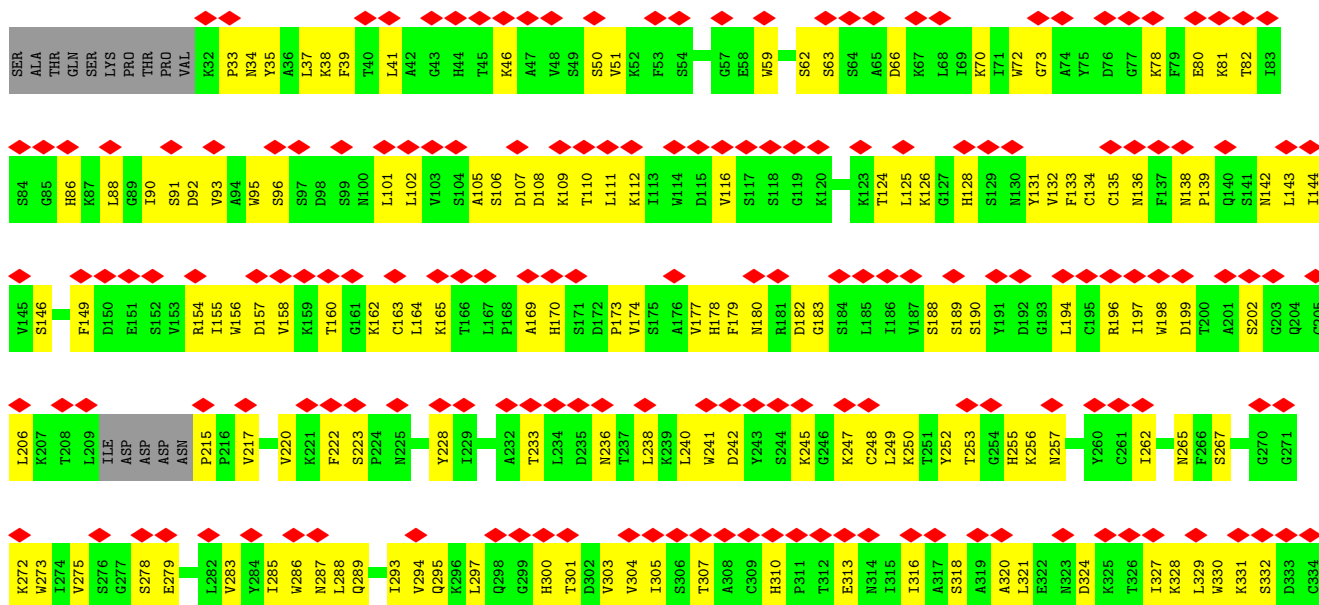
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Retinoblastoma-binding protein 5

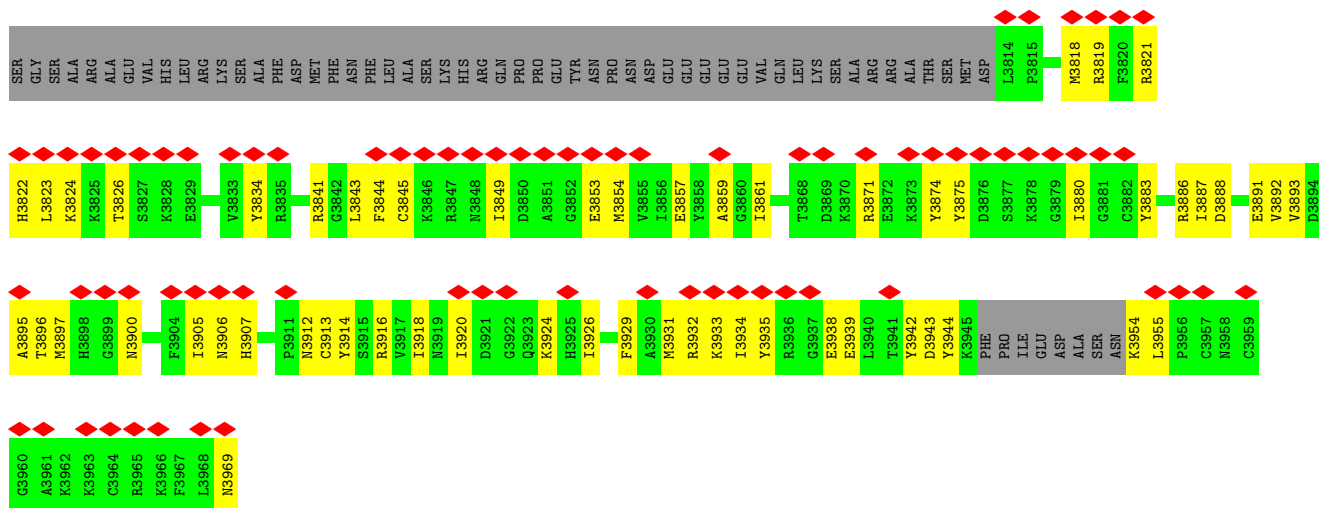
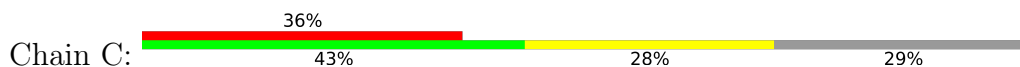


• Molecule 2: WD repeat-containing protein 5

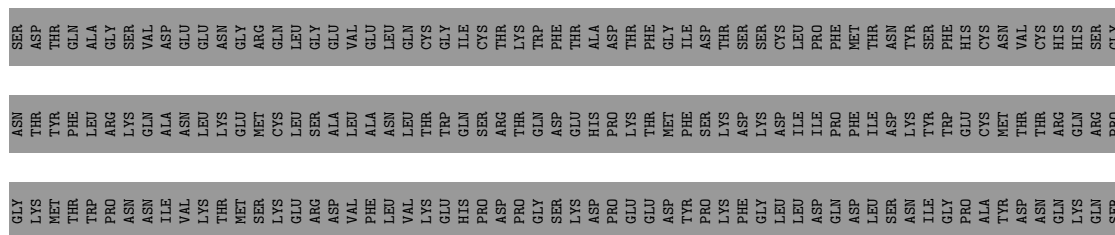


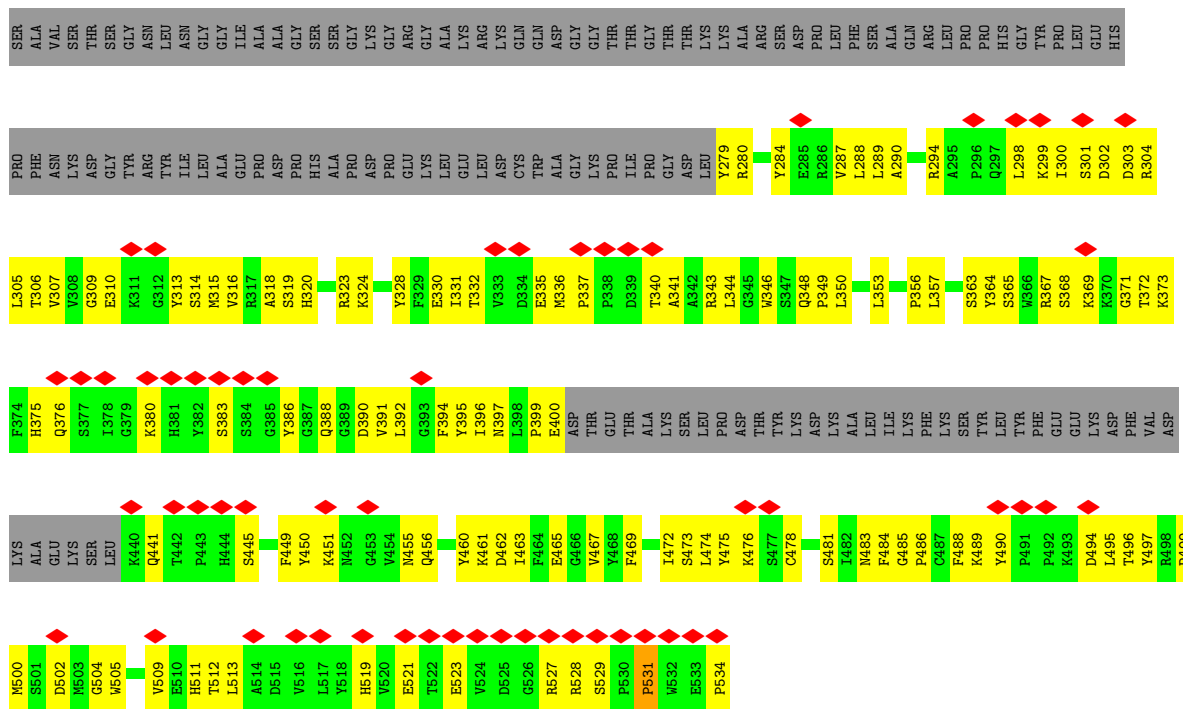


- Molecule 3: Histone-lysine N-methyltransferase 2A

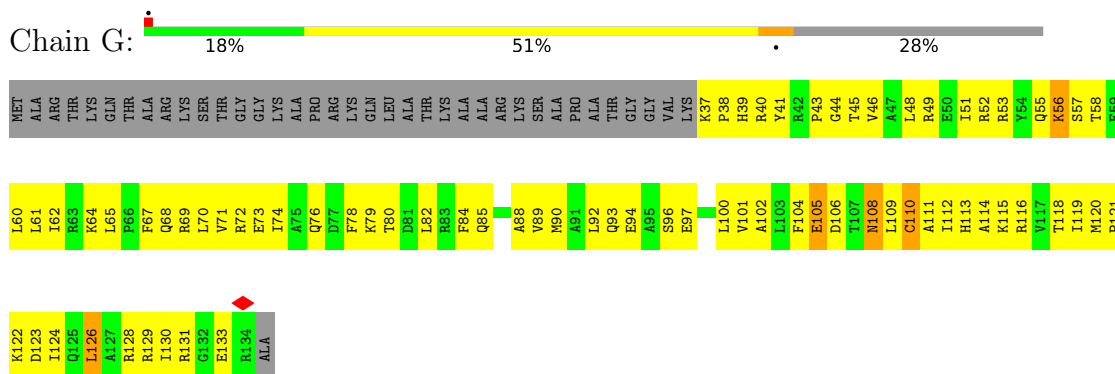


- Molecule 4: Set1/Ash2 histone methyltransferase complex subunit ASH2

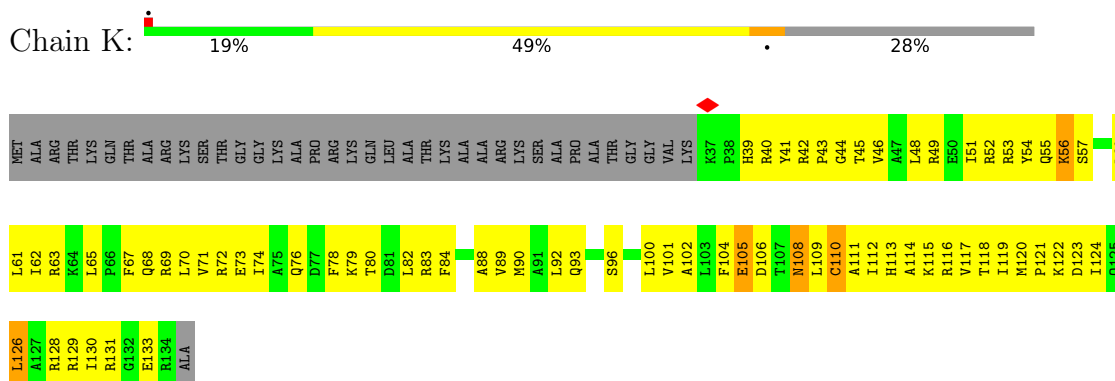




- Molecule 5: Histone H3.2

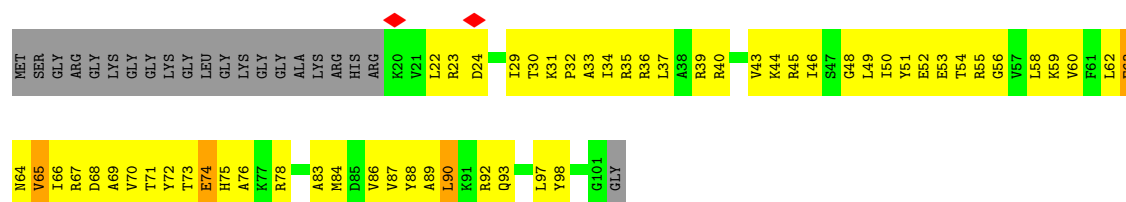


- Molecule 5: Histone H3.2

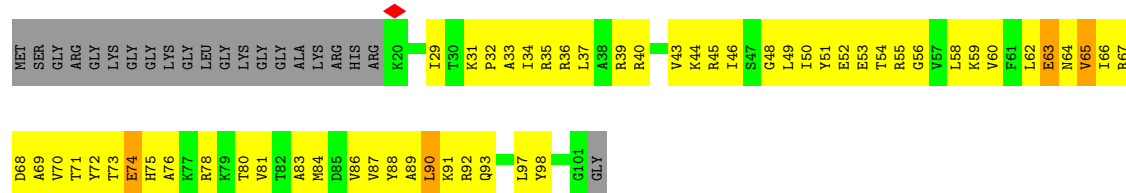


- Molecule 6: Histone H4

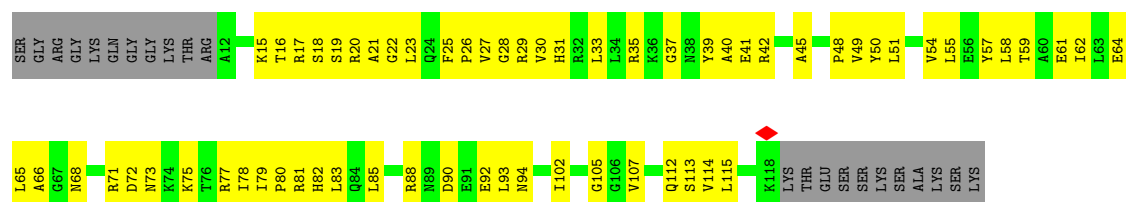




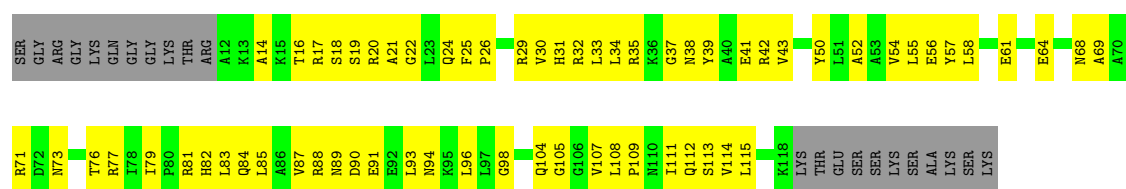
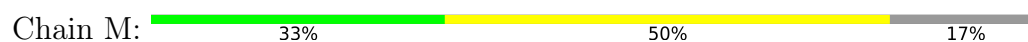
• Molecule 6: Histone H4



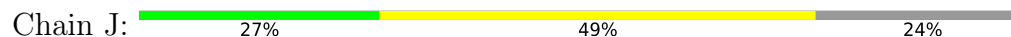
• Molecule 7: Histone H2A type 1



• Molecule 7: Histone H2A type 1



• Molecule 8: Histone H2B 1.1



• Molecule 8: Histone H2B 1.1

V66	F67	E68	A74	S75	R76	L77	H78	A79	Y80	N81	K82	R83	T87	S88	R89	E90	I91	Q92	V95	R96	L97	N98	L99	P100	H106	A107	V108	G111	T112	K117	S120	A121	LYS																					
ALA	LYS	SER	ALA	PRO	ALA	PRO	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	THR	GLN	LYS	ASP	GLY	LYS	LYS	ARG	ARG	LYS	T29	E32	S33	Y34	A35	I36	Y37	V38	Y39	K40	V41	L42	K43	Q44	I51	S52	S53	R54	A55	M56	S57	I58	M59	N60	S61	F62	V63	N64	D65

Chain O: 22% 78%

C140	C141	T142	A143	C144	C145	A146	T147	C72	G73	C74	T75	G76	T77	C78	C79	C80	C81	C82	G83	C84	G85	T86	T87	T88	T89	A90	A91	C92	G99	G100	G101	G102	A103	T104	T105	A106	C107	T108	C109	C110	C111	T112	A113	G114	T115	C118	C119	A120	A124	C125	G126	T127	G128	T129	C130	A131	G132	A133	T134	A135	T136	A137	T138	A139
DA	T2	C3	G4	A5	G6	A7	A8	T9	C10	C17	C18	G19	A20	G21	G22	C23	C24	G25	C26	T27	C28	A29	A30	T31	T32	G33	G34	T35	C36	G37	T38	A39	G40	A41	C42	C45	T46	C47	T48	A49	G50	C51	T58	A59	A60	A61	C62	G63	C64	A65	C66	G67	T68	A69	C70	C71								

Chain P: 12% 88%

C127	T128	G68	G69	A6	G5	A1
C129	G130	G70	A71	T7	A6	
G131	C132	C72	T9	G8		
A133	C134	A73	G74	A10		
C135	G75	C75	T11	A11		
G136	C77	G76	T13	A12		
G137	G78	G77	T15	A14		
A138	T140	T79	A80	C16		
T141	C81	C81	T17	A18		
C142	G82	T82	G18	A19		
T143	T83	G84	C20	A21		
C144	C85	C85	A21	C22		
G145	T87	C86	G23	G23		
A146	T88	T88	T24	G25		
DT	T89	A90	C26	C27		
	A91	G92	T28	G29		
	C93	G93	G30	A31		
	G94	G95				
	T96	G97				
	C98	C98	A36			
	T99	G99	G37	G38		
	A100	G101	G39	A40		
	A102	A103	G41	T42		
	C104	T105	A43	A44		
	T106	G106	T45	C46		
	T107	G108	C47	C48		
	T109	A110	C49	T50		
	C111	T112	T51	G52		
	A113	C114	G53	C54		
	C115	A116	G55	G56		
	A117	T118	T57	T58		
	T119	G120	A59	A60		
	A121	C122	A61	C63		
	C123	G124	G64	G65		
	G125	C126				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27730	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0073	Depositor
Map size ($\text{\AA}$)	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	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	0.18	0/2431	0.38	1/3301 (0.0%)
2	B	0.16	0/2372	0.33	0/3216
3	C	0.15	0/1208	0.32	0/1616
4	D	0.20	0/1797	0.43	0/2438
5	G	0.26	0/813	0.41	0/1093
5	K	0.25	0/813	0.41	0/1093
6	H	0.27	0/660	0.51	0/885
6	L	0.27	0/660	0.51	0/885
7	I	0.24	0/821	0.39	0/1112
7	M	0.24	0/825	0.37	0/1116
8	J	0.27	0/729	0.43	0/985
8	N	0.26	0/737	0.38	0/993
9	O	0.34	0/3333	0.44	0/5137
10	P	0.34	0/3381	0.44	0/5221
All	All	0.26	0/20580	0.41	1/29091 (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
4	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ILE	N-CA-C	-5.49	104.61	112.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	531	PRO	Peptide

5.2 Too-close contacts

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	2381	0	2394	131	0
2	B	2302	0	2269	119	0
3	C	1185	0	1190	55	0
4	D	1742	0	1685	98	0
5	G	801	0	831	144	0
5	K	801	0	831	136	0
6	H	653	0	695	99	0
6	L	653	0	695	117	0
7	I	811	0	849	82	0
7	M	815	0	860	96	0
8	J	718	0	725	96	0
8	N	726	0	747	98	0
9	O	2975	0	1639	206	0
10	P	3011	0	1639	228	0
All	All	19574	0	17049	1320	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 37.

The worst 5 of 1320 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:G:115:LYS:NZ	5:K:122:LYS:HE2	1.32	1.41
5:G:122:LYS:HE2	5:K:115:LYS:NZ	1.33	1.38
5:G:113:HIS:CE1	5:K:122:LYS:HG3	1.62	1.34
2:B:247:LYS:HB3	3:C:3834:TYR:CE1	1.64	1.31
5:G:122:LYS:CE	5:K:115:LYS:HZ3	1.48	1.27

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	304/538 (56%)	286 (94%)	18 (6%)	0	100	100
2	B	297/313 (95%)	281 (95%)	16 (5%)	0	100	100
3	C	144/209 (69%)	139 (96%)	5 (4%)	0	100	100
4	D	213/534 (40%)	194 (91%)	19 (9%)	0	100	100
5	G	96/136 (71%)	92 (96%)	4 (4%)	0	100	100
5	K	96/136 (71%)	92 (96%)	4 (4%)	0	100	100
6	H	80/103 (78%)	69 (86%)	11 (14%)	0	100	100
6	L	80/103 (78%)	70 (88%)	10 (12%)	0	100	100
7	I	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
7	M	105/129 (81%)	101 (96%)	4 (4%)	0	100	100
8	J	91/123 (74%)	86 (94%)	5 (6%)	0	100	100
8	N	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
All	All	1702/2576 (66%)	1601 (94%)	101 (6%)	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	266/462 (58%)	266 (100%)	0	100	100
2	B	258/274 (94%)	258 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	127/182 (70%)	127 (100%)	0	100	100
4	D	185/460 (40%)	185 (100%)	0	100	100
5	G	84/111 (76%)	78 (93%)	6 (7%)	13	35
5	K	84/111 (76%)	78 (93%)	6 (7%)	13	35
6	H	67/79 (85%)	62 (92%)	5 (8%)	12	33
6	L	67/79 (85%)	62 (92%)	5 (8%)	12	33
7	I	81/101 (80%)	81 (100%)	0	100	100
7	M	82/101 (81%)	82 (100%)	0	100	100
8	J	77/103 (75%)	77 (100%)	0	100	100
8	N	79/103 (77%)	78 (99%)	1 (1%)	61	72
All	All	1457/2166 (67%)	1434 (98%)	23 (2%)	54	69

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	108	ASN
6	L	49	LEU
5	K	126	LEU
6	L	63	GLU
6	H	49	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
8	J	106	HIS
7	M	112	GLN
5	K	39	HIS
7	M	31	HIS
8	N	46	HIS

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 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.

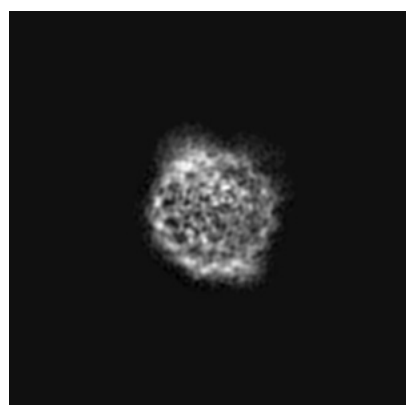
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21543. These allow visual inspection of the internal detail of the map and identification of artifacts.

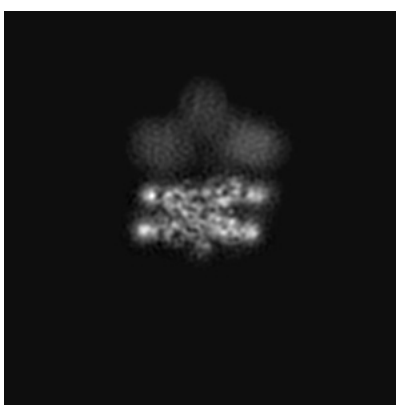
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

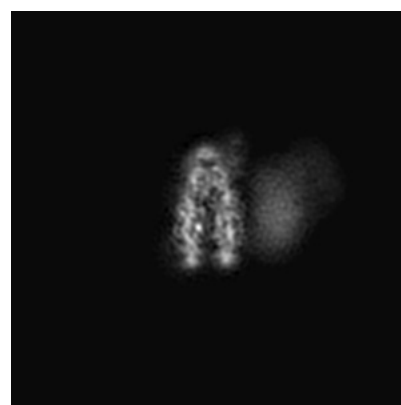
6.1.1 Primary map



X



Y

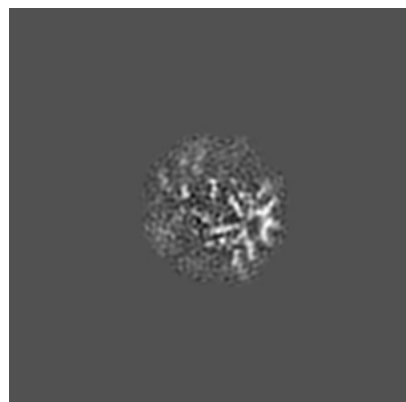


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150

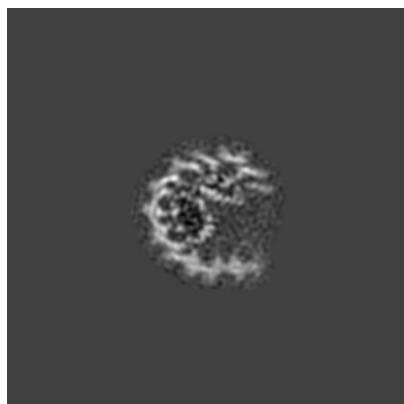


Z Index: 150

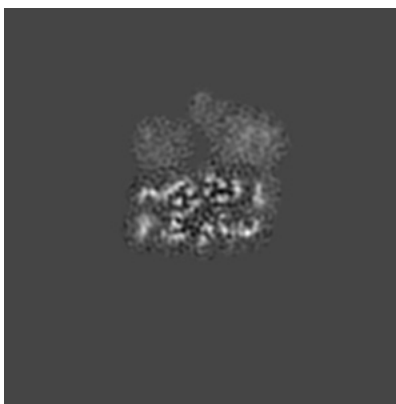
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

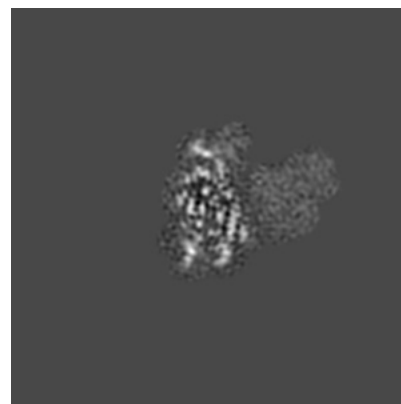
6.3.1 Primary map



X Index: 135



Y Index: 145

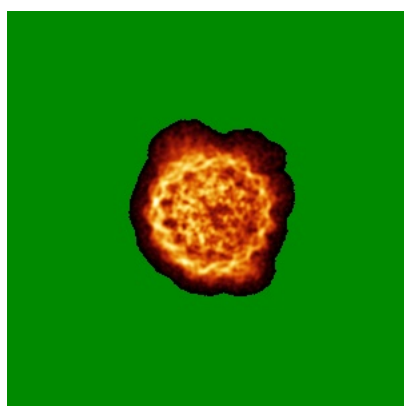


Z Index: 162

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

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

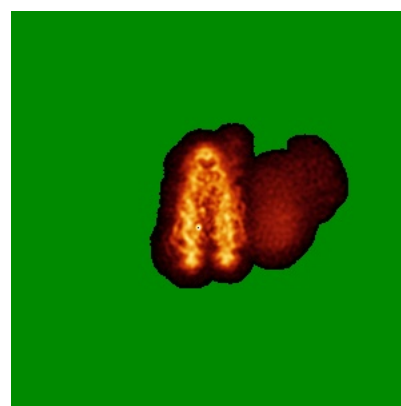
6.4.1 Primary map



X



Y

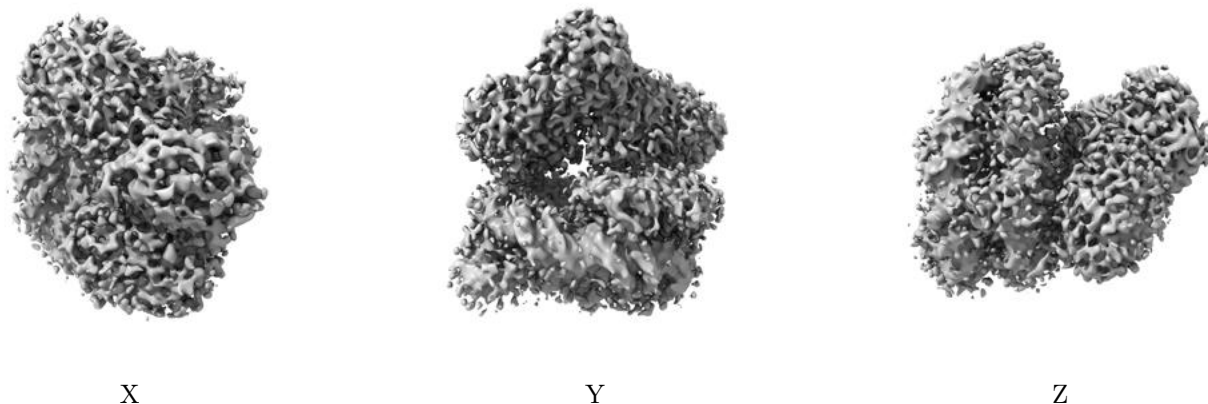


Z

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 0.0073. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

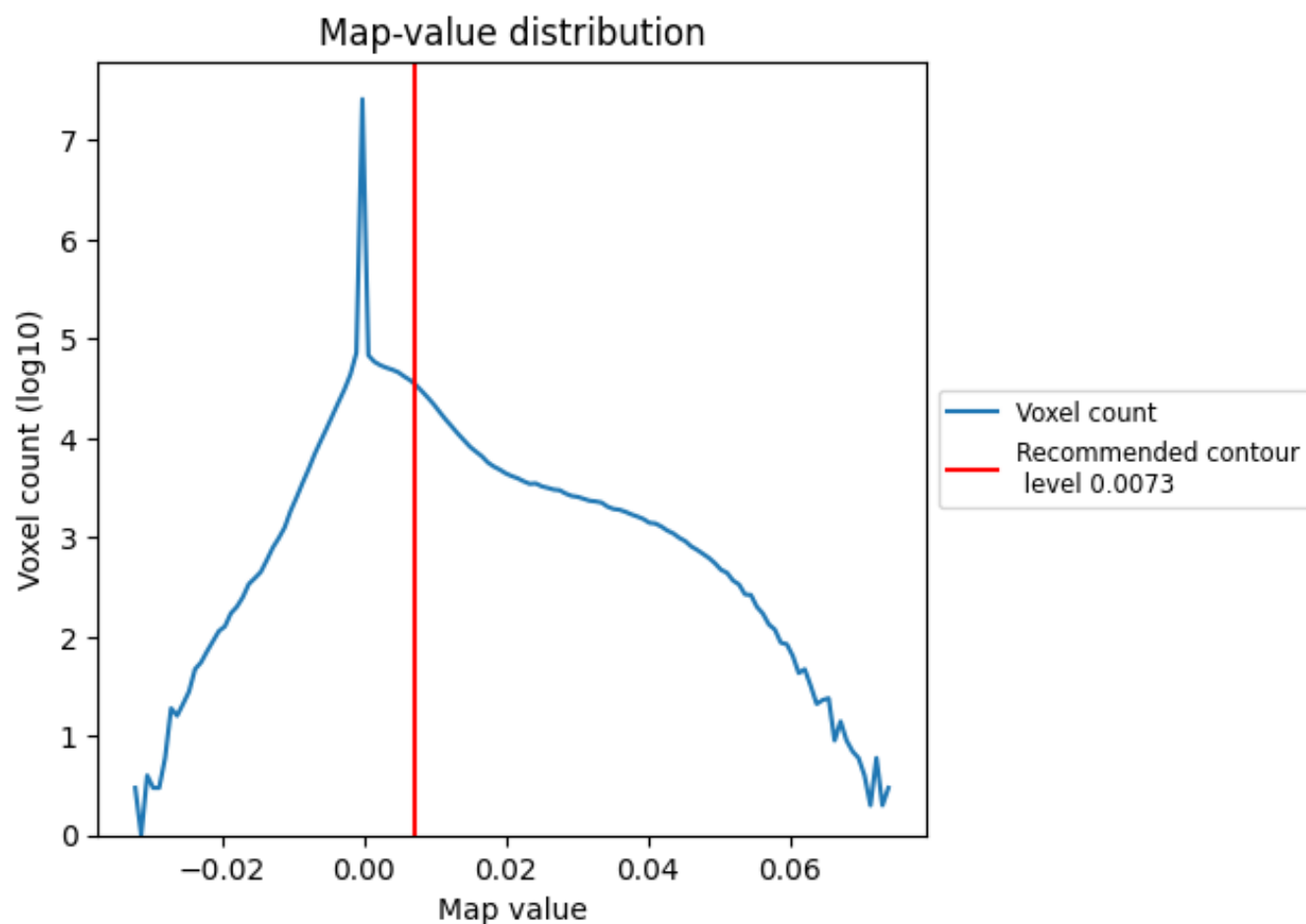
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

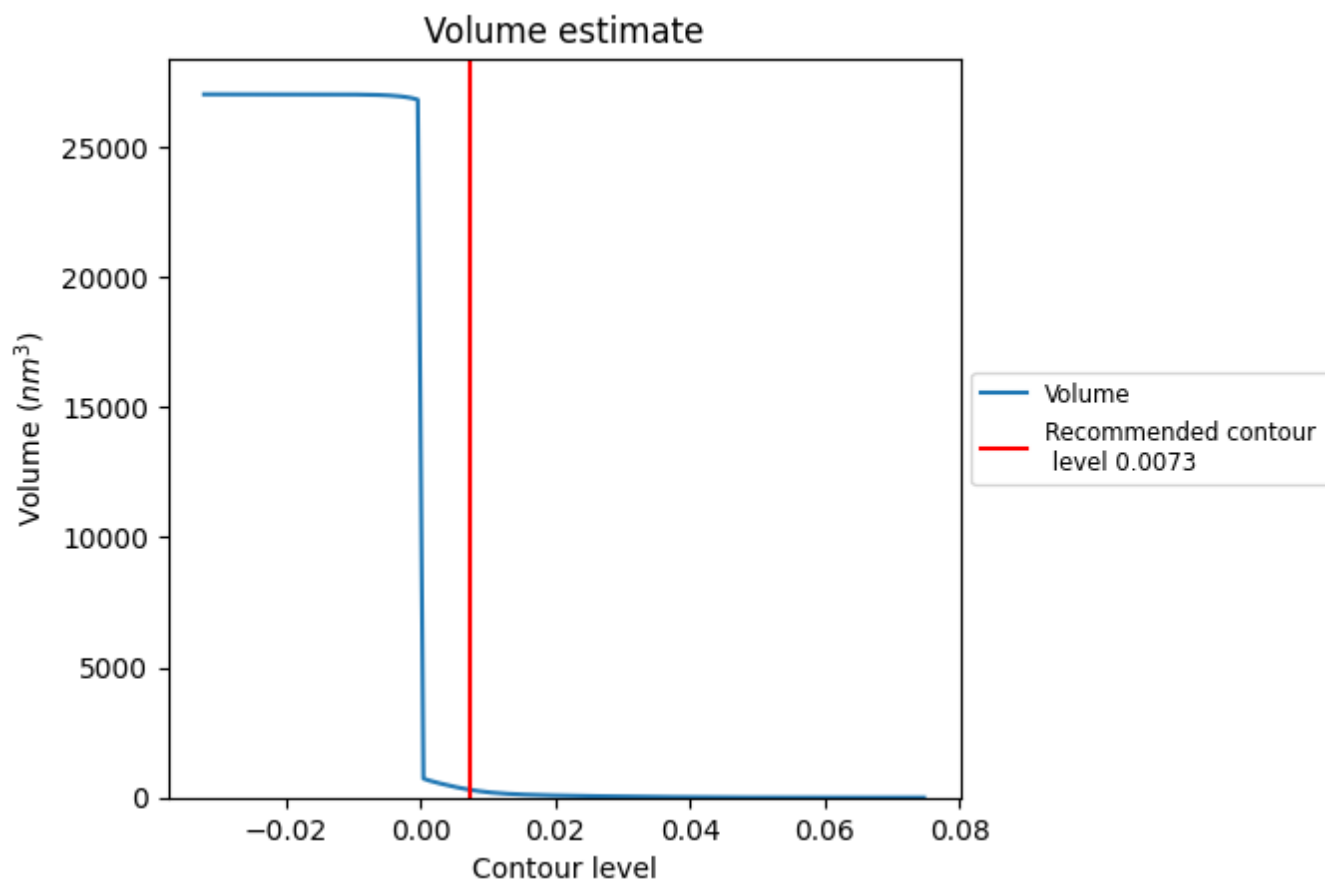
This section contains the results of statistical analysis of the map.

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.

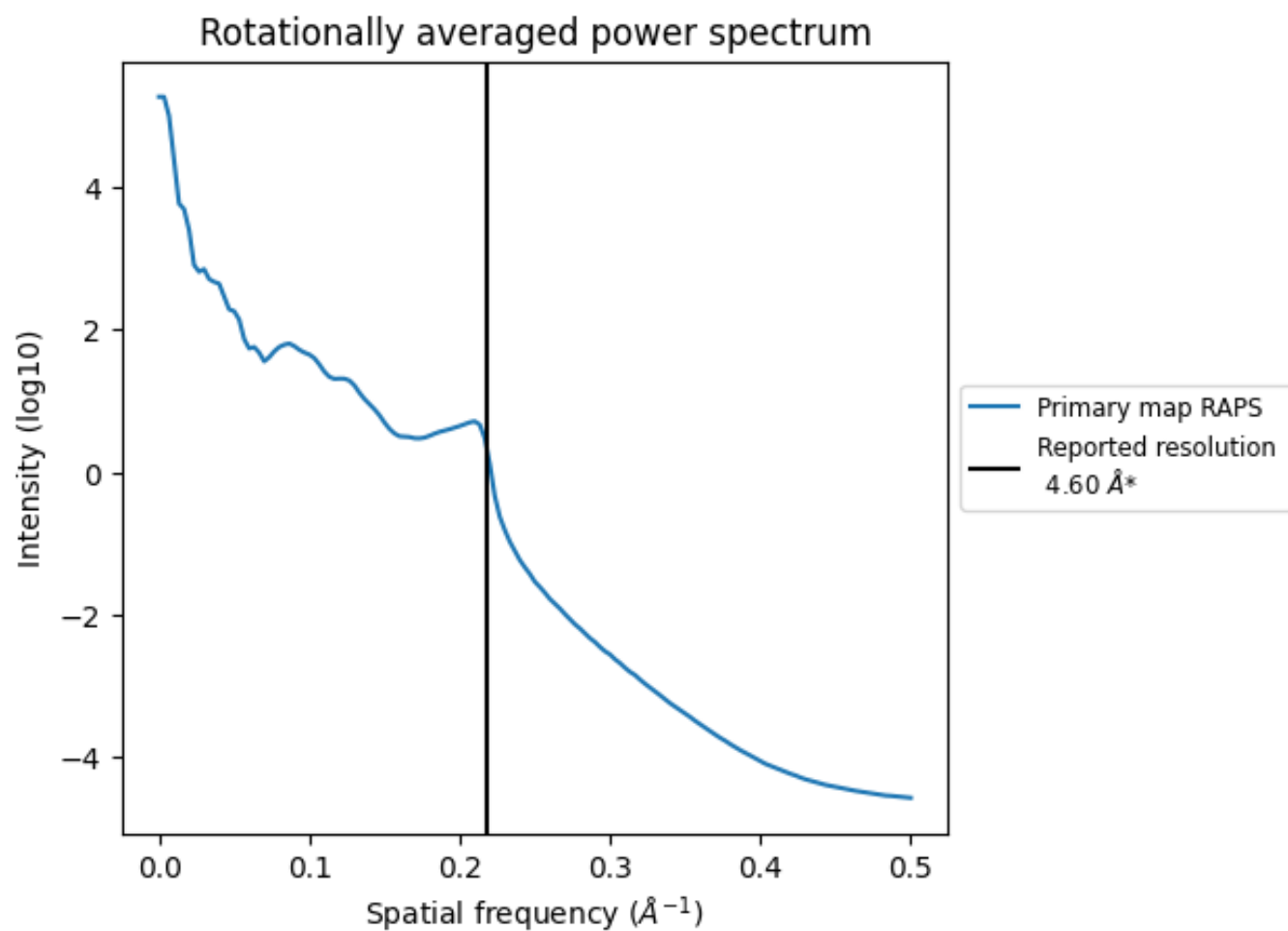
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 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 ⓘ

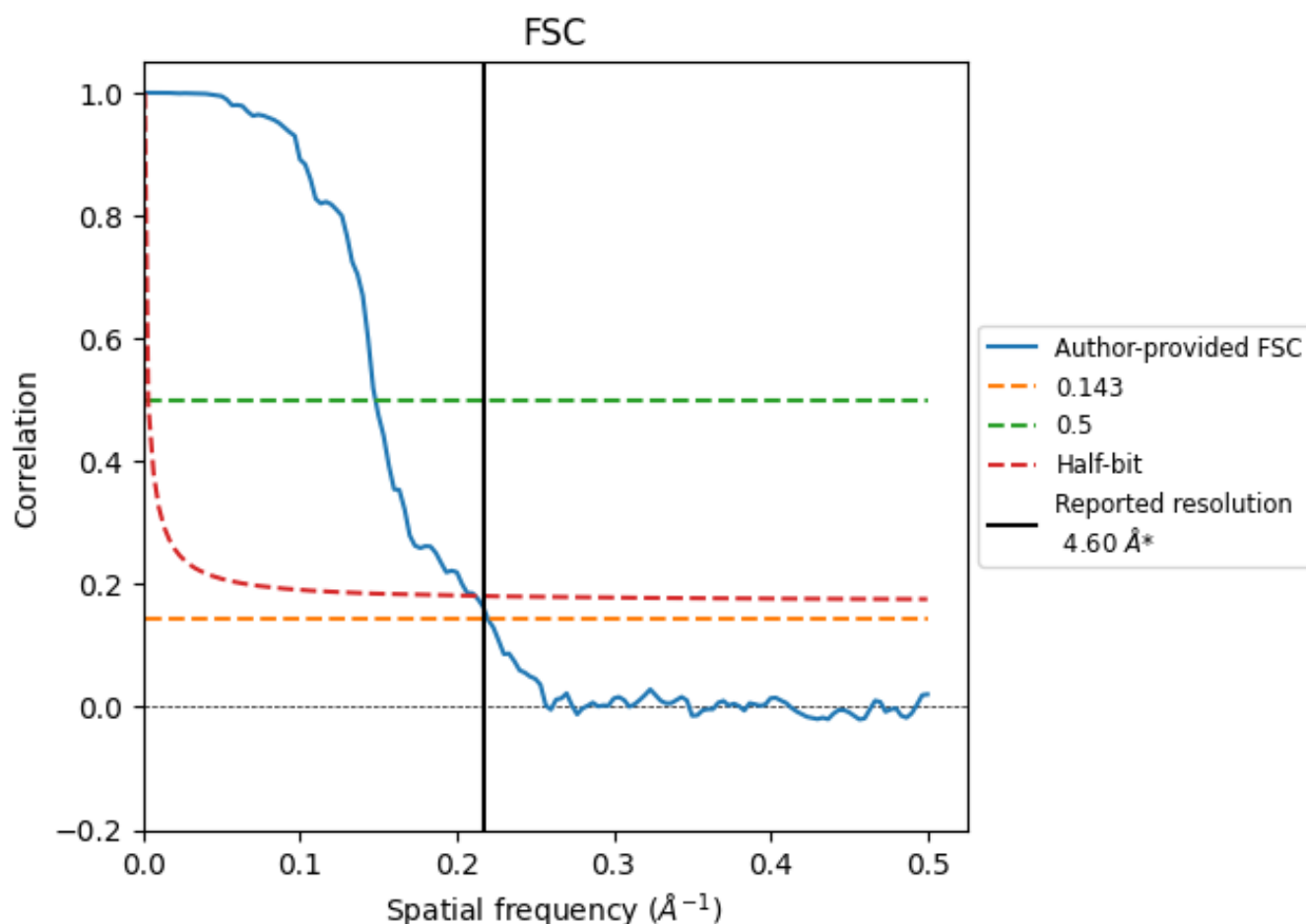


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

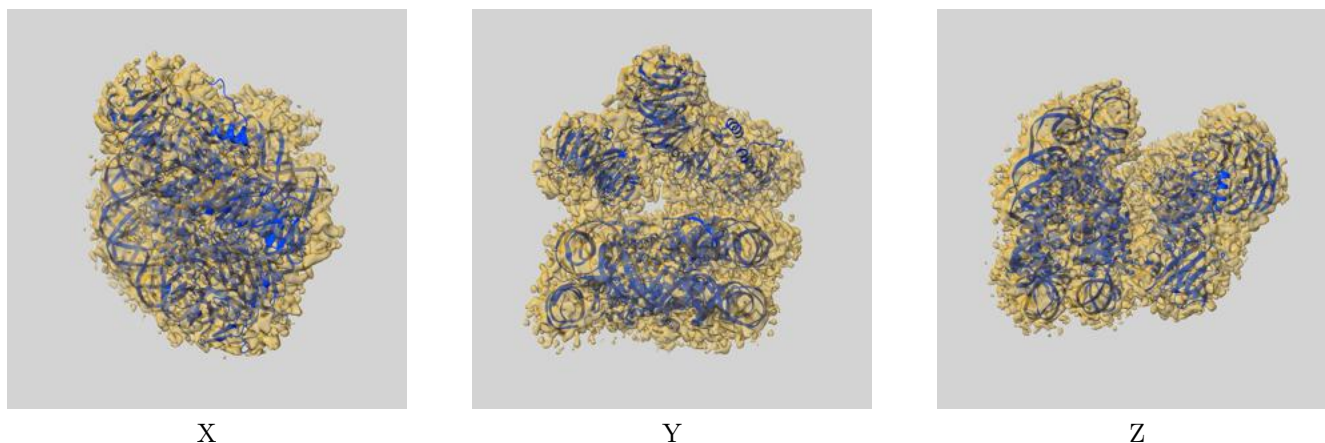
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.55	6.75	4.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

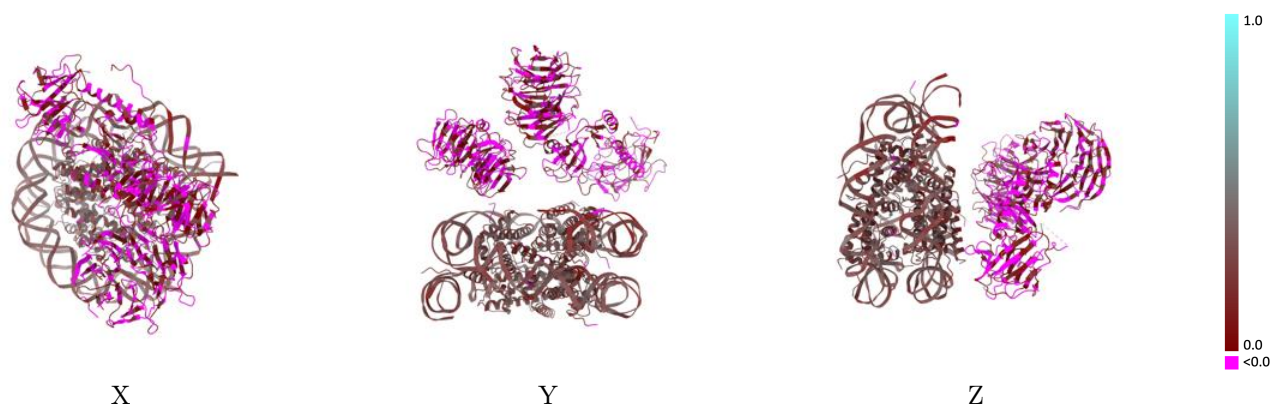
This section contains information regarding the fit between EMDB map EMD-21543 and PDB model 6W5M. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



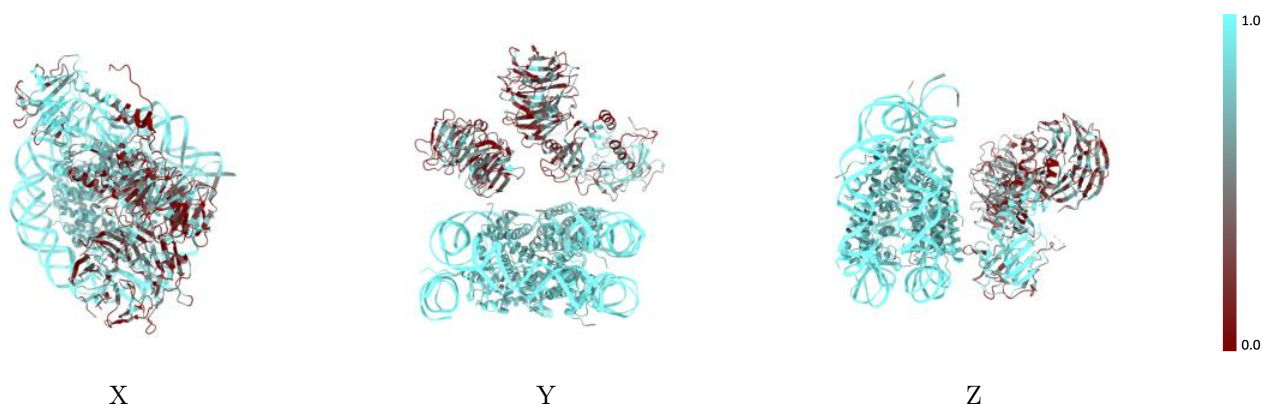
The images above show the 3D surface view of the map at the recommended contour level 0.0073 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



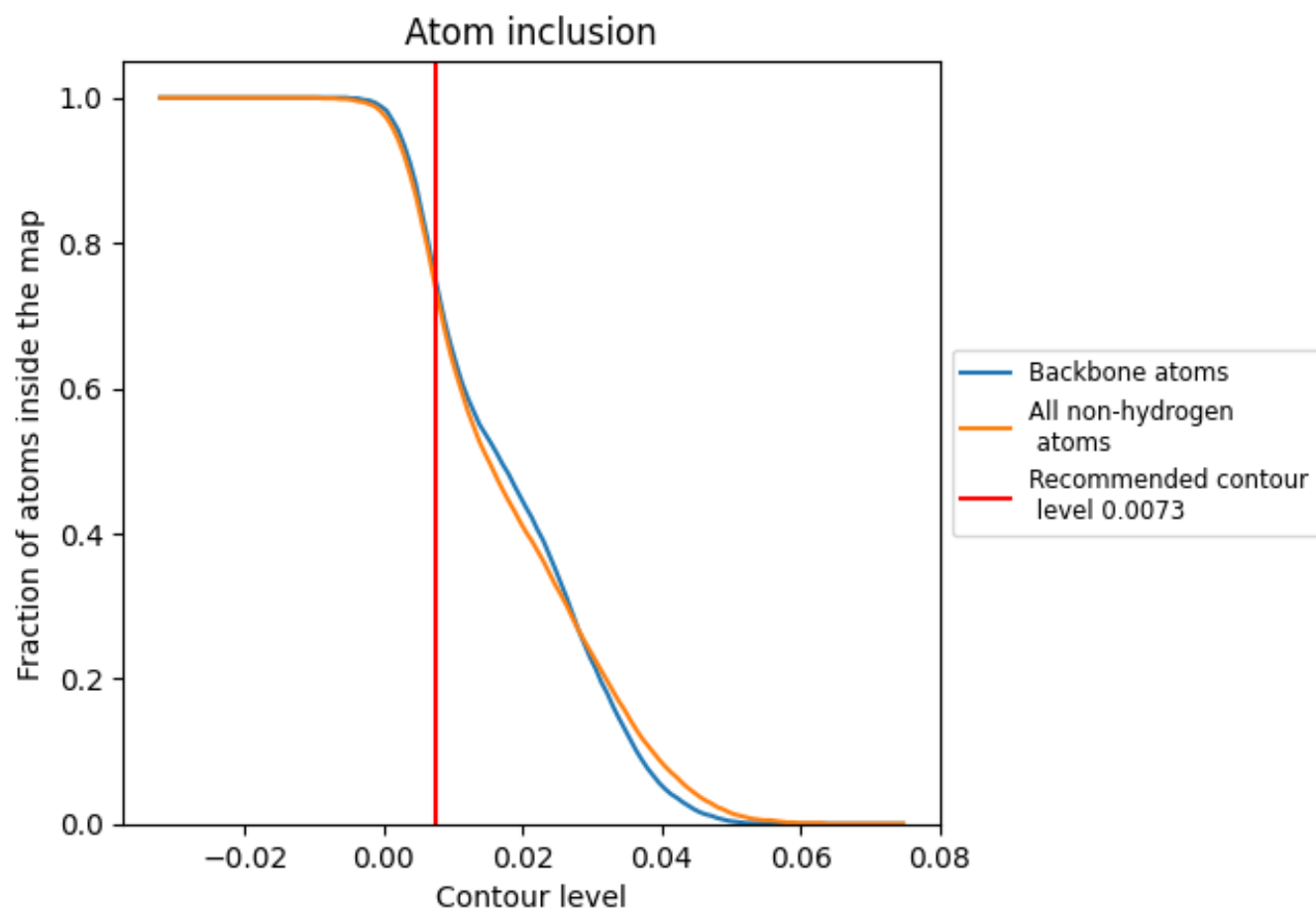
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0073).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.0073) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.1770
A	 0.3940	 -0.0000
B	 0.3860	 0.0510
C	 0.4390	 0.0070
D	 0.6570	 0.0150
G	 0.8380	 0.2660
H	 0.8710	 0.2960
I	 0.8560	 0.2810
J	 0.8760	 0.2660
K	 0.8510	 0.2630
L	 0.8840	 0.2790
M	 0.8800	 0.2670
N	 0.8750	 0.2590
O	 0.9790	 0.2820
P	 0.9790	 0.2810

