wwPDB EM Validation Summary Report

Mar 10, 2026 – 01:56 PM UTC

PDB ID	:	9Q8X / pdb_00009q8x
EMDB ID	:	EMD-52912
Title	:	Ku70/80 bound to a 153 bp H2AX nucleosome
Authors	:	Hall, C.; Chaplin, A.K.
Deposited on	:	2025-02-25
Resolution	:	2.94 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:

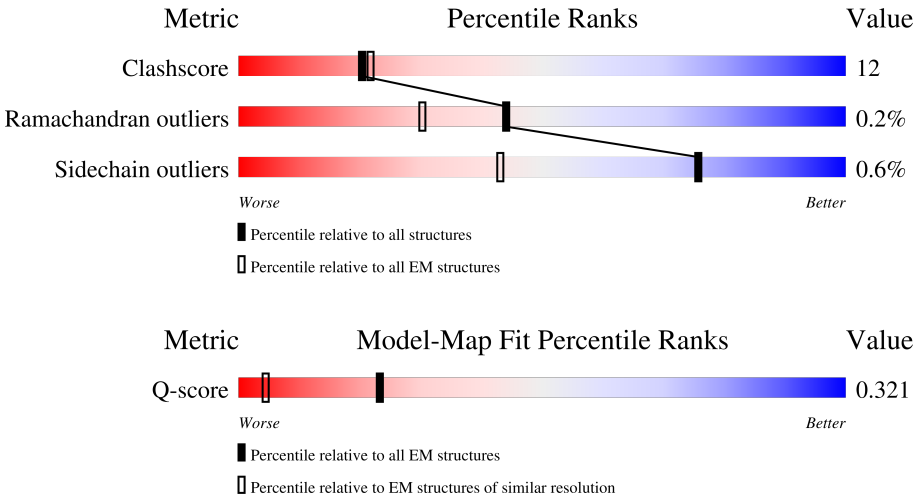
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 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	13068 (2.44 - 3.44)

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	K	609	16% 56% 25% 19%
1	M	609	59% 61% 20% 19%
2	L	732	18% 53% 19% 28%
2	N	732	48% 52% 20% 28%

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Mol	Chain	Length	Quality of chain
3	C	143	69% 27%
3	G	143	65% 9% 25%
4	D	126	64% 13% 23%
4	H	126	60% 15% 24%
5	A	136	58% 12% 29%
5	E	136	55% 15% 29%
6	B	103	69% 9% 22%
6	F	103	61% 15% 24%
7	I	153	37% 62%
8	J	153	42% 56%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 27507 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	493	Total	C	N	O	S	0	0
			3670	2348	614	696	12		
1	M	492	Total	C	N	O	S	0	0
			3844	2452	653	728	11		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	528	Total	C	N	O	S	0	0
			3874	2490	644	721	19		
2	N	530	Total	C	N	O	S	0	0
			4080	2608	683	773	16		

- Molecule 3 is a protein called Histone H2AX.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	107	Total	C	N	O	0	0
			785	497	149	139		
3	C	104	Total	C	N	O	0	0
			788	497	153	138		

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	96	Total	C	N	O	S	0	0
			726	454	132	138	2		
4	D	97	Total	C	N	O	S	0	0
			766	480	142	142	2		

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	96	Total	C	N	O	S	0	0
			782	494	148	136	4		
5	A	96	Total	C	N	O	S	0	0
			790	499	151	136	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	80	Total	C	N	O	S	0	0
			638	405	122	110	1		
6	F	78	Total	C	N	O		0	0
			620	392	120	108			

- Molecule 7 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	151	Total	C	N	O	P	0	0
			3075	1462	557	906	150		

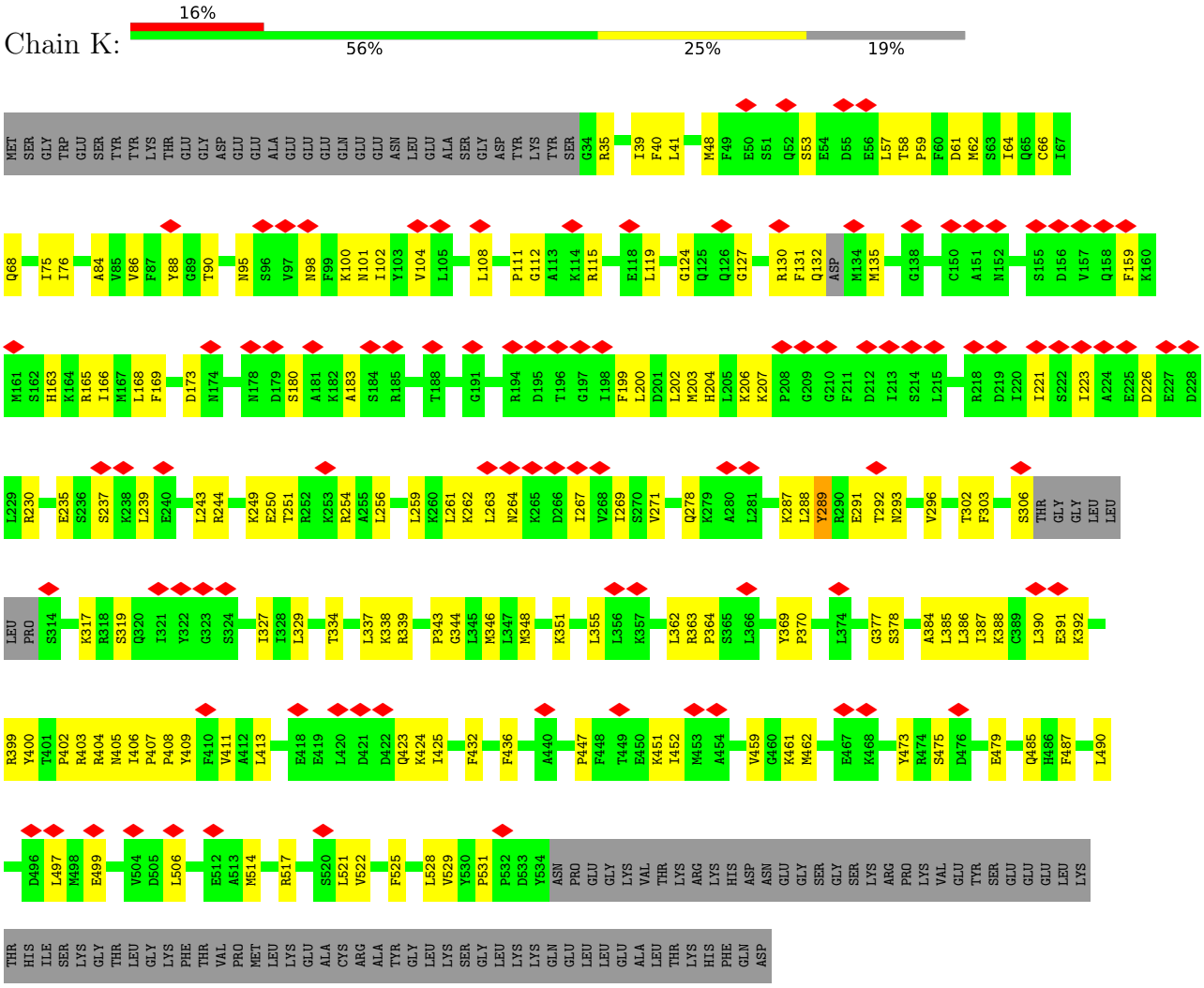
- Molecule 8 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	149	Total	C	N	O	P	0	0
			3069	1453	578	890	148		

3 Residue-property plots (i)

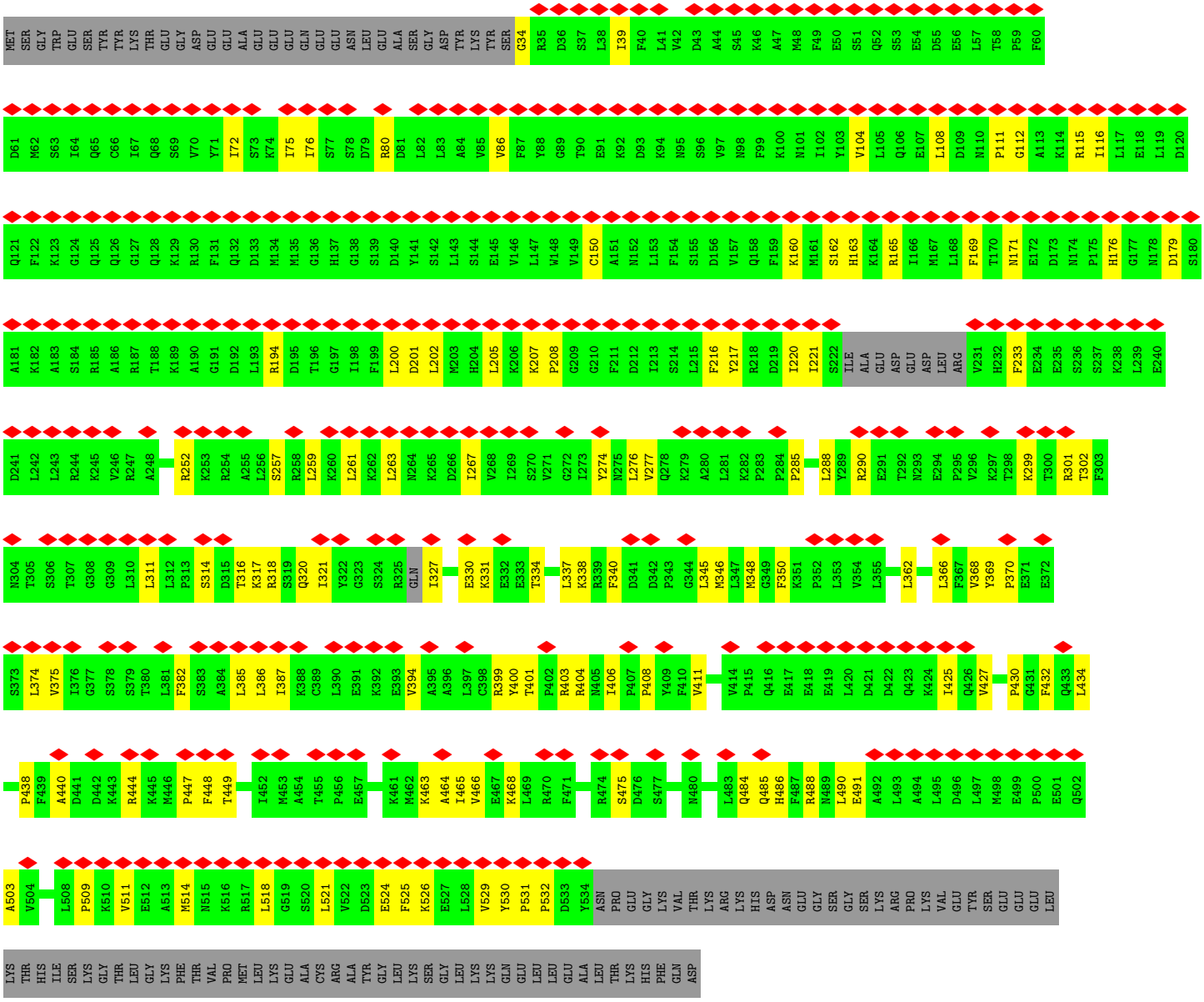
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: X-ray repair cross-complementing protein 6



• Molecule 1: X-ray repair cross-complementing protein 6

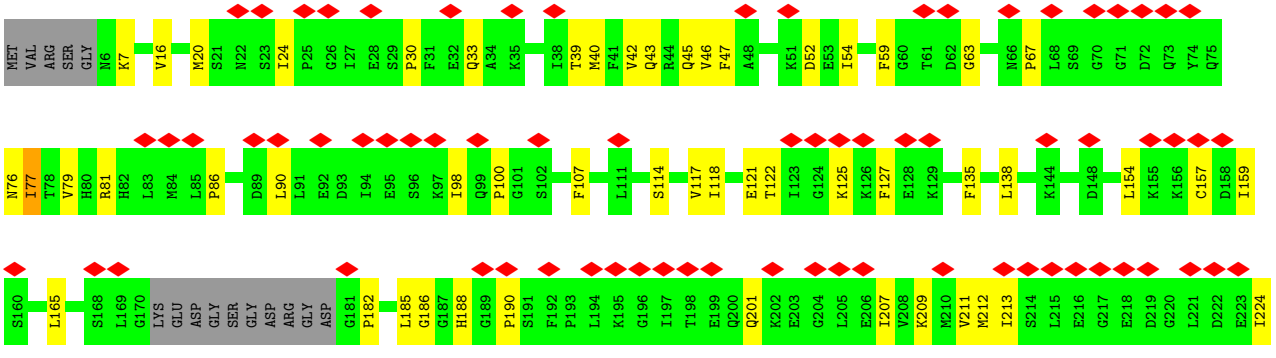


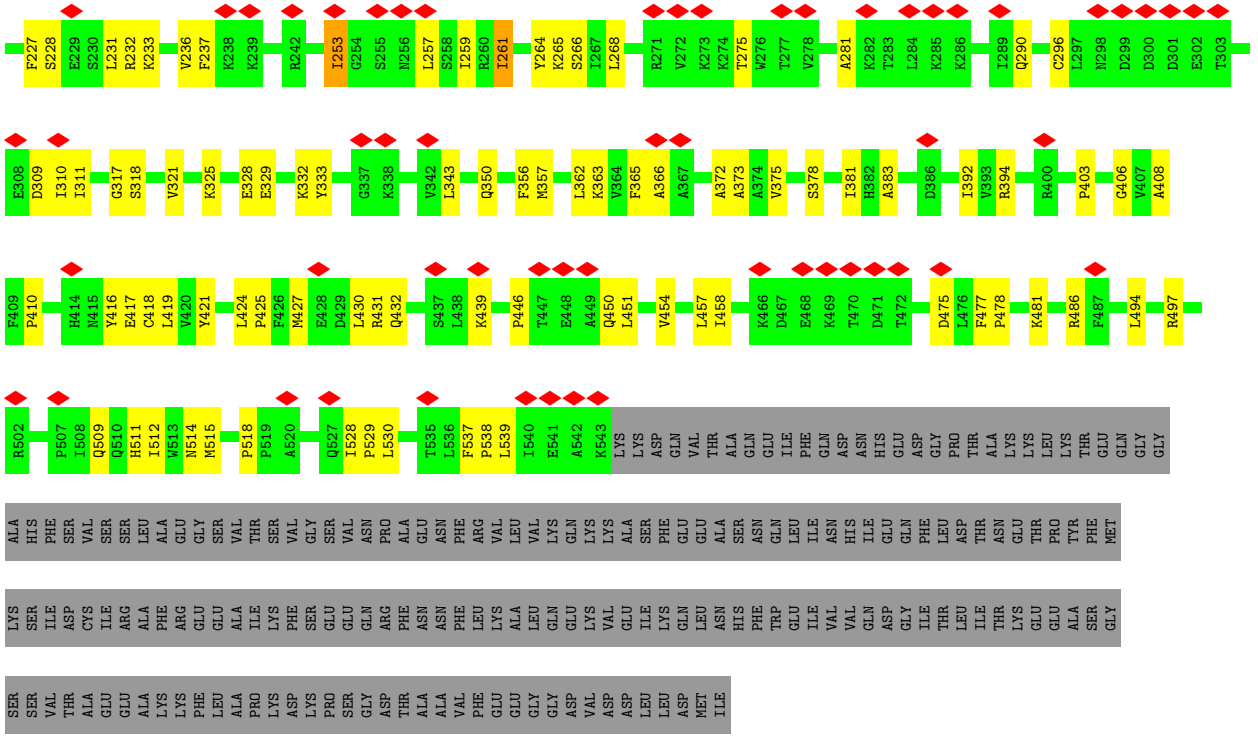


• Molecule 2: X-ray repair cross-complementing protein 5

Chain L:



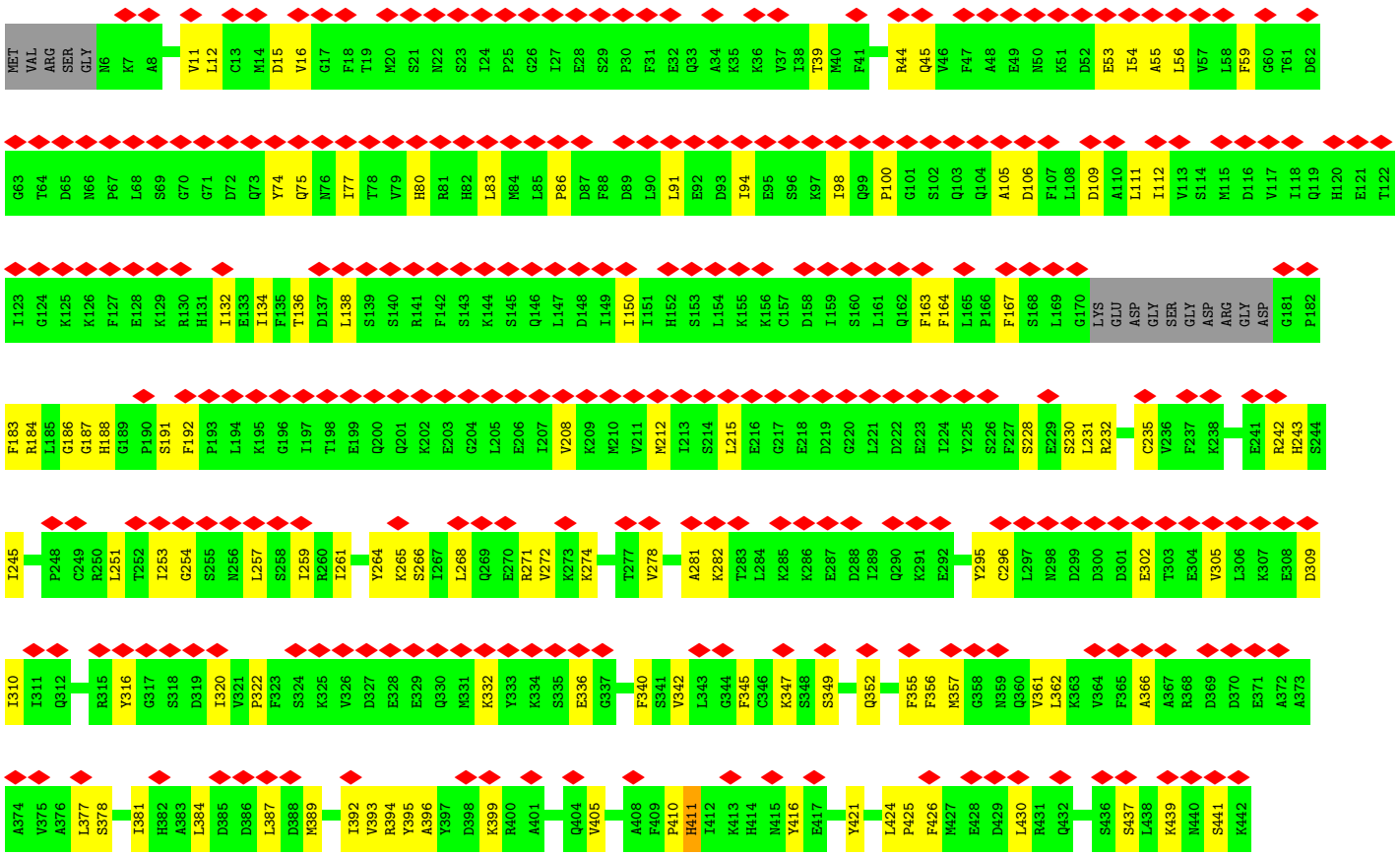


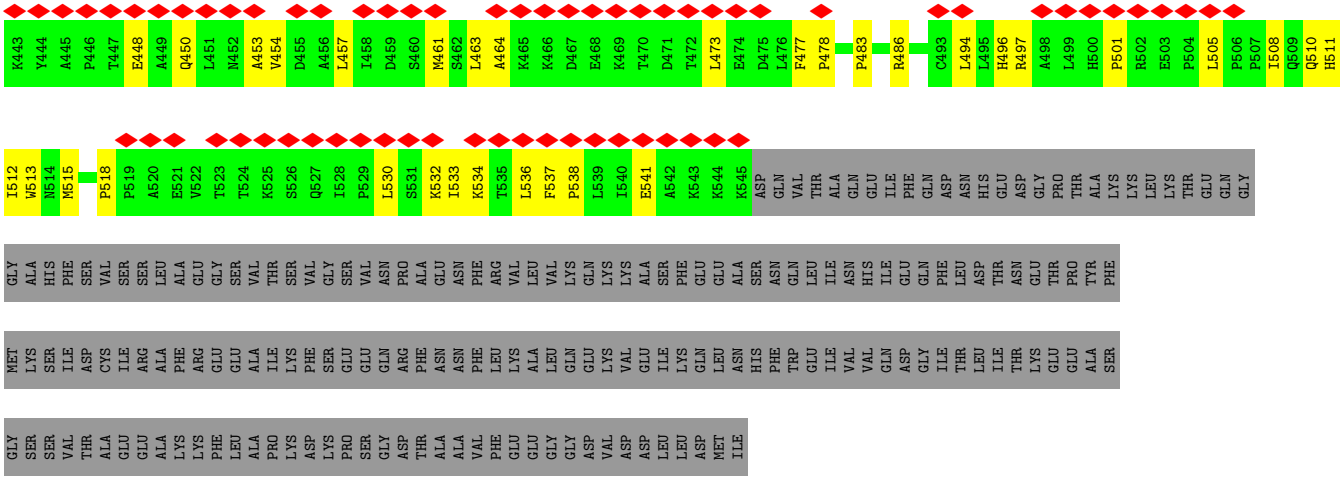


• Molecule 2: X-ray repair cross-complementing protein 5

Chain N:



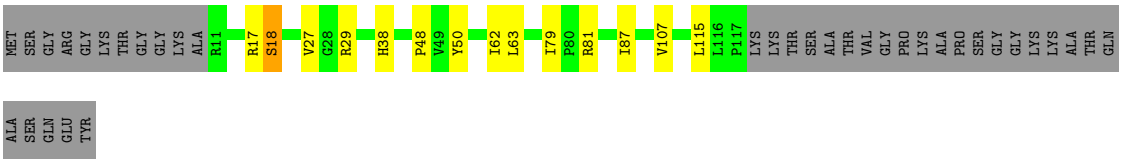




• Molecule 3: Histone H2AX

Chain G:

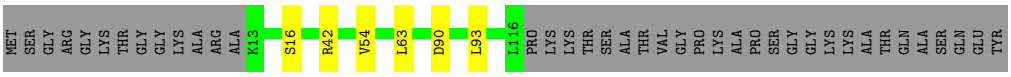




• Molecule 3: Histone H2AX

Chain C:

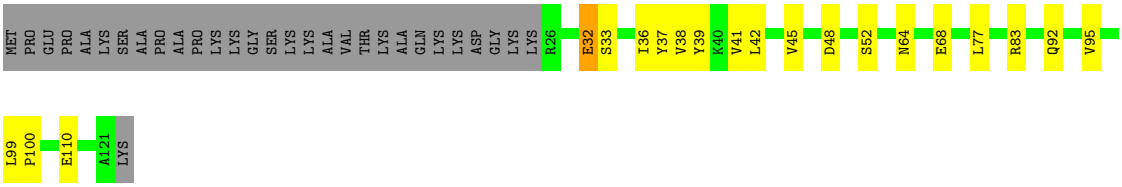




• Molecule 4: Histone H2B type 1-J

Chain H:





• Molecule 4: Histone H2B type 1-J

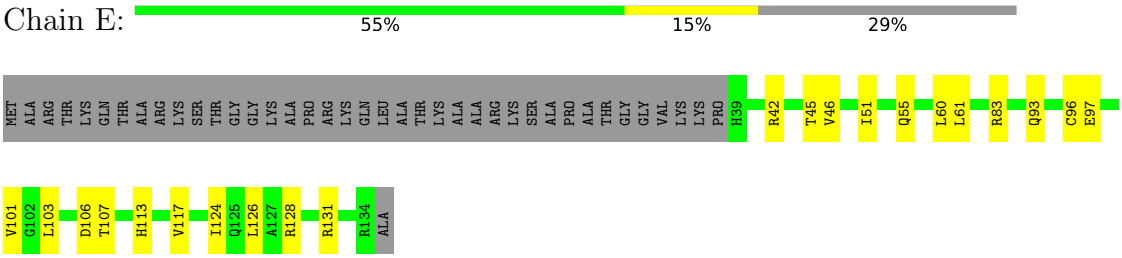
Chain D:





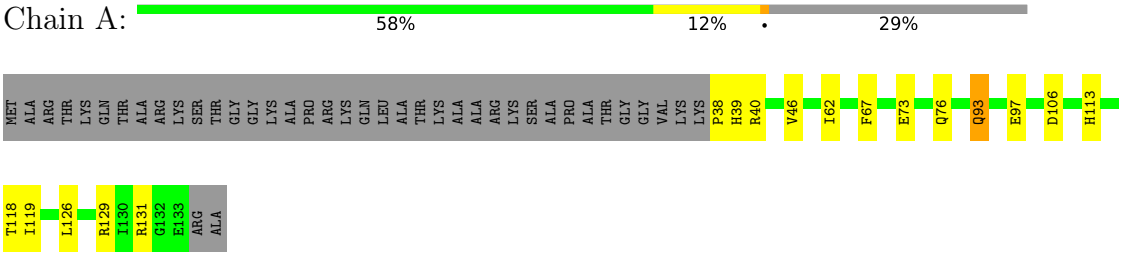
• Molecule 5: Histone H3.1

Chain E:



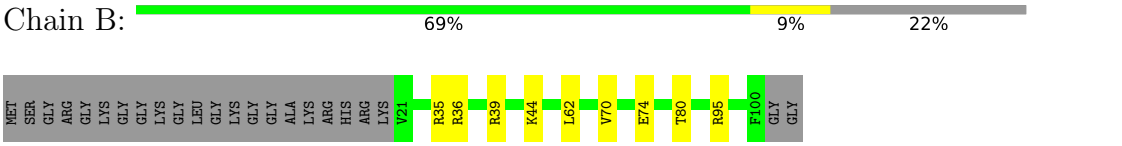
• Molecule 5: Histone H3.1

Chain A:



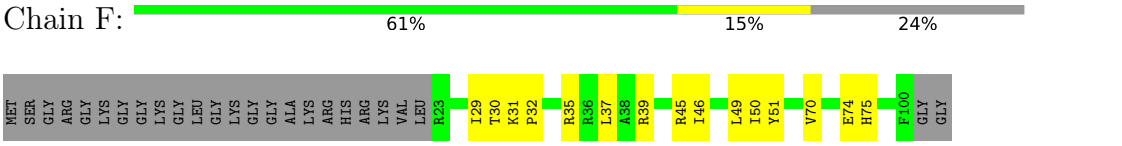
• Molecule 6: Histone H4

Chain B:



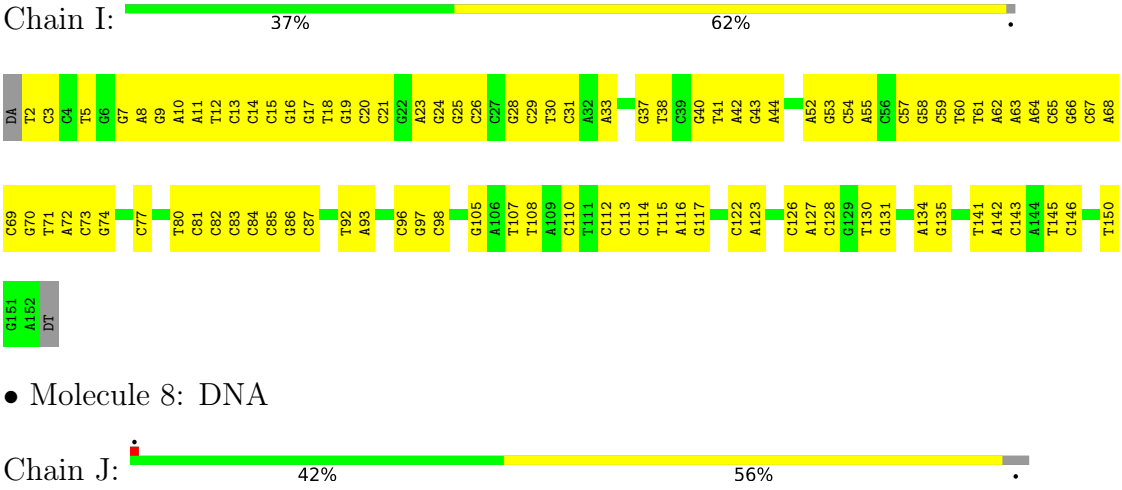
• Molecule 6: Histone H4

Chain F:



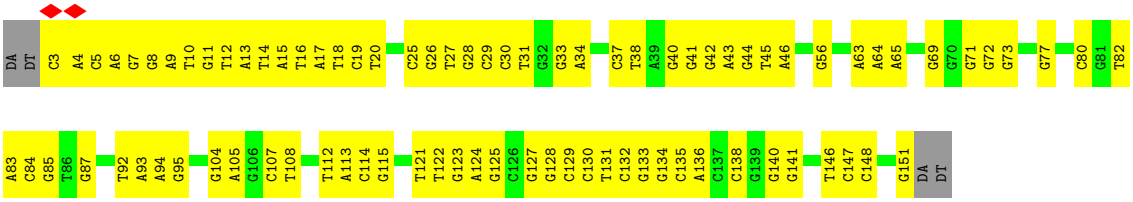
• Molecule 7: DNA

Chain I:



• Molecule 8: DNA

Chain J:


DA DT C3 A4 C5 A6 G7 G8 A9 T10 G11 T12 A13 T14 A15 T16 A17 T18 C19 T20 C25 G26 T27 G28 C29 C30 T31 G32 G33 A34 C37 T38 A39 G40 G41 G42 A43 G44 T45 A46 G56 A63 A64 A65 G69 G70 G71 G72 G73 G77 C80 G81 T82
A83 C84 G85 T86 G87 T92 A93 A94 G95 G104 A105 G106 C107 T108 T112 A113 C114 G115 T121 T122 G123 A124 G125 C126 G127 G128 C129 C130 T131 C132 G133 G134 C135 A136 C137 C138 G139 G140 G141 T146 C147 C148 G151 DA DT

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.715	Depositor
Minimum map value	-0.312	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	421.888, 421.888, 421.888	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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	K	0.12	0/3738	0.35	0/5085
1	M	0.09	0/3916	0.26	0/5295
2	L	0.13	0/3951	0.39	0/5384
2	N	0.10	0/4158	0.27	0/5633
3	C	0.14	0/798	0.27	0/1079
3	G	0.16	0/796	0.37	0/1082
4	D	0.13	0/777	0.29	0/1040
4	H	0.16	0/737	0.36	0/997
5	A	0.15	0/802	0.27	0/1076
5	E	0.16	0/793	0.34	0/1065
6	B	0.16	0/645	0.29	0/866
6	F	0.18	0/627	0.33	0/842
7	I	0.20	0/3445	0.38	0/5311
8	J	0.20	0/3447	0.37	0/5323
All	All	0.15	0/28630	0.33	0/40078

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

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	K	3670	0	3466	137	0
1	M	3844	0	3787	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	3874	0	3669	132	0
2	N	4080	0	4004	124	0
3	C	788	0	826	6	0
3	G	785	0	803	12	0
4	D	766	0	797	11	0
4	H	726	0	714	14	0
5	A	790	0	826	13	0
5	E	782	0	809	16	0
6	B	638	0	679	7	0
6	F	620	0	652	12	0
7	I	3075	0	1697	96	0
8	J	3069	0	1672	88	0
All	All	27507	0	24401	635	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 12.

The worst 5 of 635 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)
1:K:165:ARG:HG3	1:K:199:PHE:HB3	1.58	0.84
1:K:327:ILE:HG12	2:L:494:LEU:HD22	1.60	0.81
1:M:112:GLY:H	1:M:115:ARG:HG3	1.45	0.81
1:K:250:GLU:HG3	1:K:251:THR:H	1.45	0.79
2:N:464:ALA:HB1	2:N:473:LEU:HB3	1.67	0.75

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	K	416/609 (68%)	373 (90%)	42 (10%)	1 (0%)	43 65
1	M	486/609 (80%)	469 (96%)	17 (4%)	0	100 100
2	L	479/732 (65%)	436 (91%)	42 (9%)	1 (0%)	43 65
2	N	526/732 (72%)	499 (95%)	27 (5%)	0	100 100
3	C	102/143 (71%)	97 (95%)	5 (5%)	0	100 100
3	G	105/143 (73%)	100 (95%)	4 (4%)	1 (1%)	12 31
4	D	95/126 (75%)	93 (98%)	2 (2%)	0	100 100
4	H	94/126 (75%)	89 (95%)	4 (4%)	1 (1%)	11 29
5	A	94/136 (69%)	91 (97%)	3 (3%)	0	100 100
5	E	94/136 (69%)	93 (99%)	1 (1%)	0	100 100
6	B	78/103 (76%)	78 (100%)	0	0	100 100
6	F	76/103 (74%)	76 (100%)	0	0	100 100
All	All	2645/3698 (72%)	2494 (94%)	147 (6%)	4 (0%)	44 65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	18	SER
1	K	289	TYR
4	H	100	PRO
2	L	77	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	K	370/548 (68%)	369 (100%)	1 (0%)	86 93
1	M	414/548 (76%)	413 (100%)	1 (0%)	87 95
2	L	390/649 (60%)	387 (99%)	3 (1%)	73 84
2	N	437/649 (67%)	436 (100%)	1 (0%)	87 95
3	C	78/106 (74%)	78 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	G	75/106 (71%)	74 (99%)	1 (1%)	61 77
4	D	83/105 (79%)	83 (100%)	0	100 100
4	H	75/105 (71%)	73 (97%)	2 (3%)	39 64
5	A	84/111 (76%)	82 (98%)	2 (2%)	43 67
5	E	82/111 (74%)	81 (99%)	1 (1%)	63 78
6	B	66/79 (84%)	65 (98%)	1 (2%)	57 75
6	F	63/79 (80%)	63 (100%)	0	100 100
All	All	2217/3196 (69%)	2204 (99%)	13 (1%)	76 89

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	97	GLU
6	B	95	ARG
5	A	129	ARG
2	N	411	HIS
5	A	93	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	509	GLN
4	H	81	ASN
2	N	269	GLN
4	D	60	ASN
1	M	65	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 (i)

There are no chain breaks in this entry.

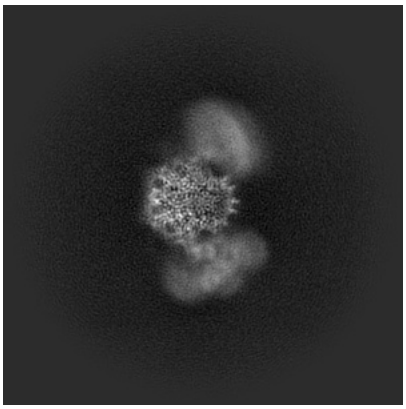
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52912. These allow visual inspection of the internal detail of the map and identification of artifacts.

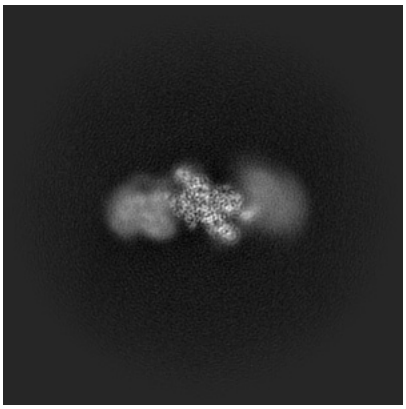
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

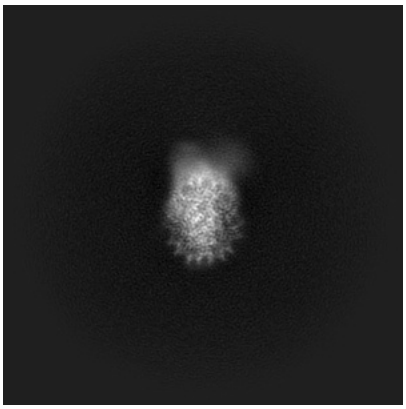
6.1.1 Primary map



X

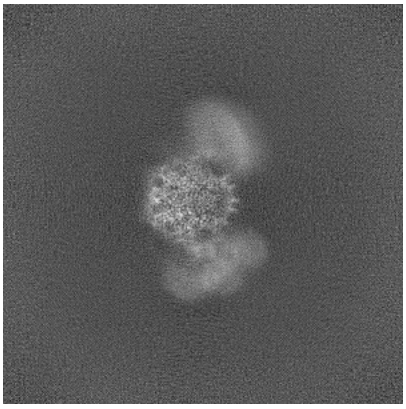


Y

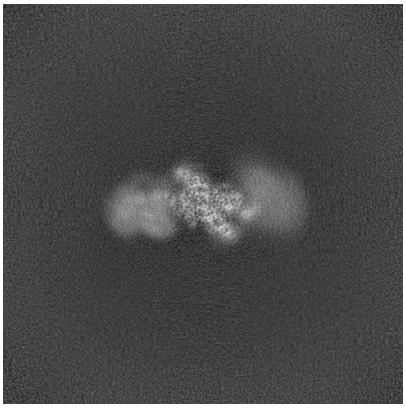


Z

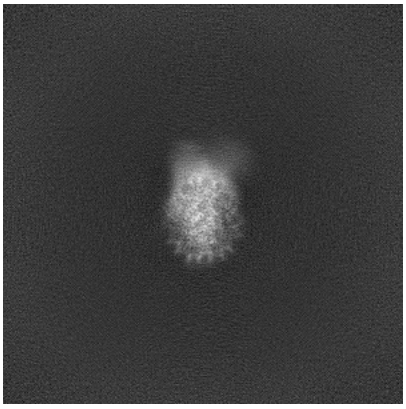
6.1.2 Raw map



X



Y



Z

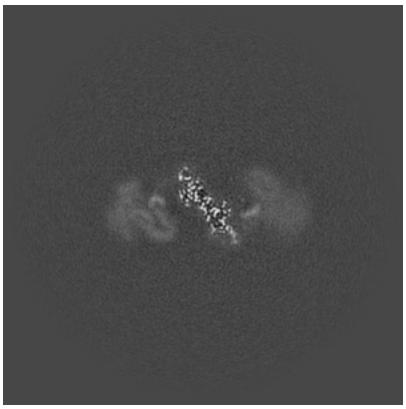
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

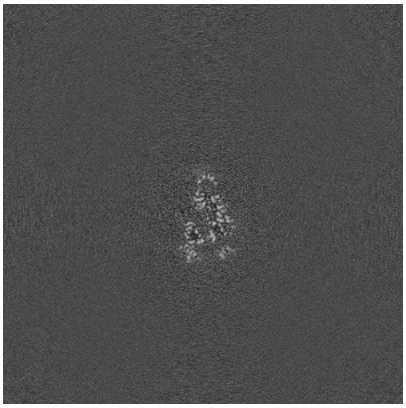
6.2.2 Raw map



X Index: 256



Y Index: 256

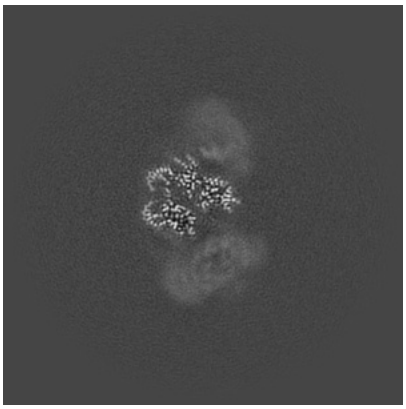


Z Index: 256

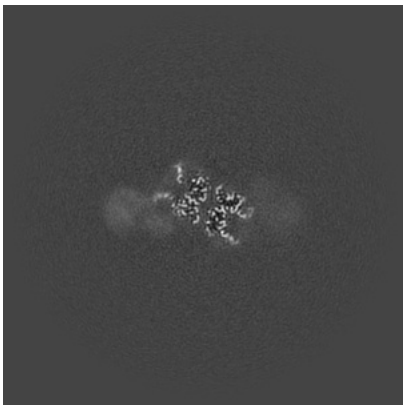
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

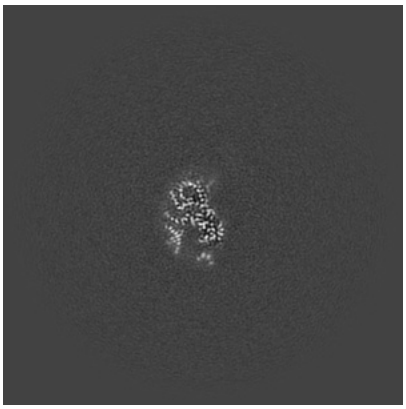
6.3.1 Primary map



X Index: 251

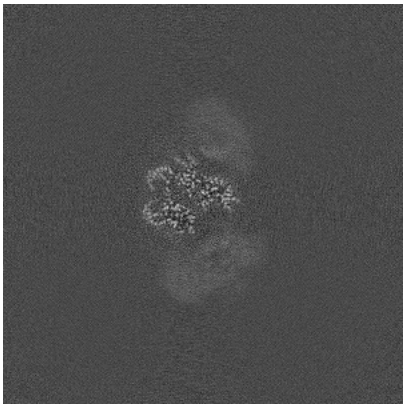


Y Index: 237

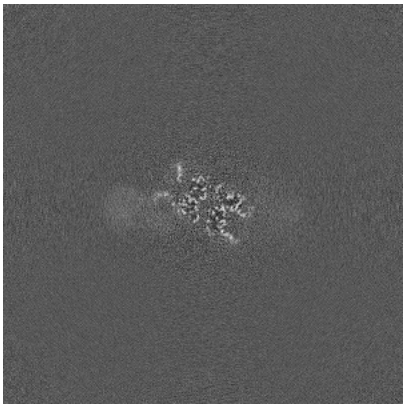


Z Index: 282

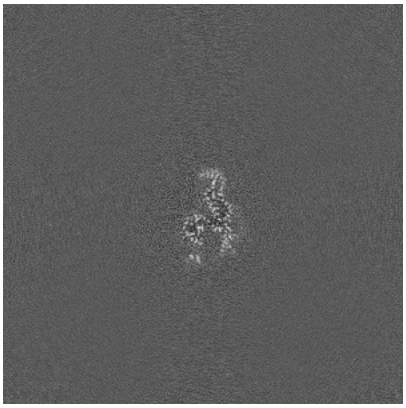
6.3.2 Raw map



X Index: 251



Y Index: 237

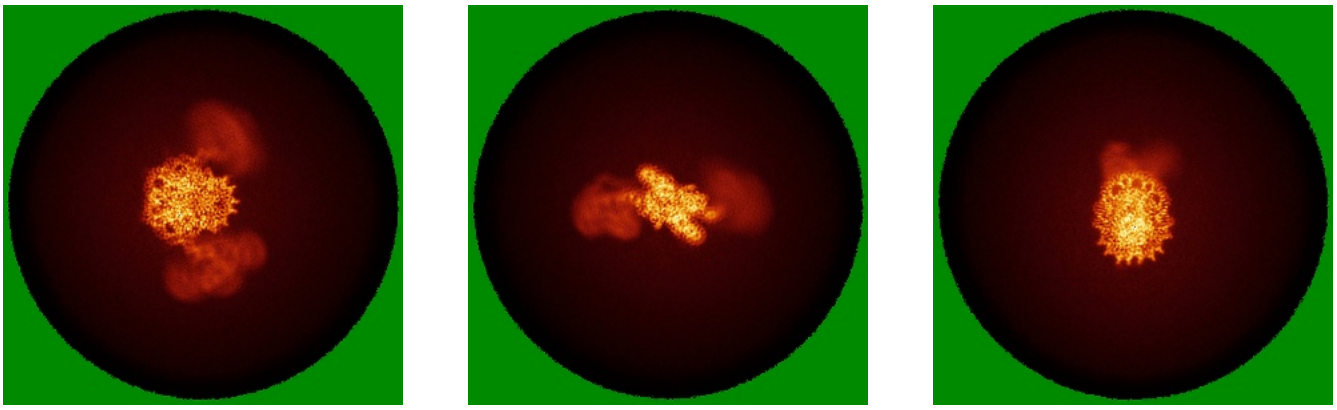


Z Index: 248

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

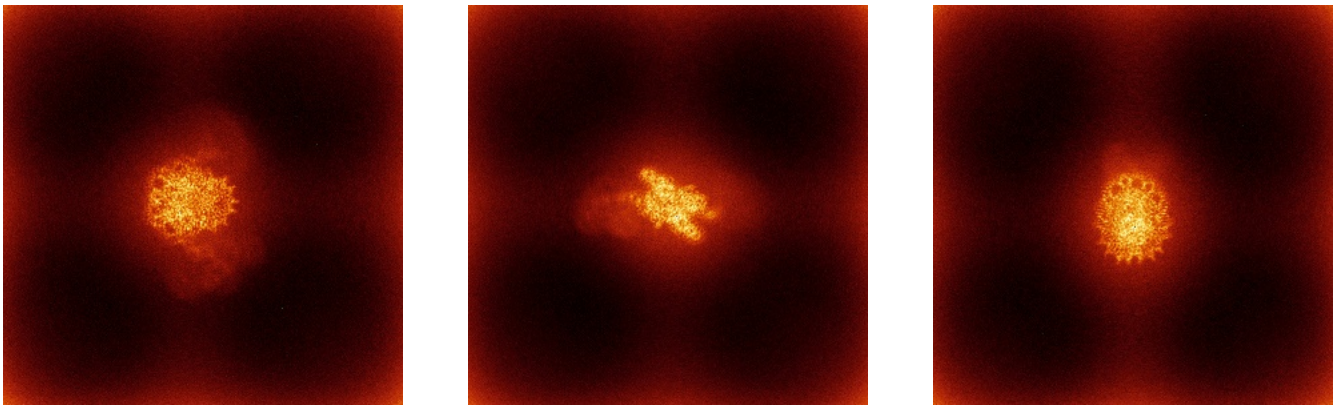
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw 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)

This section was not generated.

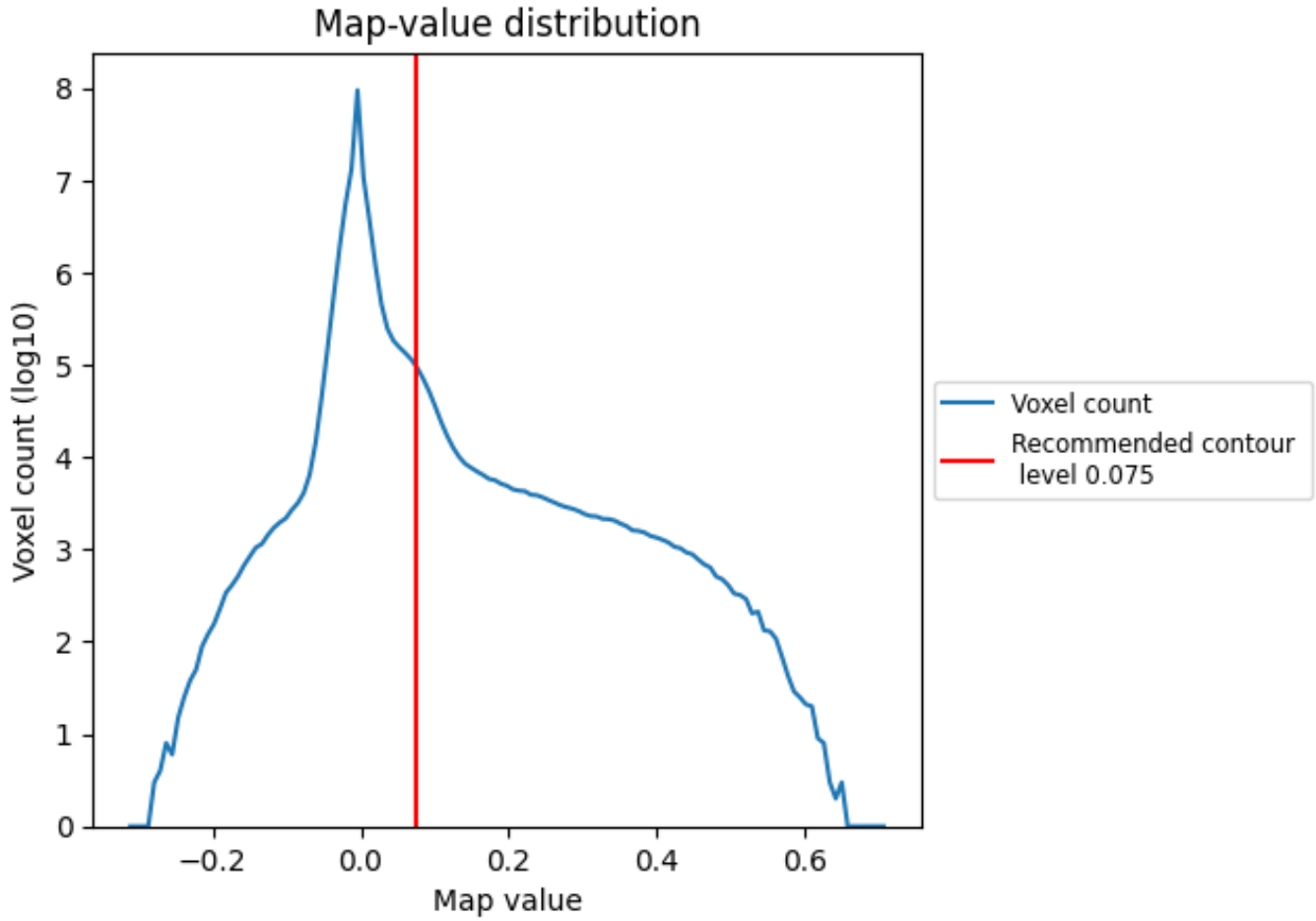
6.6 Mask visualisation (i)

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

7 Map analysis

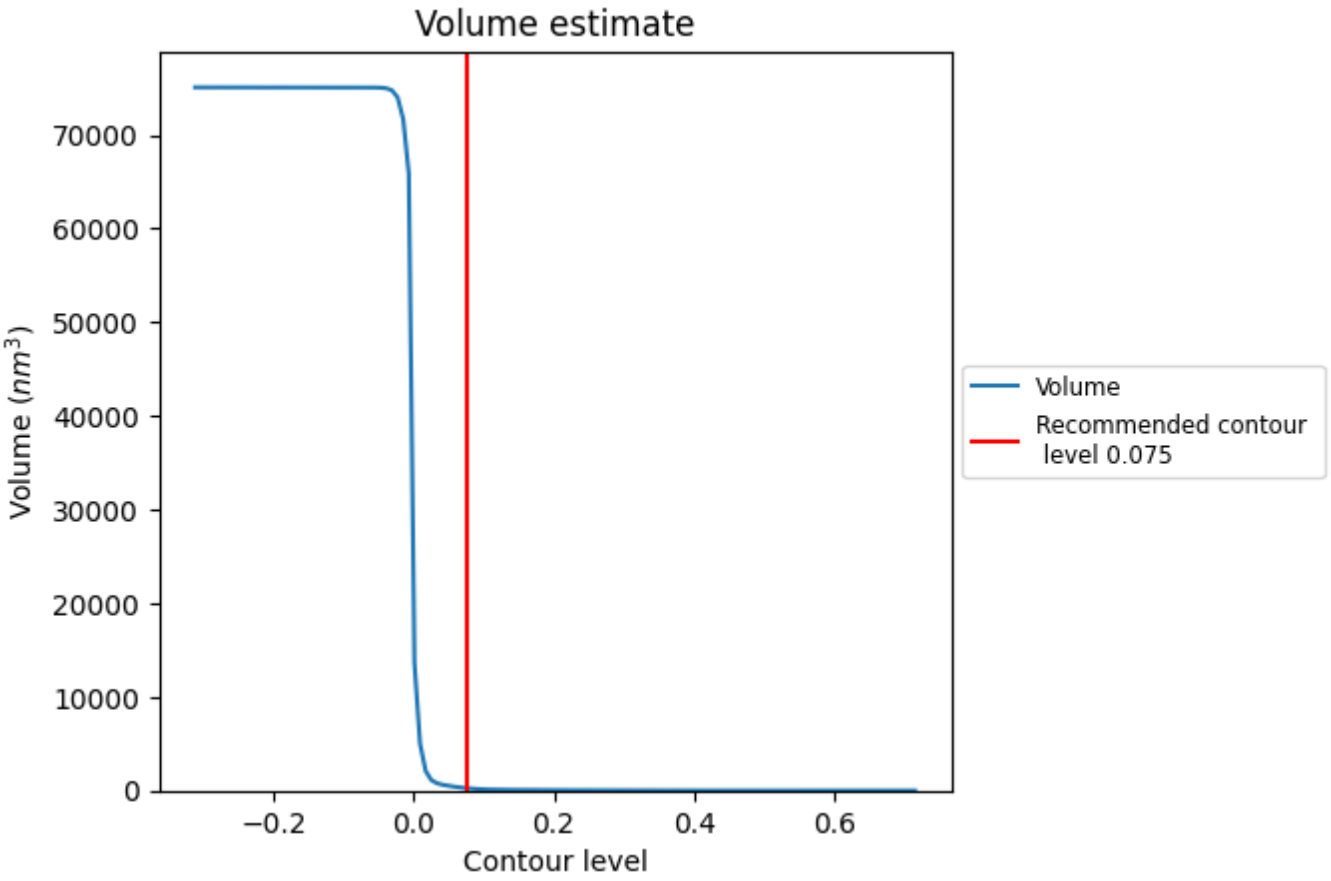
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

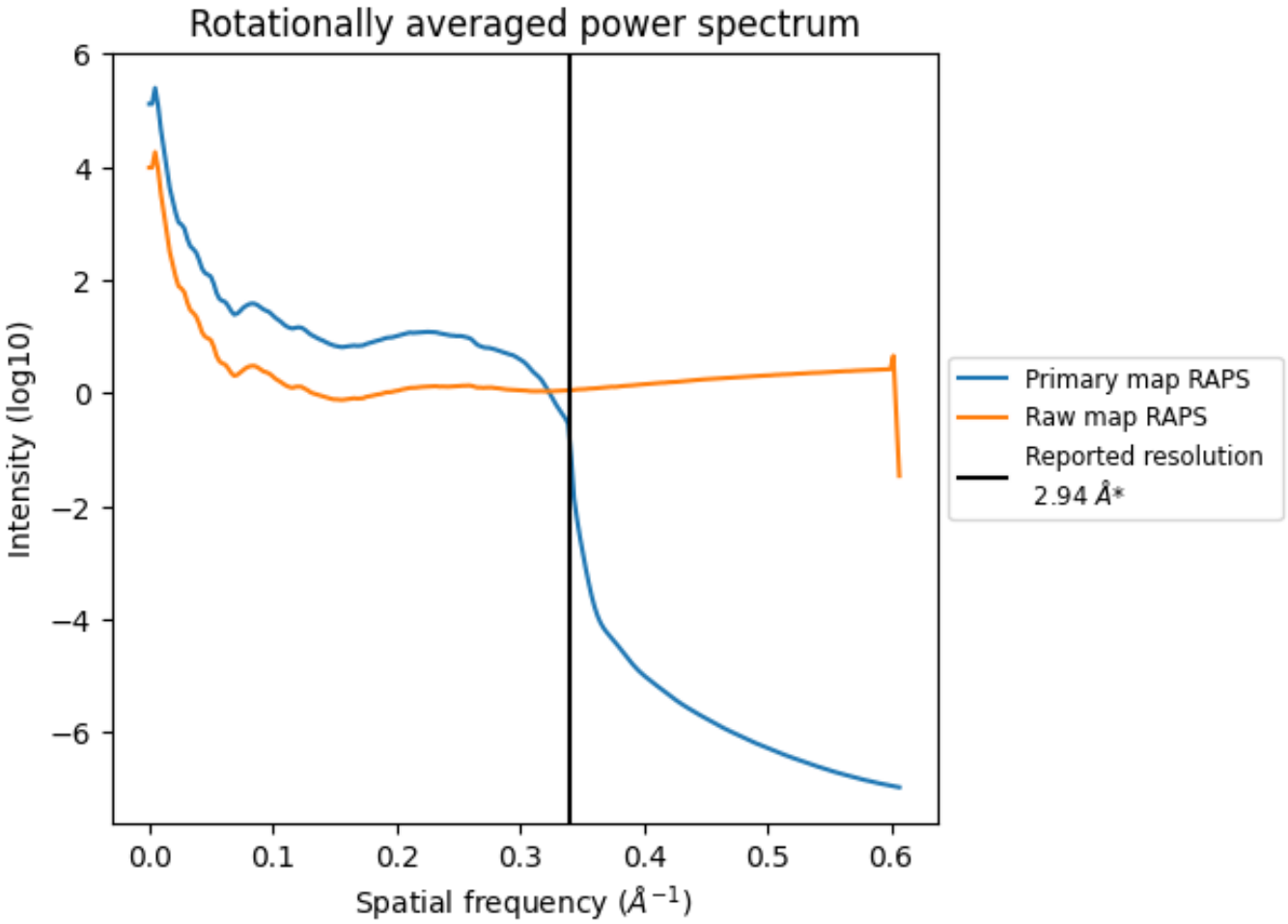
7.2 Volume estimate (i)



The volume at the recommended contour level is 260 nm^3; this corresponds to an approximate mass of 235 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)

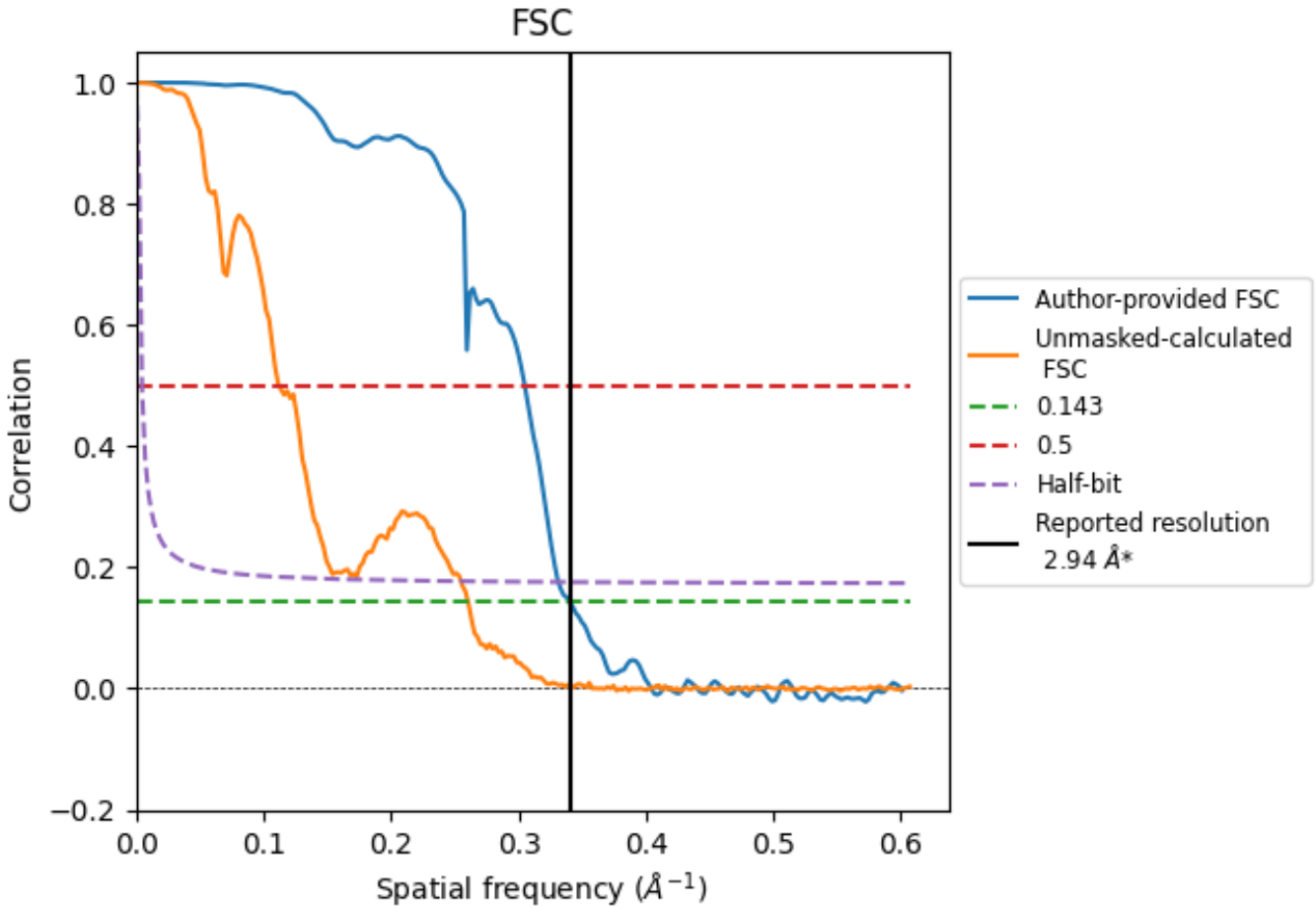


*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.340 Å^{-1}

8.2 Resolution estimates (i)

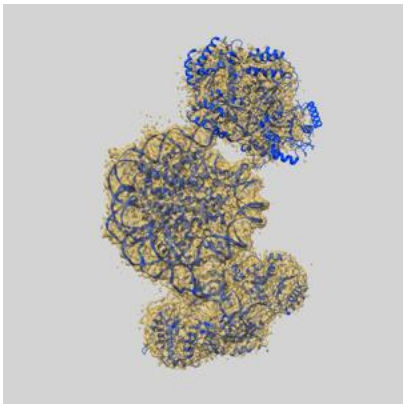
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.94	3.28	3.02
Unmasked-calculated*	3.84	8.91	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 2.94 by more than 10 %

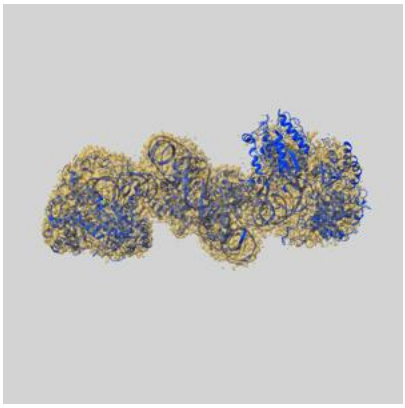
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52912 and PDB model 9Q8X. Per-residue inclusion information can be found in section 3 on page 6.

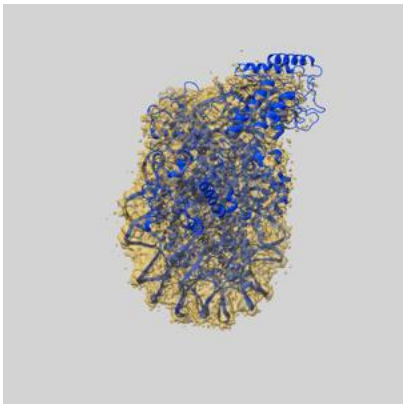
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075 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)



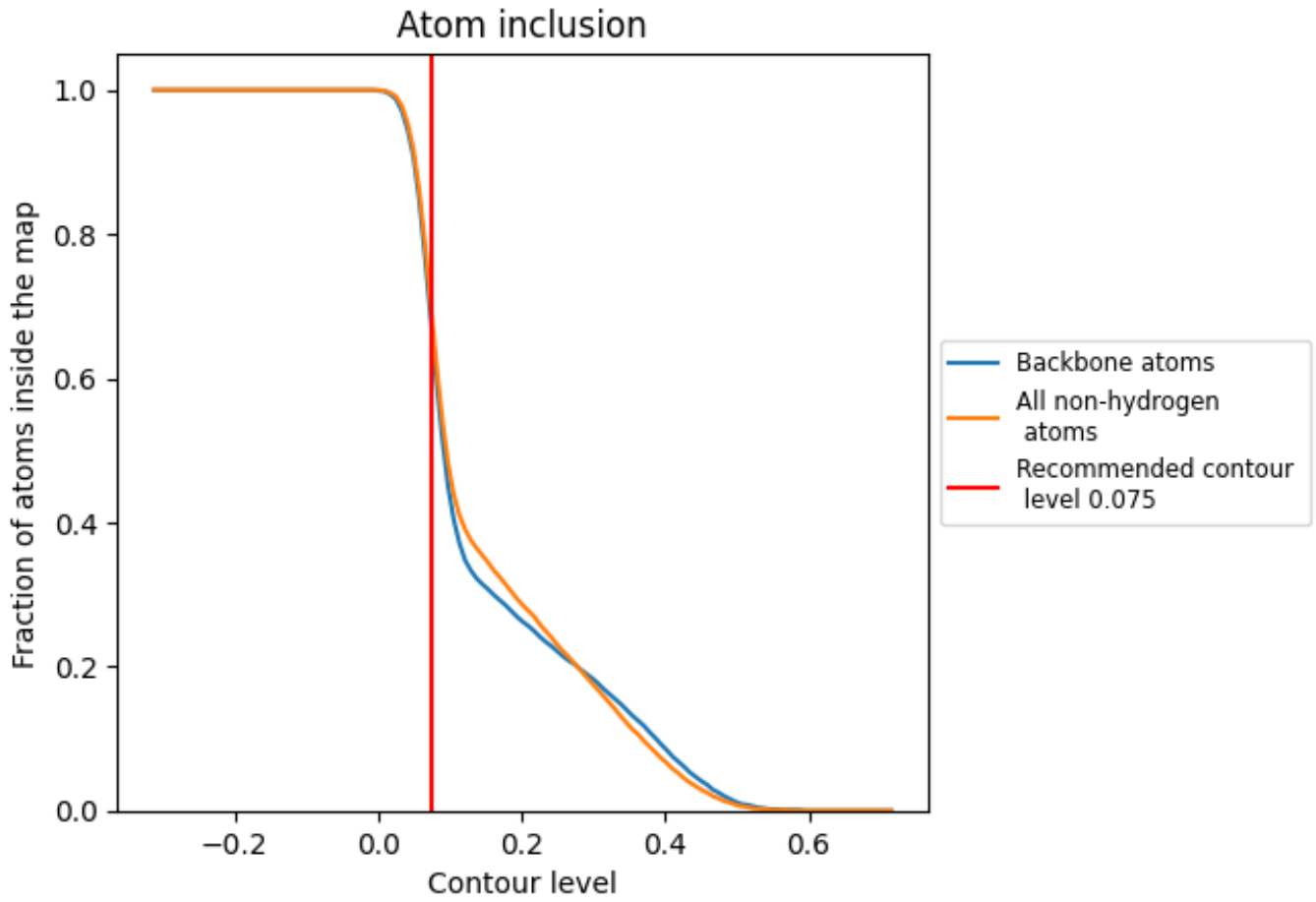
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 69% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.3210
A	0.9860	0.5820
B	0.9900	0.5880
C	0.9820	0.5790
D	0.9690	0.5580
E	0.9800	0.5780
F	0.9870	0.5870
G	0.9780	0.5740
H	0.9690	0.5570
I	0.9650	0.4740
J	0.9540	0.4620
K	0.6630	0.1720
L	0.6410	0.1710
M	0.2590	0.1700
N	0.3170	0.1540

