



wwPDB EM Validation Summary Report ⓘ

Jul 22, 2025 – 01:11 PM EDT

PDB ID : 9NQU / pdb_00009nqu
EMDB ID : EMD-49676
Title : KDM6B-nucleosome structure stabilized by H3K27C-UNC8015 covalent conjugate
Authors : Lin, C.-C.; McGinty, R.K.
Deposited on : 2025-03-13
Resolution : 3.16 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

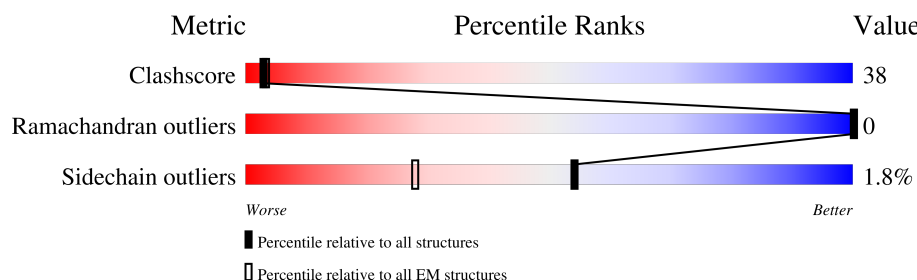
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 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	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	125	
4	H	125	

Continued on next page...

Mol	Chain	Length	Quality of chain
5	I	185	<p>10% 20% 80%</p>
6	J	185	<p>9% 28% 72%</p>
7	K	514	<p>1% 21% 65% 11%</p>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17358 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			800	505	155	138	2		
1	E	120	Total	C	N	O	S	0	0
			960	603	189	165	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	CYS	LYS	conflict	UNP Q71DI3
A	110	ALA	CYS	conflict	UNP Q71DI3
E	27	CYS	LYS	conflict	UNP Q71DI3
E	110	ALA	CYS	conflict	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	77	Total	C	N	O	S	0	0
			614	389	119	105	1		
2	F	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	108	Total	C	N	O	0	0
			832	526	163	143		
3	G	107	Total	C	N	O	0	0
			821	520	159	142		

- Molecule 4 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	94	Total	C	N	O	S	0	0
			736	461	134	139	2		
4	H	93	Total	C	N	O	S	0	0
			725	455	130	138	2		

- Molecule 5 is a DNA chain called DNA (185-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	185	Total	C	N	O	P	0	0
			3771	1791	684	1111	185		

- Molecule 6 is a DNA chain called DNA (185-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	185	Total	C	N	O	P	0	0
			3814	1805	715	1109	185		

- Molecule 7 is a protein called Lysine-specific demethylase 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	455	Total	C	N	O	S	0	0
			3649	2316	640	674	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1128	GLY	-	expression tag	UNP Q5NCY0
K	1129	SER	-	expression tag	UNP Q5NCY0

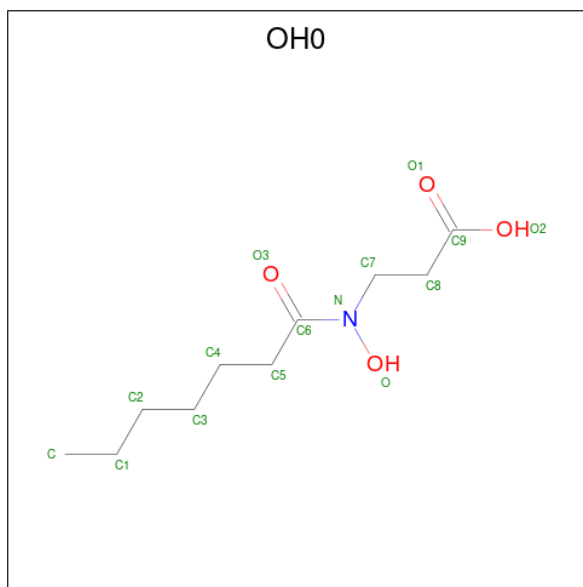
- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
8	K	1	Total	Fe	0
			1	1	

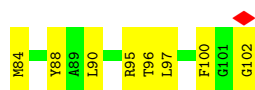
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	K	1	Total	Zn	0
			1	1	

- Molecule 10 is N-heptanoyl-N-hydroxy-beta-alanine (CCD ID: OH0) (formula: C₁₀H₁₉NO₄).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	K	1	15	10	1	4	0



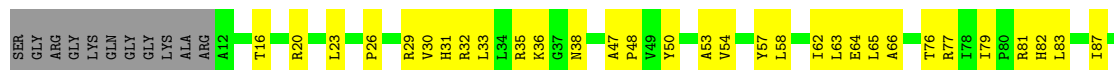
• Molecule 3: Histone H2A type 1

Chain C: 53% 31% 16%



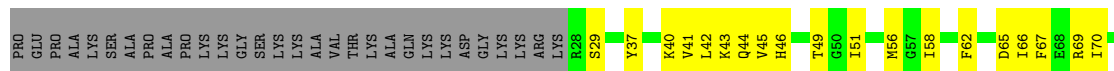
• Molecule 3: Histone H2A type 1

Chain G: 55% 28% 17%



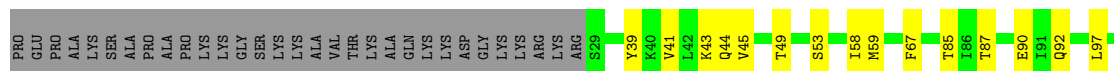
• Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain D: 50% 26% 25%



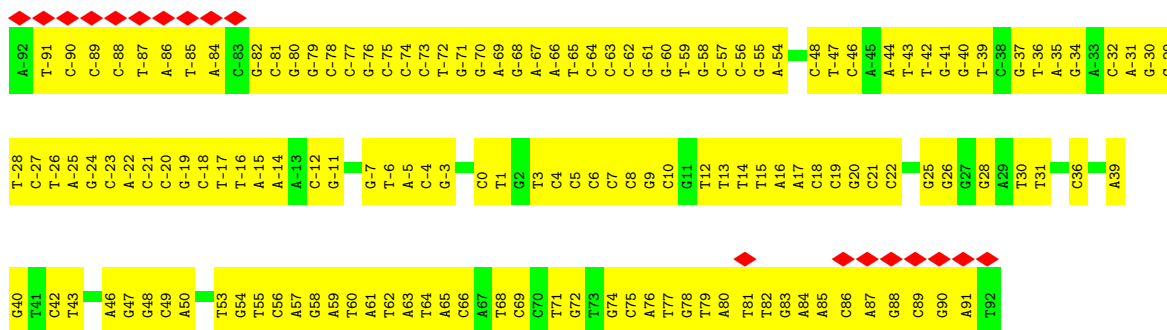
• Molecule 4: Histone H2B type 1-C/E/F/G/I

Chain H: 59% 15% 26%

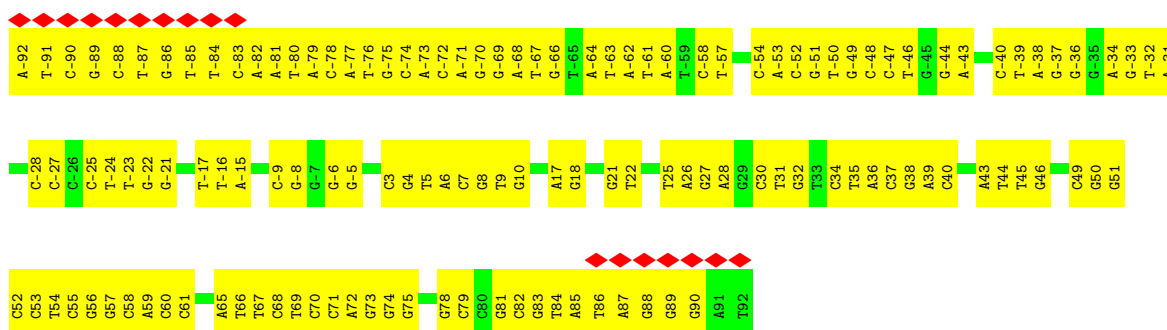


• Molecule 5: DNA (185-MER)

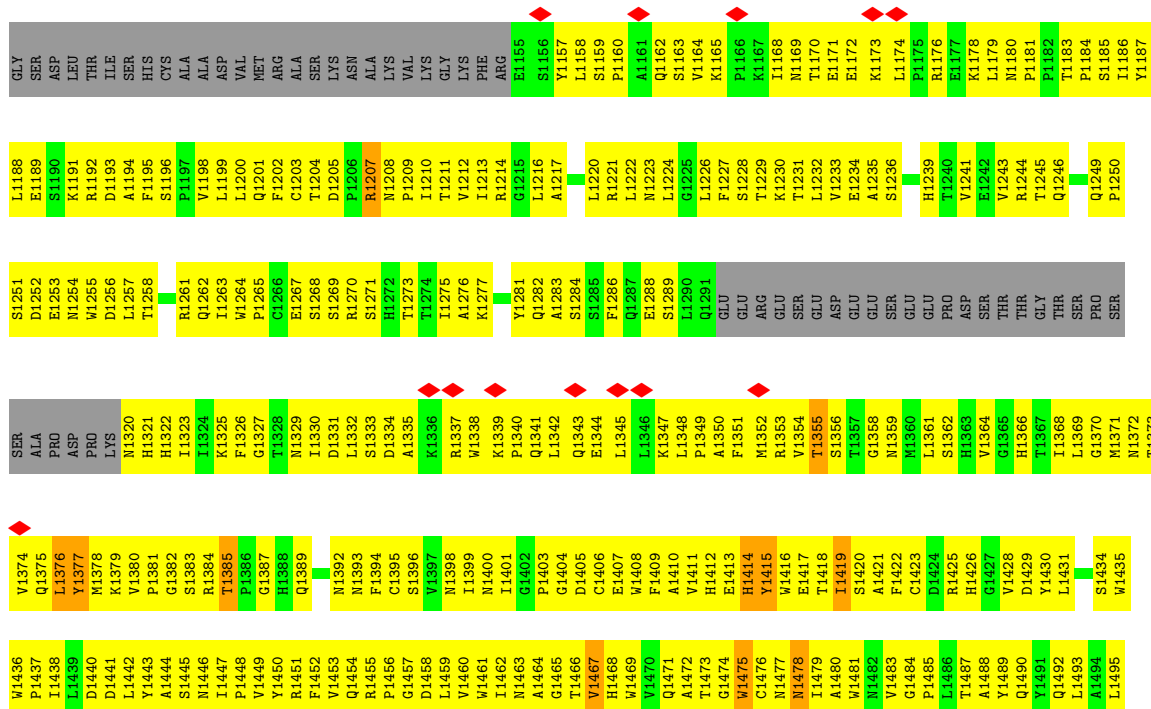
Chain I: 10% 20% 80%



• Molecule 6: DNA (185-MER)



• Molecule 7: Lysine-specific demethylase 6B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	61.240	Depositor
Minimum map value	-28.691	Depositor
Average map value	0.021	Depositor
Map value standard deviation	1.197	Depositor
Recommended contour level	5	Depositor
Map size (Å)	294.336, 294.336, 294.336	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OH0, FE

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	0.24	0/812	0.37	0/1089
1	E	0.25	0/974	0.36	0/1307
2	B	0.12	0/621	0.25	0/832
2	F	0.21	0/626	0.35	0/837
3	C	0.23	0/842	0.30	0/1135
3	G	0.21	0/831	0.36	0/1121
4	D	0.25	0/747	0.34	0/1004
4	H	0.25	0/736	0.37	0/990
5	I	0.23	0/4225	0.43	0/6513
6	J	0.29	0/4283	0.49	0/6614
7	K	0.39	0/3744	0.58	0/5096
All	All	0.28	0/18441	0.46	0/26538

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	800	0	839	47	0
1	E	960	0	1017	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	614	0	656	41	0
2	F	619	0	659	25	0
3	C	832	0	897	45	0
3	G	821	0	884	33	0
4	D	736	0	756	46	0
4	H	725	0	743	20	0
5	I	3771	0	2077	223	0
6	J	3814	0	2076	179	0
7	K	3649	0	3564	608	0
8	K	1	0	0	0	0
9	K	1	0	0	0	0
10	K	15	0	0	2	0
All	All	17358	0	14168	1211	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 38.

The worst 5 of 1211 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)
7:K:1418:THR:HB	7:K:1447:ILE:HD11	1.47	0.94
1:E:68:GLN:HG2	1:E:89:VAL:HG11	1.46	0.94
5:I:14:DT:H2''	5:I:15:DT:H71	1.49	0.94
5:I:-79:DG:H1'	5:I:-78:DC:H5'	1.50	0.94
7:K:1428:VAL:HG11	7:K:1435:TRP:HB3	1.51	0.93

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	95/135 (70%)	92 (97%)	3 (3%)	0	100	100
1	E	118/135 (87%)	110 (93%)	8 (7%)	0	100	100
2	B	75/102 (74%)	75 (100%)	0	0	100	100
2	F	76/102 (74%)	75 (99%)	1 (1%)	0	100	100
3	C	106/129 (82%)	104 (98%)	2 (2%)	0	100	100
3	G	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	D	92/125 (74%)	90 (98%)	2 (2%)	0	100	100
4	H	91/125 (73%)	88 (97%)	3 (3%)	0	100	100
7	K	451/514 (88%)	380 (84%)	71 (16%)	0	100	100
All	All	1209/1496 (81%)	1116 (92%)	93 (8%)	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	84/109 (77%)	84 (100%)	0	100	100
1	E	99/109 (91%)	98 (99%)	1 (1%)	73	85
2	B	63/78 (81%)	63 (100%)	0	100	100
2	F	63/78 (81%)	63 (100%)	0	100	100
3	C	84/98 (86%)	84 (100%)	0	100	100
3	G	83/98 (85%)	83 (100%)	0	100	100
4	D	81/105 (77%)	80 (99%)	1 (1%)	67	82
4	H	80/105 (76%)	80 (100%)	0	100	100
7	K	402/453 (89%)	385 (96%)	17 (4%)	25	53
All	All	1039/1233 (84%)	1020 (98%)	19 (2%)	54	74

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	1478	ASN
7	K	1577	ASP
7	K	1611	LEU
7	K	1521	ARG
7	K	1385	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
7	K	1490	GLN
7	K	1518	ASN
7	K	1562	GLN
7	K	1544	HIS
7	K	1162	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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	OH0	K	1703	1	14,14,14	2.28	1 (7%)	11,16,16	1.19	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	OH0	K	1703	1	-	6/15/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	1703	OH0	C6-N	7.85	1.45	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	1703	OH0	O-N-C7	2.22	118.96	113.76

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	K	1703	OH0	C7-C8-C9-O2
10	K	1703	OH0	C7-C8-C9-O1
10	K	1703	OH0	N-C7-C8-C9
10	K	1703	OH0	C8-C7-N-C6
10	K	1703	OH0	O3-C6-N-O

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	1703	OH0	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

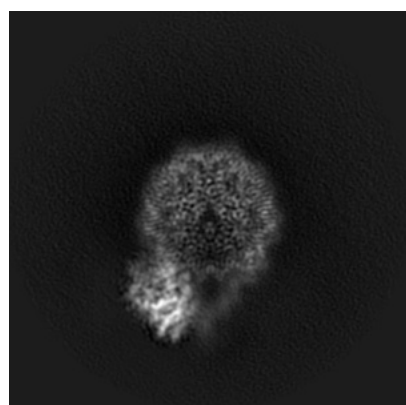
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49676. These allow visual inspection of the internal detail of the map and identification of artifacts.

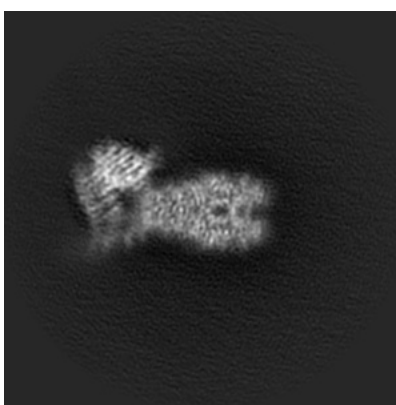
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

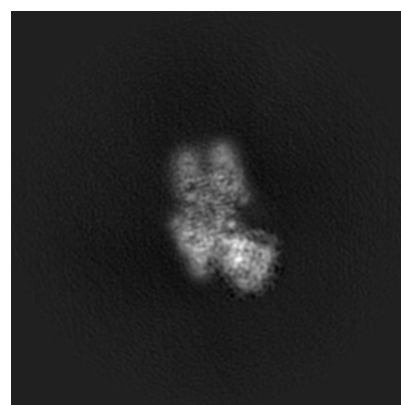
6.1.1 Primary map



X



Y

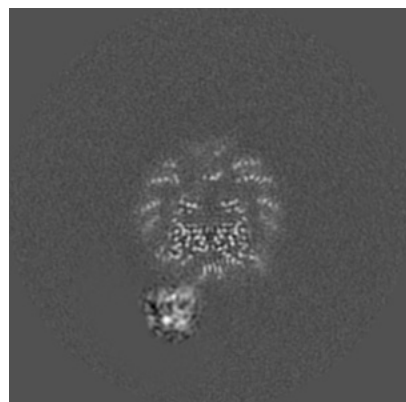


Z

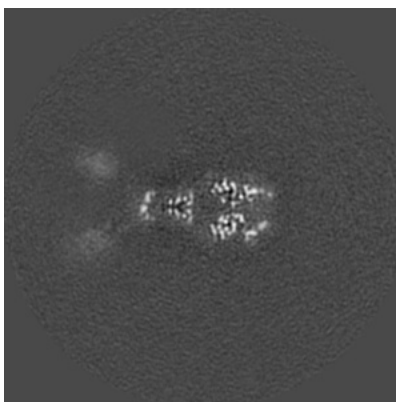
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

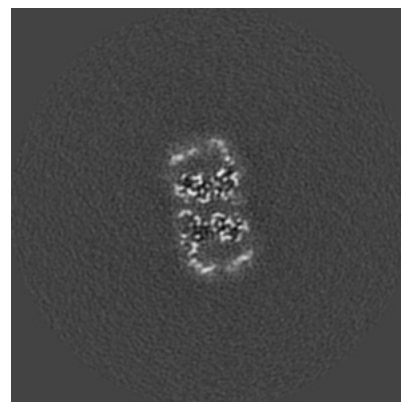
6.2.1 Primary map



X Index: 168



Y Index: 168

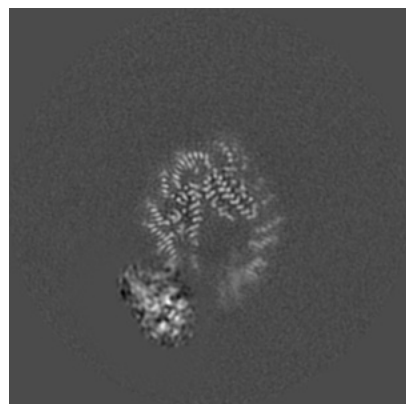


Z Index: 168

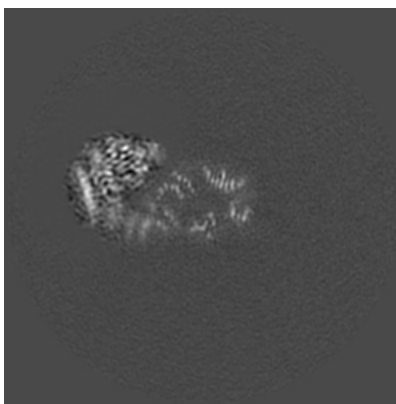
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

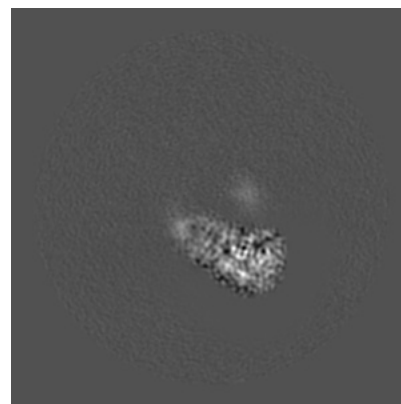
6.3.1 Primary map



X Index: 186



Y Index: 130

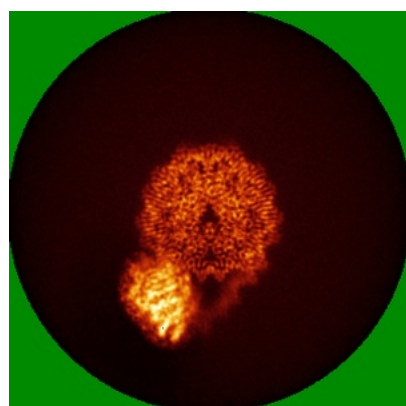


Z Index: 88

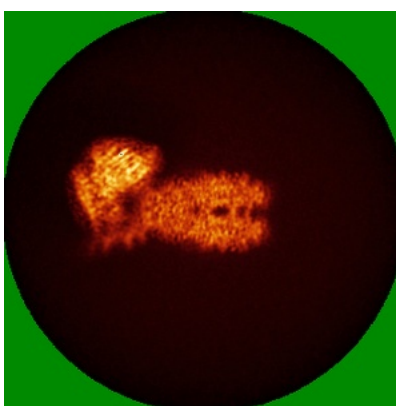
The images above show the largest variance slices of the map in three orthogonal directions.

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

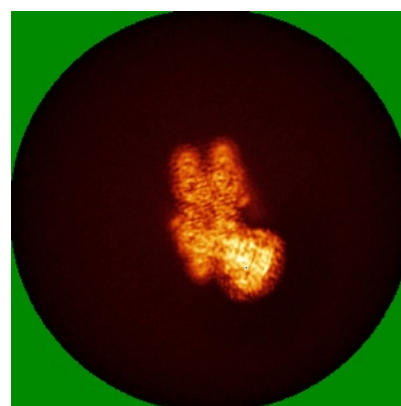
6.4.1 Primary map



X



Y

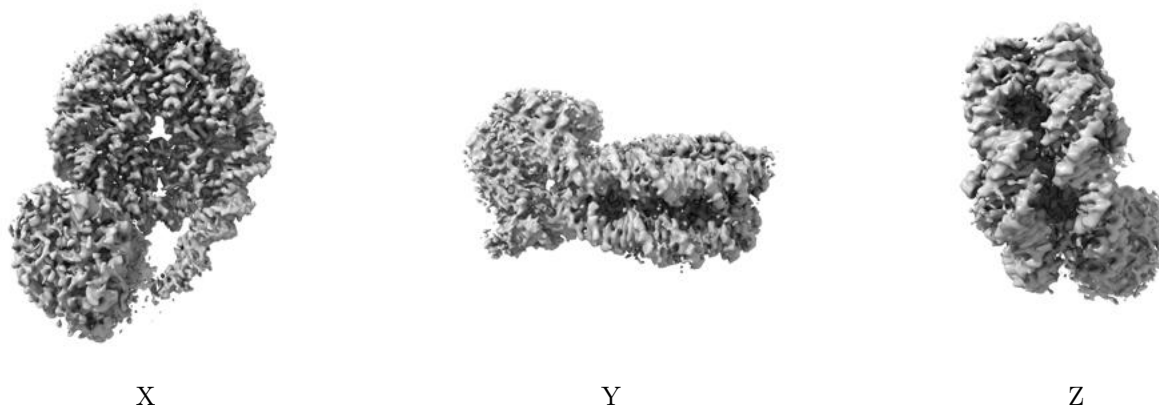


Z

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

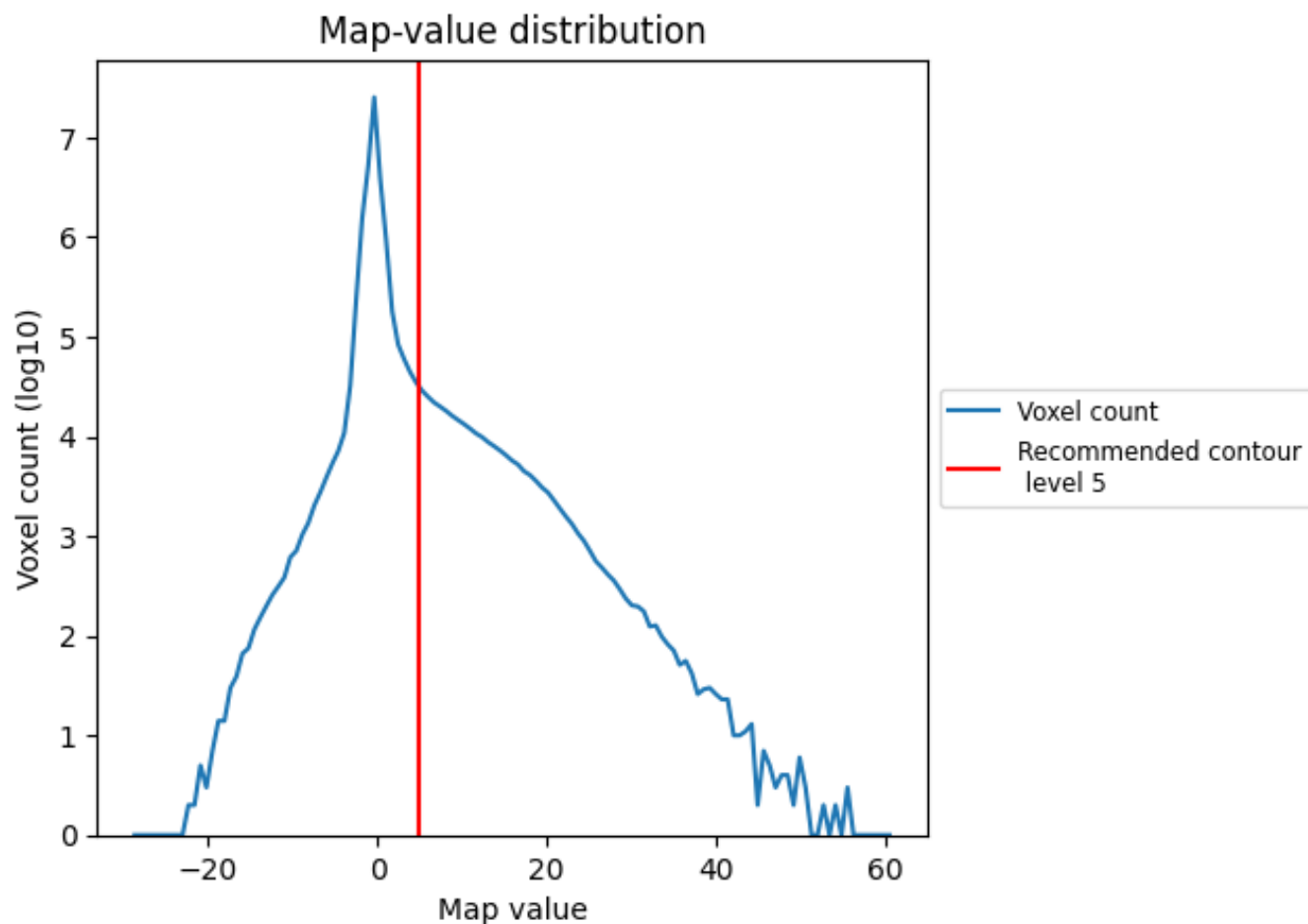
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

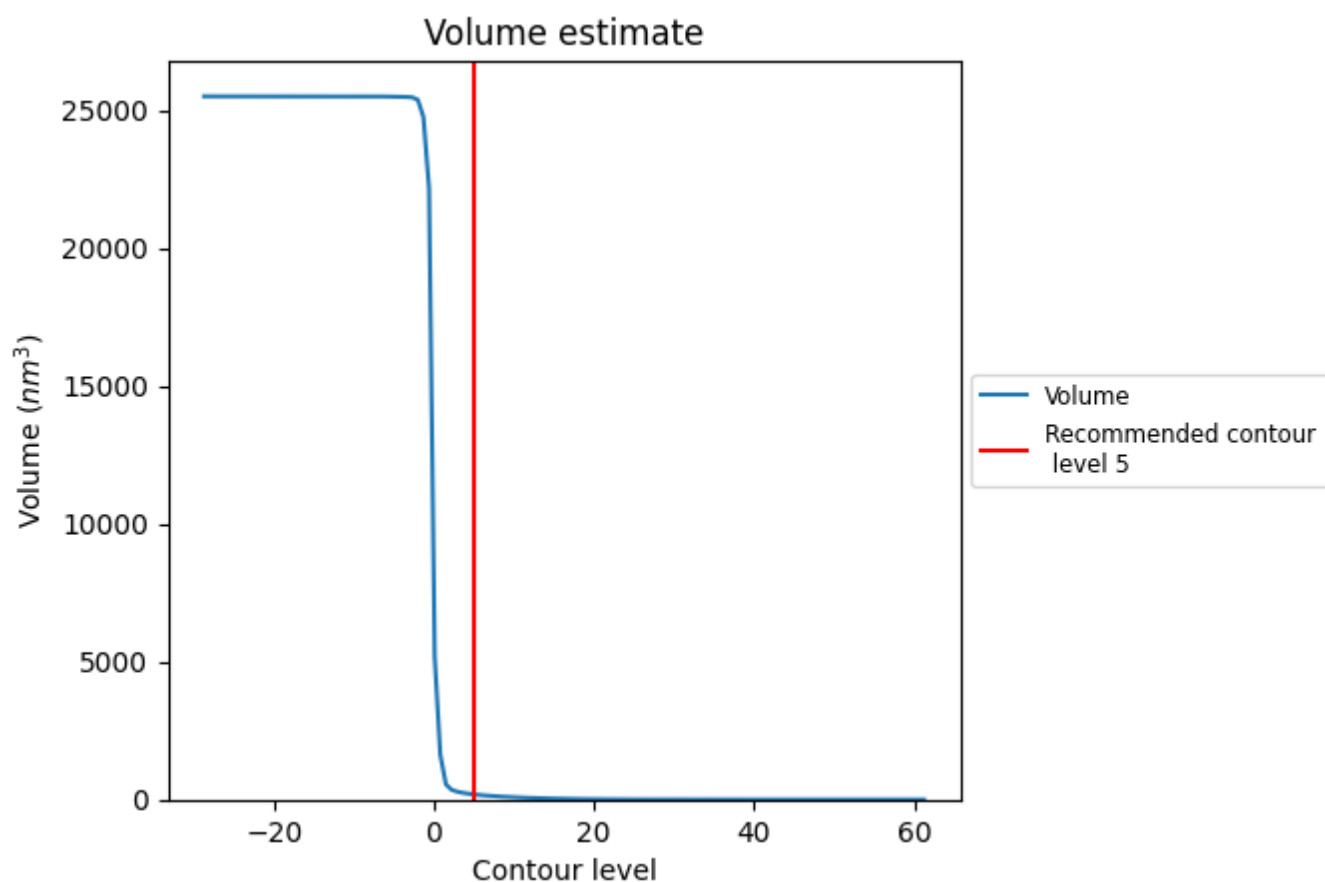
This section contains the results of statistical analysis of the map.

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.

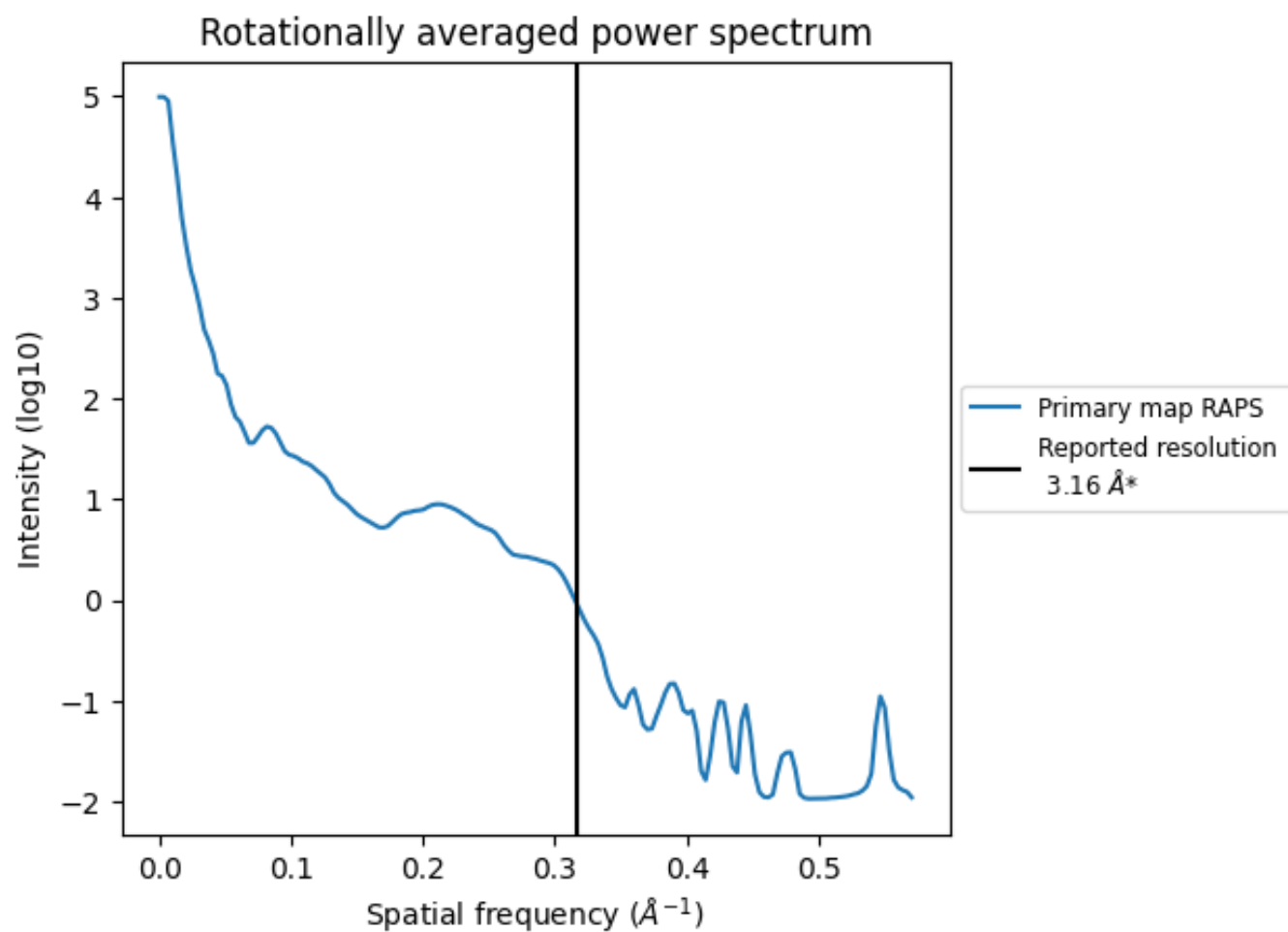
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm^3 ; this corresponds to an approximate mass of 169 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 0.316 \AA^{-1}

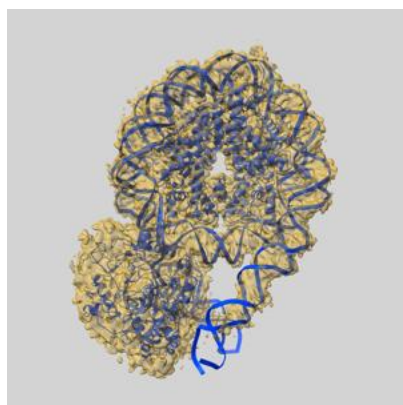
8 Fourier-Shell correlation

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

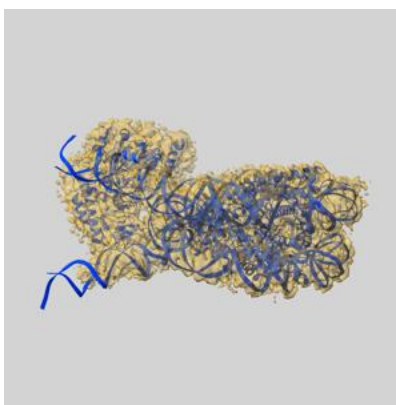
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49676 and PDB model 9NQU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

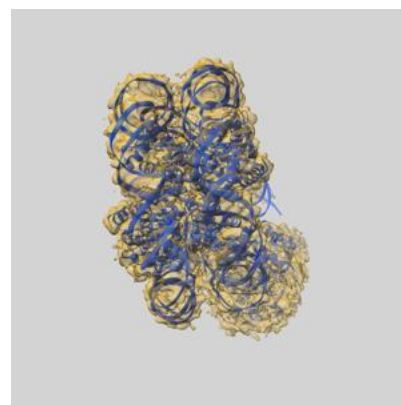
9.1 Map-model overlay [i](#)



X



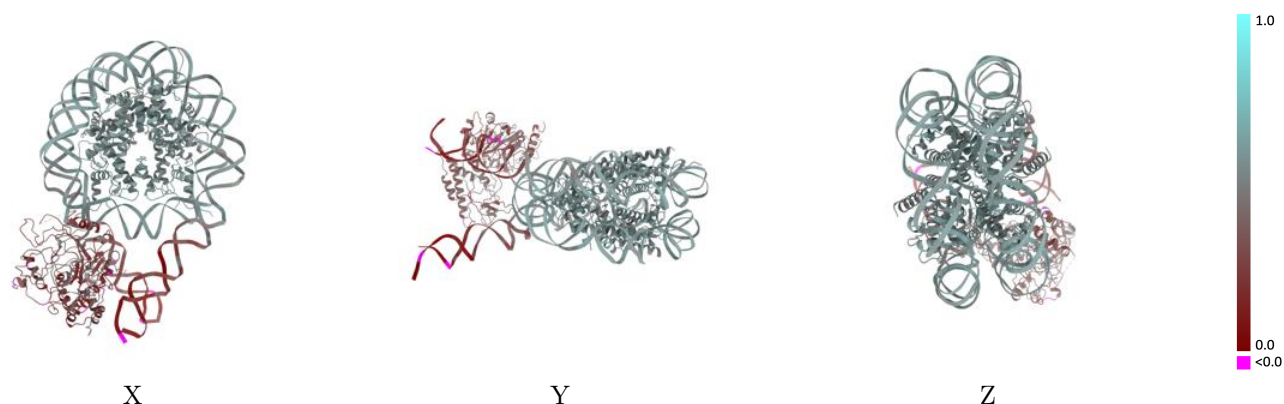
Y



Z

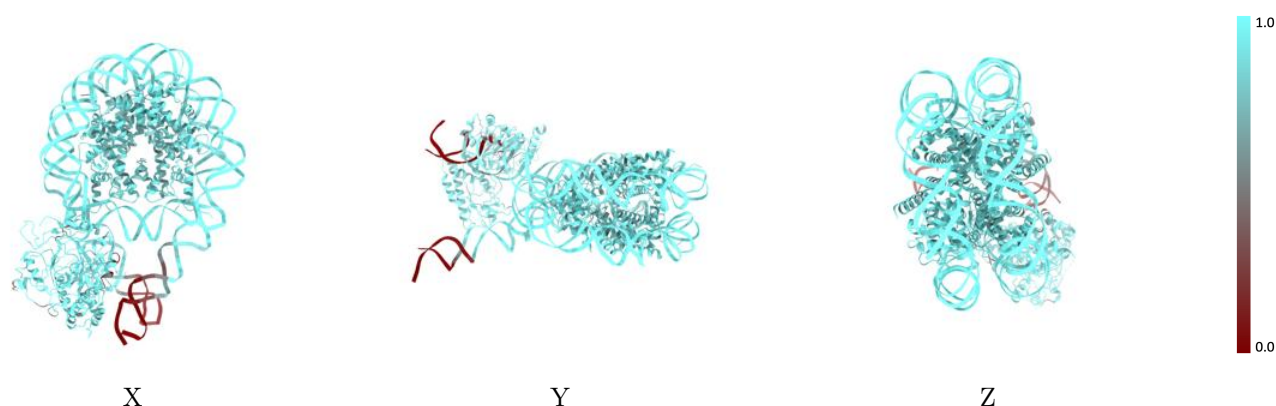
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



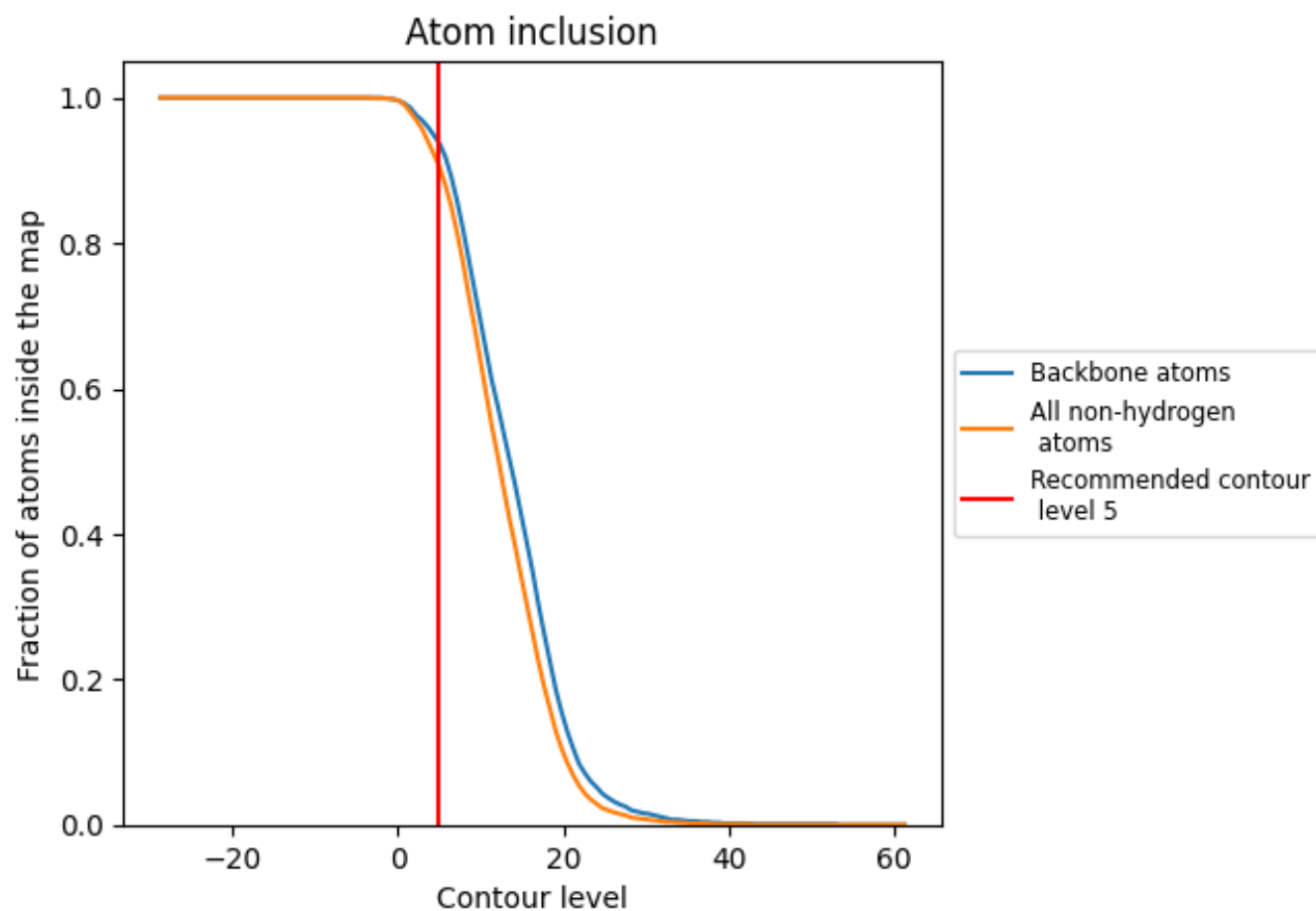
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9060	<div></div> 0.4700
A	<div></div> 0.9230	<div></div> 0.5630
B	<div></div> 0.9390	<div></div> 0.5720
C	<div></div> 0.9410	<div></div> 0.5650
D	<div></div> 0.9300	<div></div> 0.5480
E	<div></div> 0.8820	<div></div> 0.5240
F	<div></div> 0.9290	<div></div> 0.5720
G	<div></div> 0.9240	<div></div> 0.5600
H	<div></div> 0.9290	<div></div> 0.5540
I	<div></div> 0.8780	<div></div> 0.4730
J	<div></div> 0.8890	<div></div> 0.4790
K	<div></div> 0.9250	<div></div> 0.3130

1.0

0.0

<0.0