wwPDB EM Validation Summary Report ⓘ

Oct 28, 2026 – 06:13 PM JST

PDB ID	:	9M75 / pdb_00009m75
EMDB ID	:	EMD-63668
Title	:	Cryo-EM structure of human UHRF1 bound to mononucleosome with hemimethylated DNA at superhelical location -6.2.
Authors	:	Naschberger, A.; Baradaran, R.; Sayed, A.; Fischle, W.
Deposited on	:	2025-03-09
Resolution	:	2.80 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:

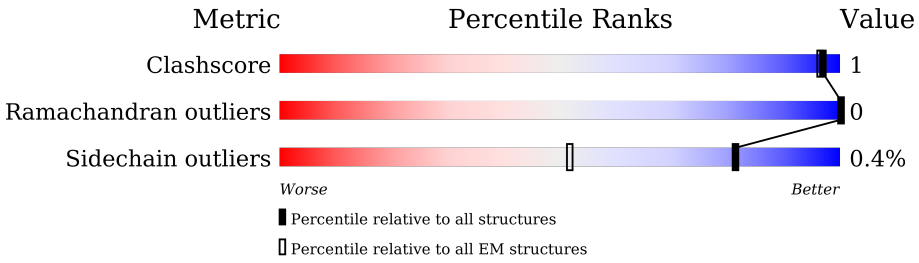
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

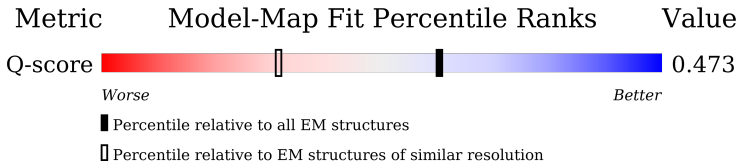
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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.





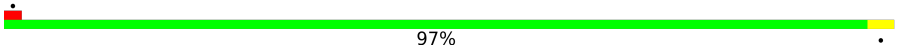
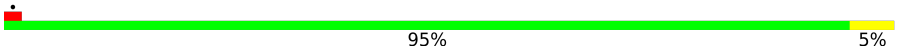
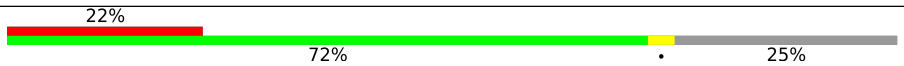
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	103	81% 19%
1	F	103	83% 17%
2	C	130	84% 16%
2	G	130	85% 15%

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Mol	Chain	Length	Quality of chain
3	D	126	
3	H	126	
4	A	136	
4	E	136	
5	I	144	
6	J	144	
7	K	793	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 31378 atoms, of which 14443 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 H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	83	Total	C	H	N	O	S	0	0
			1387	422	719	132	113	1		
1	F	86	Total	C	H	N	O	S	0	0
			1436	436	742	140	117	1		

- Molecule 2 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	109	Total	C	H	N	O	0	0
			1736	528	897	166	145		
2	G	111	Total	C	H	N	O	0	0
			1757	535	906	168	148		

- Molecule 3 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	97	Total	C	H	N	O	S	0	0
			1563	480	797	142	142	2		
3	H	96	Total	C	H	N	O	S	0	0
			1539	474	784	138	141	2		

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	99	Total	C	H	N	O	S	0	0
			1675	515	858	158	141	3		
4	A	108	Total	C	H	N	O	S	0	0
			1833	558	943	176	153	3		

- Molecule 5 is a DNA chain called DNA (144-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	144	Total	C	H	N	O	P	0	0
			4556	1395	1618	535	864	144		

- Molecule 6 is a DNA chain called DNA (144-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	144	Total	C	H	N	O	P	0	0
			4583	1404	1616	555	864	144		

- Molecule 7 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	596	Total	C	H	N	O	S	0	0
			9308	2945	4563	861	903	36		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	K	5	Total	Zn	0
			5	5	

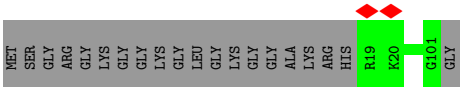
3 Residue-property plots (i)

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: Histone H4

Chain B:

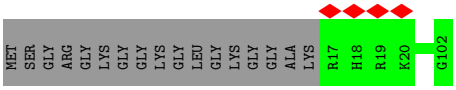




- Molecule 1: Histone H4

Chain F:

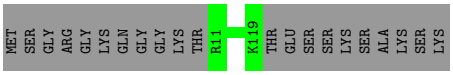




- Molecule 2: Histone H2A

Chain C:

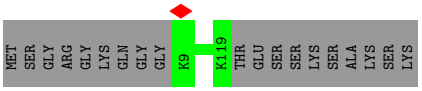




- Molecule 2: Histone H2A

Chain G:

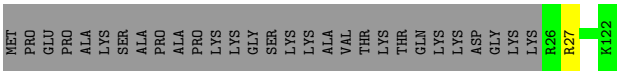




- Molecule 3: Histone H2B 1.1

Chain D:

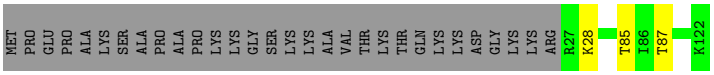




- Molecule 3: Histone H2B 1.1

Chain H:

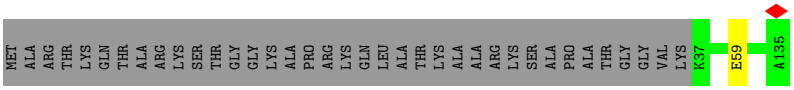




• Molecule 4: Histone H3

Chain E:

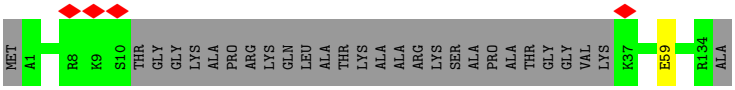




• Molecule 4: Histone H3

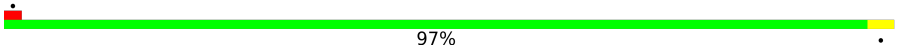
Chain A:

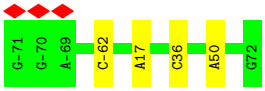




• Molecule 5: DNA (144-MER)

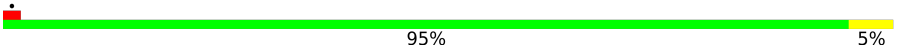
Chain I:

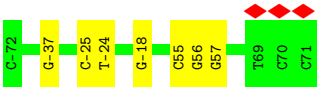




• Molecule 6: DNA (144-MER)

Chain J:





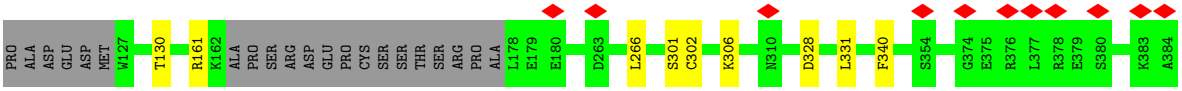
• Molecule 7: E3 ubiquitin-protein ligase UHRF1

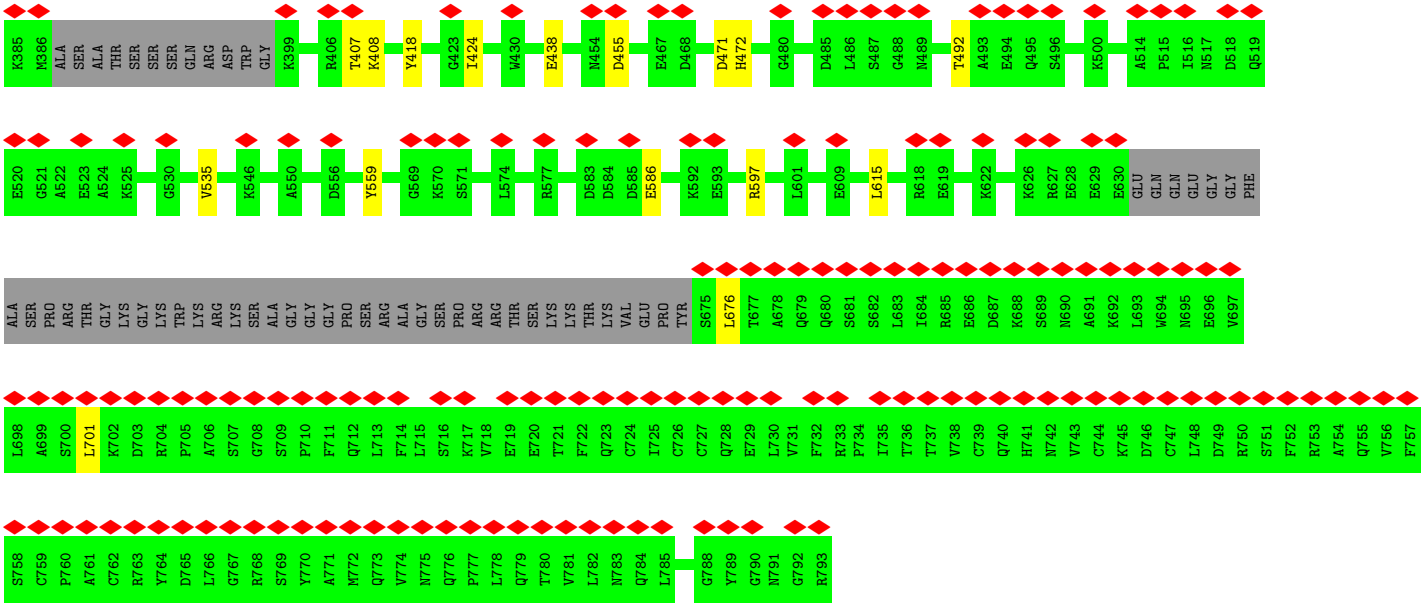
Chain K:










K385 M386 ALA SER ALA THR SER SER SER GLN ARG ASP TRP GLY K399 R406 T407 K408 Y418 G423 I424 W430 E438 N454 D455 E467 D468 D471 H472 G480 D485 L486 S487 G488 N489 T492 A493 E494 Q495 S496 K500 A514 P515 I516 N517 D518 Q519
E520 G521 A522 E523 A524 K525 G530 V535 K546 A550 D556 Y559 G569 K570 S571 L574 R577 D583 D584 D585 E586 K592 E593 R597 L601 E609 L615 R618 E619 K622 K626 R627 E628 E629 E630 GLU GLN GLN GLU GLY GLY PHE
ALA SER PRO ARG THR GLY LYS GLY LYS TRP LYS ARG LYS SER ALA GLY GLY GLY PRO SER ARG ALA GLY SER PRO ARG ARG THR SER LYS LYS THR LYS VAL GLU PRO TYR S675 L676 T677 A678 Q679 Q680 S681 S682 L683 I684 R685 E686 D687 K688 S689 N690 A691 K692 L693 W694 N695 E696 V697
L698 A699 S700 L701 K702 D703 R704 P705 A706 S707 G708 S709 P710 F711 Q712 L713 F714 L715 S716 K717 V718 E719 E720 T721 F722 Q723 C724 I725 C726 C727 Q728 E729 L730 V731 F732 R733 P734 I735 T736 T737 V738 C739 Q740 H741 N742 V743 C744 K745 D746 C747 L748 D749 R750 S751 F752 R753 A754 Q755 V756 F757
S758 C759 P760 A761 C762 R763 Y764 D765 L766 G767 R768 S769 Y770 A771 M772 Q773 V774 N775 Q776 P777 L778 Q779 T780 V781 L782 N783 Q784 L785 G788 Y789 G790 N791 G792 R793

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	603891	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	39.201	Depositor
Minimum map value	-12.972	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.014	Depositor
Recommended contour level	3.54	Depositor
Map size (Å)	279.93597, 279.93597, 279.93597	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7289999, 0.7289999, 0.7289999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5CM, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.12	0/675	0.28	0/903
1	F	0.12	0/702	0.26	0/937
2	C	0.13	0/849	0.27	0/1145
2	G	0.13	0/861	0.25	0/1162
3	D	0.11	0/777	0.26	0/1041
3	H	0.12	0/766	0.25	0/1027
4	A	0.13	0/901	0.25	0/1205
4	E	0.12	0/829	0.26	0/1111
5	I	0.71	0/3269	0.88	0/5037
6	J	0.69	0/3331	0.86	0/5143
7	K	0.11	0/4844	0.32	0/6539
All	All	0.44	0/17804	0.59	0/25250

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	B	668	719	719	0	0
1	F	694	742	742	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	839	897	897	0	0
2	G	851	906	906	0	0
3	D	766	797	797	1	0
3	H	755	784	784	1	0
4	A	890	943	944	1	0
4	E	817	858	858	1	0
5	I	2938	1618	1618	4	0
6	J	2967	1616	1616	5	0
7	K	4745	4563	4560	13	0
8	K	5	0	0	0	0
All	All	16935	14443	14441	22	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 1.

The worst 5 of 22 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:586:GLU:OE1	7:K:597:ARG:NH2	2.33	0.62
4:A:59:GLU:OE1	4:A:59:GLU:N	2.38	0.54
3:D:27:ARG:NH2	5:I:50:DA:N3	2.57	0.53
5:I:36:DC:N4	6:J:-37:DG:O6	2.42	0.52
7:K:302:CYS:O	7:K:306:LYS:N	2.42	0.51

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	81/103 (79%)	81 (100%)	0	0	100	100
1	F	84/103 (82%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	107/130 (82%)	107 (100%)	0	0	100	100
2	G	109/130 (84%)	109 (100%)	0	0	100	100
3	D	95/126 (75%)	93 (98%)	2 (2%)	0	100	100
3	H	94/126 (75%)	93 (99%)	1 (1%)	0	100	100
4	A	104/136 (76%)	104 (100%)	0	0	100	100
4	E	97/136 (71%)	96 (99%)	1 (1%)	0	100	100
7	K	588/793 (74%)	574 (98%)	14 (2%)	0	100	100
All	All	1359/1783 (76%)	1341 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	69/79 (87%)	69 (100%)	0	100	100
1	F	71/79 (90%)	71 (100%)	0	100	100
2	C	85/102 (83%)	85 (100%)	0	100	100
2	G	86/102 (84%)	86 (100%)	0	100	100
3	D	83/106 (78%)	83 (100%)	0	100	100
3	H	82/106 (77%)	81 (99%)	1 (1%)	63	87
4	A	94/111 (85%)	94 (100%)	0	100	100
4	E	86/111 (78%)	86 (100%)	0	100	100
7	K	512/687 (74%)	508 (99%)	4 (1%)	73	90
All	All	1168/1483 (79%)	1163 (100%)	5 (0%)	81	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	28	LYS

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Mol	Chain	Res	Type
7	K	266	LEU
7	K	408	LYS
7	K	676	LEU
7	K	701	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	92	GLN
3	H	81	ASN
7	K	679	GLN
7	K	784	GLN
7	K	791	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
5	5CM	I	-62	5	17,21,22	0.12	0	24,30,33	0.41	0

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
5	5CM	I	-62	5	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	-62	5CM	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

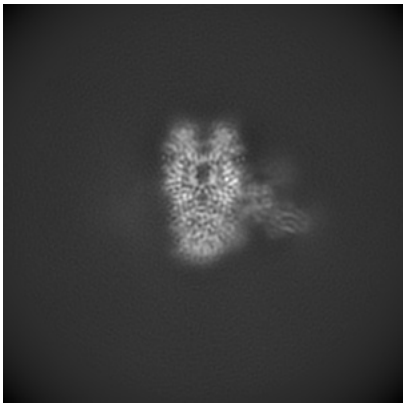
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-63668. These allow visual inspection of the internal detail of the map and identification of artifacts.

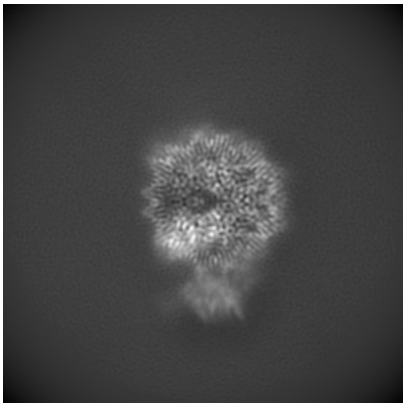
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

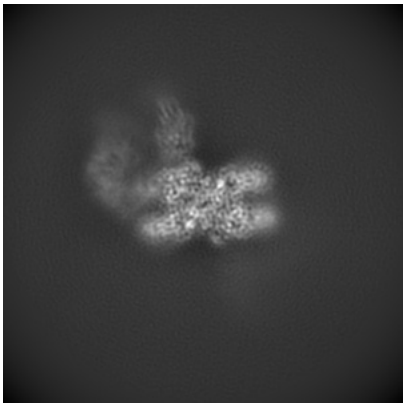
6.1.1 Primary map



X



Y

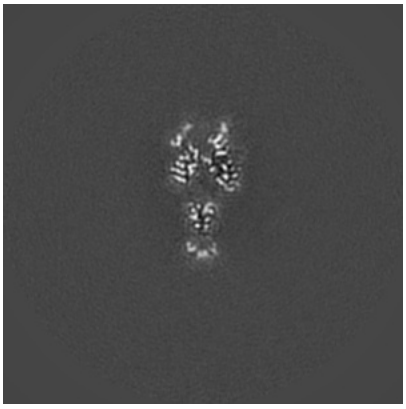


Z

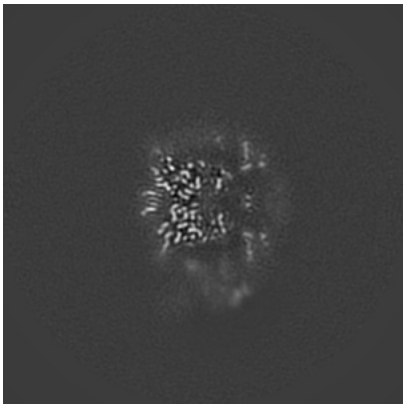
The images above show the map projected in three orthogonal directions.

6.2 Central slices

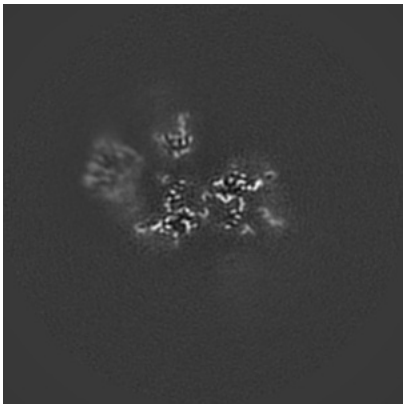
6.2.1 Primary map



X Index: 192



Y Index: 192

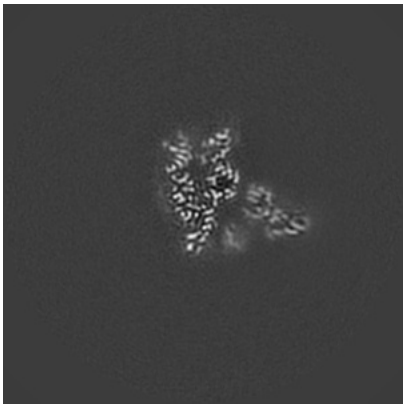


Z Index: 192

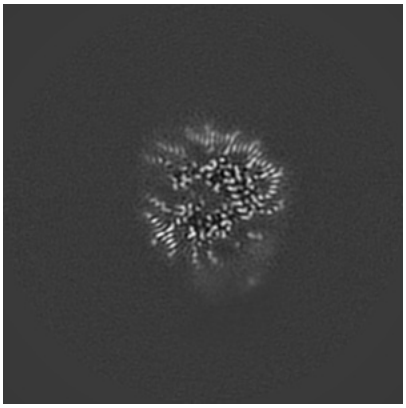
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

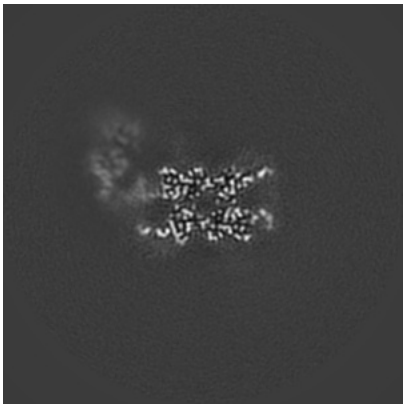
6.3.1 Primary map



X Index: 162



Y Index: 179



Z Index: 214

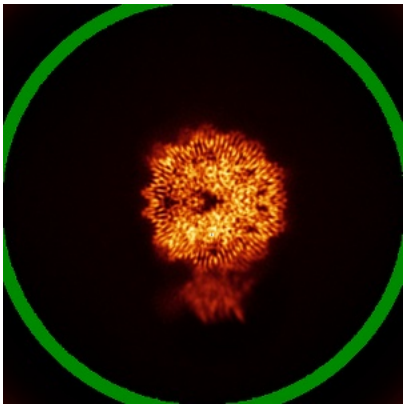
The images above show the largest variance slices of the map in three orthogonal directions.

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

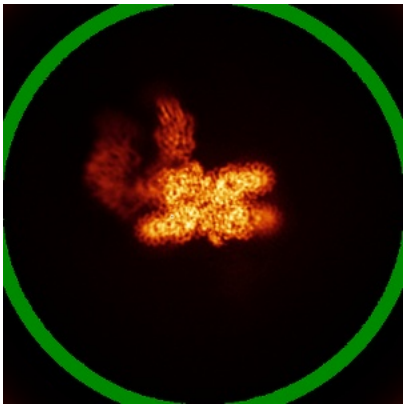
6.4.1 Primary map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.54. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

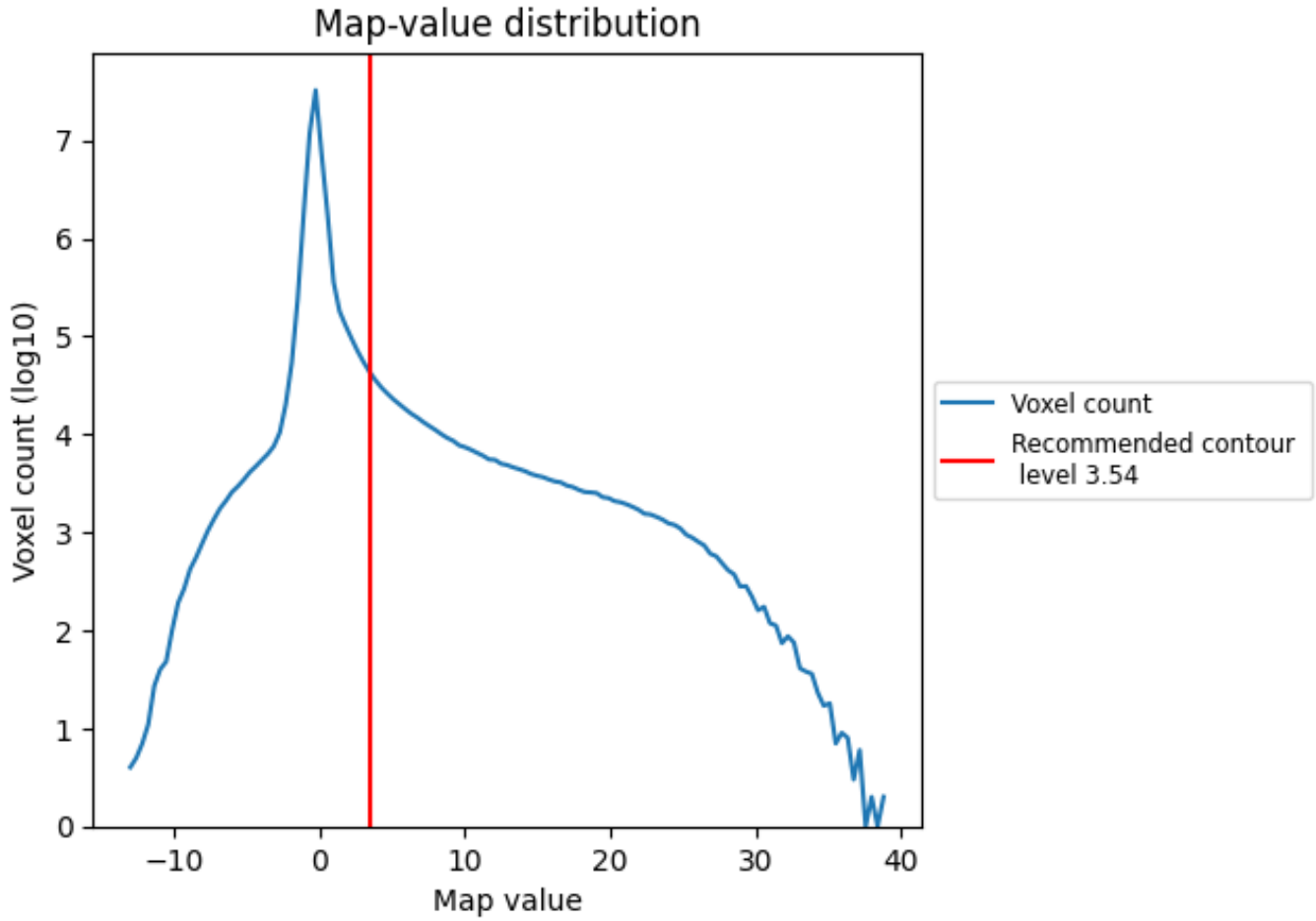
6.6 Mask visualisation (i)

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

7 Map analysis

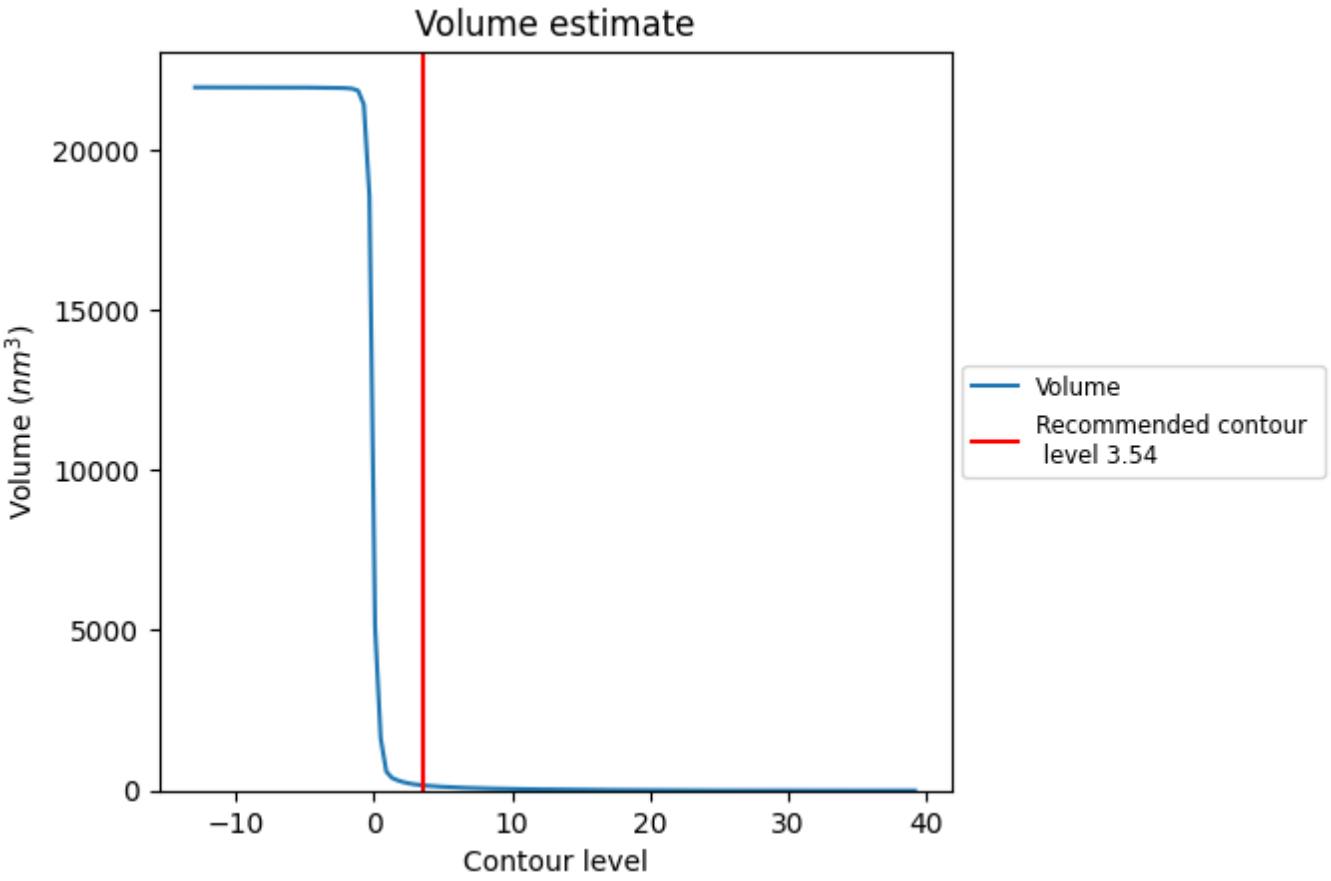
This section contains the results of statistical analysis of the map.

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.

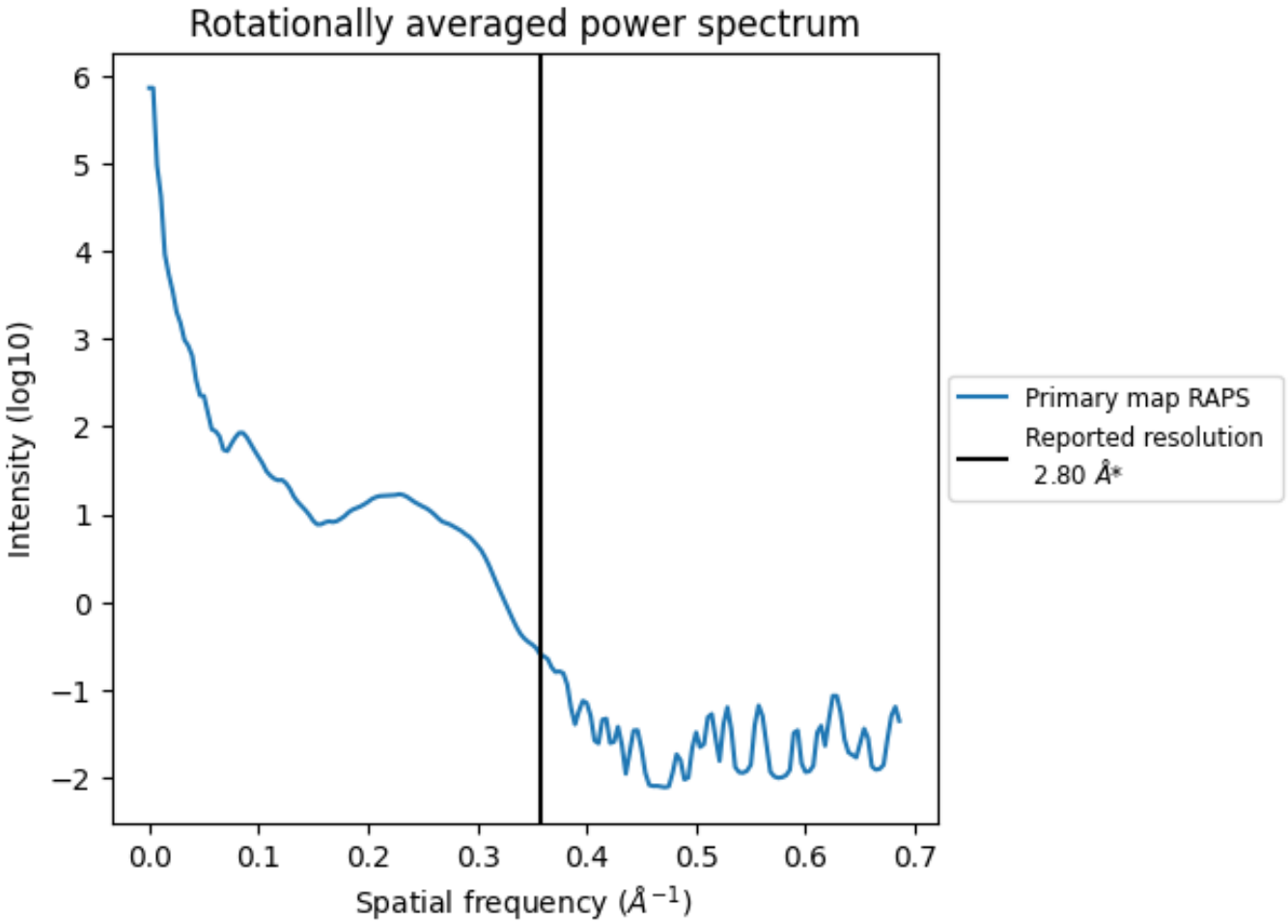
7.2 Volume estimate (i)



The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 148 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 0.357 Å^{-1}

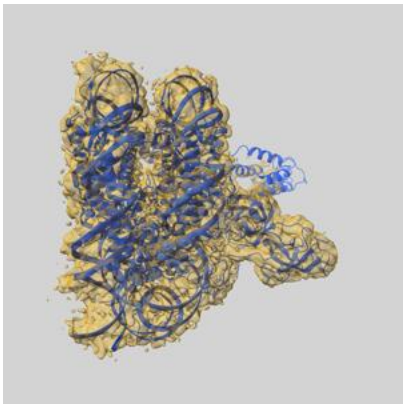
8 Fourier-Shell correlation (i)

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

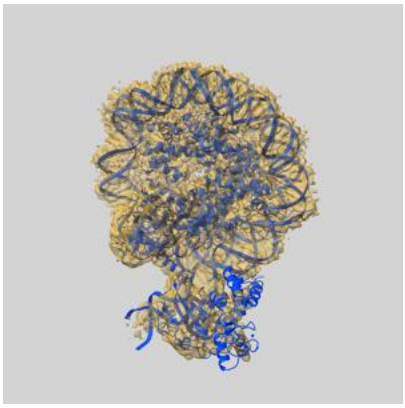
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63668 and PDB model 9M75. Per-residue inclusion information can be found in section 3 on page 6.

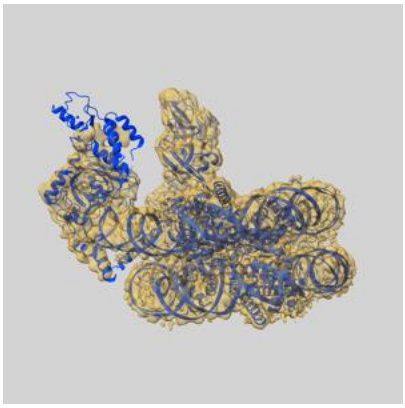
9.1 Map-model overlay



X



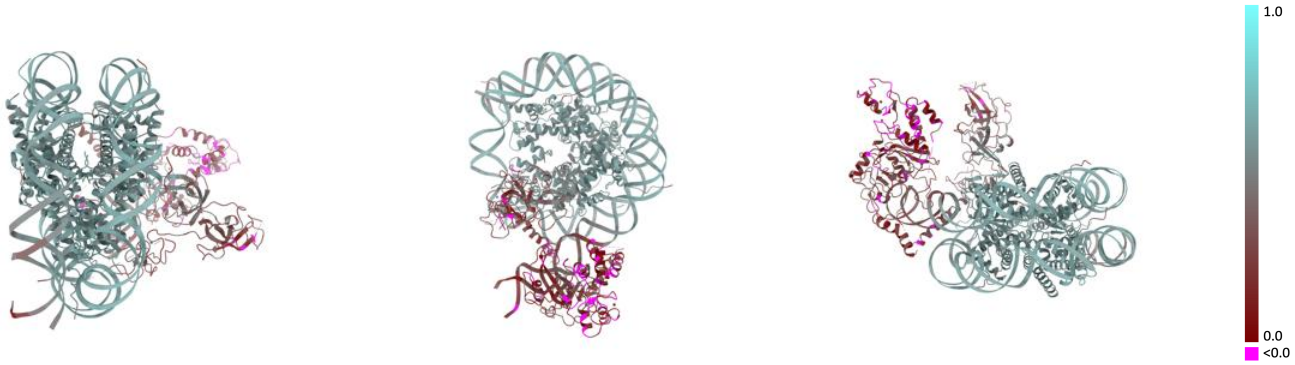
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.54 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.

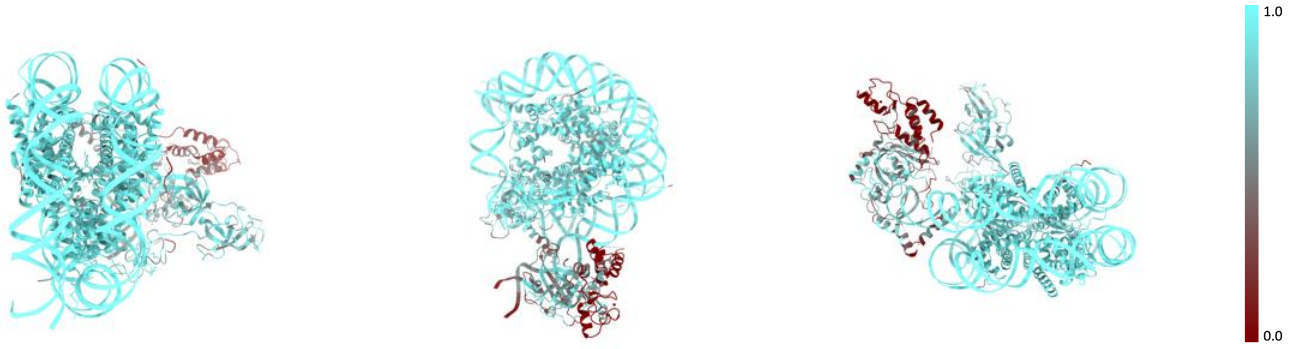
9.2 Q-score mapped to coordinate model



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.

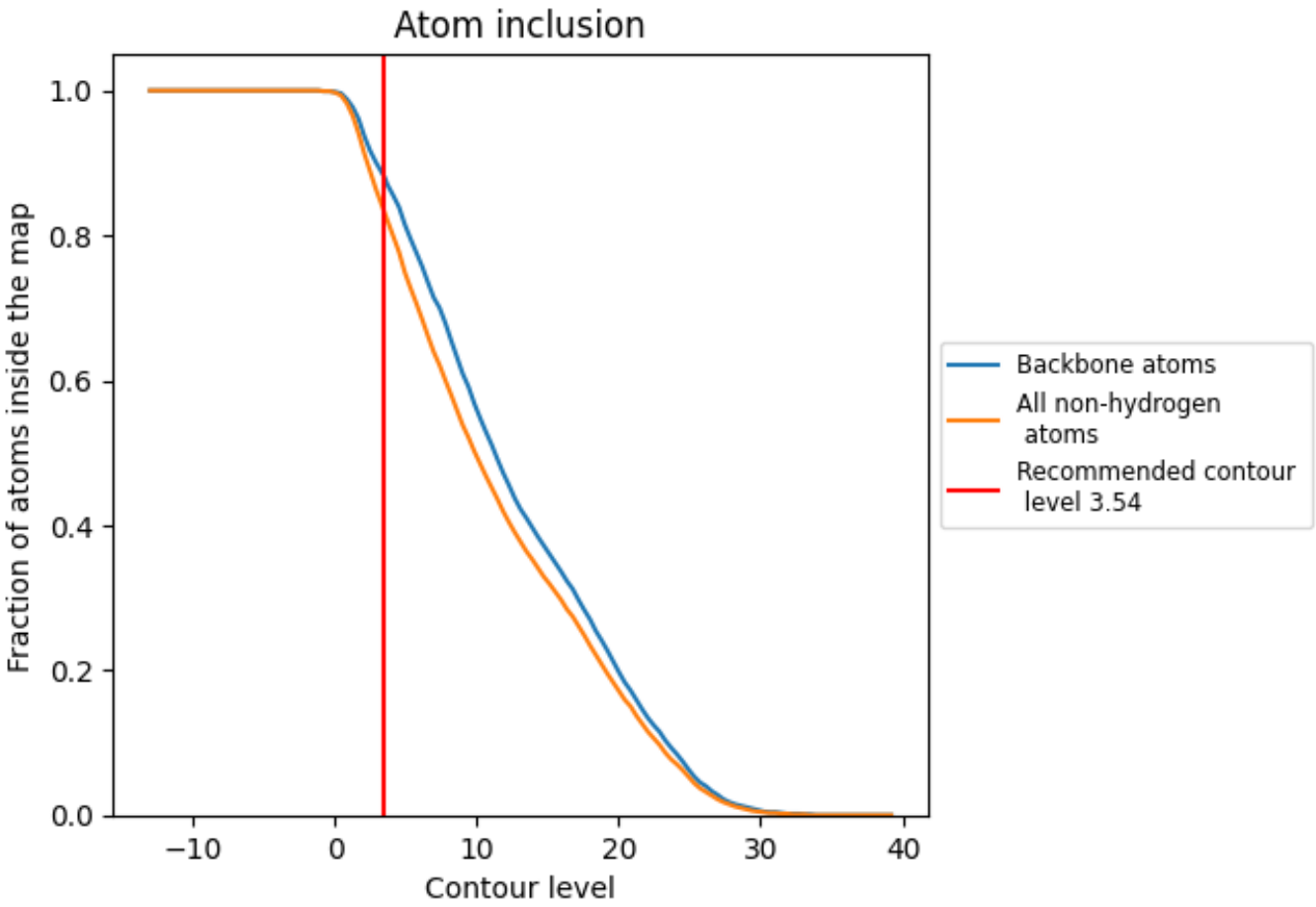
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (3.54).

9.4 Atom inclusion (i)



At the recommended contour level, 88% 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 (3.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8310	0.4730
A	0.9460	0.5680
B	0.9580	0.5880
C	0.9700	0.6010
D	0.9730	0.5850
E	0.9810	0.5960
F	0.9290	0.5890
G	0.9590	0.5800
H	0.9660	0.5800
I	0.9560	0.5530
J	0.9690	0.5510
K	0.5900	0.2260

