



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 06:14 AM UTC

PDB ID : 8OF4 / pdb\_00008of4  
EMDB ID : EMD-16845  
Title : Nucleosome Bound human SIRT6 (Composite)  
Authors : Smirnova, E.; Bignon, E.; Schultz, P.; Papai, G.; Ben-Shem, A.  
Deposited on : 2023-03-13  
Resolution : 2.94 Å(reported)  
Based on initial models : 3LZ0, 5X16

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

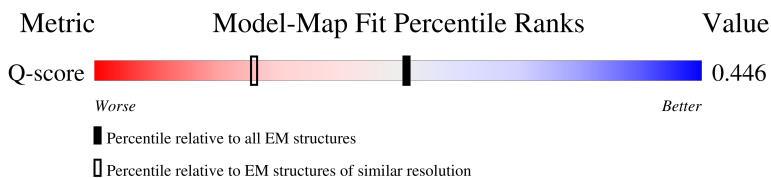
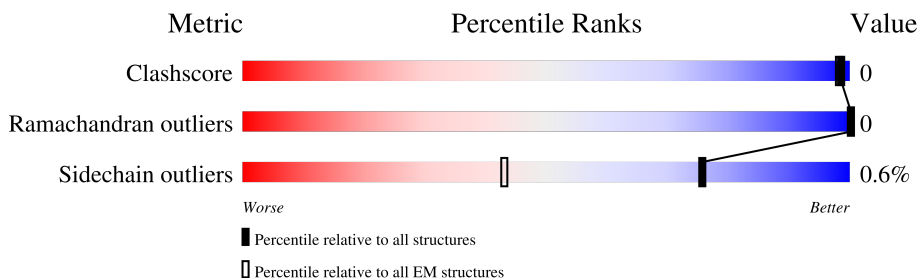
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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  $\geq 3$ , 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	136	69% (with 5% red bar above)
1	E	136	68% (with 5% red bar above)
2	B	103	80% (with 5% red bar above)
2	F	103	83% (with 8% red bar above)

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Mol	Chain	Length	Quality of chain
3	C	130	<p>10% 88% 8%</p>
3	G	130	<p>1% 82% 17%</p>
4	D	126	<p>5% 76% 21%</p>
4	H	126	<p>6% 77% 21%</p>
5	I	145	<p>6% 61% 37% 6%</p>
6	J	145	<p>7% 65% 28% 7%</p>
7	L	355	<p>22% 64% 33%</p>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14087 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
			Total	C	N	O	S		
1	A	98	807	508	156	140	3	0	0
1	E	98	807	508	156	140	3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	83	662	418	129	114	1	0	0
2	F	87	703	442	142	118	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	120	916	573	181	162	0	0
3	G	108	832	525	163	144	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	99	785	493	146	144	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	99	Total	C	N	O	S	0	0
			785	493	146	144	2		

- Molecule 5 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	145	Total	C	N	O	P	0	0
			2952	1404	537	867	144		

- Molecule 6 is a DNA chain called DNA (145-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	P	0	0
			2987	1416	558	869	144		

- Molecule 7 is a protein called NAD-dependent protein deacylase sirtuin-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	237	Total	C	N	O	S	0	0
			1850	1153	350	338	9		

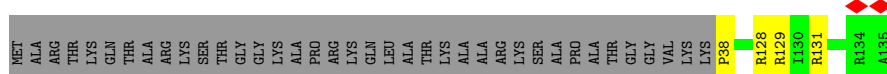
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	L	1	Total	Zn	0
			1	1	

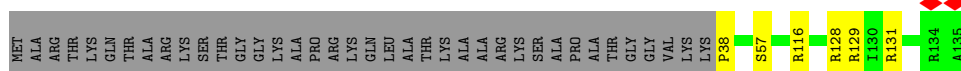
### 3 Residue-property plots [i](#)

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.

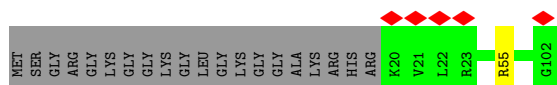
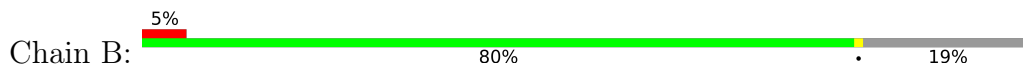
- Molecule 1: Histone H3.2



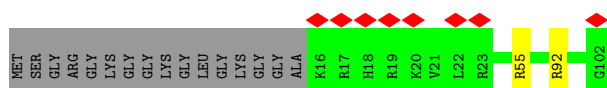
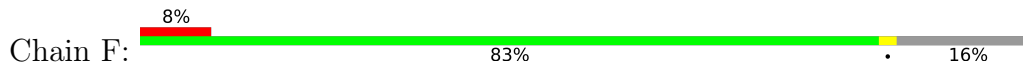
- Molecule 1: Histone H3.2



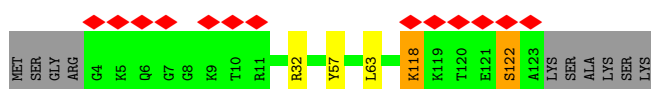
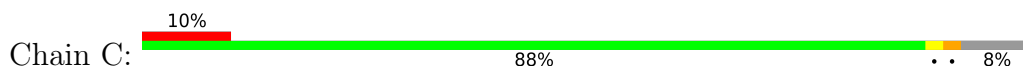
- Molecule 2: Histone H4



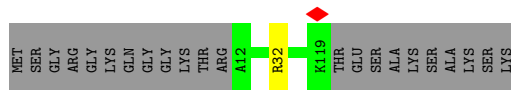
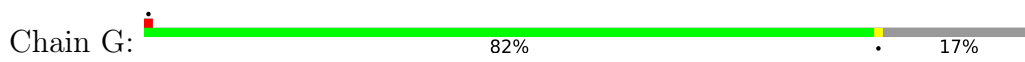
- Molecule 2: Histone H4



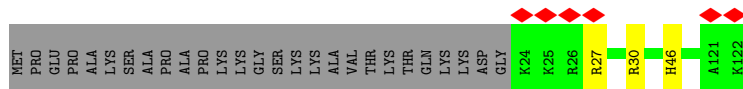
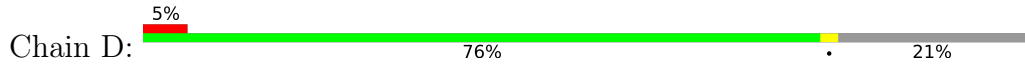
- Molecule 3: Histone H2A type 1



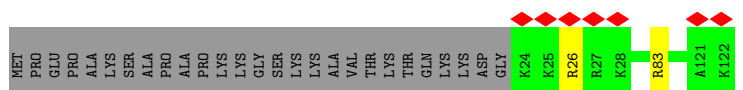
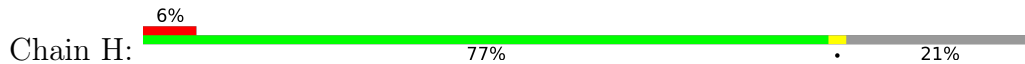
• Molecule 3: Histone H2A type 1



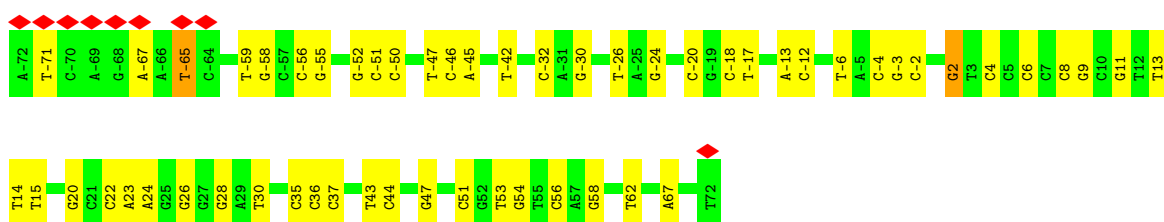
• Molecule 4: Histone H2B



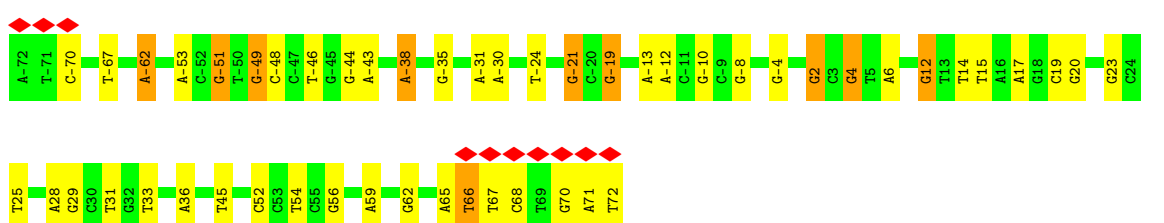
• Molecule 4: Histone H2B



• Molecule 5: DNA (145-MER)

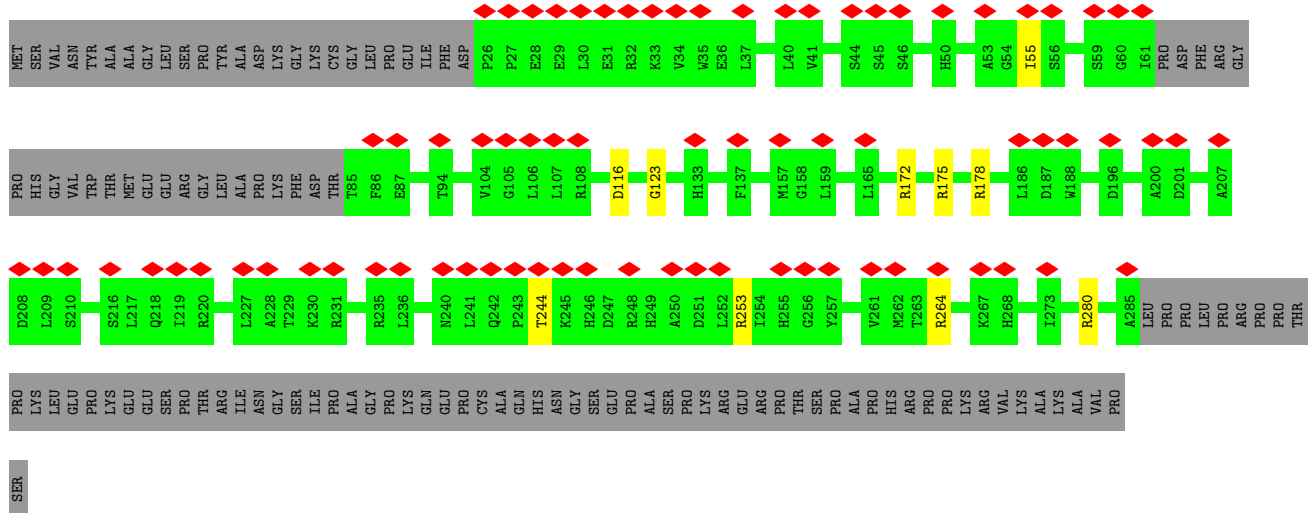


• Molecule 6: DNA (145-MER)



• Molecule 7: NAD-dependent protein deacylase sirtuin-6





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	439796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS, TFS KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50, 55	Depositor
Minimum defocus (nm)	1200, 1200	Depositor
Maximum defocus (nm)	2600, 2600	Depositor
Magnification	270000, 180000	Depositor
Image detector	FEI FALCON IV (4k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.603	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.28	Depositor
Map size ( $\text{\AA}$ )	205.184, 205.184, 205.184	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.916, 0.916, 0.916	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

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	0.80	0/819	1.31	3/1097 (0.3%)
1	E	0.76	0/819	1.32	5/1097 (0.5%)
2	B	0.78	0/669	1.31	1/894 (0.1%)
2	F	0.81	0/711	1.32	1/948 (0.1%)
3	C	0.80	0/926	2.09	8/1245 (0.6%)
3	G	0.76	0/842	1.32	1/1135 (0.1%)
4	D	0.74	0/796	1.31	3/1065 (0.3%)
4	H	0.76	0/796	1.32	1/1065 (0.1%)
5	I	0.76	2/3308 (0.1%)	1.33	11/5099 (0.2%)
6	J	0.71	0/3354	1.33	15/5180 (0.3%)
7	L	0.82	0/1881	1.39	8/2542 (0.3%)
All	All	0.76	2/14921 (0.0%)	1.39	57/21367 (0.3%)

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
1	A	0	1
3	C	0	3
4	H	0	1
5	I	0	43
6	J	0	45
7	L	0	1
All	All	0	94

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	-65	DT	C5-C7	15.86	1.82	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	-59	DT	C5-C7	8.09	1.66	1.50

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	118	LYS	O-C-N	-49.62	60.44	122.96
3	C	122	SER	O-C-N	-20.01	95.03	122.04
1	E	38	PRO	CA-N-CD	-8.01	100.79	112.00
3	C	118	LYS	CA-C-O	-7.71	112.88	121.51
3	C	122	SER	CA-C-N	7.21	134.68	121.70

There are no chirality outliers.

5 of 94 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
3	C	118	LYS	Mainchain
3	C	122	SER	Mainchain
3	C	57	TYR	Sidechain
4	H	83	ARG	Sidechain

## 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	807	0	844	0	0
1	E	807	0	844	0	0
2	B	662	0	709	0	0
2	F	703	0	755	0	0
3	C	916	0	981	0	0
3	G	832	0	895	0	0
4	D	785	0	825	0	0
4	H	785	0	825	0	0
5	I	2952	0	1629	4	0
6	J	2987	0	1630	1	0
7	L	1850	0	1880	1	0
8	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14087	0	11817	5	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 0.

All (5) 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:I:-65:DT:C5	5:I:-65:DT:C7	1.82	1.62
5:I:-65:DT:C7	5:I:-65:DT:C6	2.76	0.52
5:I:-65:DT:C7	5:I:-65:DT:C4	2.83	0.41
7:L:123:GLY:HA3	7:L:280:ARG:HB3	2.02	0.41
5:I:62:DT:H3	6:J:-62:DA:H61	1.69	0.40

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	96/136 (71%)	96 (100%)	0	0	100	100
1	E	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
2	B	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
2	F	85/103 (82%)	84 (99%)	1 (1%)	0	100	100
3	C	118/130 (91%)	111 (94%)	7 (6%)	0	100	100
3	G	106/130 (82%)	102 (96%)	4 (4%)	0	100	100
4	D	97/126 (77%)	94 (97%)	3 (3%)	0	100	100
4	H	97/126 (77%)	94 (97%)	3 (3%)	0	100	100
7	L	233/355 (66%)	218 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1009/1345 (75%)	973 (96%)	36 (4%)	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	A	85/111 (77%)	85 (100%)	0	100	100
1	E	85/111 (77%)	84 (99%)	1 (1%)	63	78
2	B	68/79 (86%)	68 (100%)	0	100	100
2	F	72/79 (91%)	71 (99%)	1 (1%)	59	76
3	C	93/101 (92%)	92 (99%)	1 (1%)	65	80
3	G	85/101 (84%)	85 (100%)	0	100	100
4	D	85/106 (80%)	85 (100%)	0	100	100
4	H	85/106 (80%)	85 (100%)	0	100	100
7	L	199/298 (67%)	197 (99%)	2 (1%)	68	81
All	All	857/1092 (78%)	852 (99%)	5 (1%)	76	89

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

Mol	Chain	Res	Type
3	C	63	LEU
1	E	57	SER
2	F	92	ARG
7	L	55	ILE
7	L	244	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	L	246	HIS
7	L	133	HIS
7	L	93	GLN
3	G	104	GLN
7	L	113	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 1 ligands modelled in this entry, 1 is 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.

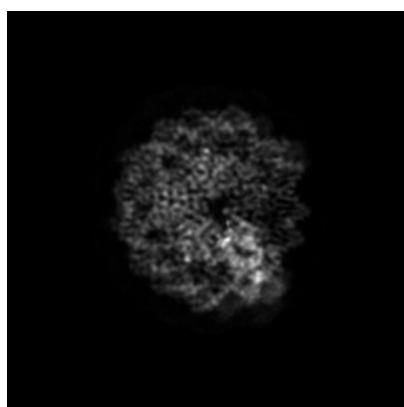
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16845. These allow visual inspection of the internal detail of the map and identification of artifacts.

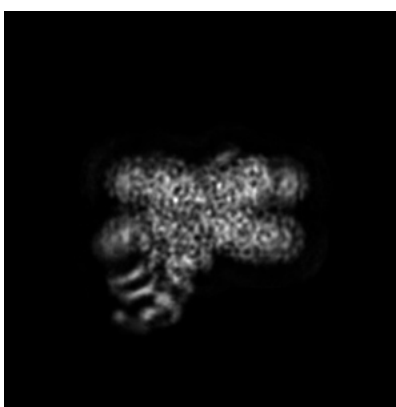
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

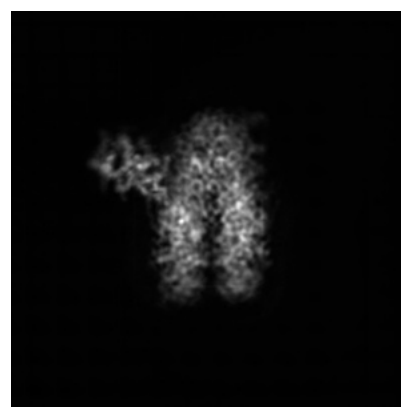
#### 6.1.1 Primary map



X



Y

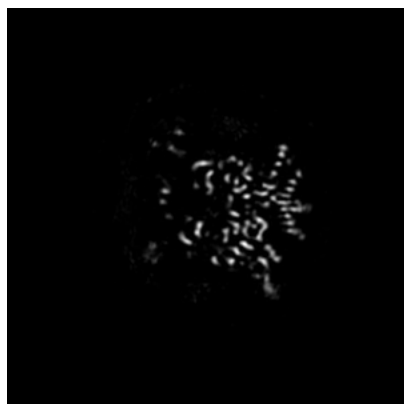


Z

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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 112



Y Index: 112

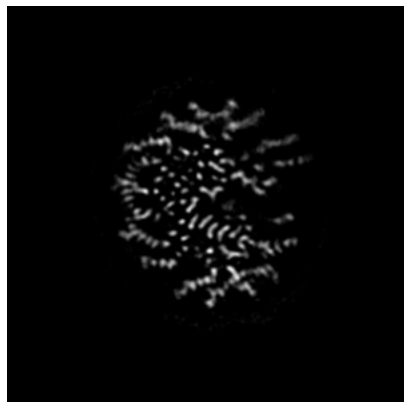


Z Index: 112

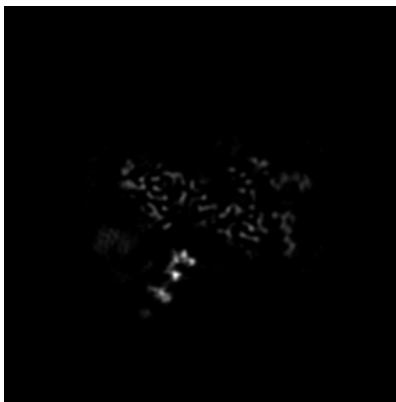
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

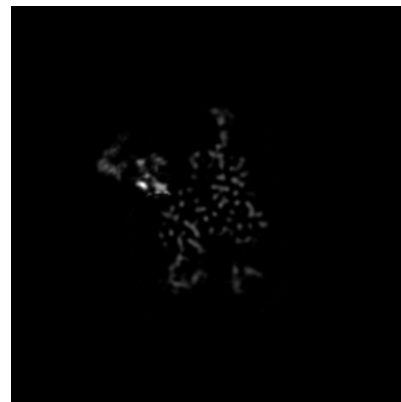
### 6.3.1 Primary map



X Index: 126



Y Index: 124

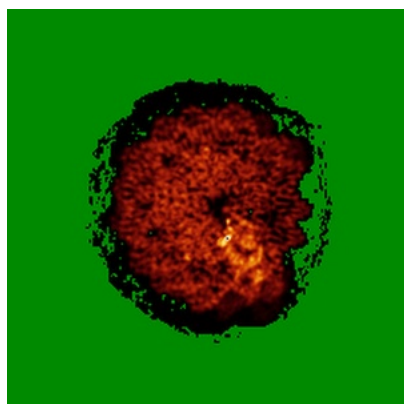


Z Index: 95

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

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

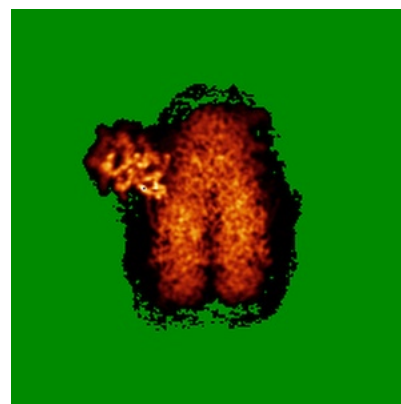
### 6.4.1 Primary map



X



Y

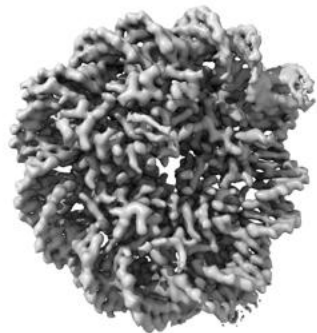


Z

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](#)

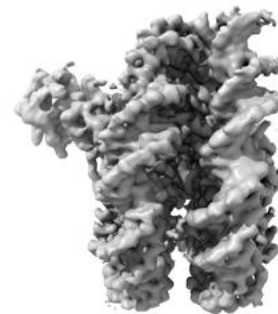
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

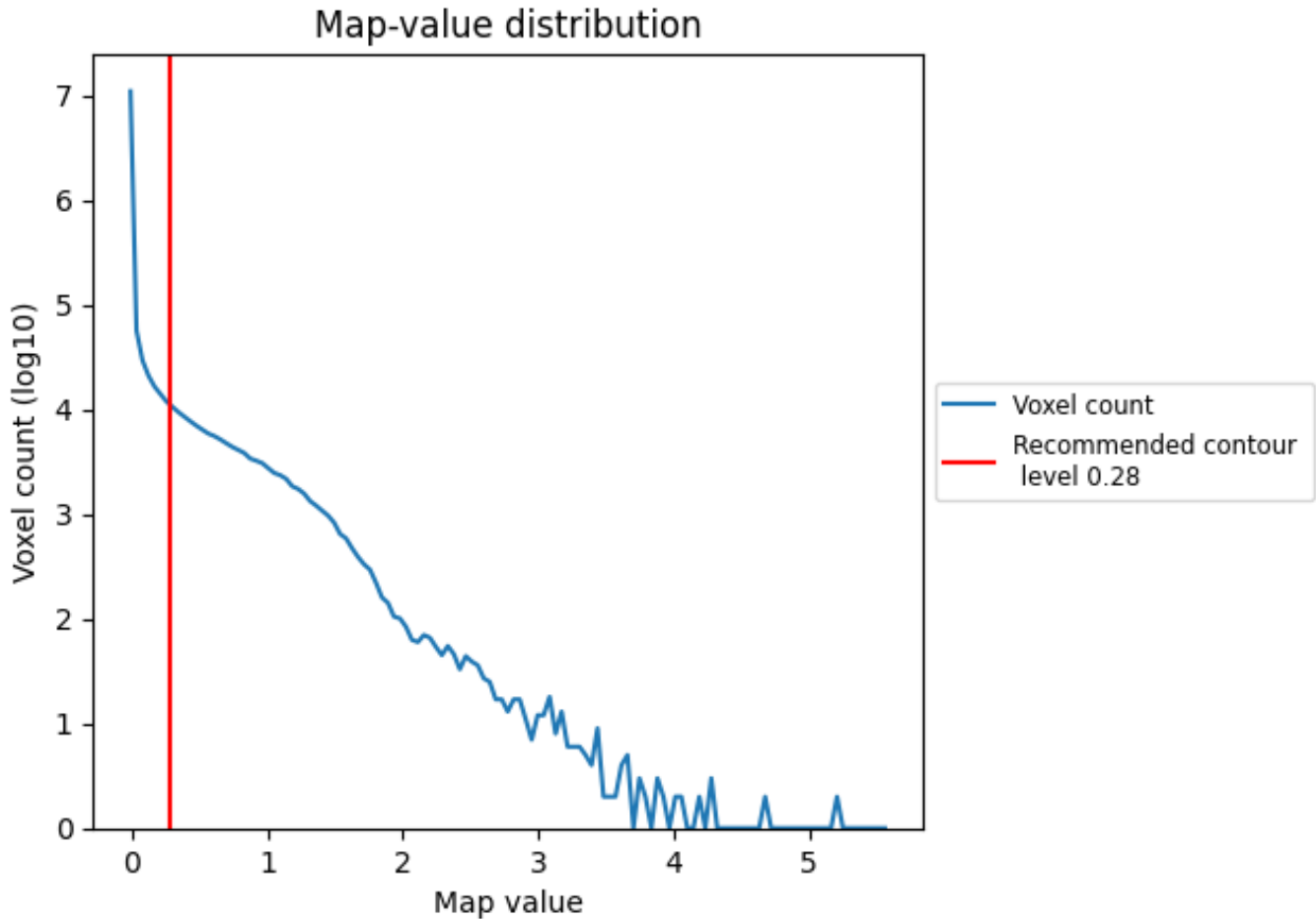
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

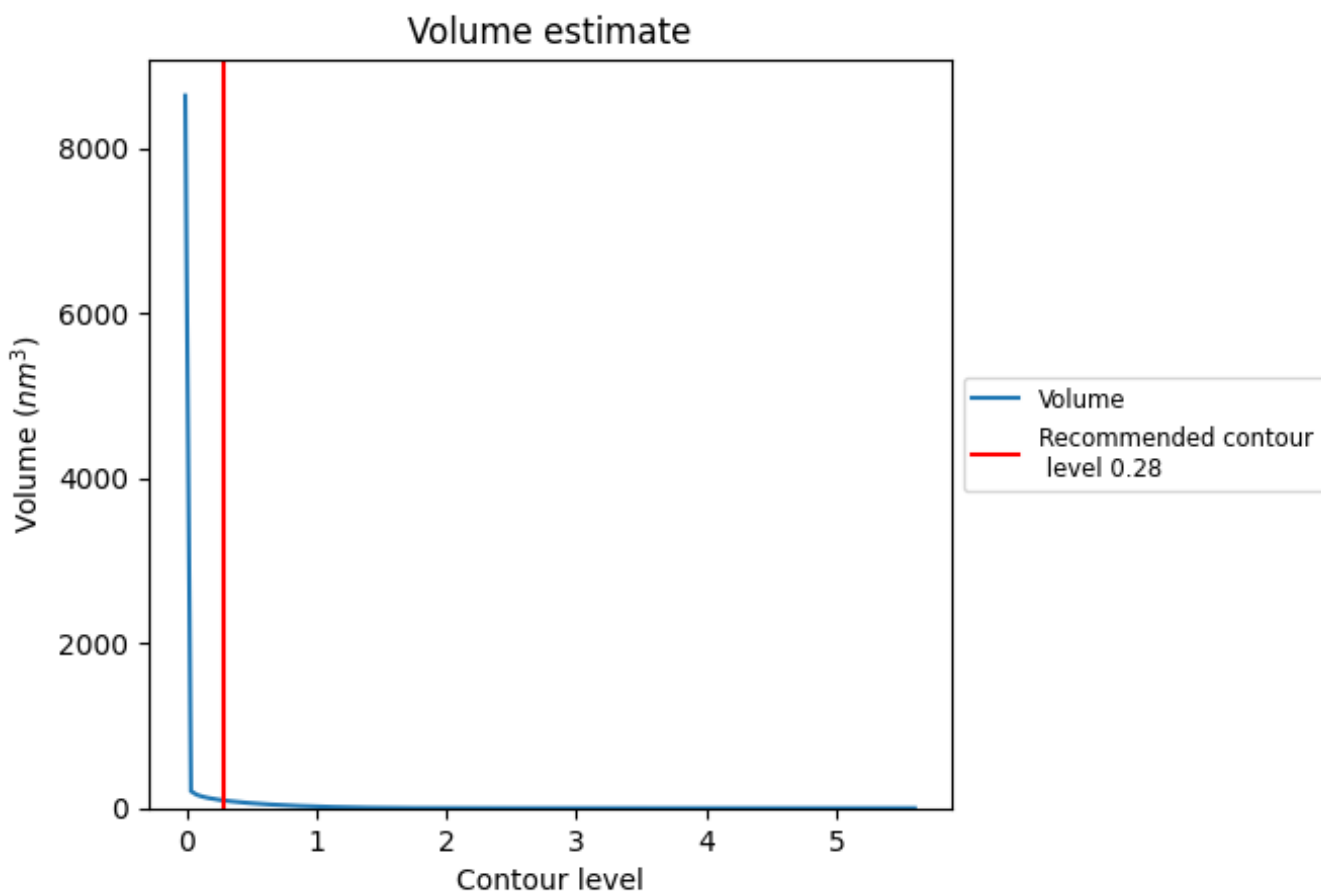
This section contains the results of statistical analysis of the map.

### 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.

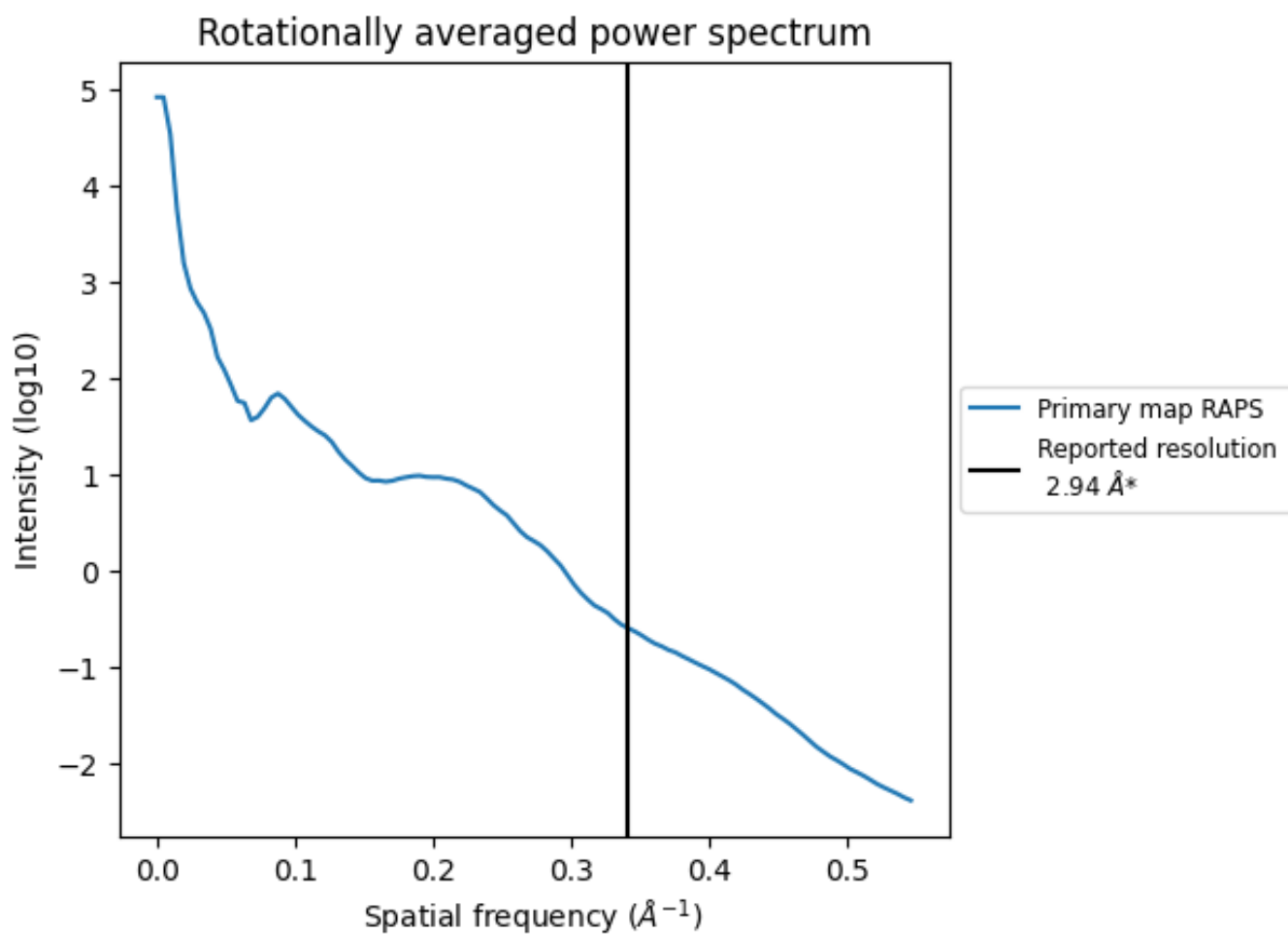
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 95 nm<sup>3</sup>; this corresponds to an approximate mass of 86 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<sup>-1</sup>

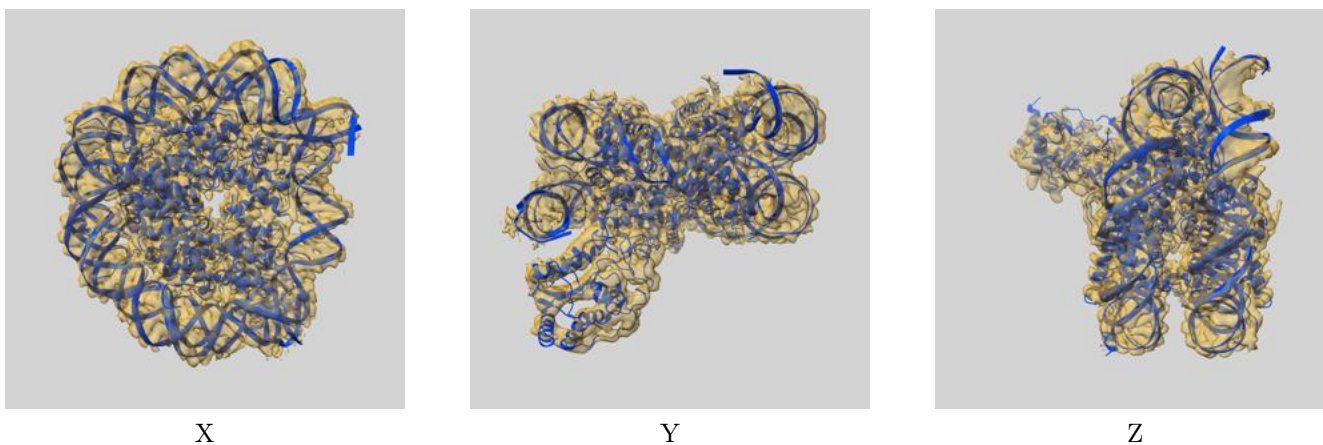
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

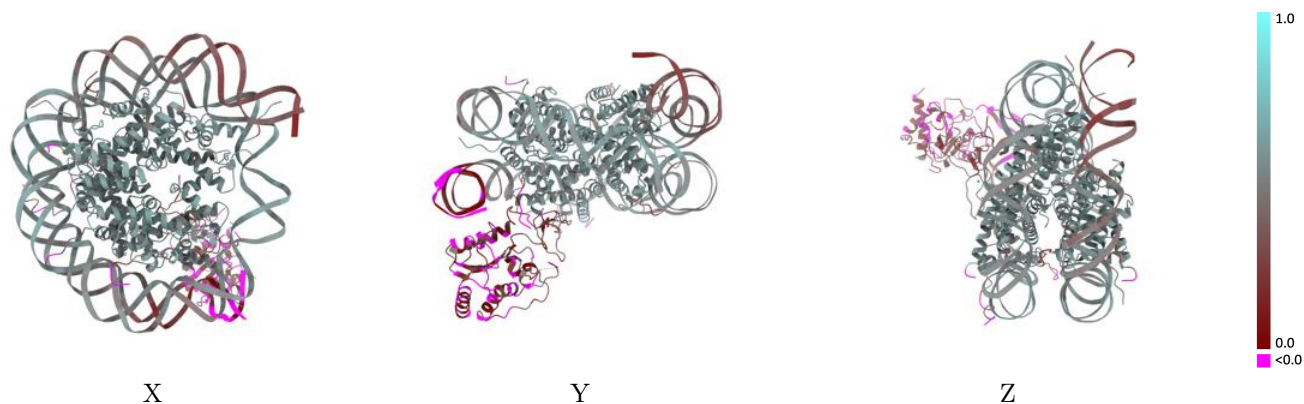
This section contains information regarding the fit between EMDB map EMD-16845 and PDB model 8OF4. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.28 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](#)

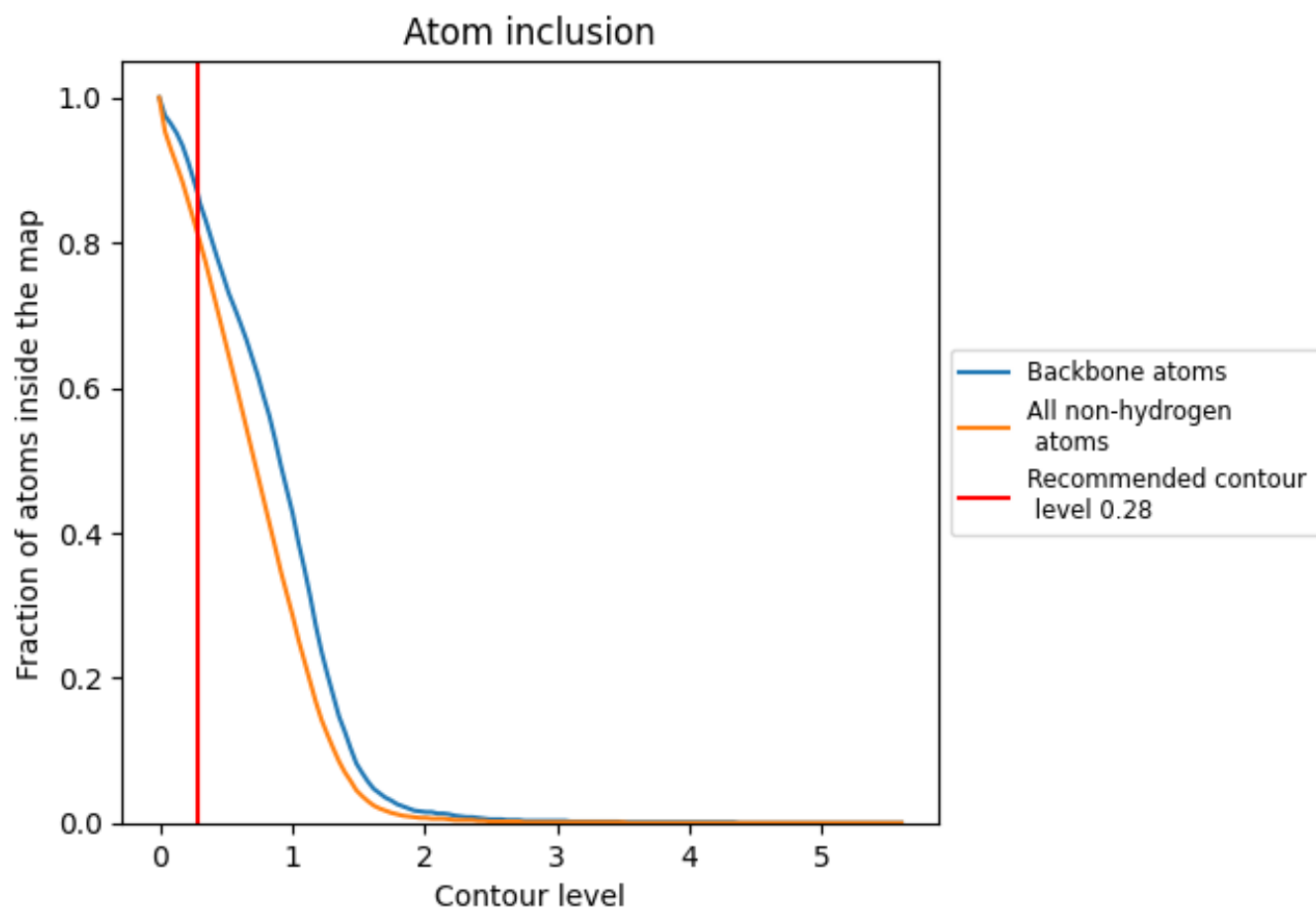


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.4460
A	 0.8800	 0.5440
B	 0.8550	 0.5390
C	 0.7850	 0.4810
D	 0.8250	 0.5090
E	 0.8930	 0.5540
F	 0.8310	 0.5200
G	 0.8710	 0.5470
H	 0.8260	 0.5110
I	 0.8580	 0.4510
J	 0.8660	 0.4510
L	 0.5450	 0.1620

