



wwPDB EM Validation Summary Report ⓘ

Apr 6, 2026 – 01:03 AM UTC

PDB ID : 9ZQA / pdb_00009zqa
EMDB ID : EMD-74562
Title : Nucleosome with an SSB at SHL -2.8 in complex with the WGR domain of human PARP2, Class 2
Authors : Kim, T.H.; Jayathilake, C.; Virk, R.K.; Gregory-Lott, E.R.
Deposited on : 2025-12-18
Resolution : 3.28 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

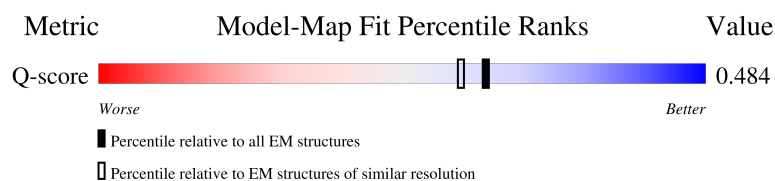
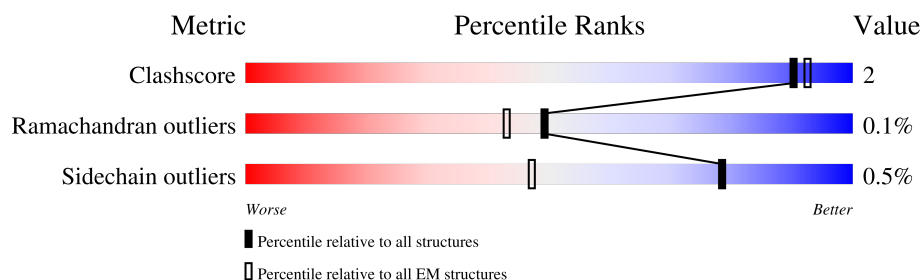
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.28 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.








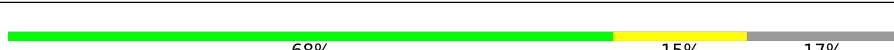
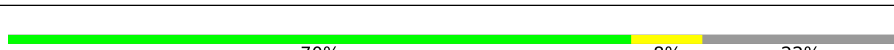
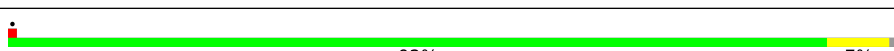
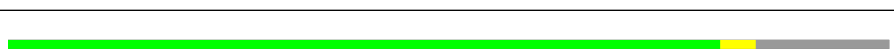

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14492 (2.78 - 3.78)

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	124	
1	B	124	
2	C	125	
2	D	125	

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Mol	Chain	Length	Quality of chain
3	E	136	
3	F	136	
4	G	104	
4	H	104	
5	K	69	
6	L	128	
7	M	197	
8	P	123	
9	I	274	
9	J	274	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31704 atoms, of which 14563 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 H2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	109	Total	C	H	N	O	S	0	0
			1730	526	896	163	144	1		
1	B	109	Total	C	H	N	O	S	0	0
			1730	526	896	163	144	1		

- Molecule 2 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	99	Total	C	H	N	O	S	0	0
			1627	498	838	145	144	2		
2	D	98	Total	C	H	N	O	S	0	0
			1605	492	825	143	143	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P02283
C	2	ILE	-	insertion	UNP P02283
D	0	GLY	-	expression tag	UNP P02283
D	2	ILE	-	insertion	UNP P02283

- Molecule 3 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	100	Total	C	H	N	O	S	0	0
			1700	522	874	160	142	2		
3	F	100	Total	C	H	N	O	S	0	0
			1695	520	870	160	143	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	111	SER	CYS	conflict	UNP P02299

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Chain	Residue	Modelled	Actual	Comment	Reference
F	111	SER	CYS	conflict	UNP P02299

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
4	H	85	Total	C	H	N	O	S	0	0
			1413	430	730	136	116	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	ILE	-	insertion	UNP P84040
H	2	ILE	-	insertion	UNP P84040

- Molecule 5 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	47	Total	C	H	N	O	P	0	0
			1489	455	529	172	286	47		

- Molecule 6 is a DNA chain called DNA (128-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	106	Total	C	H	N	O	P	0	0
			3345	1025	1191	385	638	106		

- Molecule 7 is a DNA chain called DNA (197-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	M	153	Total	C	H	N	O	P	0	0
			4874	1494	1714	600	913	153		

- Molecule 8 is a protein called Poly [ADP-ribose] polymerase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	122	Total	C	H	N	O	S	0	0
			1972	630	972	174	188	8		


- Molecule 9 is a protein called mAb PL2-6 antibody.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	233	Total	C	H	N	O	S	0	0
			3583	1144	1762	300	367	10		
9	I	232	Total	C	H	N	O	S	0	0
			3569	1140	1756	298	365	10		

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.

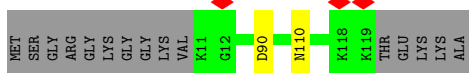
- Molecule 1: Histone H2A

Chain A:  85% 12%




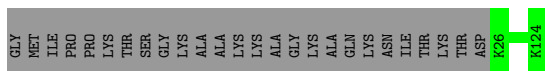
- Molecule 1: Histone H2A

Chain B:  86% 12%




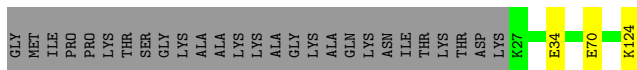
- Molecule 2: Histone H2B

Chain C:  79% 21%



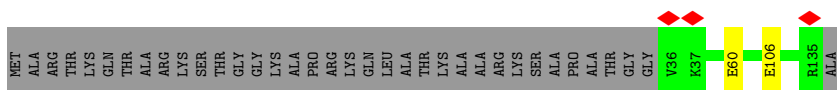
- Molecule 2: Histone H2B

Chain D:  76% 22%



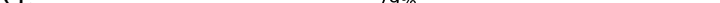
- Molecule 3: Histone H3

Chain E:  72% 26%



- Molecule 3: Histone H3

MET	ALA	ARG	THR	LYS	GLN	THR	ALA	ARG	LYS	SER	THR	GLY	GLY	LYS	ALA	ALA	PRO	ARG	LYS	GLN	LEU	THR	LYS	ALA	ALA	ALA	ARG	LYS	SER	ALA	ALA	PRO	THR	ALA	GLY	GLY	VAL	K37	R41	E74	E95	R185	A196
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- Chain G:  79% 20%

MET ILE THR GLY ARG GLY LYS GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG
 K22 D26 G104

- Chain H: 80% 18%

Sequence logo for the 1000bp upstream region of the H2O gene. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows amino acid positions from 1 to 104. The sequence is: MET, ILE, THR, GLY, ARG, GLY, LYS, GLY, GLY, LYS, GLY, LEU, GLY, LYS, GLY, ALA, LYS, ARG, H2O, R21, K22, V23, L24, E54, G104. A red diamond is above the H2O position, and a red diamond is above the G104 position.

- Chain K: 57% 12% 32%

DG	DG	DG	DC	DT	DG	DG	DA	DC	DT	DC	DT	DT	DA	DT	DA	DC	DC	DG	DC	DG	DC	DC	DC	A1	A11	T12	T34	T35	G40	T41	G42	T43	G47
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- Chain L:  68% 15% 17%

[illegible]

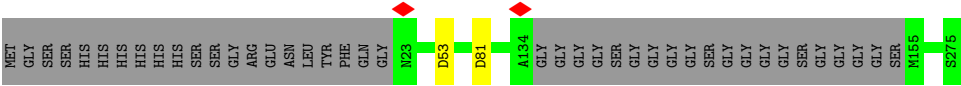
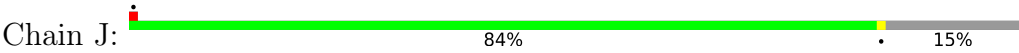
- Chain M: 70% 8% 22%

[illegible]

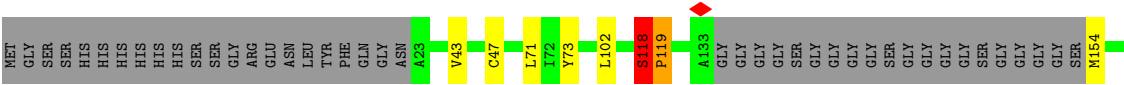
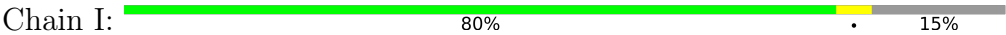
- Chain P: 92% 7%



• Molecule 9: mAb PL2-6 antibody



• Molecule 9: mAb PL2-6 antibody



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0259	Depositor
Map size (Å)	273.0, 273.0, 273.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91, 0.91, 0.91	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/844	0.27	0/1135
1	B	0.10	0/844	0.25	0/1135
2	C	0.09	0/800	0.25	0/1068
2	D	0.11	0/791	0.27	0/1057
3	E	0.13	0/838	0.34	0/1123
3	F	0.11	0/837	0.26	0/1120
4	G	0.11	0/669	0.26	0/894
4	H	0.11	0/691	0.27	0/923
5	K	0.16	0/1074	0.42	0/1655
6	L	0.18	0/2411	0.44	0/3712
7	M	0.17	0/3551	0.42	0/5484
8	P	0.10	0/1021	0.27	0/1372
9	I	0.10	0/1855	0.28	1/2510 (0.0%)
9	J	0.09	0/1863	0.22	0/2521
All	All	0.14	0/18089	0.34	1/25709 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	118	SER	C-N-CD	-6.94	96.53	125.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	118	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	834	896	895	3	0
1	B	834	896	895	1	0
2	C	789	838	837	0	0
2	D	780	825	824	3	0
3	E	826	874	873	2	0
3	F	825	870	869	3	0
4	G	662	710	709	1	0
4	H	683	730	729	2	0
5	K	960	529	529	5	0
6	L	2154	1191	1192	15	0
7	M	3160	1714	1715	11	0
8	P	1000	972	971	5	0
9	I	1813	1756	1754	5	0
9	J	1821	1762	1760	2	0
All	All	17141	14563	14552	55	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 2.

The worst 5 of 55 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:M:52:DC:H2''	7:M:53:DT:H71	1.85	0.58
8:P:98:CYS:O	8:P:102:VAL:HG23	2.04	0.58
5:K:42:DG:H2''	5:K:43:DT:H71	1.88	0.56
2:D:34:GLU:HA	2:D:34:GLU:OE1	2.07	0.54
3:F:95:GLU:HA	3:F:95:GLU:OE1	2.08	0.53

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/124 (86%)	105 (98%)	2 (2%)	0	100	100
1	B	107/124 (86%)	106 (99%)	1 (1%)	0	100	100
2	C	97/125 (78%)	97 (100%)	0	0	100	100
2	D	96/125 (77%)	96 (100%)	0	0	100	100
3	E	98/136 (72%)	94 (96%)	4 (4%)	0	100	100
3	F	98/136 (72%)	96 (98%)	2 (2%)	0	100	100
4	G	81/104 (78%)	79 (98%)	2 (2%)	0	100	100
4	H	83/104 (80%)	79 (95%)	4 (5%)	0	100	100
8	P	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
9	I	228/274 (83%)	221 (97%)	6 (3%)	1 (0%)	30	60
9	J	229/274 (84%)	222 (97%)	7 (3%)	0	100	100
All	All	1344/1649 (82%)	1309 (97%)	34 (2%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	119	PRO

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	84/94 (89%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	84/94 (89%)	83 (99%)	1 (1%)	63	75
2	C	86/105 (82%)	86 (100%)	0	100	100
2	D	85/105 (81%)	85 (100%)	0	100	100
3	E	88/111 (79%)	88 (100%)	0	100	100
3	F	87/111 (78%)	87 (100%)	0	100	100
4	G	68/80 (85%)	68 (100%)	0	100	100
4	H	70/80 (88%)	70 (100%)	0	100	100
8	P	108/108 (100%)	106 (98%)	2 (2%)	50	69
9	I	203/226 (90%)	200 (98%)	3 (2%)	57	73
9	J	204/226 (90%)	204 (100%)	0	100	100
All	All	1167/1340 (87%)	1161 (100%)	6 (0%)	78	83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	47	CYS
9	I	71	LEU
9	I	154	MET
8	P	113	ASP
1	B	110	ASN

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

Mol	Chain	Res	Type
1	A	19	ASN
1	A	112	GLN
4	G	77	HIS
4	H	77	HIS
9	I	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

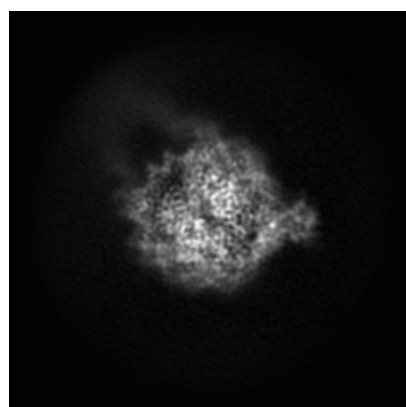
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74562. These allow visual inspection of the internal detail of the map and identification of artifacts.

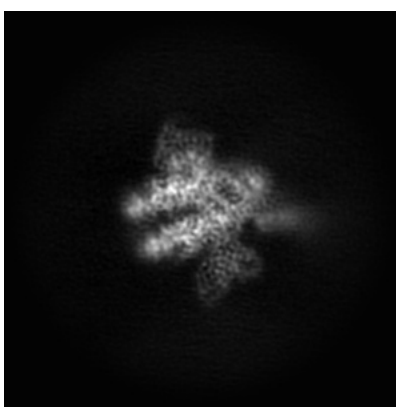
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

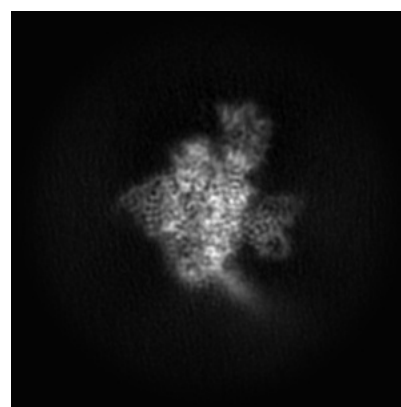
6.1.1 Primary map



X



Y

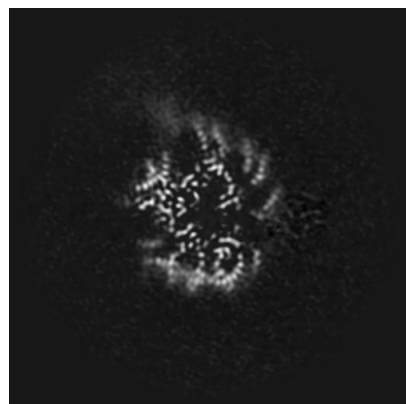


Z

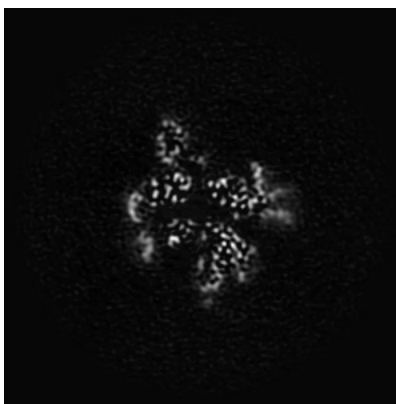
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

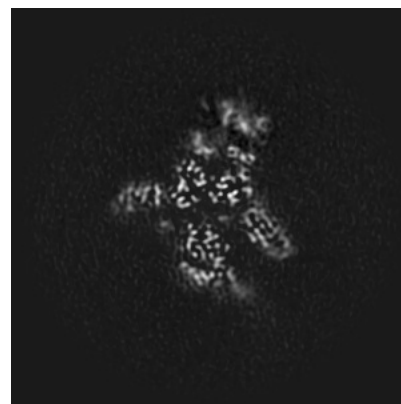
6.2.1 Primary map



X Index: 150



Y Index: 150

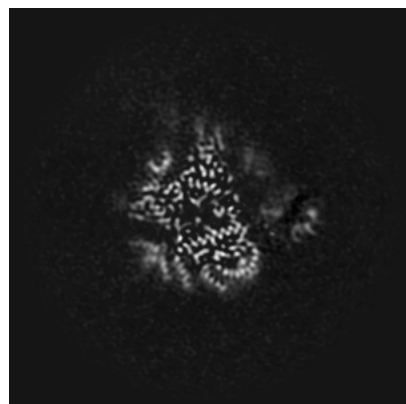


Z Index: 150

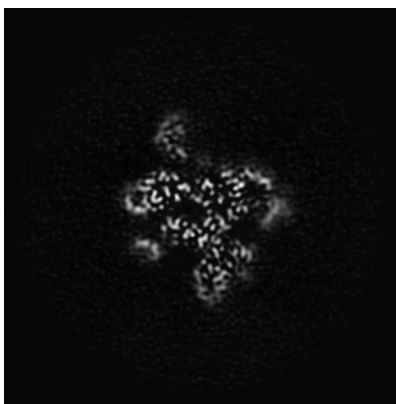
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

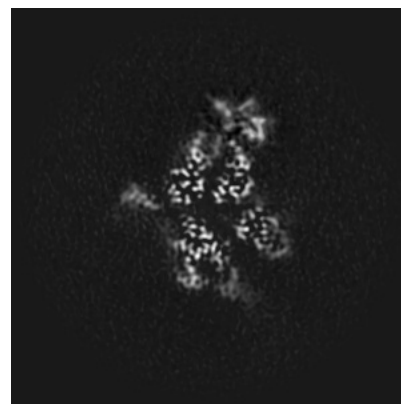
6.3.1 Primary map



X Index: 155



Y Index: 156

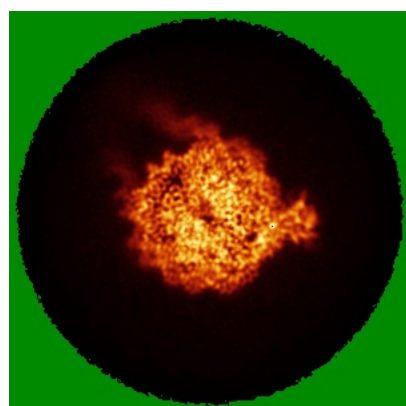


Z Index: 146

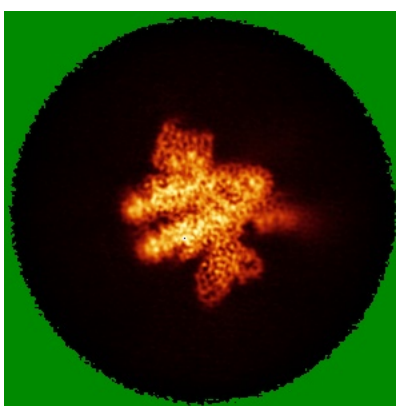
The images above show the largest variance slices of the map in three orthogonal directions.

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

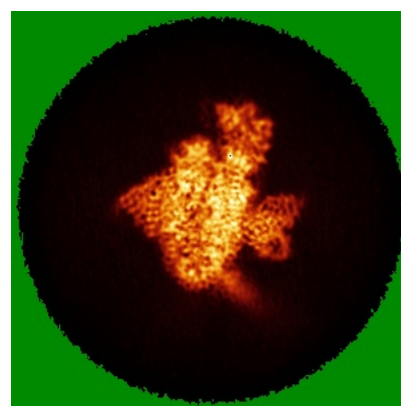
6.4.1 Primary map



X



Y

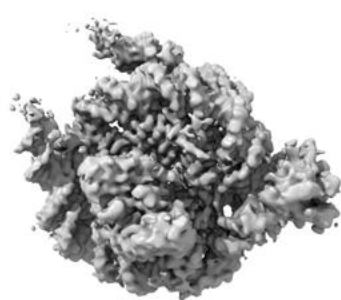


Z

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 0.0259. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

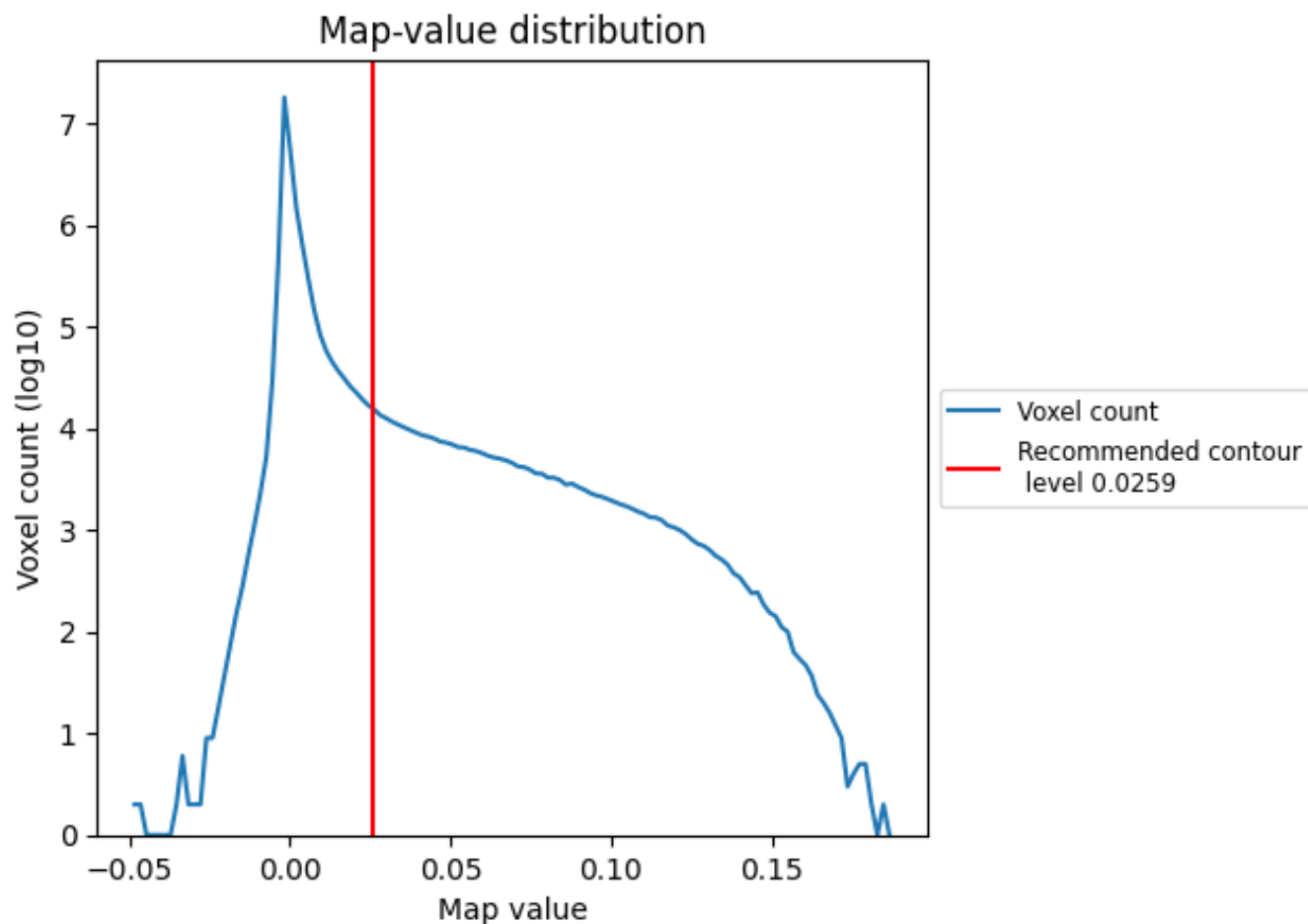
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

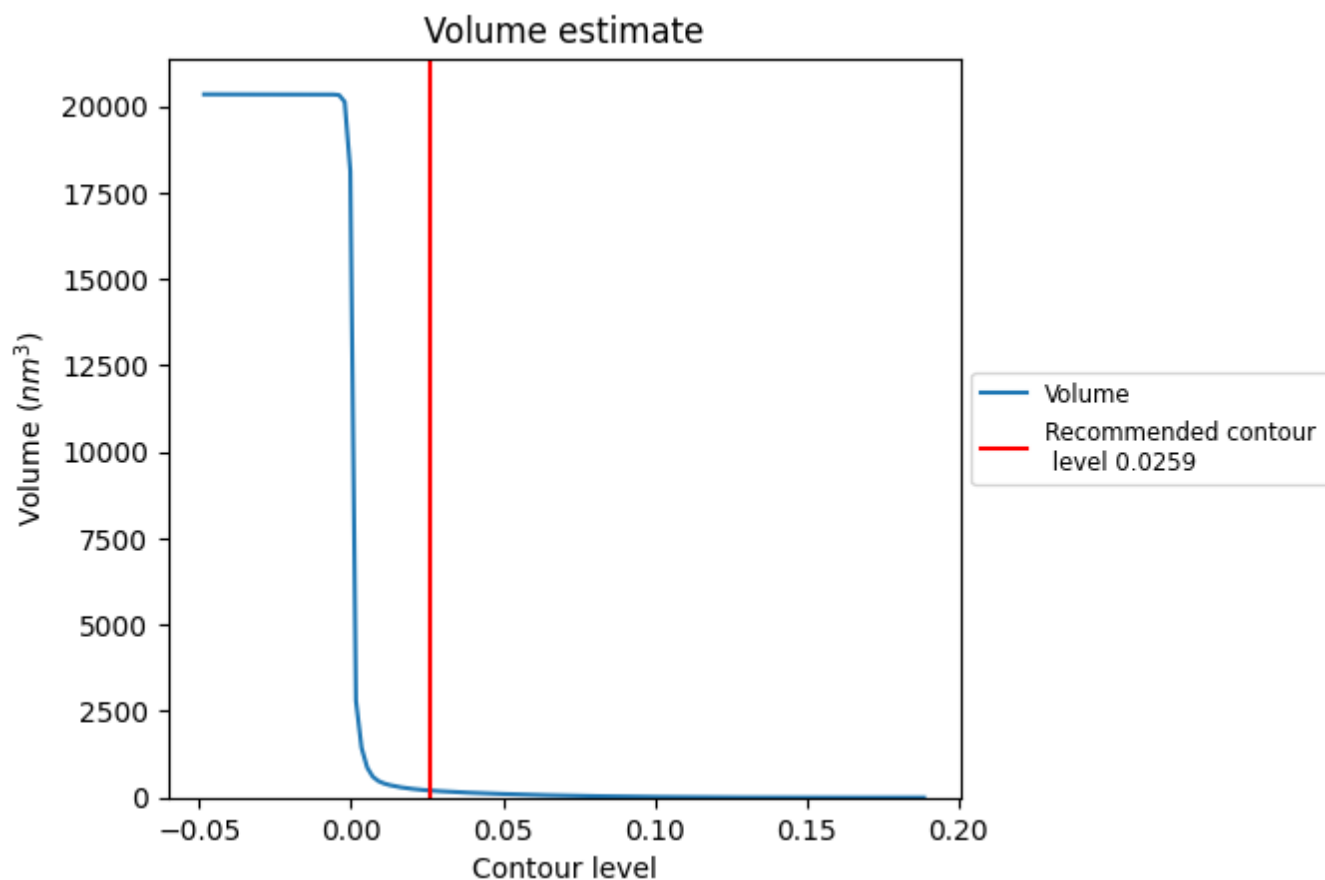
This section contains the results of statistical analysis of the map.

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.

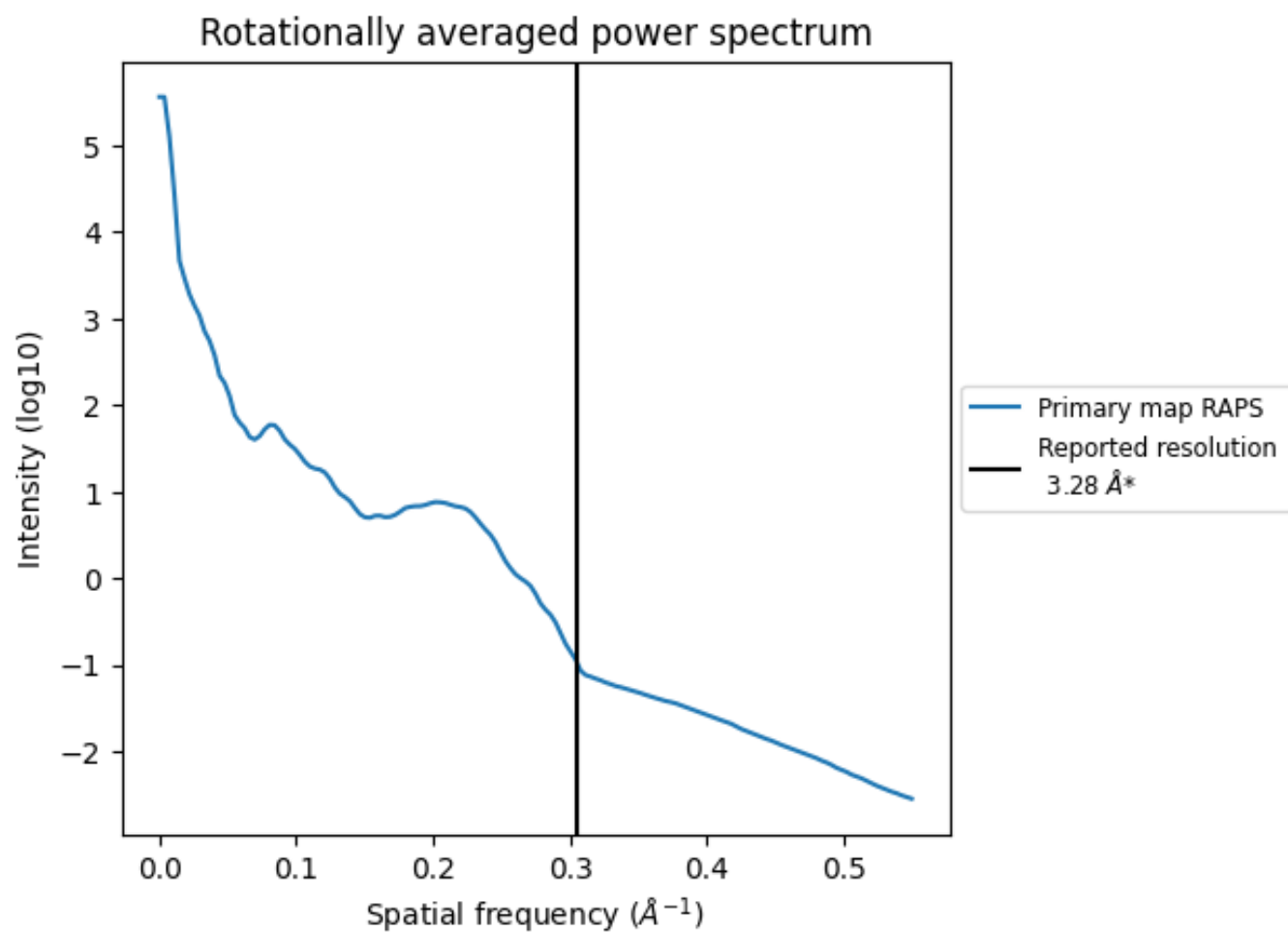
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm^3 ; this corresponds to an approximate mass of 185 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 0.305 Å⁻¹

8 Fourier-Shell correlation

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

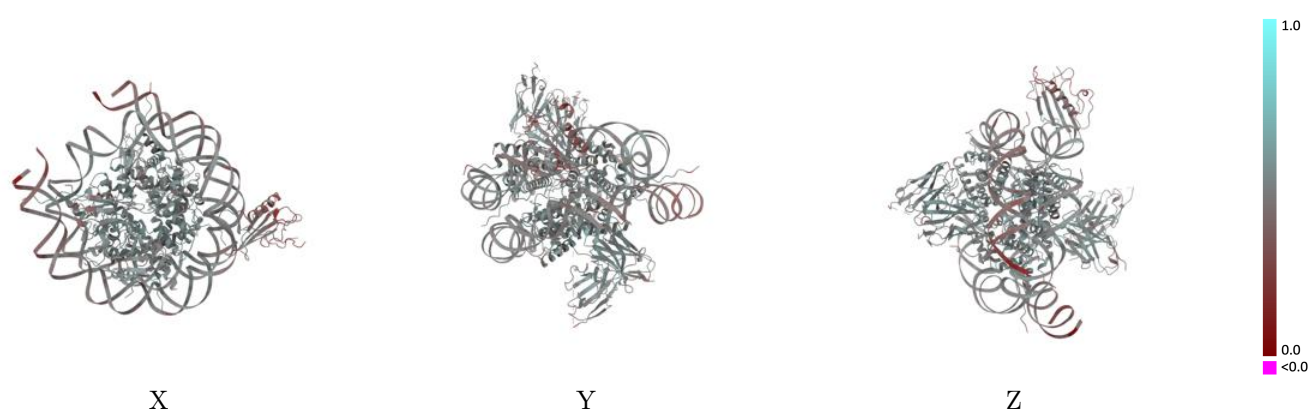
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-74562 and PDB model 9ZQA. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

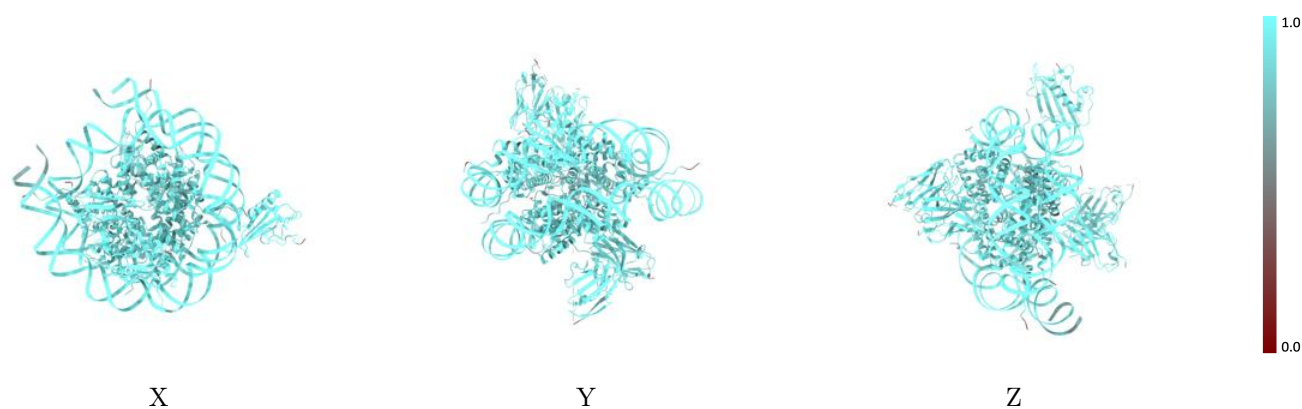
This section was not generated.

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



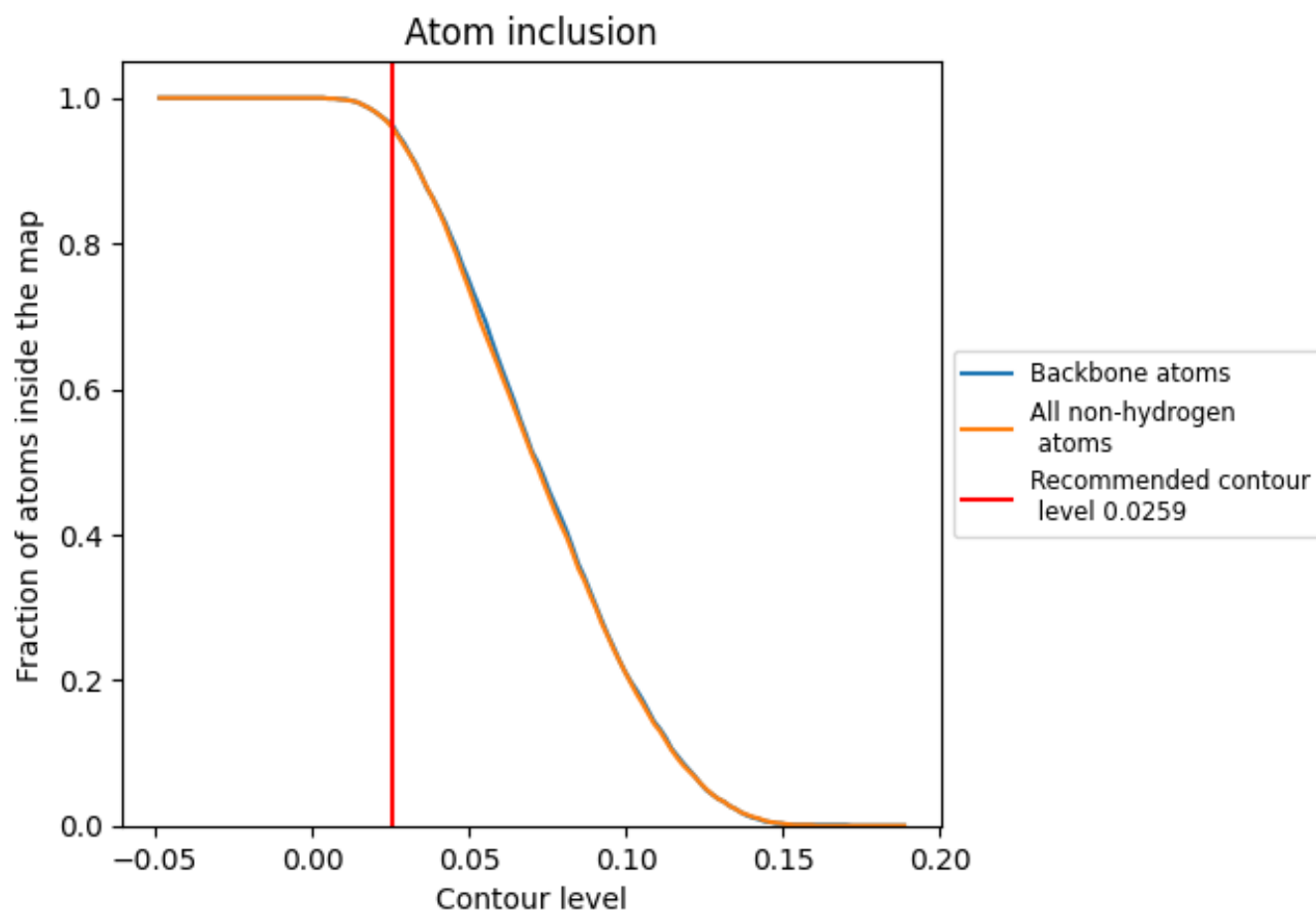
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0259).































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.0259) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.4840
A	 0.9630	 0.5300
B	 0.9490	 0.5290
C	 0.9510	 0.5110
D	 0.9610	 0.5140
E	 0.9460	 0.5210
F	 0.9410	 0.5140
G	 0.9420	 0.5230
H	 0.9450	 0.5140
I	 0.9520	 0.5030
J	 0.9560	 0.5070
K	 0.9560	 0.4360
L	 0.9950	 0.4630
M	 0.9810	 0.4500
P	 0.9510	 0.3760

