



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 10:32 PM UTC

PDB ID : 6OKT / pdb_00006okt
EMDB ID : EMD-20104
Title : CDTb Double Heptamer Long Form Mask 1 Modeled from Cryo-EM Map
Reconstructed using C7 Symmetry
Authors : Lacy, D.B.; Sheedlo, M.J.; Anderson, D.M.
Deposited on : 2019-04-15
Resolution : 4.20 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

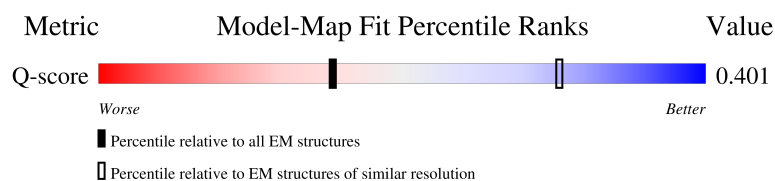
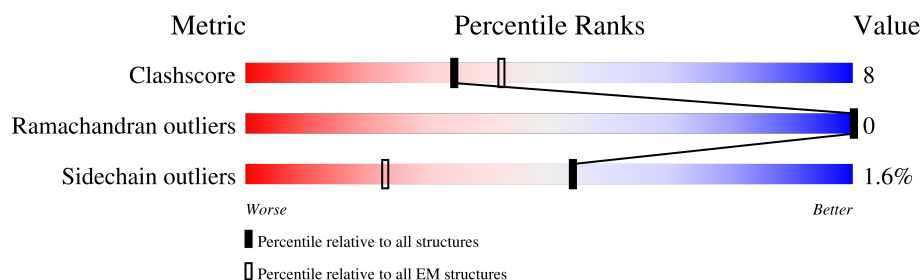
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



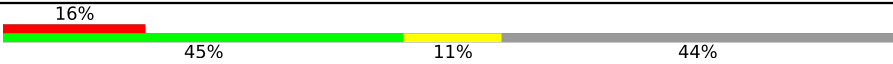
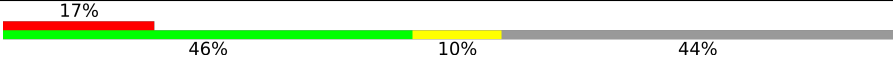
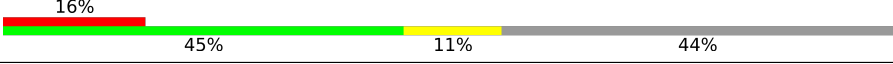
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	H	876	16% 45% 11% 44%
1	I	876	16% 45% 11% 44%
1	J	876	17% 45% 11% 44%
1	K	876	16% 45% 11% 44%

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Mol	Chain	Length	Quality of chain
1	L	876	
1	M	876	
1	N	876	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27048 atoms, of which 0 are hydrogens and 0 are deuteriums.

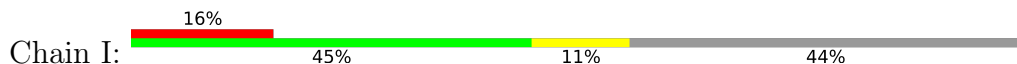
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ADP-ribosyltransferase binding component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	493	Total	C	N	O	S	0	0
			3864	2418	624	816	6		
1	I	493	Total	C	N	O	S	0	0
			3864	2418	624	816	6		
1	J	493	Total	C	N	O	S	0	0
			3864	2418	624	816	6		
1	K	493	Total	C	N	O	S	0	0
			3864	2418	624	816	6		
1	L	493	Total	C	N	O	S	0	0
			3864	2418	624	816	6		
1	M	493	Total	C	N	O	S	0	0
			3864	2418	624	816	6		
1	N	493	Total	C	N	O	S	0	0
			3864	2418	624	816	6		

ILE	TYR	ALA	ILE	THR	PRO	ASP	ASP	GLU	ARG	LEU	VAL	LEU	SER	LEU	VAL	ASP	LYS	ASP	ASP	GLY	GLY	GLY	THR	THR	LYS	LYS	ASP	LYS	LEU	ASN	ARG	MET	GLU	LYS	ASP	ASP	GLY	LEU	TYR	TYR	GLN	PRO	LYS	THR	THR	ASN	VAL	VAL	ASN	LEU	ARG	SER	TYR	THR	THR	ASN	GLY	THR	THR	GLY	GLU	ASN	LYS	LYS	TYR	THR	THR	MET	ILE	LYS	LYS	ASP	LEU	ASP
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- Molecule 1: ADP-ribosyltransferase binding component



MET	LYS	ILE	GLN	MET	ARG	ASN	LYS	LYS	VAL	LEU	SER	PHE	LEU	THR	LEU	LEU	THR	ALA	ALA	ILE	VAL	SER	GLN	LEU	ALA	LEU	VAL	TYR	PRO	TYR	THR	VAL	TYR	THR	SER	ASN	ASN	HIS	SER	ASN	ASN	LYS	LYS	LYS	GLU	ILE	VAL	ASN	GLU	ASP	ILE	LEU	PRO	ASN	GLY	LEU	MET	GLY	TYR	THR	PHE
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THR	ASP	GLU	HIS	PHE	LYS	ASP	LEU	LEU	LEU	MET	ALA	PRO	PRO	ILE	LYS	ASP	ASN	GLY	LEU	LYS	PHE	GLU	GLU	LYS	LYS	VAL	ASP	LYS	LEU	LEU	ASP	LYS	ASP	SER	VAL	LYS	SER	ILE	ILE	ARG	TRP	THR	GLY	ARG	ILE	ILE	PRO	PRO	ASP	LYS	ASP	GLY	GLU	TYR	THR	SER	THR	ASP	ARG
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ASP	ASP	VAL	ASP	VAL	LEU	LEU	GLN	GLN	VAL	VAL	THR	THR	GLU	GLU	SER	SER	THR	THR	THR	THR	LEU	LEU	LYS	LYS	VAL	VAL	ASN	ASN	MET	MET	LYS	LYS	GLY	GLY	LYS	LYS	GLU	GLU	TYR	TYR	LYS	LYS	VAL	VAL	ARG	ARG	ILE	ILE	GLU	GLU	LEU	LEU	GLN	GLN	ASP	ASP	LYS	LYS	ASN	ASN	LEU	LEU	GLY	GLY	SER	SER	SER	SER	PRO	PRO	ASN	ASN	LEU	LEU	LEU	LEU	TYR	TYR	TRP	TRP	GLU	GLU	LEU	LEU	ASP	ASP	ASP	ASP	GLY	GLY	MET	MET	LYS	LYS	LYS	LYS	ILE	ILE	ILE	ILE
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PRO	GLU	GLU	ASN	LEU	PHE	LEU	ARG	ASP	TYP	SER	ASN	ILE	GLU	LYS	ASP	PRO	PHE	ILE	PRO	ASN	ASN	ASN	PHE	PHE	ASP	PRO	LYS	LEU	MET	SER	SER	ASP	TRP	GLU

F249	A250	E251	K255	K256	S259	M260	T261	L262	Y271	T272	D273	K276	A277	S278	R290	D291	A295	T308	E313	H314	K321	T322	V323	K324	R325	A326	T327	T328	ASN	ASN	SER	SER	LYS	THR	GLU	THR	ASN	ASN	THR	ALA	GLY	VAL	SER	VAL	ASN	VAL	VAL	GLY	TYR	GLN	ASN	GLY	PRO
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[illegible]

Node Type	Number of Nodes (approx.)
D471	95
A472	90
G473	85
K477	80
L478	75
L496	70
N501	65
S512	60
T521	55
E522	50
N523	45
E524	40
E527	35
R528	30
R529	25
N534	20
L535	15
Q536	10
E539	5
D540	5
E544	5
L545	5
T546	5
E549	5
E552	5
K553	5
A557	5
L583	5
D588	5
L578	5
I579	5
F580	5
D581	5
T584	5

Category	Count
L595	1000
S596	1000
D597	1000
K598	1000
K599	1000
M602	1000
R607	1000
G608	1000
M609	1000
M610	1000
T611	1000
L612	1000
L613	1000
Y618	1000
F622	1000
D623	1000
D624	1000
Y625	1000
M626	1000
M627	1000
S630	1000
T631	1000
W632	1000
S633	1000
S634	1000
W635	1000
W636	1000
T637	1000
T638	1000
W639	1000
G642	1000
L643	1000
Q644	1000
G645	1000
S646	1000
A647	1000
M648	1000
K649	1000
L650	1000
M651	1000
G652	1000
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S661	1000
E662	1000
L663	1000
K664	1000
P665	1000
Y666	1000

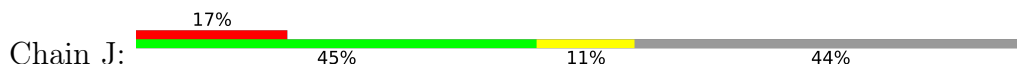
F671	F672	G673	G674	G675	G676	D677	D678	D679	T680	S681	M682	S683	F684	F685	F686	K687	F688	K689	A690	K691	E692	E693	K694	T695	D696	F697	L698	F699	P700	E701	Q702	G703	Y704	T705	K706	F707	S708	Y709	E710	F711	E712	T713	T714	E715	K716	D717	S718	S719	N720	I721	L725	I726	G727	S728	G729	T730
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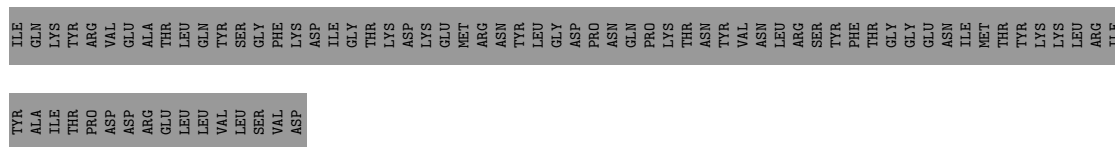
L736 S737 T738 T739 E740 L741 N742 S743 E746 T747 LEU ASP GLU GLU PRO GLU VAL LYS LYS ILE PRO THR ASP ASN GLN GLN ILE ILE NET ASP ALA ALA HIS LYS LYS ILE TYR PHE ALA ASP LEU ASN ASN PHE PRO SER THR GLY ASN THR TYR ILE ASN GLY NET TYR PHE ALA PRO THR GLN THR ASN LYS

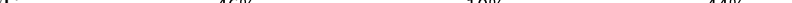
ALA LEU LEU ASP TYR ILE GLN LYS TYR ARG VAL GLU ALA THR LEU GLN TYR SER GLY PHE LYS ASP ASP ILE GLY THR LYS ASP ASN TYR TYR LEU GLY ASP PRO GLN GLN PRO PRO TYR LYS THR ASN TYR VAL ASN ASN LEU LEU ARG SER TYR PHE THR GLY GLY GLU ASN ILE MET MET THR TYR

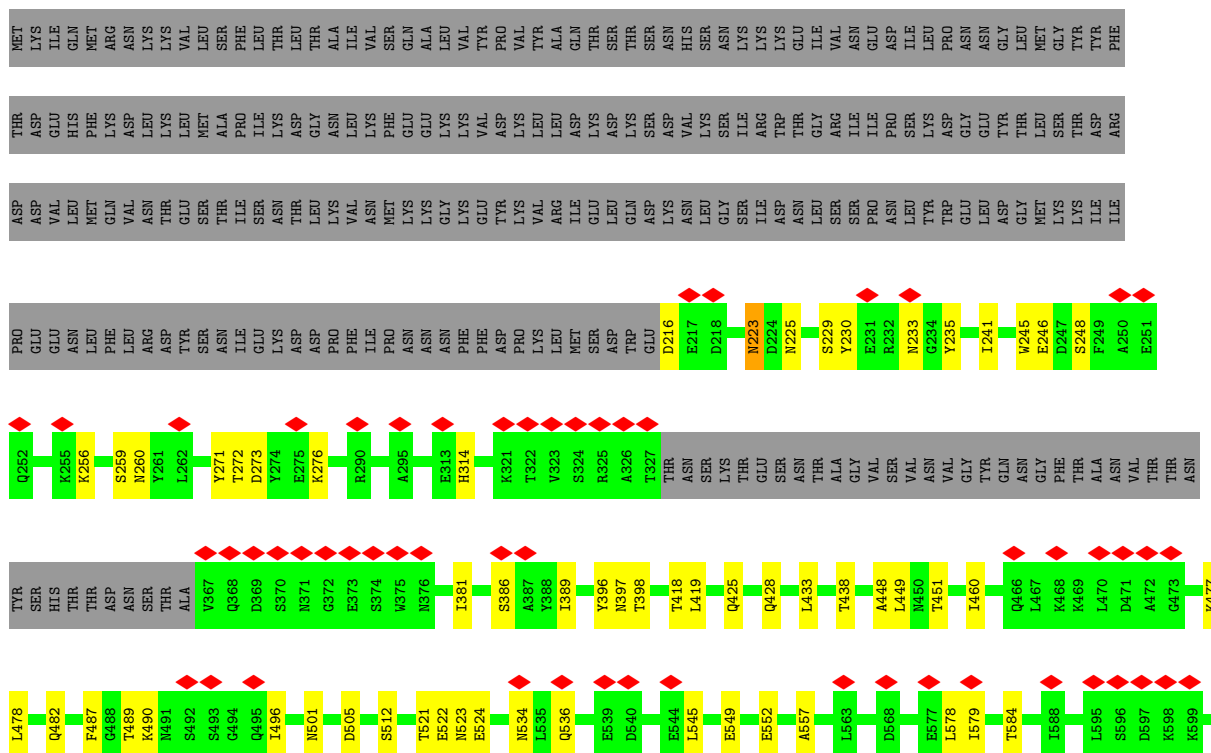
LYS
LEU
ARG
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TYR
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PRO
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ASP
ARG
GLU
LEU
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VAL
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VAL
ASP

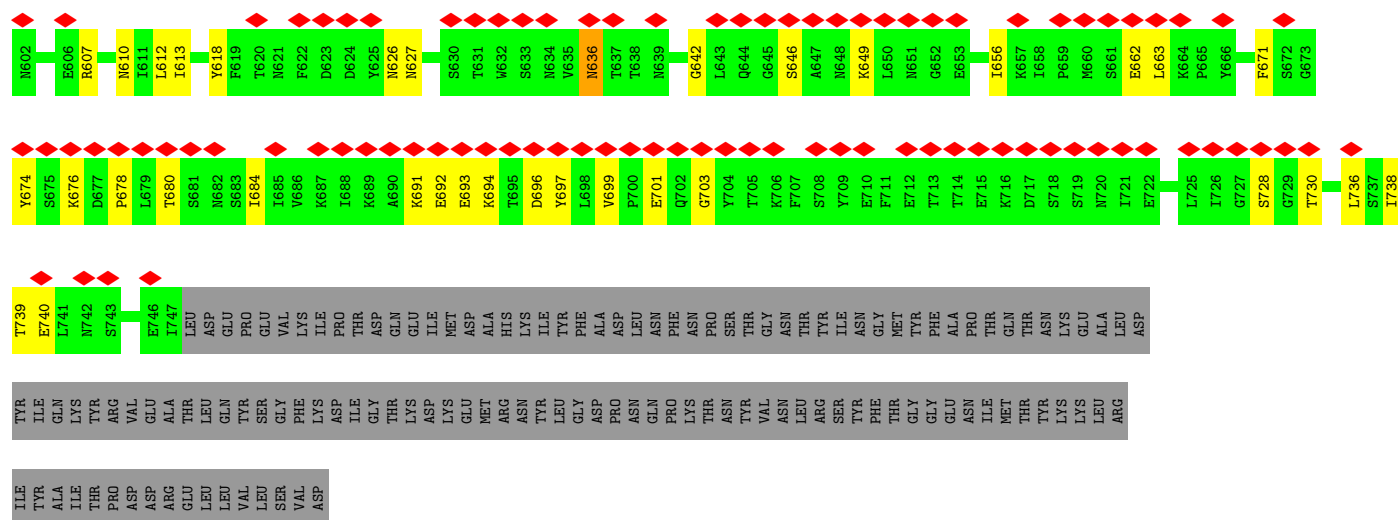
- Molecule 1: ADP-ribosyltransferase binding component



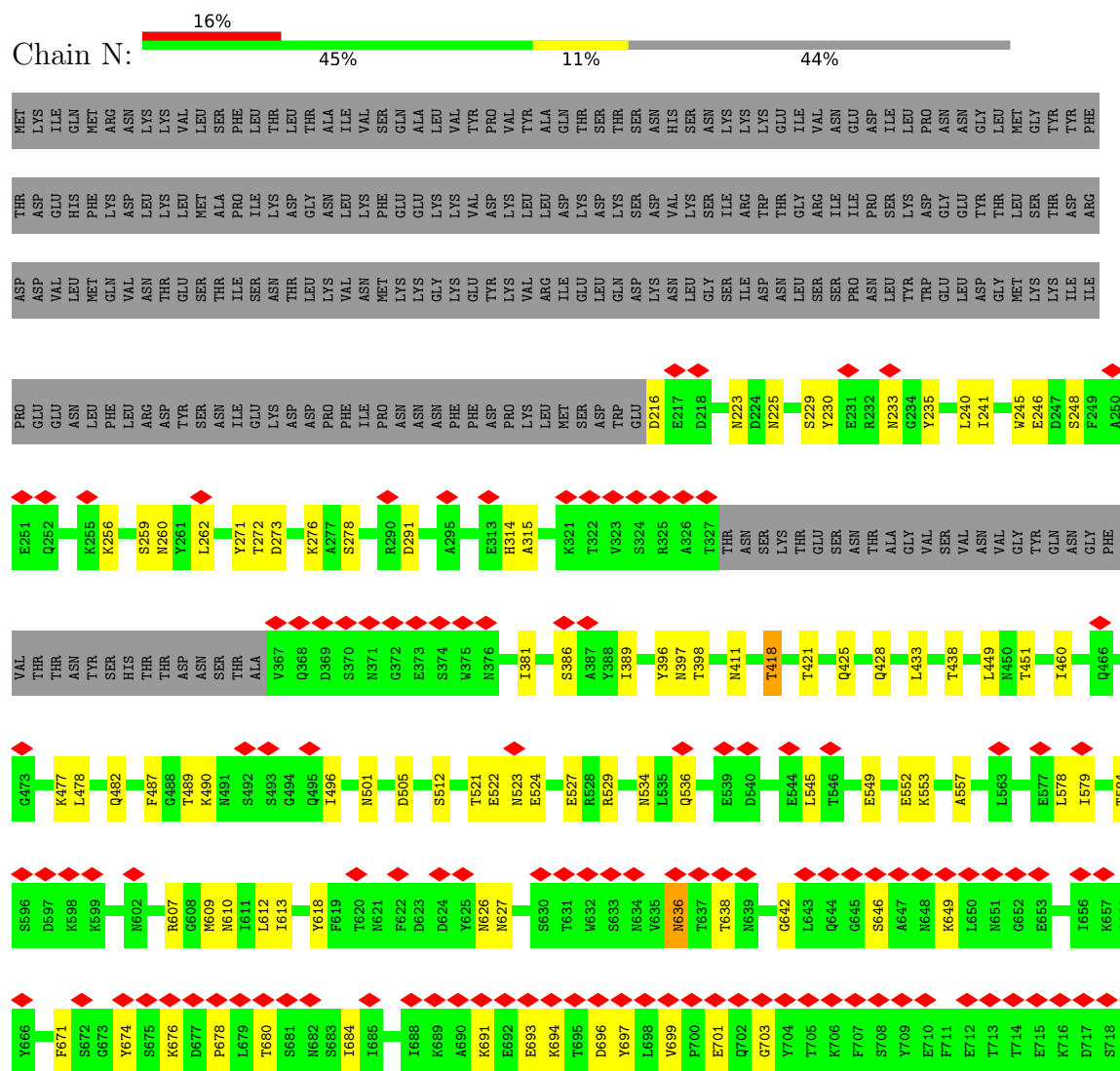


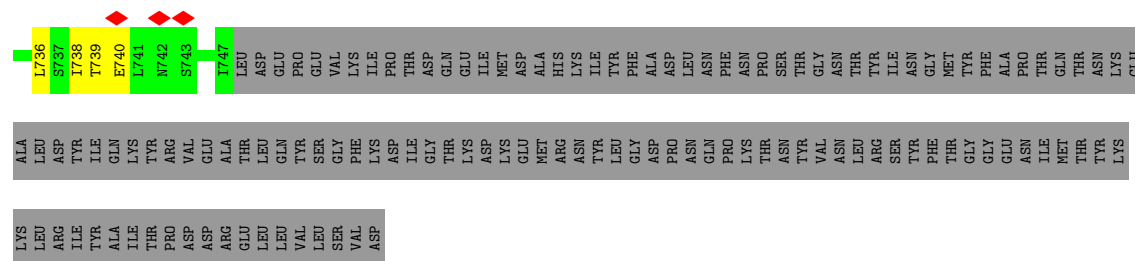
Chain M: 





• Molecule 1: ADP-ribosyltransferase binding component





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13266	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	110.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	362.5, 362.5, 362.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.45, 1.45, 1.45	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	H	0.34	0/3931	0.57	0/5331
1	I	0.34	0/3931	0.57	0/5331
1	J	0.34	0/3931	0.57	0/5331
1	K	0.34	0/3931	0.57	0/5331
1	L	0.34	0/3931	0.57	0/5331
1	M	0.34	0/3931	0.57	0/5331
1	N	0.34	0/3931	0.57	0/5331
All	All	0.34	0/27517	0.57	0/37317

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	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	223	ASN	Peptide
1	I	223	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	J	223	ASN	Peptide
1	K	223	ASN	Peptide
1	L	223	ASN	Peptide

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	H	3864	0	3760	65	0
1	I	3864	0	3760	63	0
1	J	3864	0	3760	64	0
1	K	3864	0	3760	62	0
1	L	3864	0	3760	63	0
1	M	3864	0	3760	59	0
1	N	3864	0	3760	62	0
All	All	27048	0	26320	430	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 8.

The worst 5 of 430 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:701:GLU:HG2	1:N:703:GLY:H	1.58	0.69
1:H:701:GLU:HG2	1:H:703:GLY:H	1.58	0.69
1:J:701:GLU:HG2	1:J:703:GLY:H	1.58	0.68
1:K:701:GLU:HG2	1:K:703:GLY:H	1.58	0.68
1:L:701:GLU:HG2	1:L:703:GLY:H	1.58	0.68

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	H	489/876 (56%)	431 (88%)	58 (12%)	0	100	100
1	I	489/876 (56%)	431 (88%)	58 (12%)	0	100	100
1	J	489/876 (56%)	431 (88%)	58 (12%)	0	100	100
1	K	489/876 (56%)	431 (88%)	58 (12%)	0	100	100
1	L	489/876 (56%)	431 (88%)	58 (12%)	0	100	100
1	M	489/876 (56%)	431 (88%)	58 (12%)	0	100	100
1	N	489/876 (56%)	431 (88%)	58 (12%)	0	100	100
All	All	3423/6132 (56%)	3017 (88%)	406 (12%)	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	H	438/790 (55%)	431 (98%)	7 (2%)	55	69
1	I	438/790 (55%)	431 (98%)	7 (2%)	55	69
1	J	438/790 (55%)	431 (98%)	7 (2%)	55	69
1	K	438/790 (55%)	431 (98%)	7 (2%)	55	69
1	L	438/790 (55%)	431 (98%)	7 (2%)	55	69
1	M	438/790 (55%)	431 (98%)	7 (2%)	55	69
1	N	438/790 (55%)	431 (98%)	7 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3066/5530 (55%)	3017 (98%)	49 (2%)	54 69

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	386	SER
1	M	386	SER
1	L	418	THR
1	L	636	ASN
1	M	482	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	425	GLN
1	N	425	GLN
1	L	312	ASN
1	N	648	ASN
1	M	523	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

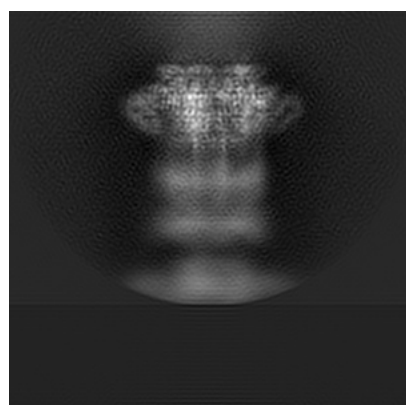
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20104. These allow visual inspection of the internal detail of the map and identification of artifacts.

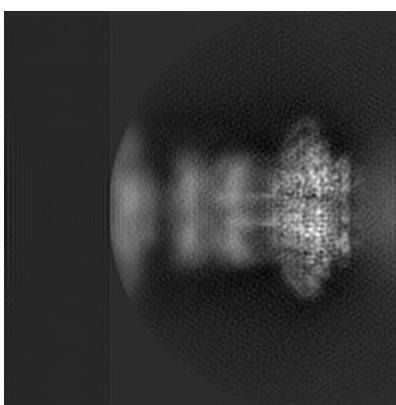
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

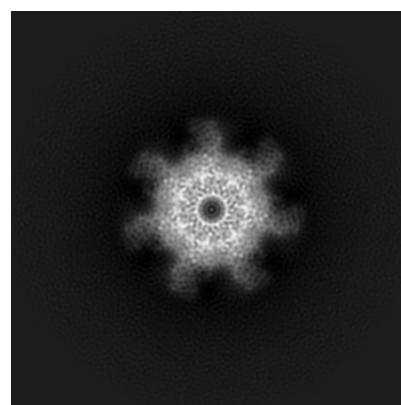
6.1.1 Primary map



X



Y

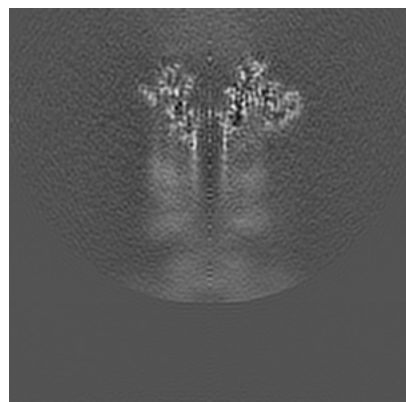


Z

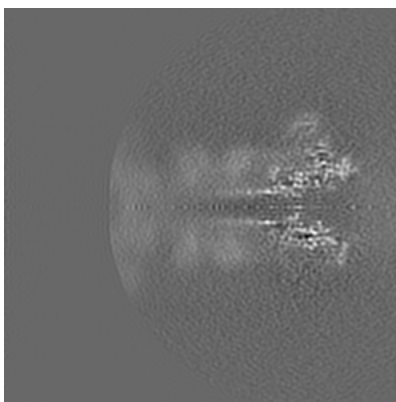
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

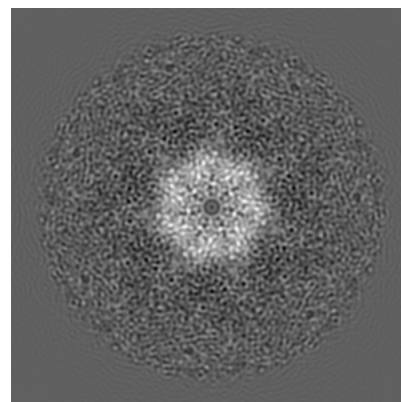
6.2.1 Primary map



X Index: 125



Y Index: 125

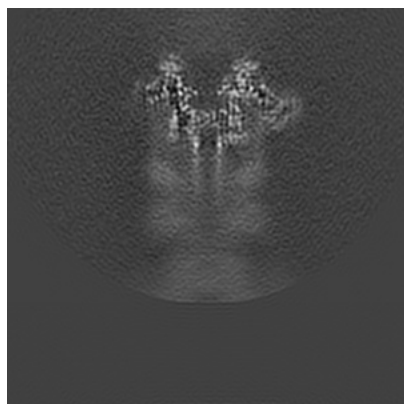


Z Index: 125

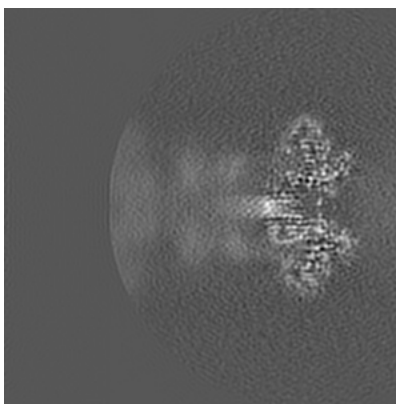
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

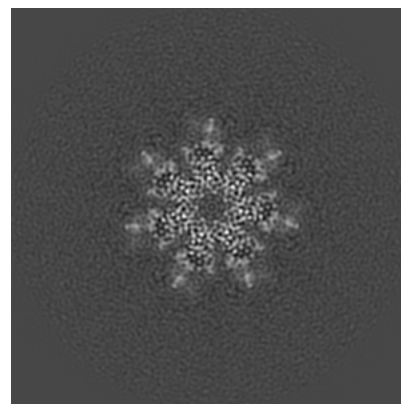
6.3.1 Primary map



X Index: 119



Y Index: 116

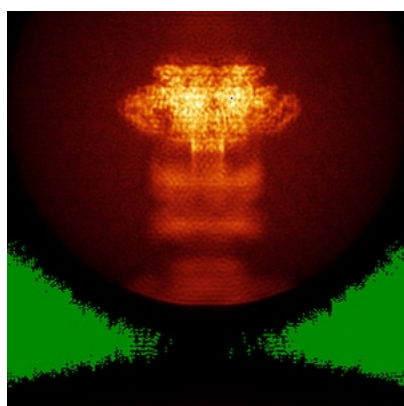


Z Index: 196

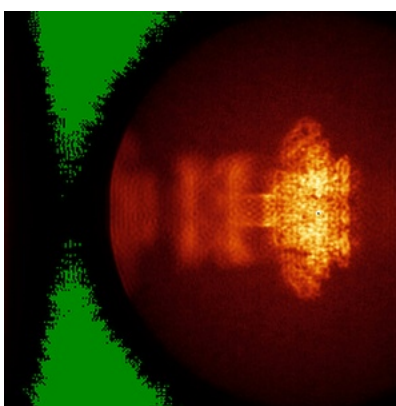
The images above show the largest variance slices of the map in three orthogonal directions.

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

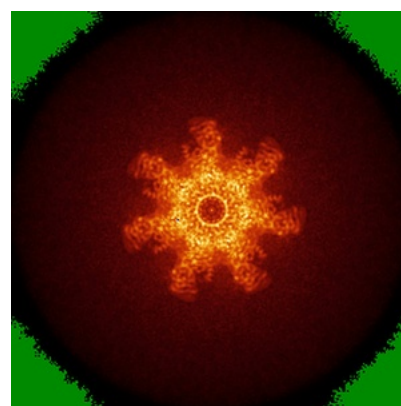
6.4.1 Primary map



X



Y

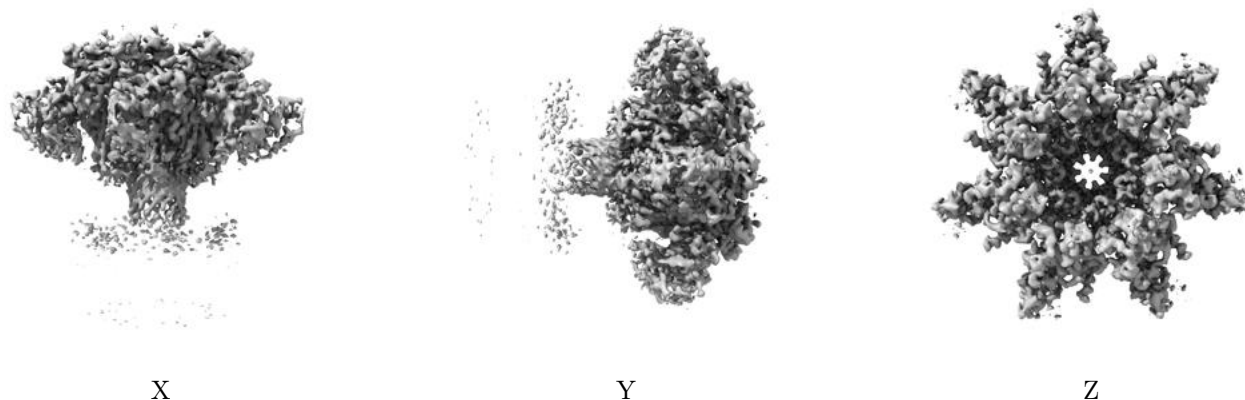


Z

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

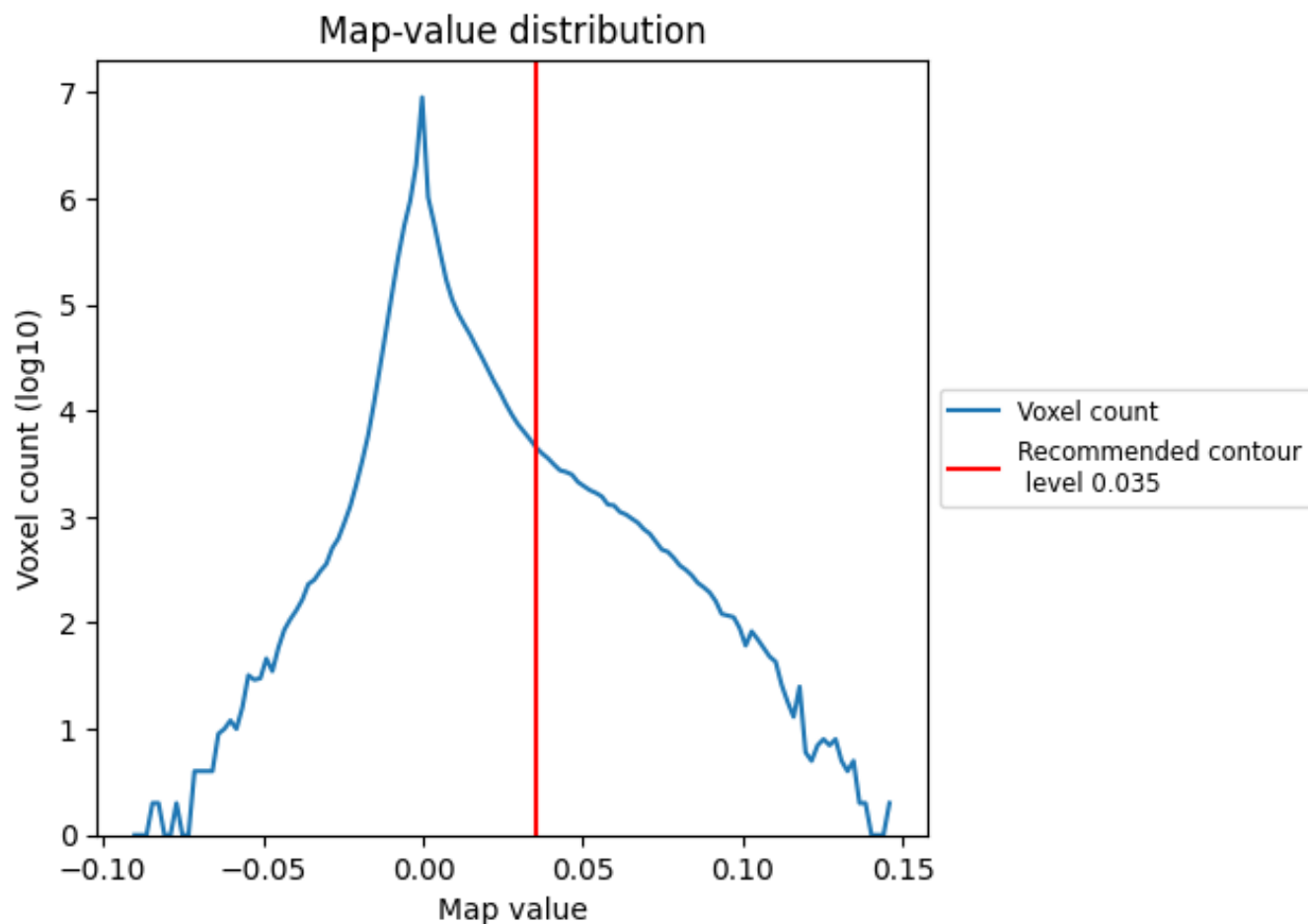
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

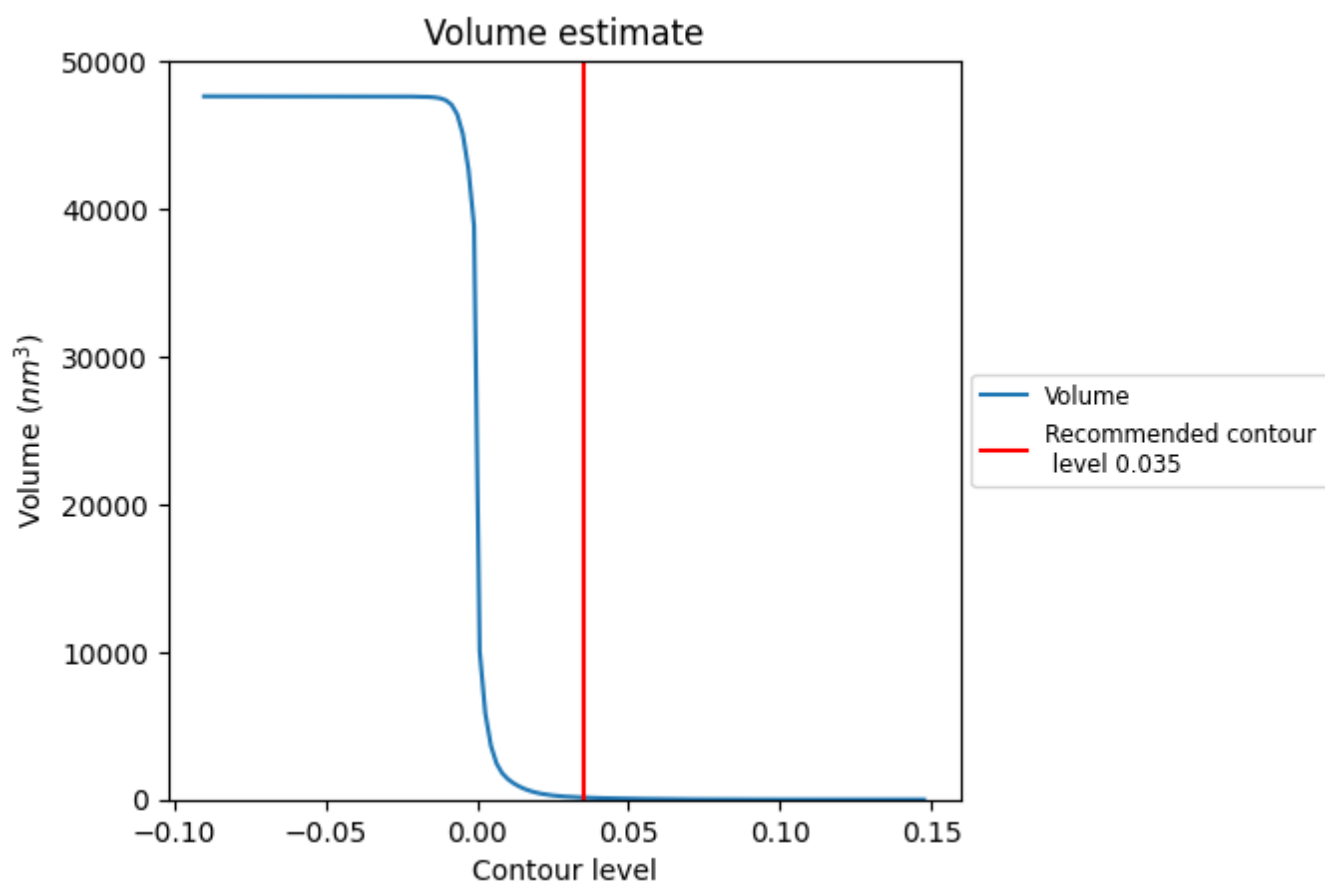
This section contains the results of statistical analysis of the map.

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.

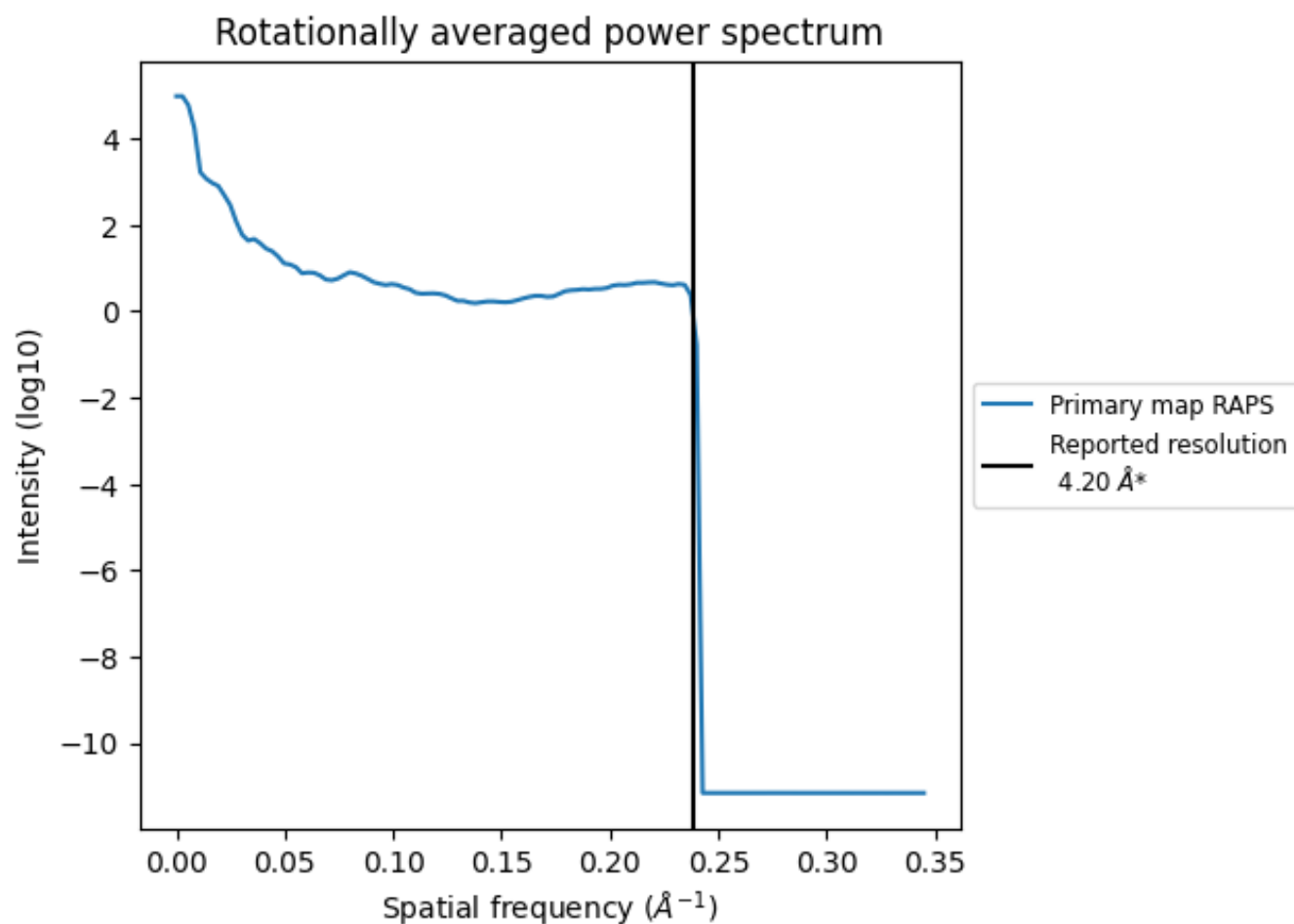
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 126 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 ⓘ

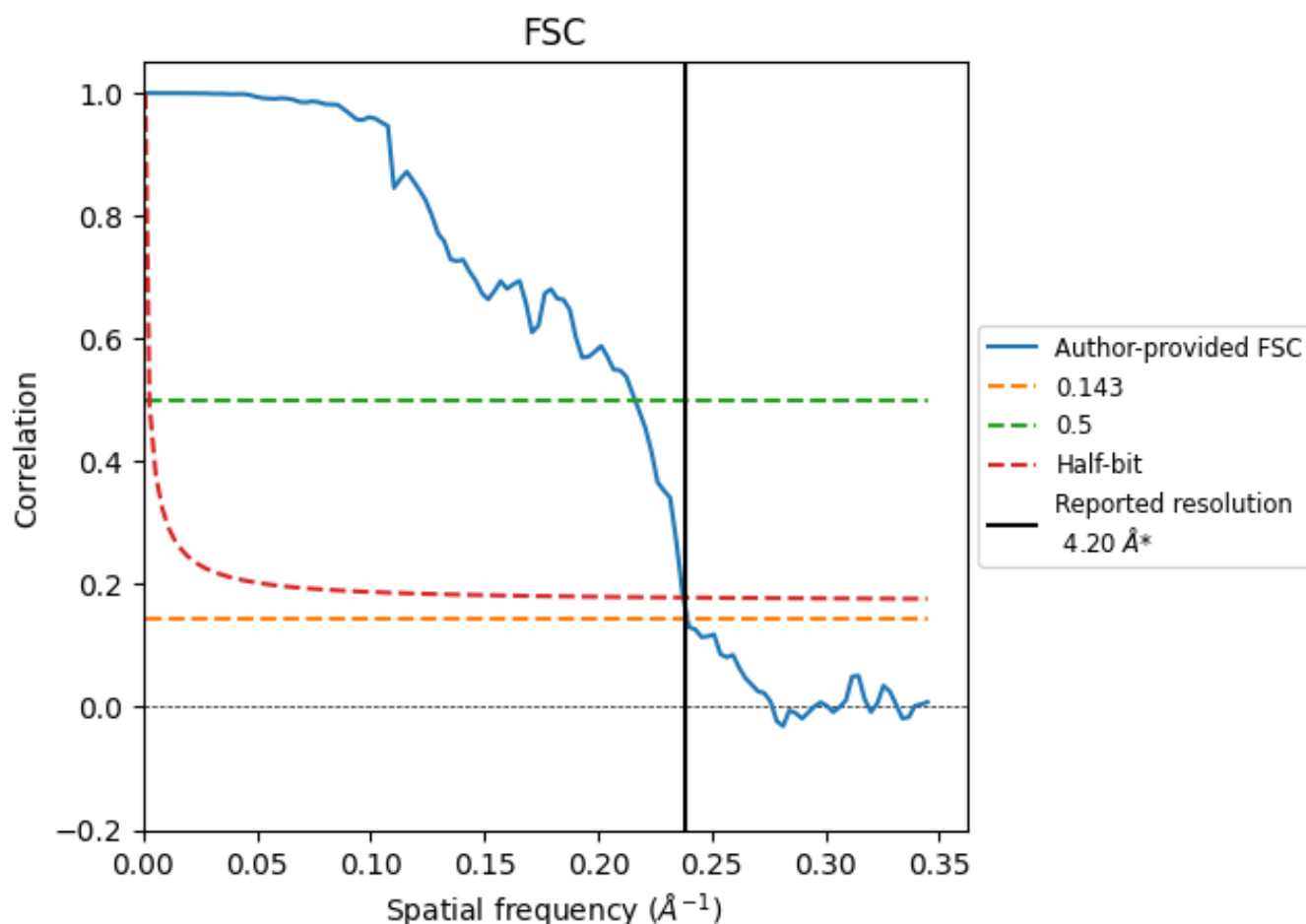


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

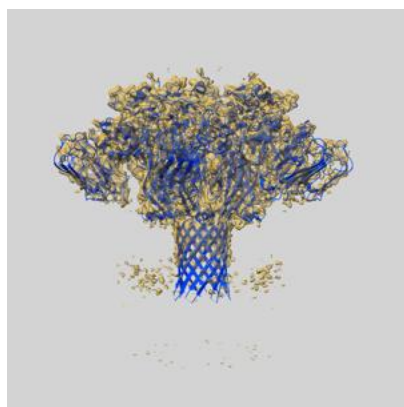
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	4.62	4.21
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

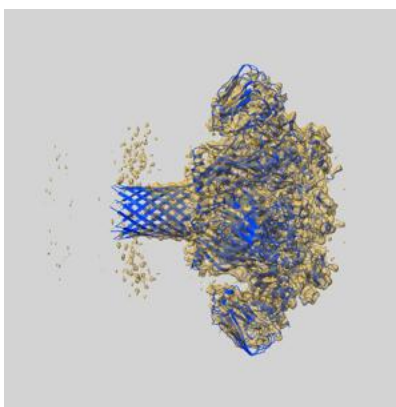
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20104 and PDB model 6OKT. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

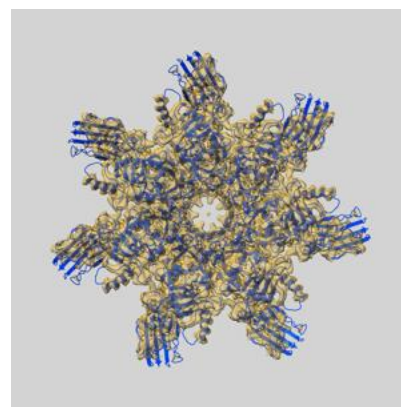
9.1 Map-model overlay [i](#)



X



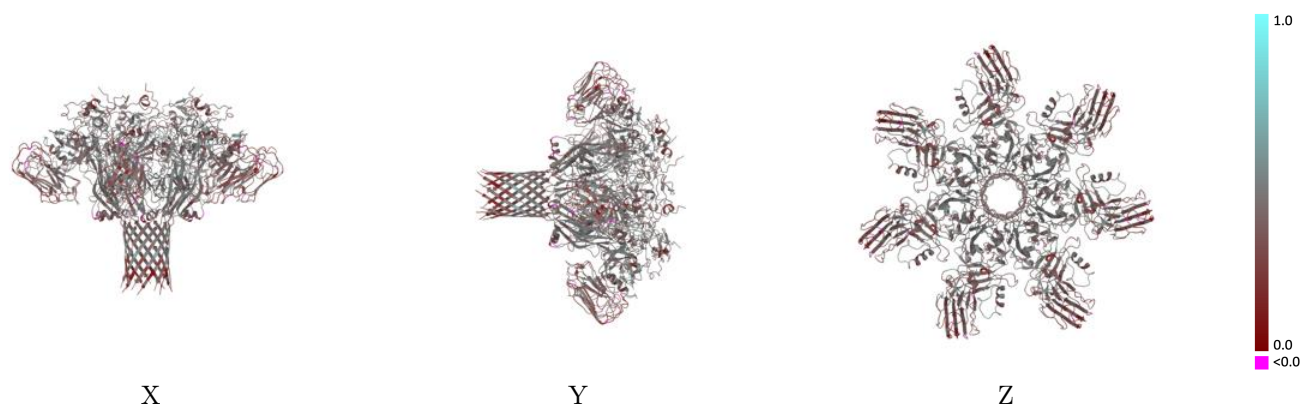
Y



Z

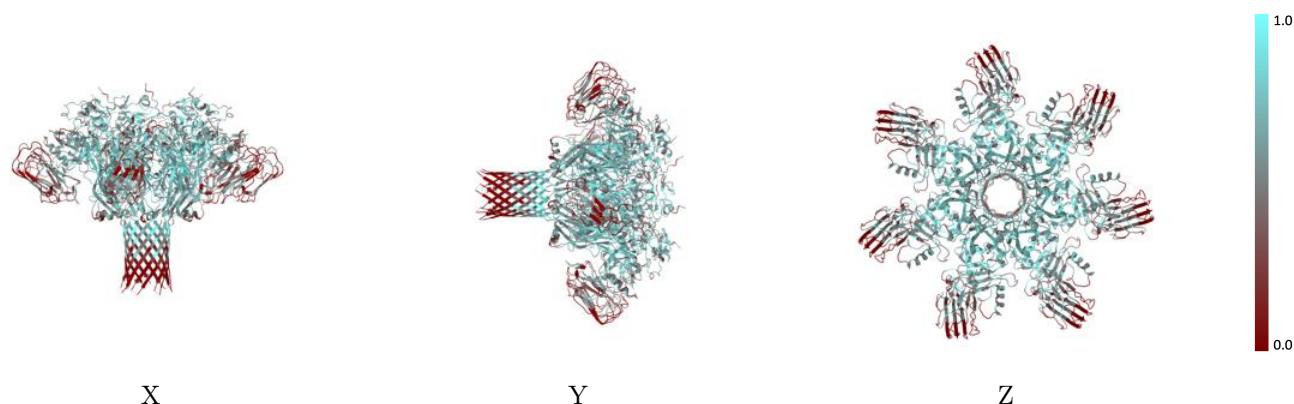
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



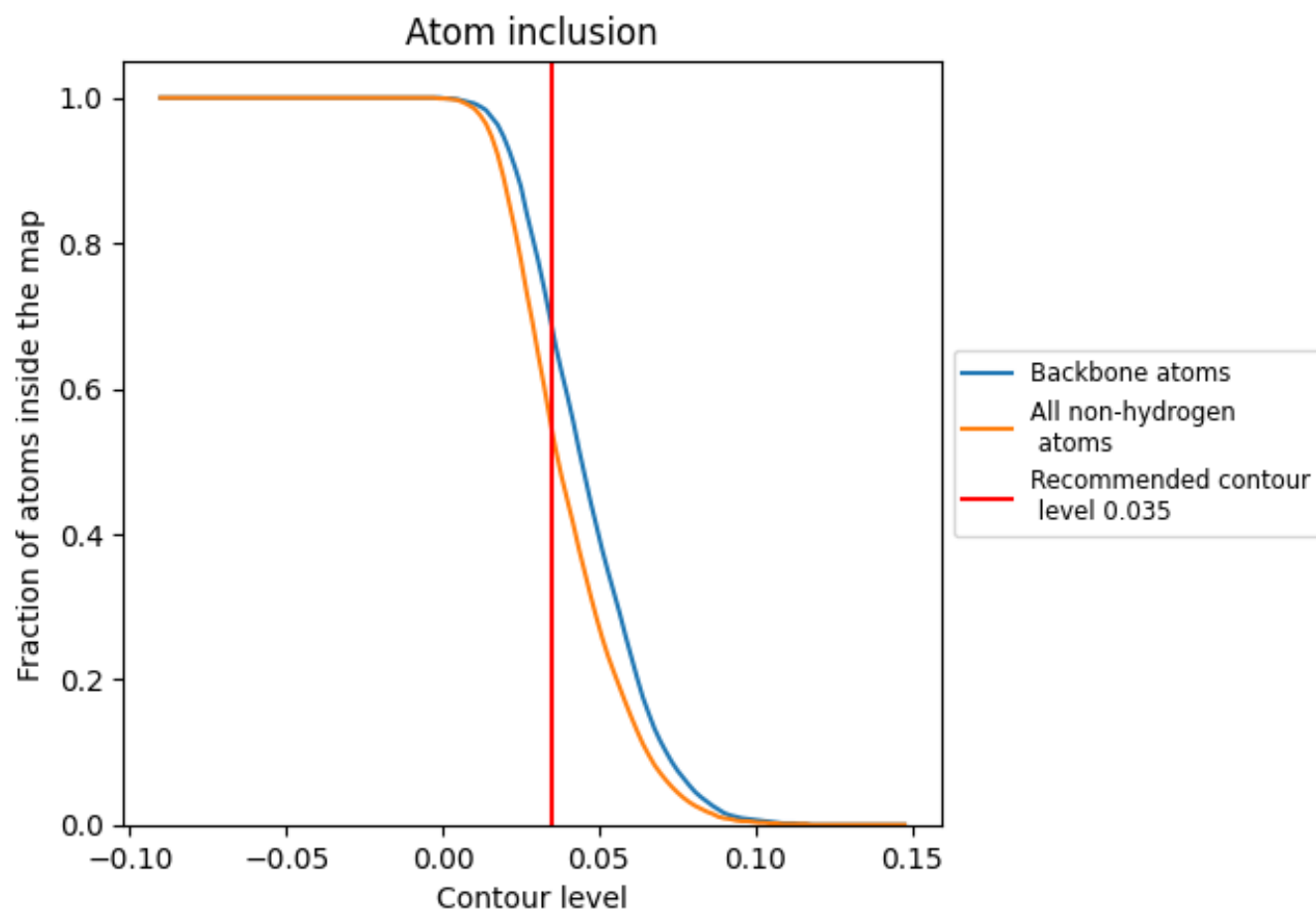
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 54% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.4010
H	0.5440	0.4020
I	0.5450	0.4010
J	0.5380	0.3990
K	0.5420	0.3990
L	0.5420	0.4000
M	0.5420	0.4010
N	0.5370	0.4020

1.0

0.0

<0.0