



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:58 AM UTC

PDB ID : 7R77 / pdb_00007r77
EMDB ID : EMD-24294
Title : Cryo-EM structure of DNMT5 binary complex with hemimethylated DNA
Authors : Wang, J.; Patel, D.J.
Deposited on : 2021-06-24
Resolution : 3.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

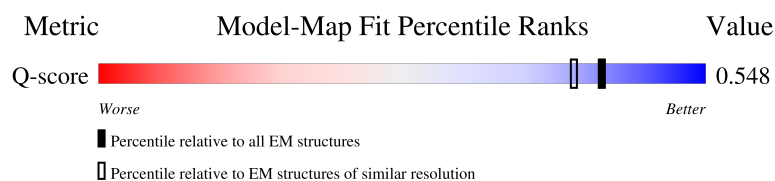
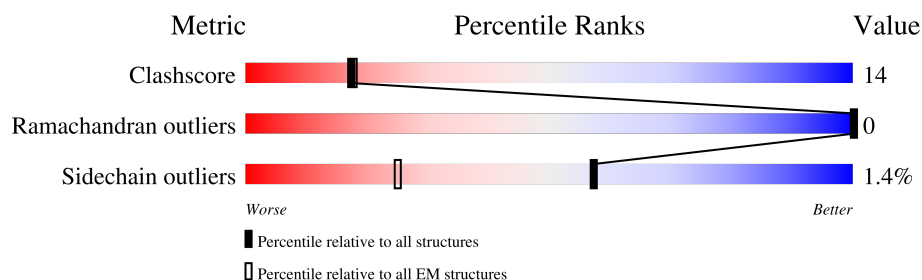
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	2348	
2	B	36	
3	D	36	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14980 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 DNA repair protein Rad8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1830	Total	C	N	O	S	0	0
			14464	9095	2612	2687	70		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP J9VI03
A	31	SER	-	expression tag	UNP J9VI03
A	32	TYR	-	expression tag	UNP J9VI03
A	33	TYR	-	expression tag	UNP J9VI03
A	34	HIS	-	expression tag	UNP J9VI03
A	35	HIS	-	expression tag	UNP J9VI03
A	36	HIS	-	expression tag	UNP J9VI03
A	37	HIS	-	expression tag	UNP J9VI03
A	38	HIS	-	expression tag	UNP J9VI03
A	39	HIS	-	expression tag	UNP J9VI03
A	40	ASP	-	expression tag	UNP J9VI03
A	41	TYR	-	expression tag	UNP J9VI03
A	42	ASP	-	expression tag	UNP J9VI03
A	43	ILE	-	expression tag	UNP J9VI03
A	44	PRO	-	expression tag	UNP J9VI03
A	45	THR	-	expression tag	UNP J9VI03
A	46	THR	-	expression tag	UNP J9VI03
A	47	GLU	-	expression tag	UNP J9VI03
A	48	ASN	-	expression tag	UNP J9VI03
A	49	LEU	-	expression tag	UNP J9VI03
A	50	TYR	-	expression tag	UNP J9VI03
A	51	PHE	-	expression tag	UNP J9VI03
A	52	GLN	-	expression tag	UNP J9VI03
A	53	GLY	-	expression tag	UNP J9VI03
A	54	ALA	-	expression tag	UNP J9VI03
A	55	MET	-	expression tag	UNP J9VI03
A	56	GLY	-	expression tag	UNP J9VI03
A	57	SER	-	expression tag	UNP J9VI03

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	12	Total	C	N	O	P	0	0
			250	118	48	72	12		

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3').

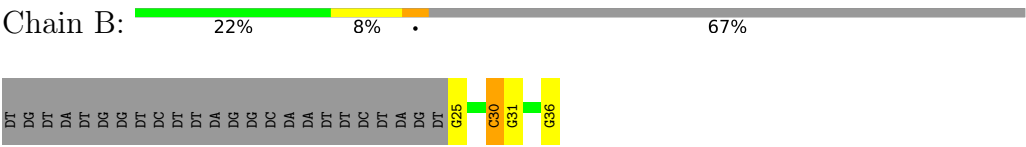
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	13	Total	C	N	O	P	0	0
			261	125	49	75	12		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

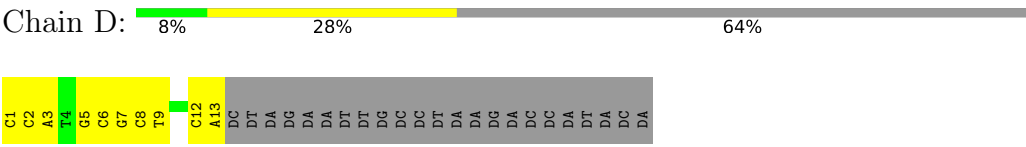
Mol	Chain	Residues	Atoms		AltConf
4	A	5	Total	Zn	0
			5	5	



● Molecule 2: DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3')



● Molecule 3: DNA (5'-D(P*GP*TP*CP*AP*GP*(5CM)P*GP*CP*AP*TP*GP*G)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78477	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	47262	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.071	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	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	A	0.47	0/14759	0.57	4/19976 (0.0%)
2	B	0.52	0/257	0.49	0/393
3	D	0.53	0/292	0.49	0/448
All	All	0.47	0/15308	0.56	4/20817 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	847	PRO	N-CA-C	-6.23	99.64	112.47
1	A	847	PRO	CA-C-N	-5.88	114.00	123.23
1	A	847	PRO	C-N-CA	-5.88	114.00	123.23
1	A	1533	ASP	N-CA-C	-5.43	108.43	114.62

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	A	14464	0	14458	392	0
2	B	250	0	137	8	0
3	D	261	0	147	9	0
4	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14980	0	14742	403	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 14.

The worst 5 of 403 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)
2:B:30:5CM:O4'	2:B:30:5CM:C1'	1.63	1.20
1:A:2011:PRO:HG2	1:A:2012:PRO:CD	1.70	1.19
1:A:2011:PRO:CG	1:A:2012:PRO:HD2	1.72	1.18
1:A:2011:PRO:HG2	1:A:2012:PRO:HD2	1.07	1.05
1:A:846:ARG:HB3	1:A:847:PRO:HD3	1.46	0.94

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	1806/2348 (77%)	1661 (92%)	145 (8%)	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	1569/2015 (78%)	1547 (99%)	22 (1%)	59 80

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1554	ILE
1	A	1963	PHE
1	A	1775	GLU
1	A	2010	ILE
1	A	1105	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2066	GLN
1	A	2193	HIS
1	A	2101	HIS
1	A	2131	ASN
1	A	2254	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
2	5CM	B	30	2,3	18,21,22	5.06	13 (72%)	24,30,33	1.25	2 (8%)

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
2	5CM	B	30	2,3	-	6/7/21/22	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	30	5CM	O4'-C1'	9.60	1.63	1.42
2	B	30	5CM	C6-C5	8.35	1.48	1.34
2	B	30	5CM	O4'-C4'	-7.68	1.27	1.45
2	B	30	5CM	C2'-C1'	-7.58	1.31	1.52
2	B	30	5CM	C4-N3	6.40	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	5CM	C5-C6-N1	-2.91	120.16	123.31
2	B	30	5CM	C5A-C5-C6	-2.35	119.67	122.85

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	30	5CM	C3'-C4'-C5'-O5'
2	B	30	5CM	O4'-C4'-C5'-O5'
2	B	30	5CM	C2'-C1'-N1-C6
2	B	30	5CM	C2'-C1'-N1-C2
2	B	30	5CM	O4'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	30	5CM	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

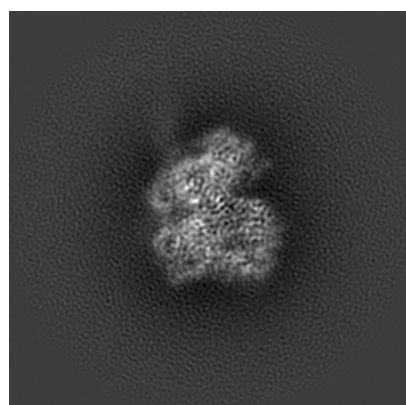
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24294. These allow visual inspection of the internal detail of the map and identification of artifacts.

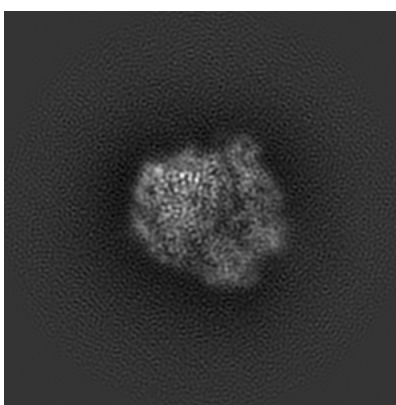
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

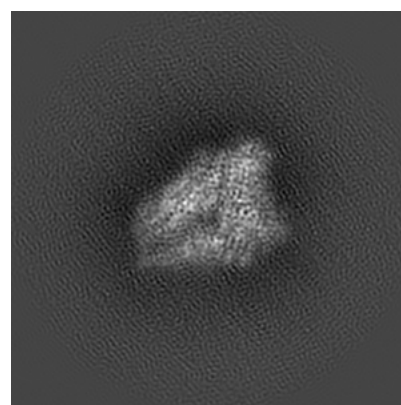
6.1.1 Primary map



X



Y

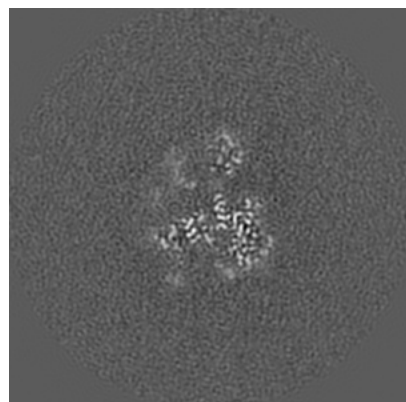


Z

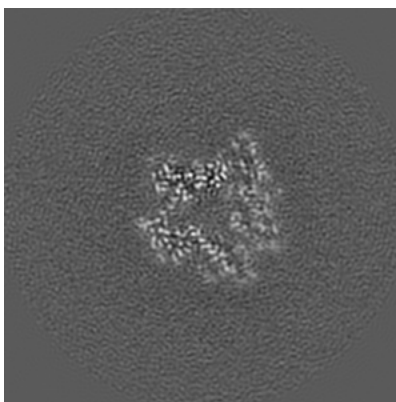
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

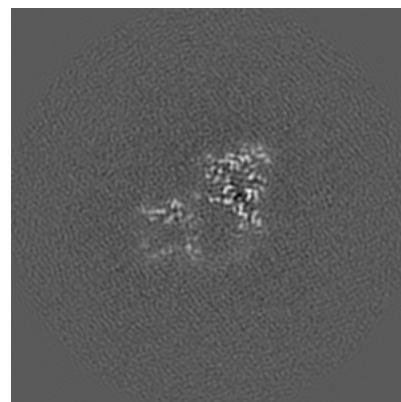
6.2.1 Primary map



X Index: 128



Y Index: 128

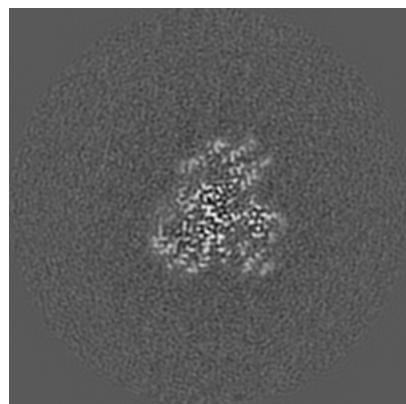


Z Index: 128

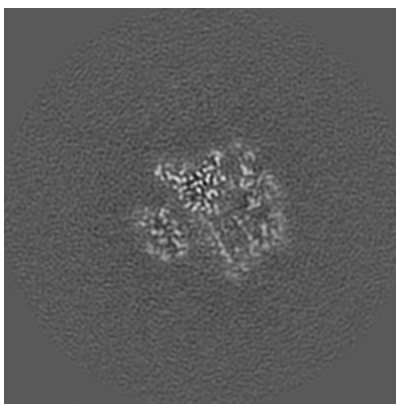
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

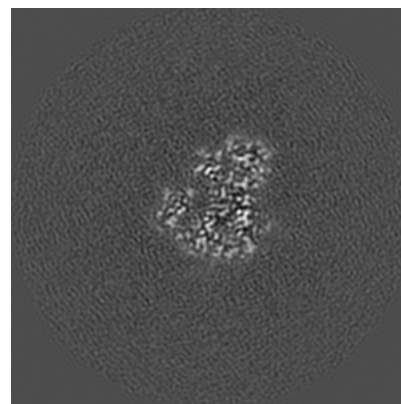
6.3.1 Primary map



X Index: 147



Y Index: 134

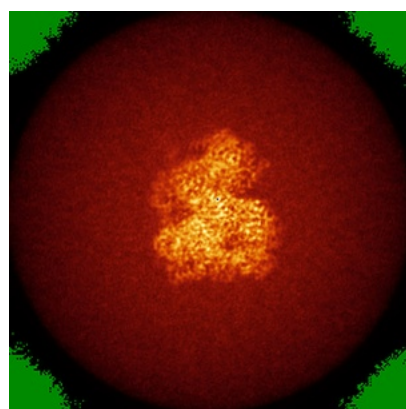


Z Index: 114

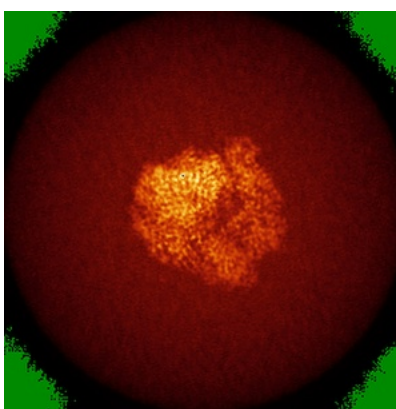
The images above show the largest variance slices of the map in three orthogonal directions.

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

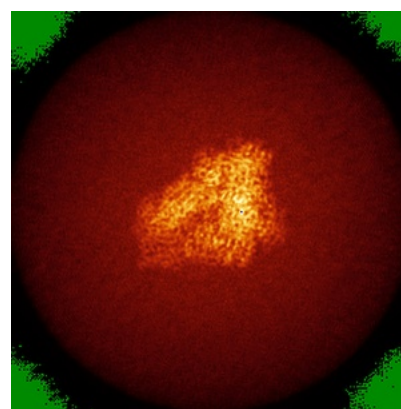
6.4.1 Primary map



X



Y

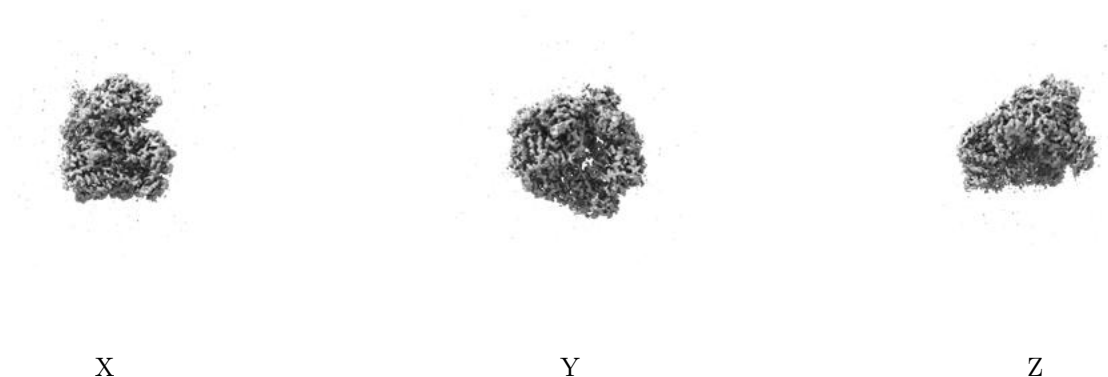


Z

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

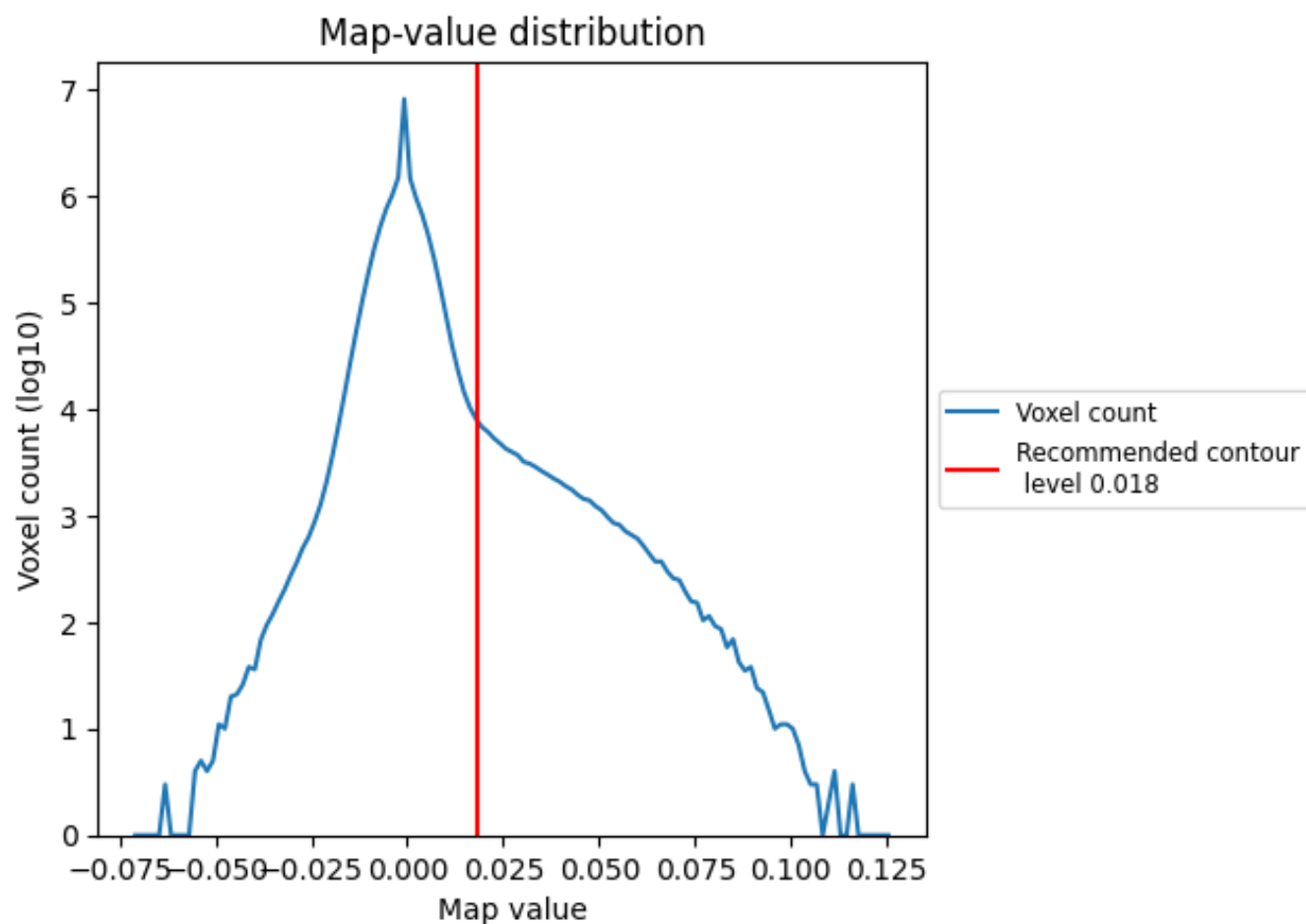
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

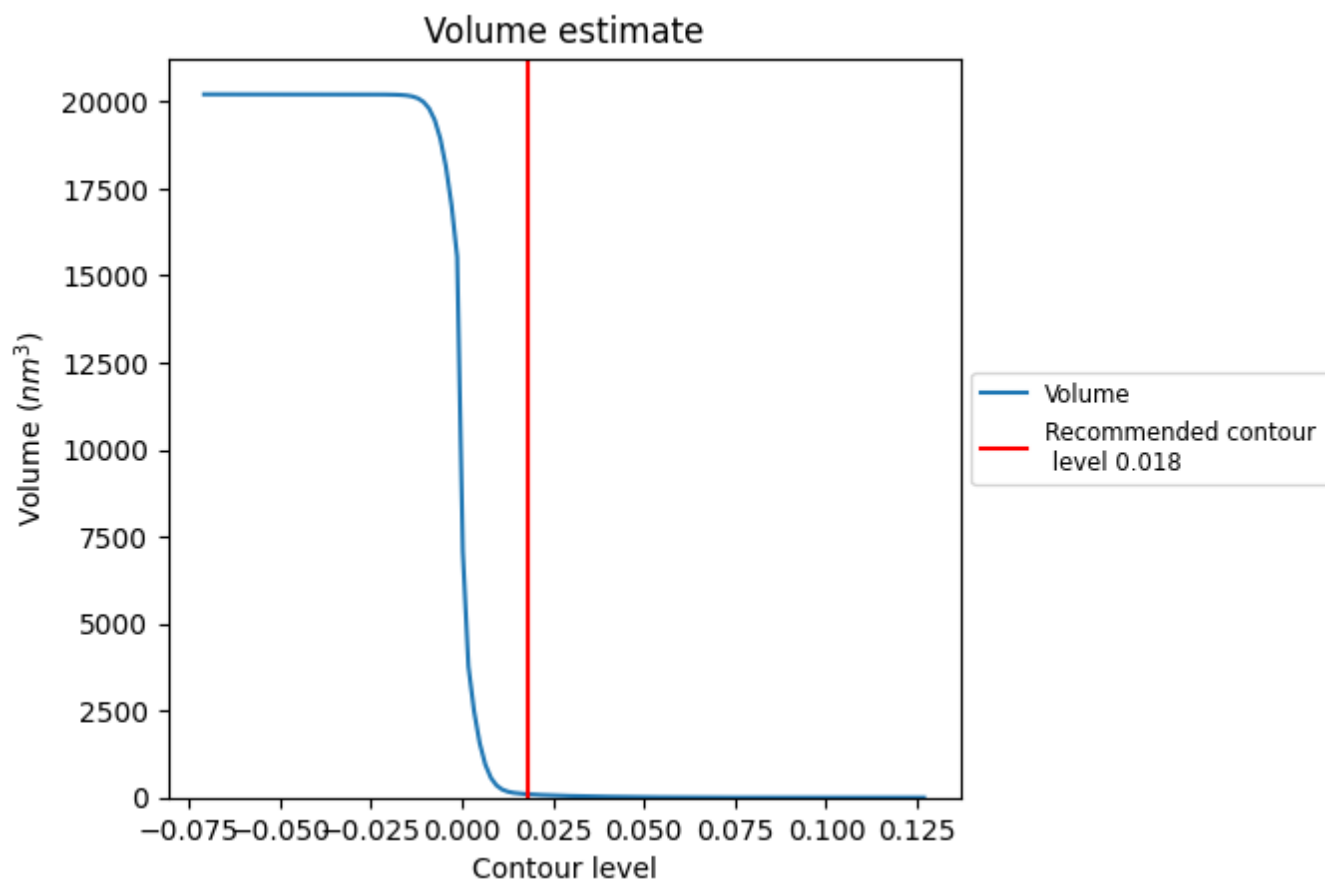
This section contains the results of statistical analysis of the map.

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.

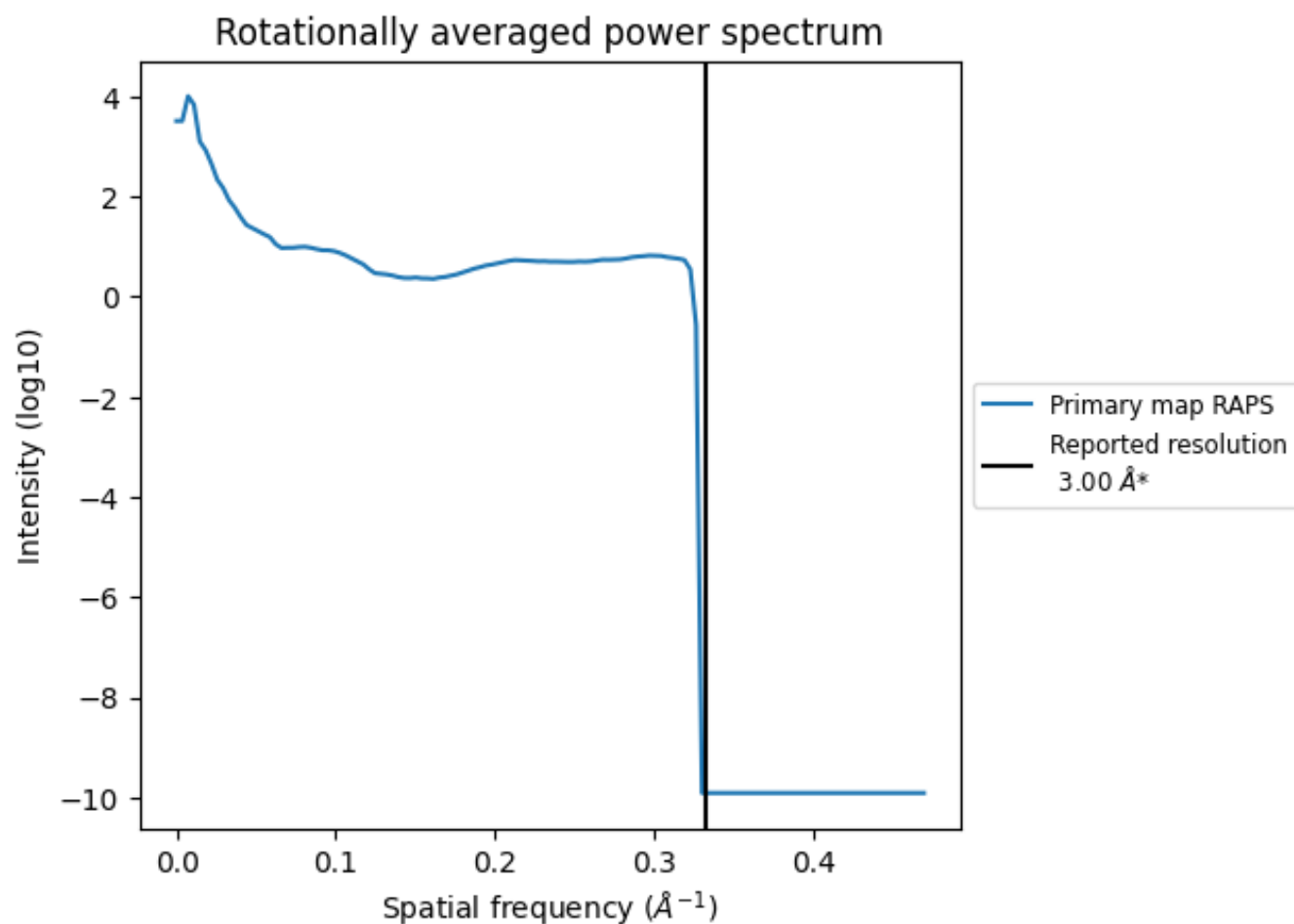
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm^3 ; this corresponds to an approximate mass of 87 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 0.333 Å⁻¹

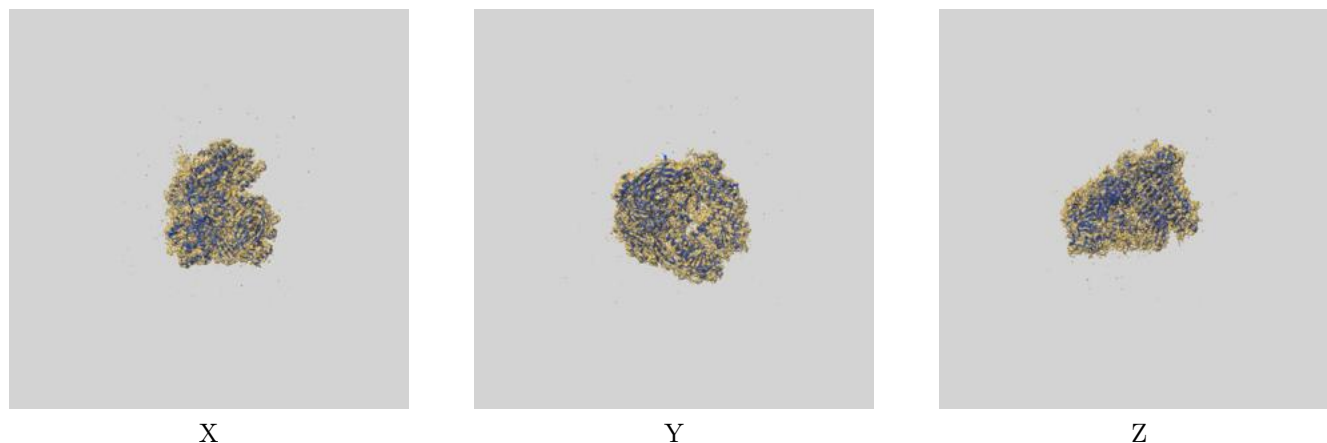
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

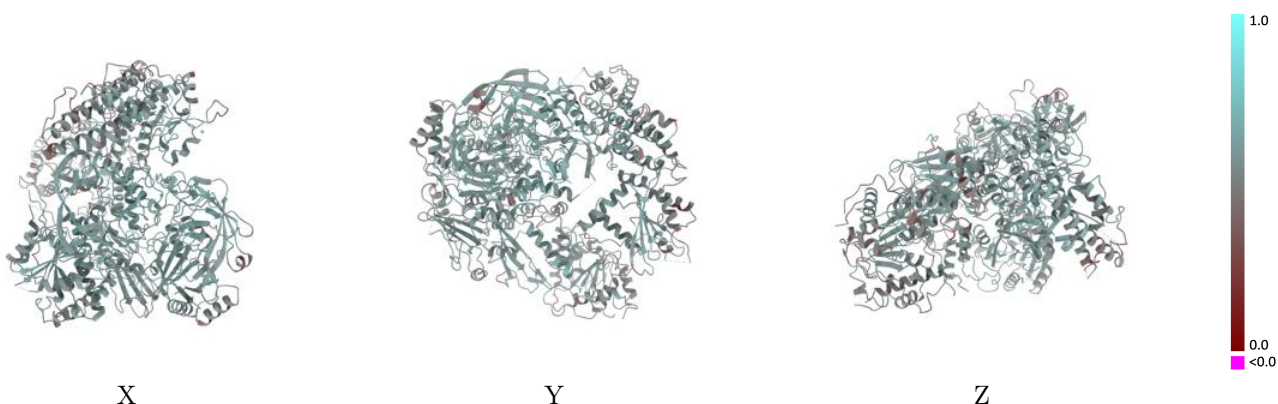
This section contains information regarding the fit between EMDB map EMD-24294 and PDB model 7R77. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



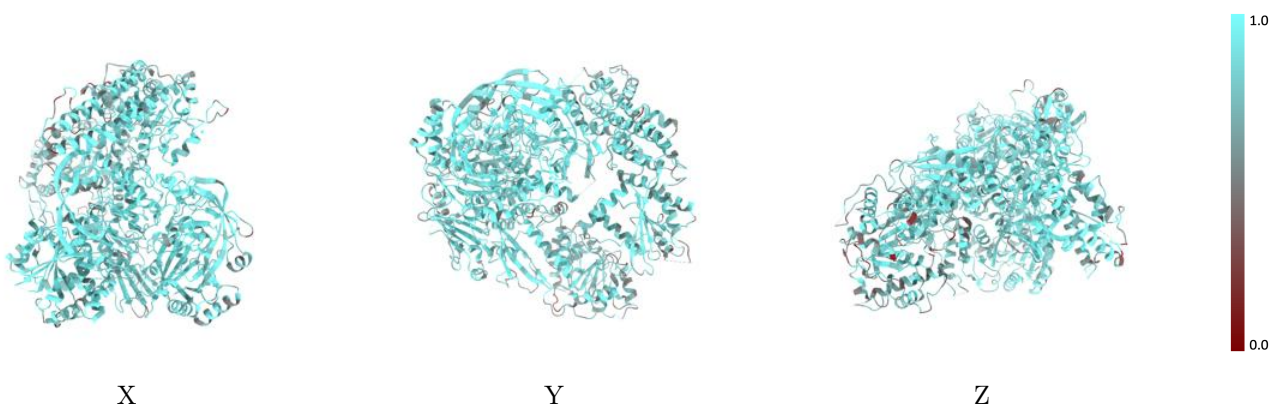
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



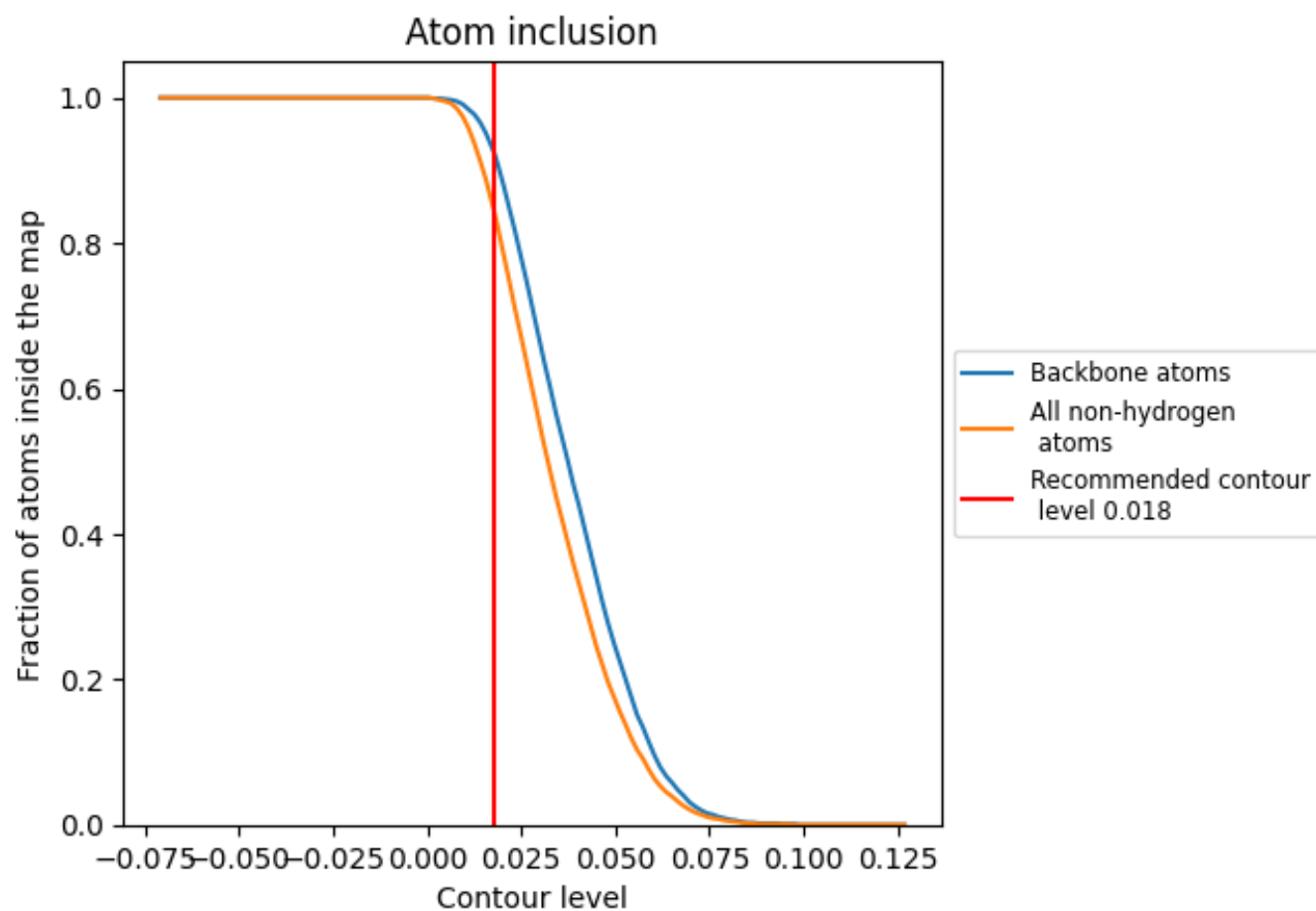
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.5480
A	0.8370	0.5470
B	0.9440	0.5910
D	0.9350	0.5770

