



wwPDB EM Validation Summary Report ⓘ

Aug 31, 2026 – 10:22 AM EDT

PDB ID : 9MYS / pdb_00009mys
EMDB ID : EMD-48749
Title : The cryo-EM structure of the mutant MHKKKQ DNMT1-umNCP complex
Authors : Fang, J.; Song, J.
Deposited on : 2025-01-22
Resolution : 3.93 Å(reported)
Based on initial models : 7XI9, 3pt6, 7JZV

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

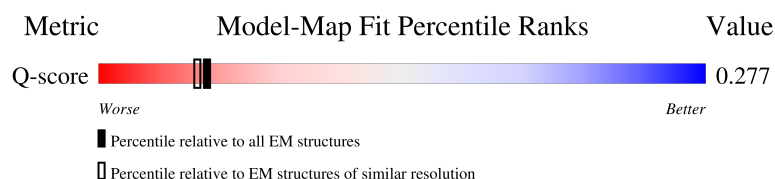
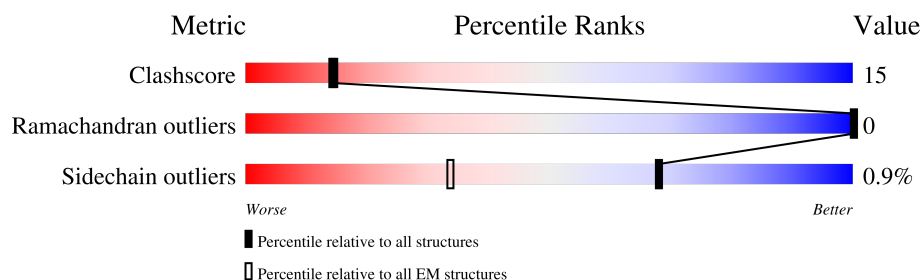
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

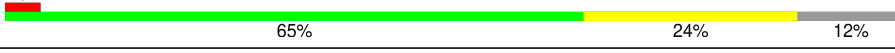
The reported resolution of this entry is 3.93 Å.

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.



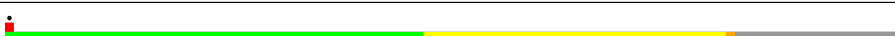
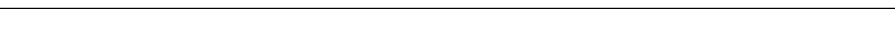
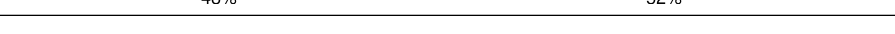
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7811 (3.43 - 4.43)

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	1250	
2	N	130	
2	n	130	
3	O	123	

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Mol	Chain	Length	Quality of chain
3	o	123	
4	P	136	
4	p	136	
5	Q	103	
5	q	103	
6	X	149	
7	Y	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	A	1703	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19120 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 (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	887	Total	C	N	O	S	0	0
			6832	4318	1201	1261	52		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	718	ALA	MET	engineered mutation	UNP P26358
A	719	ALA	HIS	engineered mutation	UNP P26358
A	723	ALA	LYS	engineered mutation	UNP P26358
A	724	ALA	LYS	engineered mutation	UNP P26358
A	725	ALA	LYS	engineered mutation	UNP P26358
A	726	ALA	GLN	engineered mutation	UNP P26358

- Molecule 2 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	111	Total	C	N	O	0	0
			849	533	167	149		
2	n	115	Total	C	N	O	0	0
			863	541	168	154		

- Molecule 3 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	94	Total	C	N	O	S	0	0
			735	463	132	138	2		
3	o	98	Total	C	N	O	S	0	0
			772	484	143	143	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	MET	-	initiating methionine	UNP P02281

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Chain	Residue	Modelled	Actual	Comment	Reference
O	29	THR	SER	engineered mutation	UNP P02281
o	0	MET	-	initiating methionine	UNP P02281
o	29	THR	SER	engineered mutation	UNP P02281

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	100	Total	C	N	O	S	0	0
			812	512	155	143	2		
4	p	100	Total	C	N	O	S	0	0
			827	523	160	142	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	18	CYS	LYS	conflict	UNP A0A310TTQ1
P	23	CYS	LYS	conflict	UNP A0A310TTQ1
P	110	SER	CYS	conflict	UNP A0A310TTQ1
p	18	CYS	LYS	conflict	UNP A0A310TTQ1
p	23	CYS	LYS	conflict	UNP A0A310TTQ1
p	110	SER	CYS	conflict	UNP A0A310TTQ1

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	82	Total	C	N	O	S	0	0
			647	409	124	113	1		
5	q	84	Total	C	N	O	S	0	0
			670	423	130	115	2		

- Molecule 6 is a DNA chain called Nucleosome 601 DNA (149-MER).

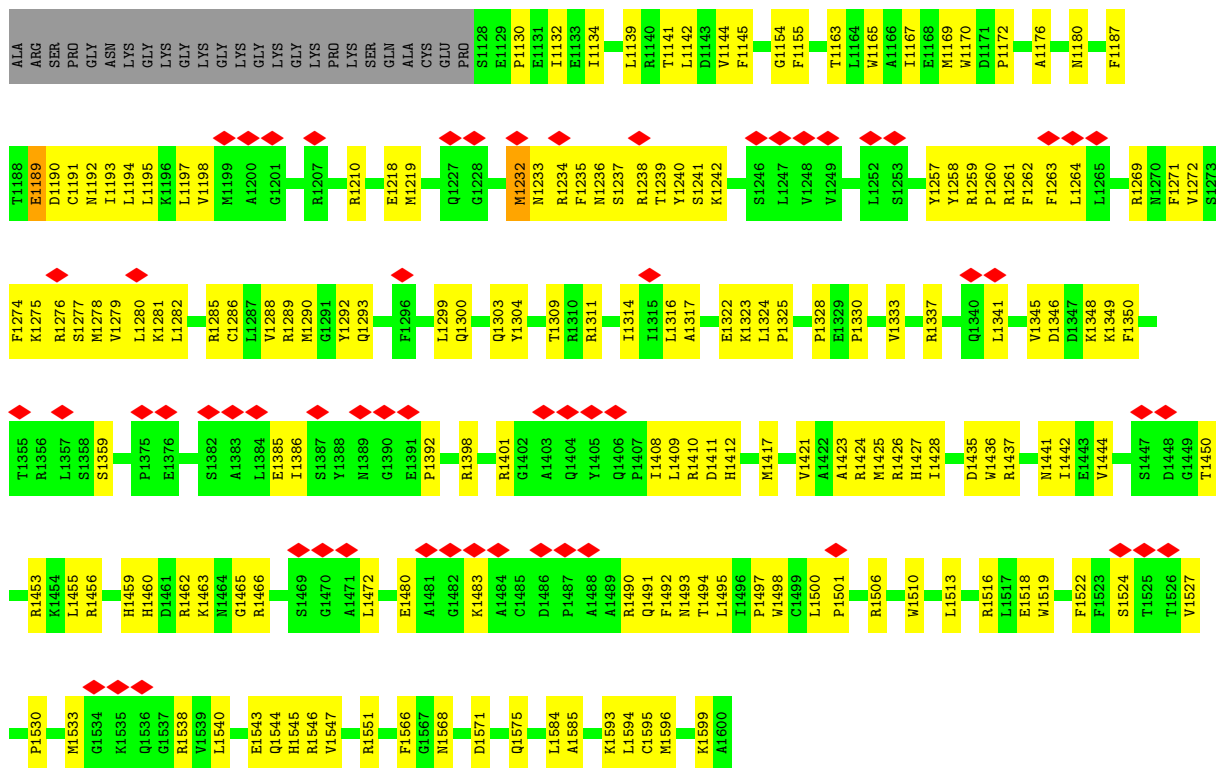
Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	149	Total	C	N	O	P	0	0
			3073	1454	580	890	149		

- Molecule 7 is a DNA chain called Nucleosome 601 DNA (149-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	149	Total	C	N	O	P	0	0
			3036	1443	546	898	149		

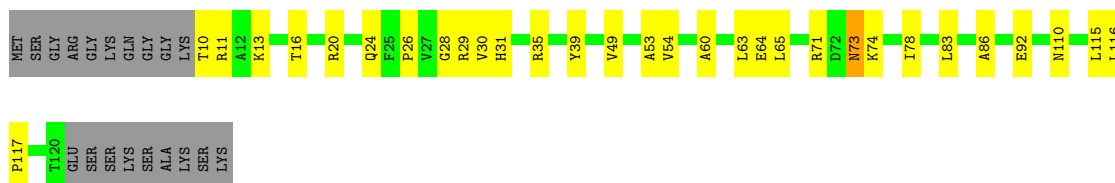
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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



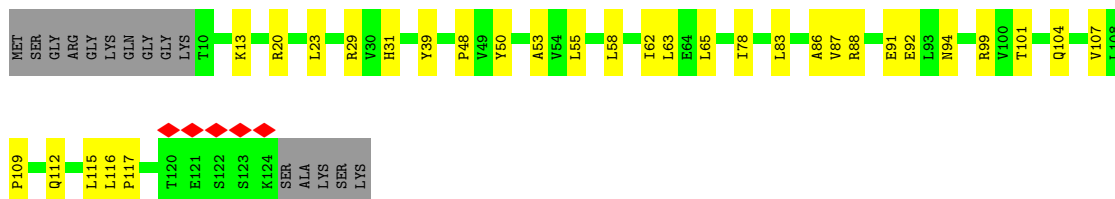
• Molecule 2: Histone H2A

Chain N: 62% 23% 15%



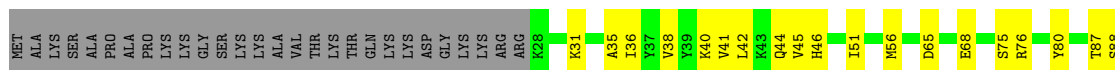
• Molecule 2: Histone H2A

Chain n: 65% 24% 12%



• Molecule 3: Histone H2B 1.1

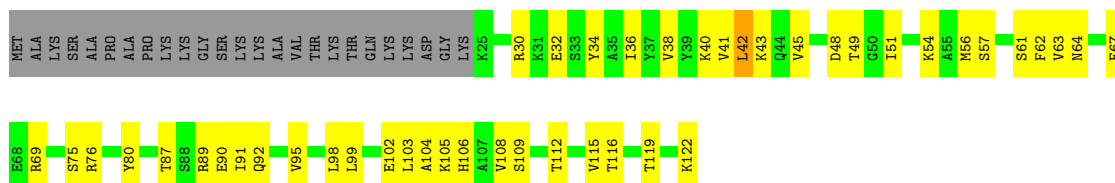
Chain O: 51% 25% 24%





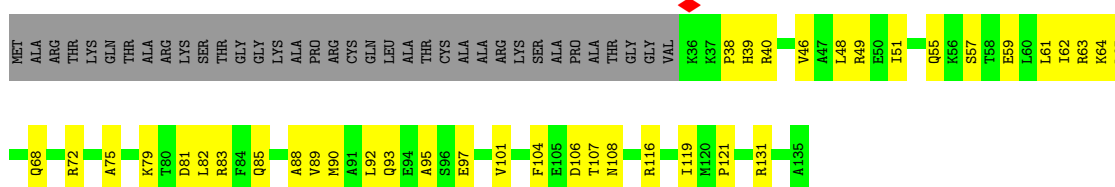
• Molecule 3: Histone H2B 1.1

Chain o: 43% 36% 20%



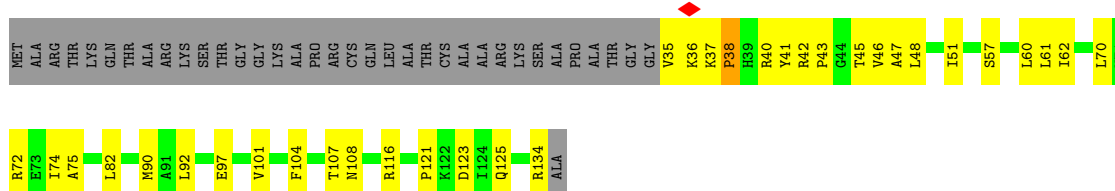
• Molecule 4: Histone H3

Chain P: 45% 29% 26%



• Molecule 4: Histone H3

Chain p: 49% 24% 26%



• Molecule 5: Histone H4

Chain Q: 45% 35% 20%



• Molecule 5: Histone H4

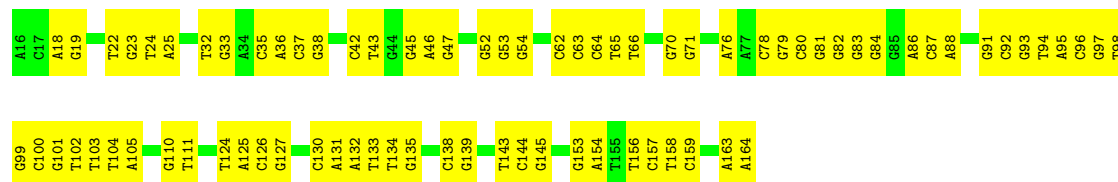
Chain q: 47% 34% 18%





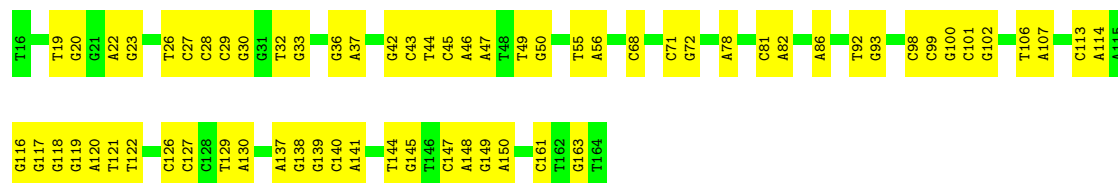
- Molecule 6: Nucleosome 601 DNA (149-MER)

Chain X: 48% 52%



- Molecule 7: Nucleosome 601 DNA (149-MER)

Chain Y: 56% 44%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287638	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	65.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	59.619	Depositor
Minimum map value	-30.046	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.978	Depositor
Recommended contour level	2.8	Depositor
Map size (Å)	380.8768, 380.8768, 380.8768	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4878, 1.4878, 1.4878	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ML3, 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	0.17	0/6994	0.48	0/9483
2	N	0.21	0/859	0.55	0/1161
2	n	0.22	0/873	0.52	0/1181
3	O	0.18	0/746	0.44	0/1004
3	o	0.18	0/783	0.48	0/1050
4	P	0.17	0/824	0.44	0/1107
4	p	0.22	0/839	0.54	1/1125 (0.1%)
5	Q	0.19	0/654	0.49	0/876
5	q	0.19	0/664	0.45	0/887
6	X	0.17	0/3452	0.37	0/5330
7	Y	0.17	0/3400	0.36	0/5241
All	All	0.18	0/20088	0.45	1/28445 (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
4	p	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	38	PRO	CA-N-CD	-8.74	99.77	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	p	134	ARG	Sidechain

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	6832	0	6521	221	0
2	N	849	0	900	35	0
2	n	863	0	898	31	0
3	O	735	0	760	38	0
3	o	772	0	801	42	0
4	P	812	0	838	37	0
4	p	827	0	875	38	0
5	Q	647	0	685	40	0
5	q	670	0	714	36	0
6	X	3073	0	1671	69	0
7	Y	3036	0	1675	50	0
8	A	4	0	0	2	0
All	All	19120	0	16338	540	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 15.

The worst 5 of 540 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)
4:p:37:LYS:HB3	4:p:38:PRO:HD3	1.50	0.94
1:A:656:CYS:HG	8:A:1703:ZN:ZN	0.77	0.94
1:A:1436:TRP:HZ2	1:A:1510:TRP:HB2	1.38	0.88
1:A:651:ARG:HE	1:A:652:ARG:H	1.20	0.86
5:q:24:ASP:OD1	5:q:24:ASP:N	2.16	0.78

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	877/1250 (70%)	846 (96%)	31 (4%)	0	100	100
2	N	109/130 (84%)	104 (95%)	5 (5%)	0	100	100
2	n	113/130 (87%)	109 (96%)	4 (4%)	0	100	100
3	O	92/123 (75%)	87 (95%)	5 (5%)	0	100	100
3	o	96/123 (78%)	92 (96%)	4 (4%)	0	100	100
4	P	98/136 (72%)	97 (99%)	1 (1%)	0	100	100
4	p	98/136 (72%)	93 (95%)	5 (5%)	0	100	100
5	Q	80/103 (78%)	77 (96%)	3 (4%)	0	100	100
5	q	81/103 (79%)	78 (96%)	3 (4%)	0	100	100
All	All	1644/2234 (74%)	1583 (96%)	61 (4%)	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	A	709/1078 (66%)	702 (99%)	7 (1%)	68	76
2	N	86/102 (84%)	85 (99%)	1 (1%)	63	73
2	n	86/102 (84%)	85 (99%)	1 (1%)	63	73
3	O	80/103 (78%)	80 (100%)	0	100	100
3	o	83/103 (81%)	81 (98%)	2 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P	84/111 (76%)	84 (100%)	0	100	100
4	p	88/111 (79%)	88 (100%)	0	100	100
5	Q	66/78 (85%)	66 (100%)	0	100	100
5	q	67/78 (86%)	66 (98%)	1 (2%)	57	71
All	All	1349/1866 (72%)	1337 (99%)	12 (1%)	68	76

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	73	ASN
2	n	101	THR
5	q	24	ASP
3	o	42	LEU
1	A	1189	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	24	GLN
2	N	94	ASN
5	q	75	HIS
2	n	104	GLN
3	o	81	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
5	ML3	q	20	5	10,11,12	0.37	0	11,14,16	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ML3	q	20	5	-	3/8/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	q	20	ML3	N-CA-CB-SG
5	q	20	ML3	C-CA-CB-SG
5	q	20	ML3	SG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

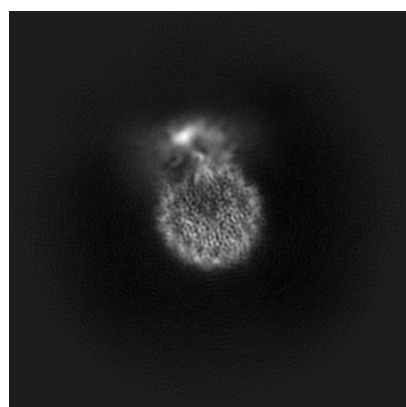
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48749. These allow visual inspection of the internal detail of the map and identification of artifacts.

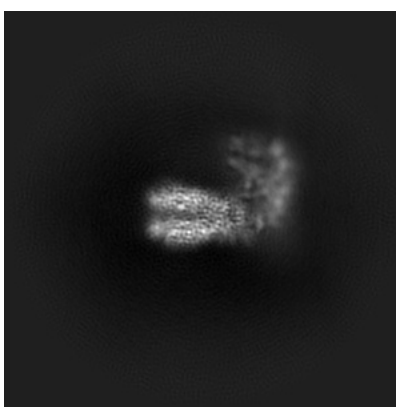
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

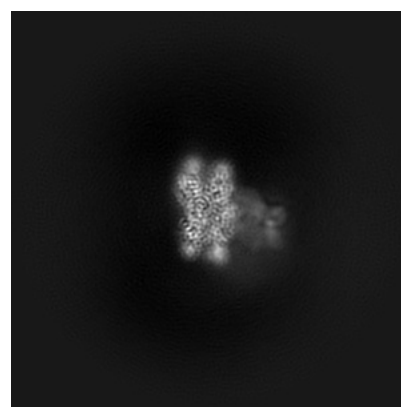
6.1.1 Primary map



X



Y

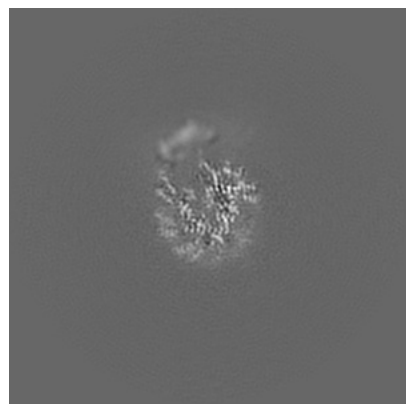


Z

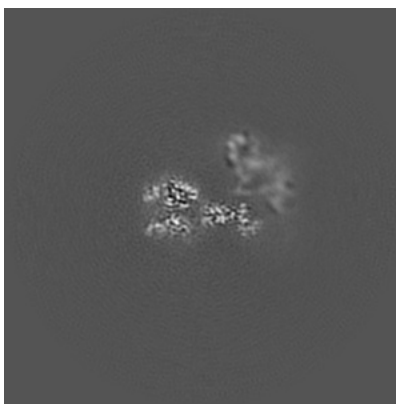
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

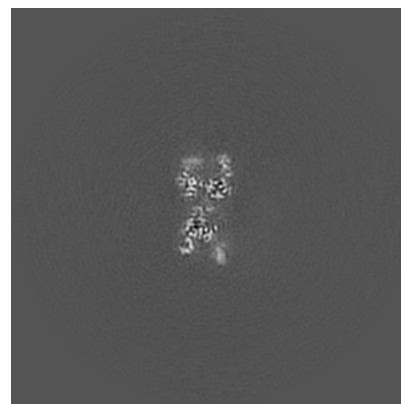
6.2.1 Primary map



X Index: 128



Y Index: 128

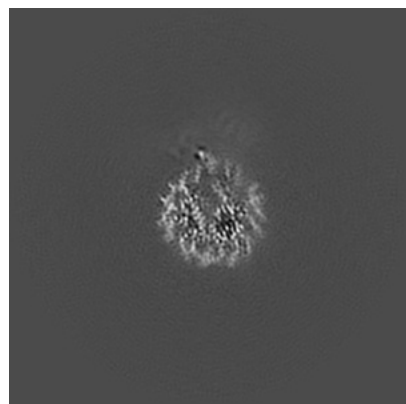


Z Index: 128

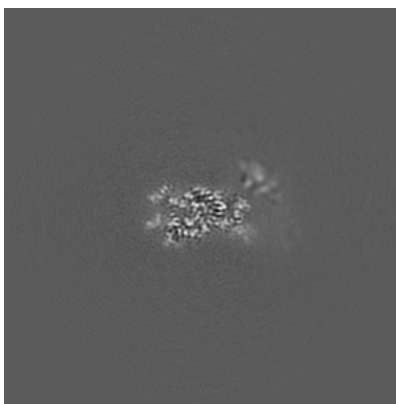
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

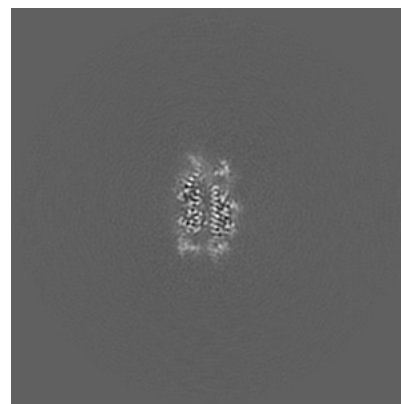
6.3.1 Primary map



X Index: 115



Y Index: 140

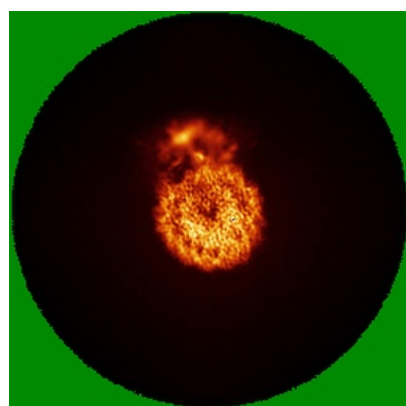


Z Index: 113

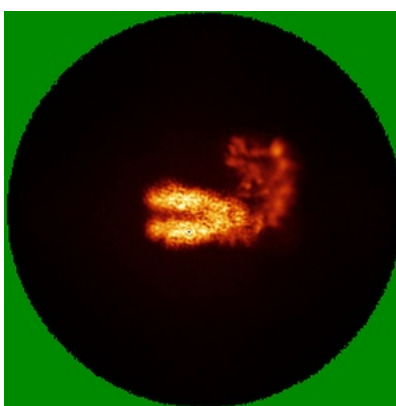
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

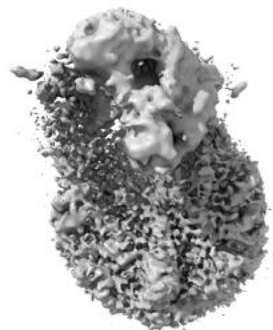


Z

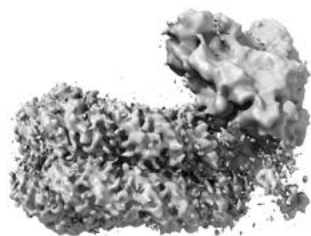
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

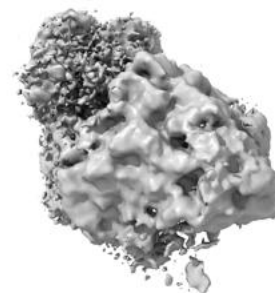
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

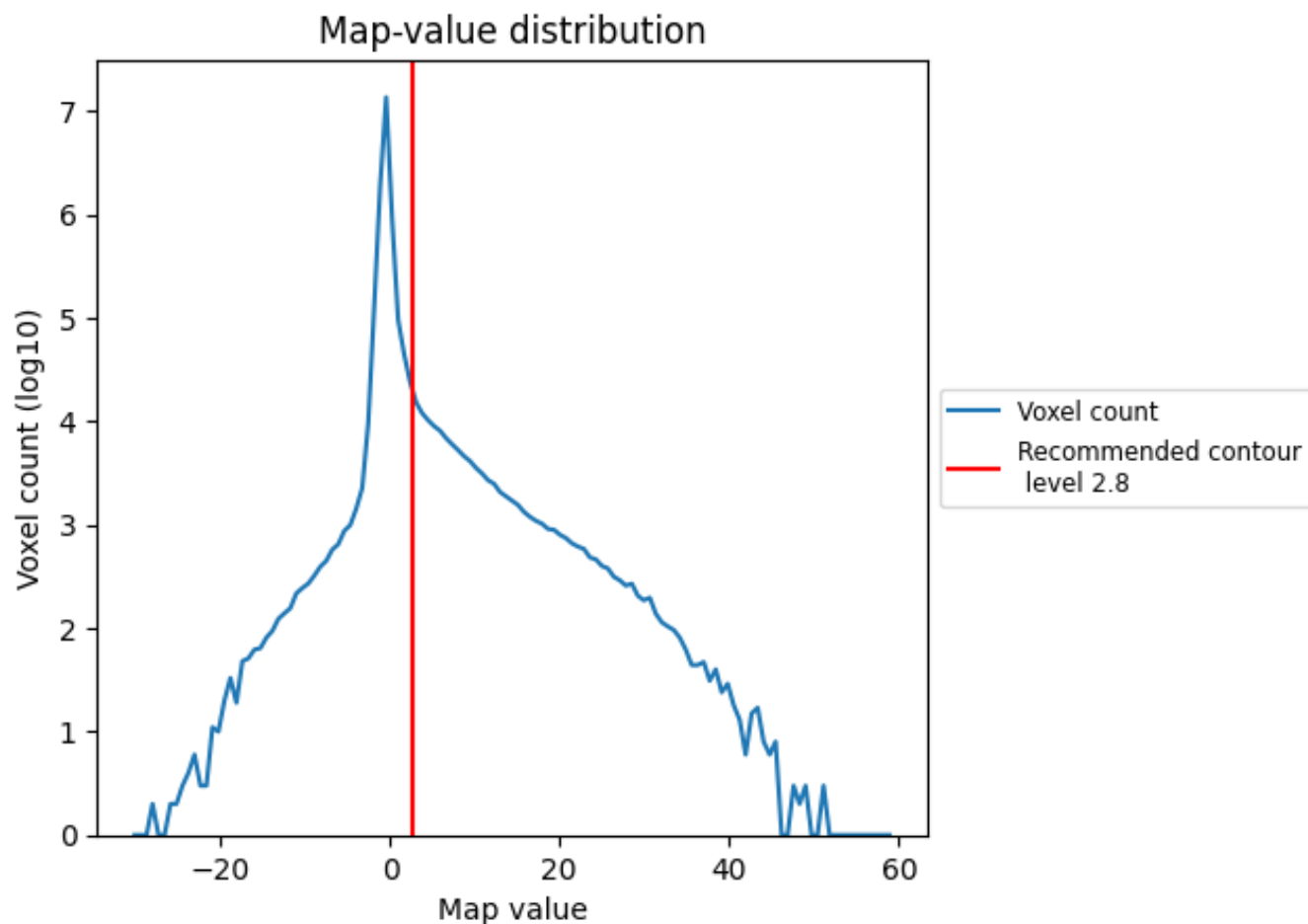
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

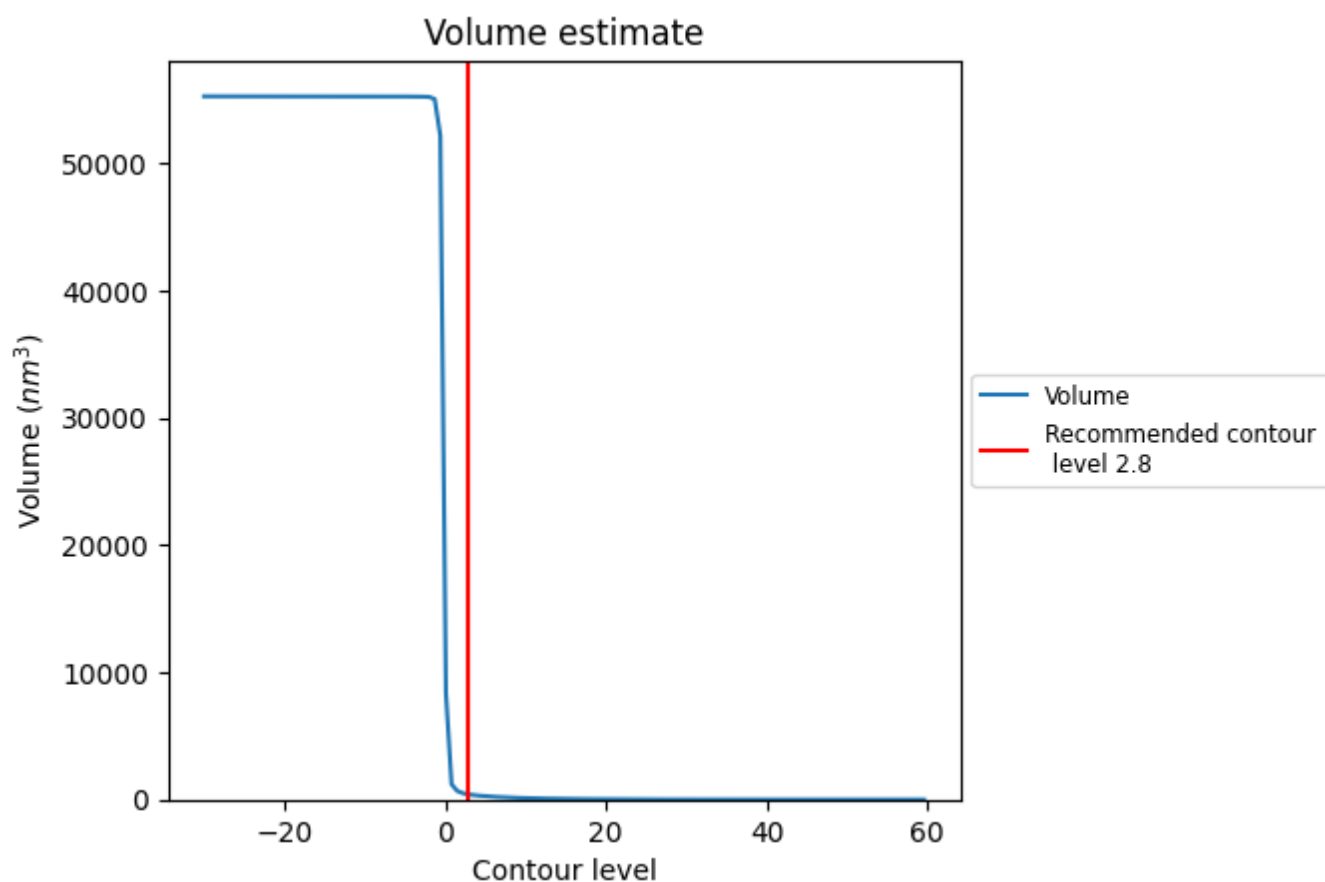
This section contains the results of statistical analysis of the map.

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.

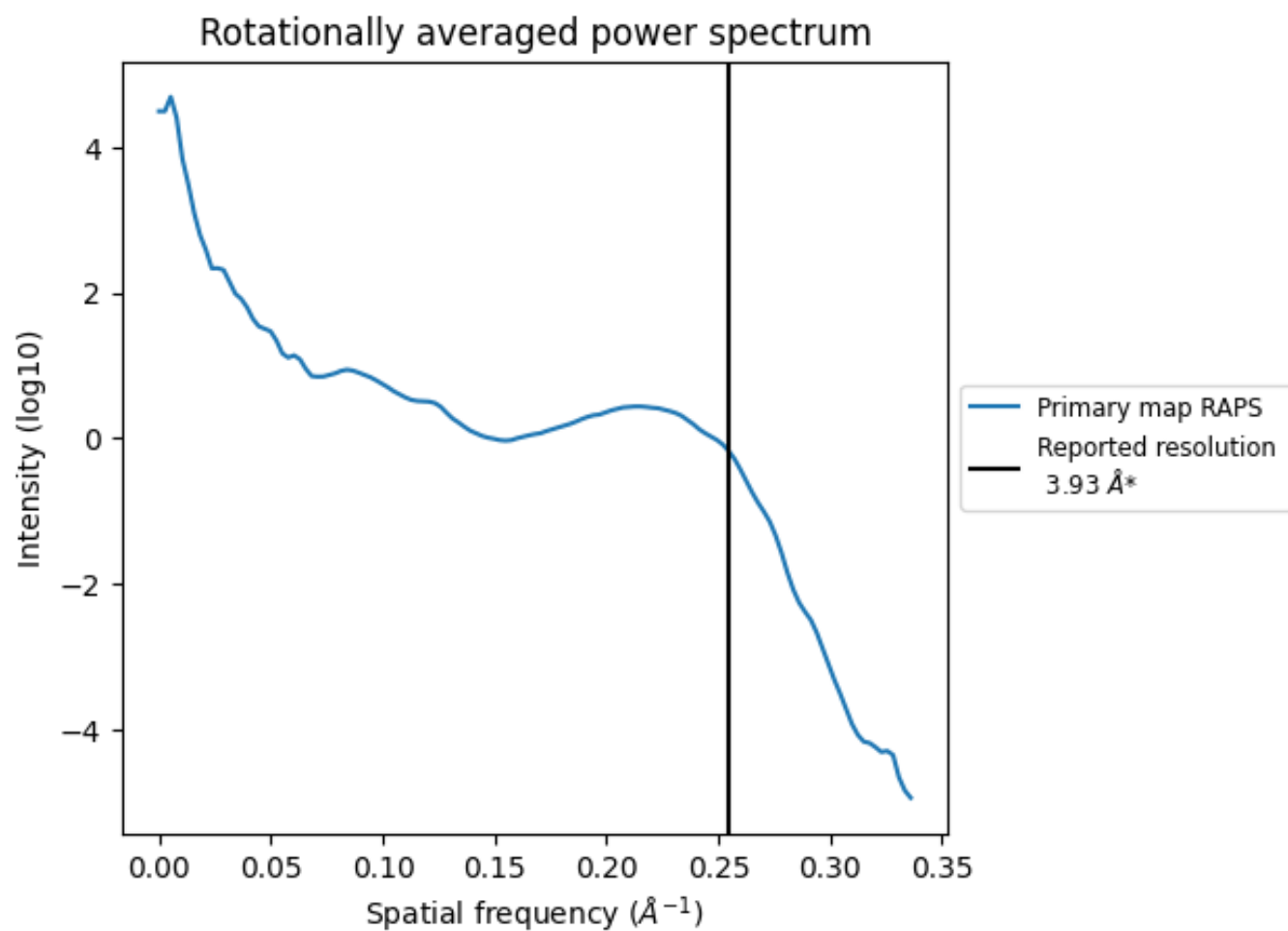
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm^3 ; this corresponds to an approximate mass of 372 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 0.254 Å⁻¹

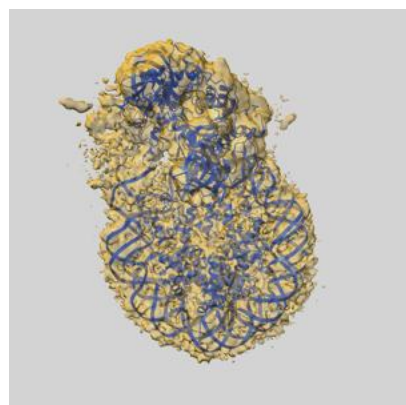
8 Fourier-Shell correlation

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

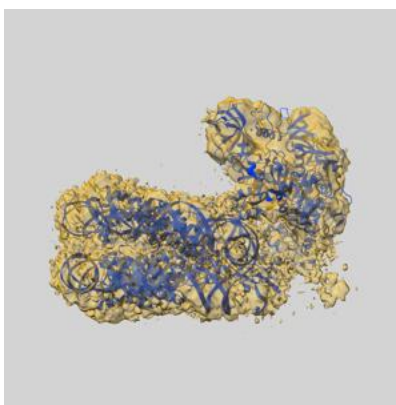
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48749 and PDB model 9MYS. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

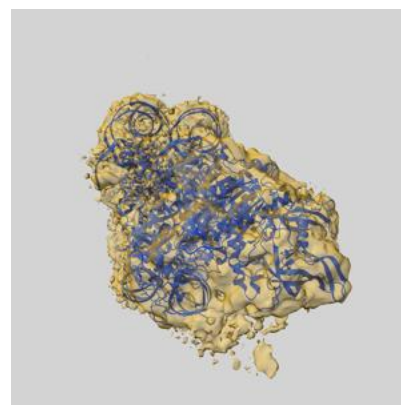
9.1 Map-model overlay [i](#)



X



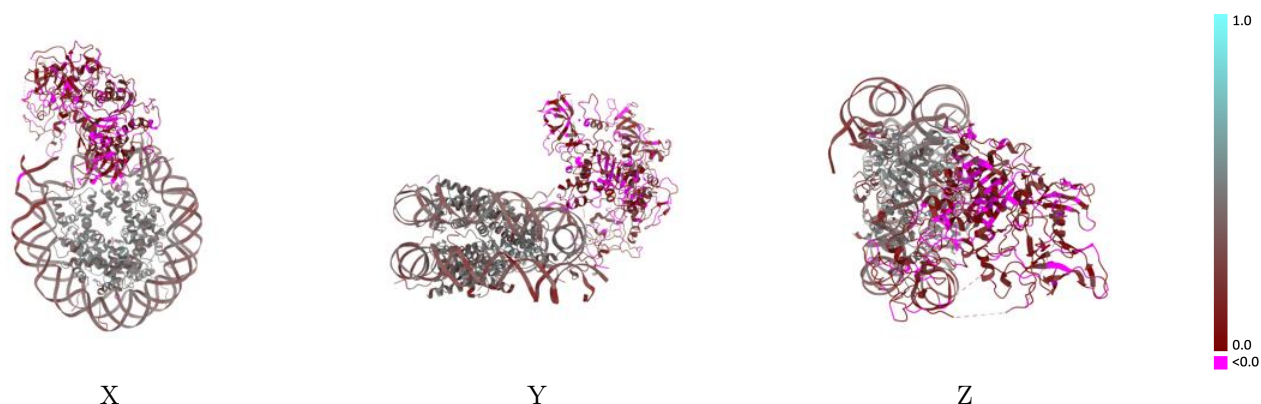
Y



Z

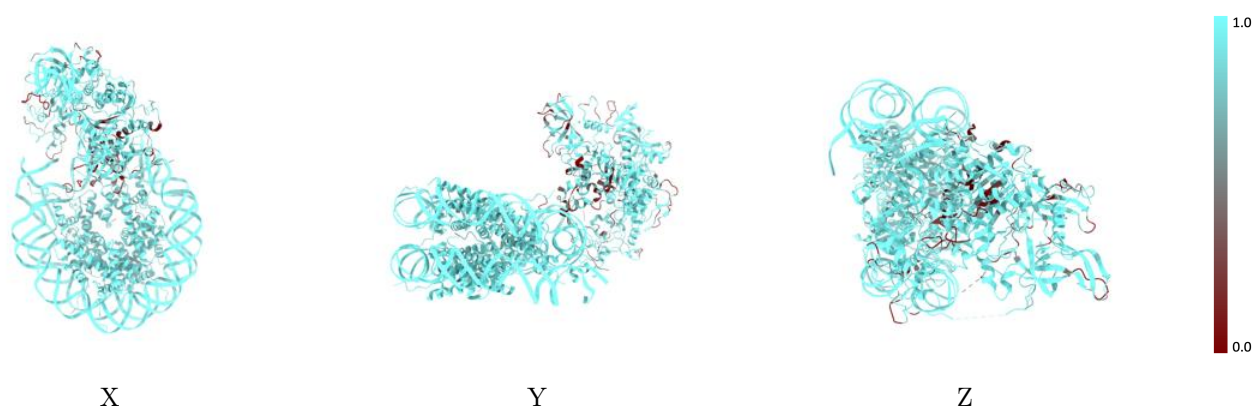
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



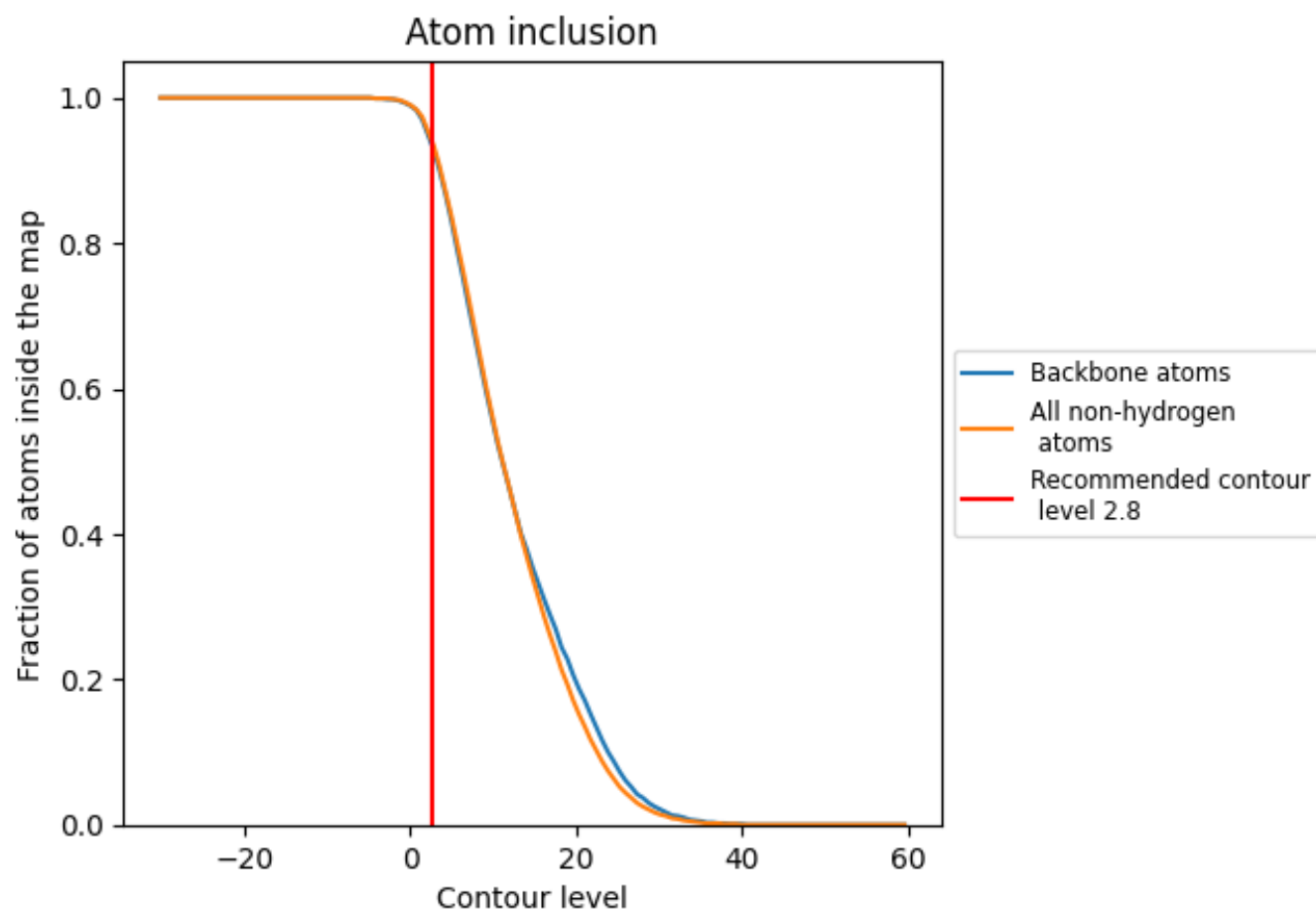
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9360	0.2770
A	0.8480	0.0850
N	0.9810	0.4320
O	0.9810	0.4230
P	0.9780	0.4390
Q	0.9840	0.4370
X	0.9940	0.3320
Y	0.9910	0.3400
n	0.9570	0.4290
o	0.9800	0.4230
p	0.9750	0.4270
q	0.9740	0.4430

1.0

0.0

<0.0