



wwPDB EM Validation Summary Report ⓘ

Apr 13, 2026 – 01:24 pm BST

PDB ID : 9S4Q / pdb_00009s4q
EMDB ID : EMD-54579
Title : Cryo-EM structure of the *Saccharomyces cerevisiae* KMN junction complex lacking the Mis12c(Mtw1c) head 2 domain
Authors : Turner, N.N.; Barford, D.
Deposited on : 2025-07-28
Resolution : 4.90 Å(reported)
Based on initial model : .

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:

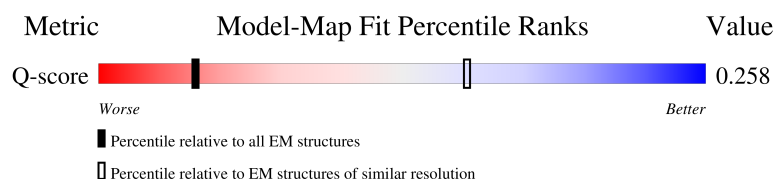
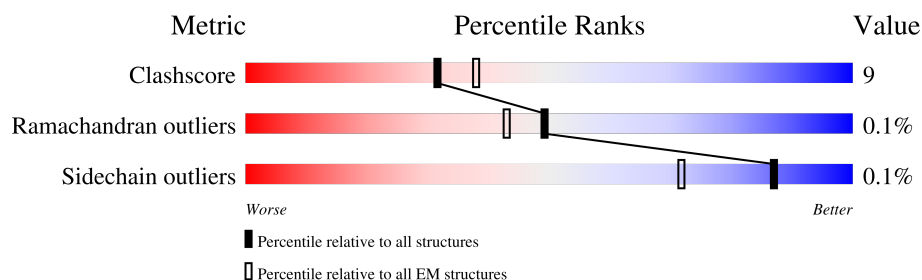
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.90 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	1274 (4.40 - 5.40)

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	Nn	201	<div> <div>12%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
2	Mt	289	<div> <div>12%</div> <div>80%</div> <div>11%</div> <div>9%</div> </div>
3	Zw	420	<div> <div>9%</div> <div>20%</div> <div>5%</div> <div>75%</div> </div>
4	Kl	474	<div> <div>32%</div> <div>10%</div> <div>58%</div> </div>

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Mol	Chain	Length	Quality of chain
5	Ds	576	<div><div><div></div><div></div><div></div><div></div></div><div>5%19%5%76%</div></div>
6	24	213	<div><div><div></div><div></div><div></div><div></div></div><div>8%27%6%67%</div></div>
7	25	221	<div><div><div></div><div></div><div></div><div></div></div><div>11%29%16%56%</div></div>
8	Ns	216	<div><div><div></div><div></div><div></div><div></div></div><div>6%46%9%44%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19471 atoms, of which 9782 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 Kinetochore-associated protein NNF1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	Nn	198	Total	C	H	N	O	S	0	0
			3233	1013	1598	283	329	10		

- Molecule 2 is a protein called Kinetochore-associated protein MTW1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	Mt	263	Total	C	H	N	O	S	0	0
			4358	1349	2225	356	420	8		

- Molecule 3 is a protein called Outer kinetochore KNL1 complex subunit KRE28.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	Zw	106	Total	C	H	N	O	S	0	0
			1760	558	897	140	162	3		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Zw	386	GLU	-	expression tag	UNP Q04431
Zw	387	ASN	-	expression tag	UNP Q04431
Zw	388	LEU	-	expression tag	UNP Q04431
Zw	389	TYR	-	expression tag	UNP Q04431
Zw	390	PHE	-	expression tag	UNP Q04431
Zw	391	GLN	-	expression tag	UNP Q04431
Zw	392	SER	-	expression tag	UNP Q04431
Zw	393	TRP	-	expression tag	UNP Q04431
Zw	394	SER	-	expression tag	UNP Q04431
Zw	395	HIS	-	expression tag	UNP Q04431
Zw	396	PRO	-	expression tag	UNP Q04431
Zw	397	GLN	-	expression tag	UNP Q04431
Zw	398	PHE	-	expression tag	UNP Q04431
Zw	399	GLU	-	expression tag	UNP Q04431
Zw	400	LYS	-	expression tag	UNP Q04431

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Chain	Residue	Modelled	Actual	Comment	Reference
Zw	401	GLY	-	expression tag	UNP Q04431
Zw	402	GLY	-	expression tag	UNP Q04431
Zw	403	GLY	-	expression tag	UNP Q04431
Zw	404	SER	-	expression tag	UNP Q04431
Zw	405	GLY	-	expression tag	UNP Q04431
Zw	406	GLY	-	expression tag	UNP Q04431
Zw	407	GLY	-	expression tag	UNP Q04431
Zw	408	SER	-	expression tag	UNP Q04431
Zw	409	GLY	-	expression tag	UNP Q04431
Zw	410	GLY	-	expression tag	UNP Q04431
Zw	411	GLY	-	expression tag	UNP Q04431
Zw	412	SER	-	expression tag	UNP Q04431
Zw	413	TRP	-	expression tag	UNP Q04431
Zw	414	SER	-	expression tag	UNP Q04431
Zw	415	HIS	-	expression tag	UNP Q04431
Zw	416	PRO	-	expression tag	UNP Q04431
Zw	417	GLN	-	expression tag	UNP Q04431
Zw	418	PHE	-	expression tag	UNP Q04431
Zw	419	GLU	-	expression tag	UNP Q04431
Zw	420	LYS	-	expression tag	UNP Q04431

- Molecule 4 is a protein called Outer kinetochore KNL1 complex subunit SPC105.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	Kl	199	Total	C	H	N	O	S	0	0
			3301	1052	1671	274	297	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Kl	444	MET	-	initiating methionine	UNP P53148

- Molecule 5 is a protein called Kinetochore-associated protein DSN1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	Ds	138	Total	C	H	N	O	S	0	0
			2216	686	1123	183	223	1		

- Molecule 6 is a protein called Kinetochore protein SPC24.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	24	71	Total	C	H	N	O	0	0
			1168	369	587	97	115		

- Molecule 7 is a protein called Kinetochore protein SPC25.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	25	98	Total	C	H	N	O	S	0	0
			1499	474	744	140	138	3		

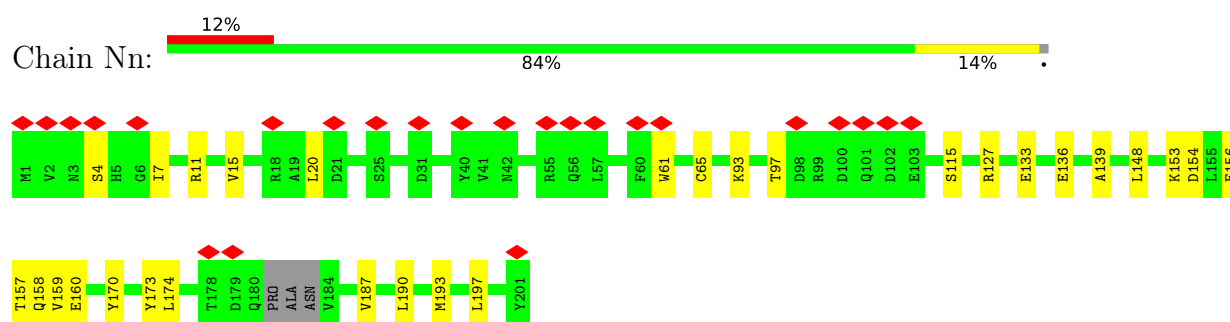
- Molecule 8 is a protein called Kinetochore-associated protein NSL1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Ns	120	Total	C	H	N	O	S	0	0
			1936	615	937	174	206	4		

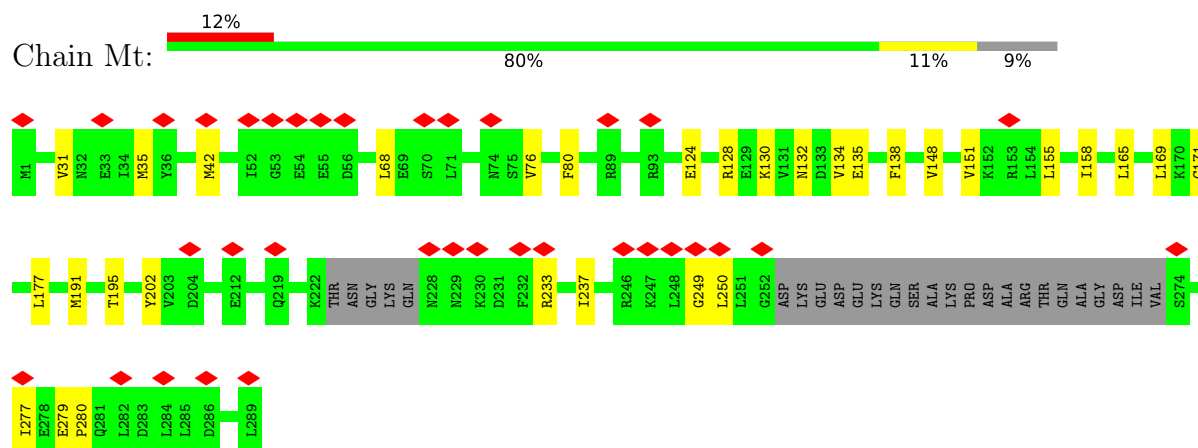
3 Residue-property plots [i](#)

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.

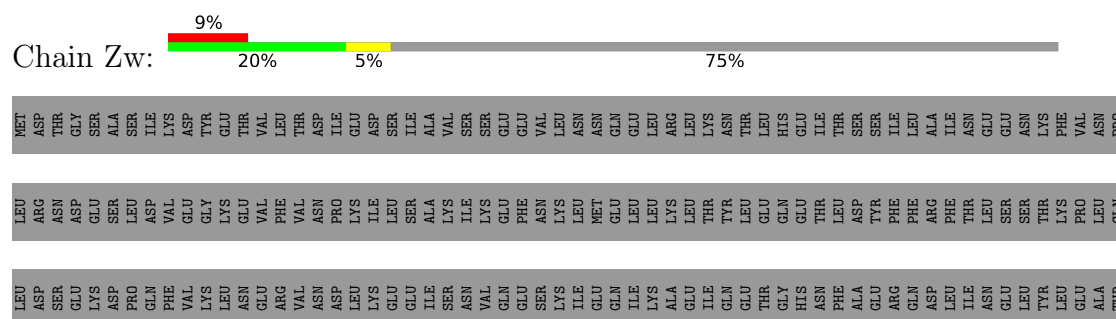
- Molecule 1: Kinetochore-associated protein NNF1



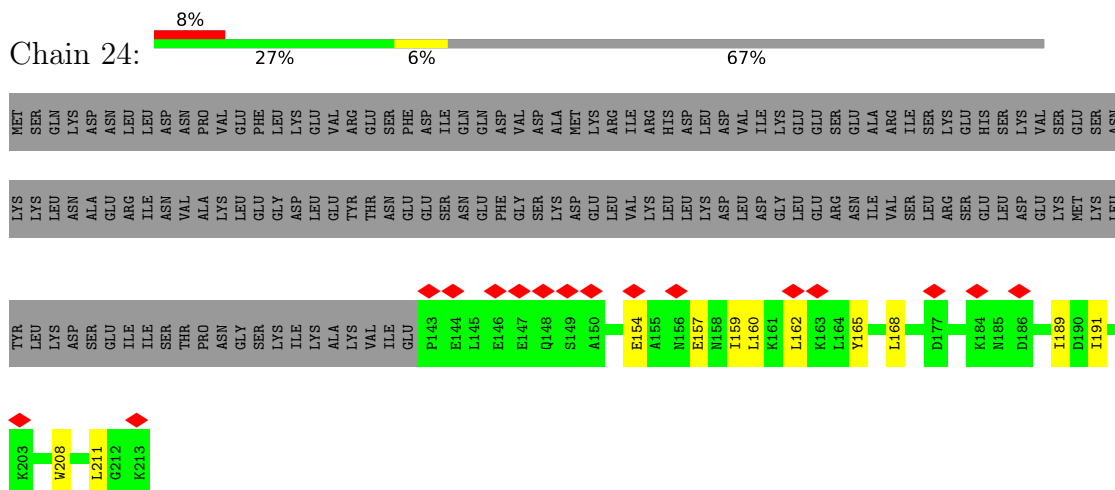
- Molecule 2: Kinetochore-associated protein MTW1



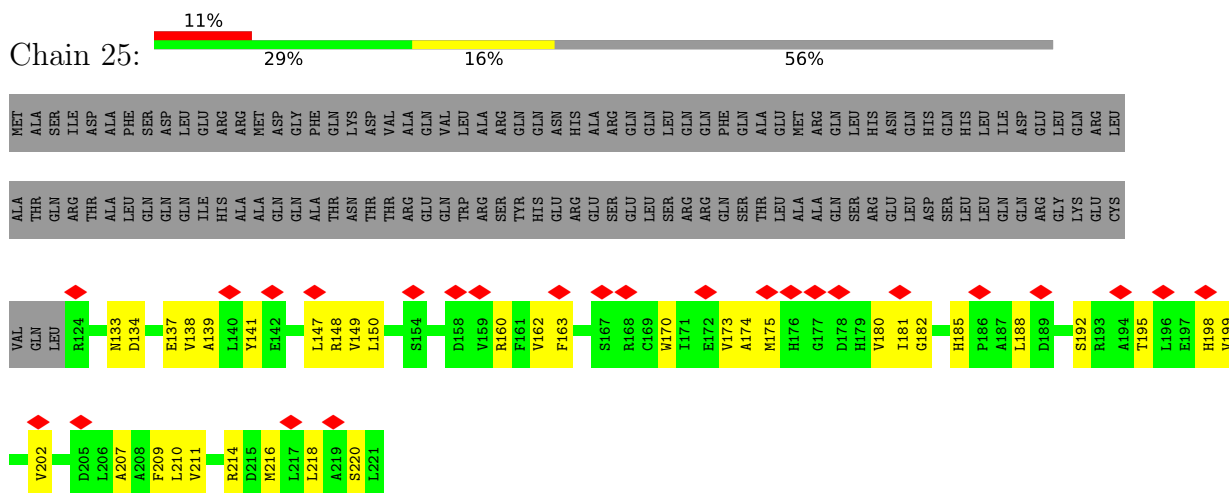
- Molecule 3: Outer kinetochore KNL1 complex subunit KRE28



- Molecule 6: Kinetochore protein SPC24

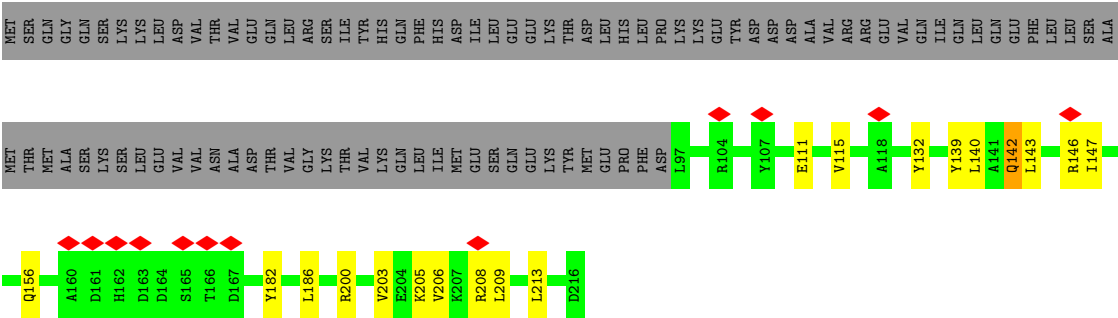


- Molecule 7: Kinetochore protein SPC25



- Molecule 8: Kinetochore-associated protein NSL1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.230	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0394	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.65, 1.65, 1.65	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	Nn	0.15	0/1655	0.32	0/2224
2	Mt	0.14	0/2151	0.30	0/2888
3	Zw	0.17	0/875	0.47	0/1175
4	Kl	0.19	0/1662	0.43	0/2237
5	Ds	0.15	0/1106	0.34	0/1498
6	24	0.16	0/589	0.35	0/796
7	25	0.19	0/770	0.40	0/1047
8	Ns	0.23	0/1014	0.38	0/1369
All	All	0.17	0/9822	0.37	0/13234

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	Nn	1635	1598	1597	22	0
2	Mt	2133	2225	2223	30	0
3	Zw	863	897	896	19	0
4	Kl	1630	1671	1670	40	0
5	Ds	1093	1123	1121	26	0
6	24	581	587	587	12	0
7	25	755	744	743	30	0
8	Ns	999	937	945	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9689	9782	9782	169	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 9.

The worst 5 of 169 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Ds:537:LEU:O	5:Ds:541:THR:HG23	1.83	0.79
1:Nn:156:GLU:O	1:Nn:159:VAL:HG22	1.85	0.77
2:Mt:134:VAL:HG11	8:Ns:143:LEU:HD23	1.71	0.72
4:Kl:781:MET:HE2	4:Kl:819:ILE:HG21	1.74	0.70
2:Mt:130:LYS:O	2:Mt:134:VAL:HG23	1.94	0.68

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	Nn	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	24	63
2	Mt	257/289 (89%)	254 (99%)	3 (1%)	0	100	100
3	Zw	104/420 (25%)	100 (96%)	4 (4%)	0	100	100
4	Kl	197/474 (42%)	180 (91%)	17 (9%)	0	100	100
5	Ds	134/576 (23%)	130 (97%)	4 (3%)	0	100	100
6	24	69/213 (32%)	67 (97%)	2 (3%)	0	100	100
7	25	96/221 (43%)	82 (85%)	14 (15%)	0	100	100
8	Ns	118/216 (55%)	114 (97%)	4 (3%)	0	100	100
All	All	1169/2610 (45%)	1114 (95%)	54 (5%)	1 (0%)	49	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Nn	115	SER

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	Nn	185/187 (99%)	185 (100%)	0	100	100
2	Mt	248/269 (92%)	248 (100%)	0	100	100
3	Zw	99/389 (25%)	99 (100%)	0	100	100
4	Kl	187/444 (42%)	187 (100%)	0	100	100
5	Ds	132/527 (25%)	132 (100%)	0	100	100
6	24	66/199 (33%)	66 (100%)	0	100	100
7	25	78/186 (42%)	78 (100%)	0	100	100
8	Ns	110/200 (55%)	109 (99%)	1 (1%)	70	77
All	All	1105/2401 (46%)	1104 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Ns	142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
8	Ns	162	HIS
8	Ns	177	HIS
8	Ns	193	GLN
4	Kl	764	ASN
4	Kl	797	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

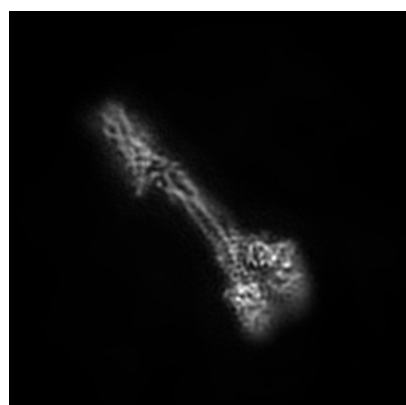
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54579. These allow visual inspection of the internal detail of the map and identification of artifacts.

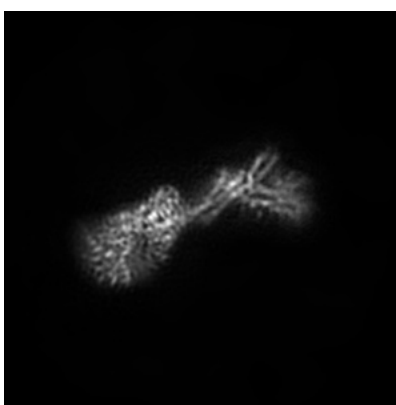
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

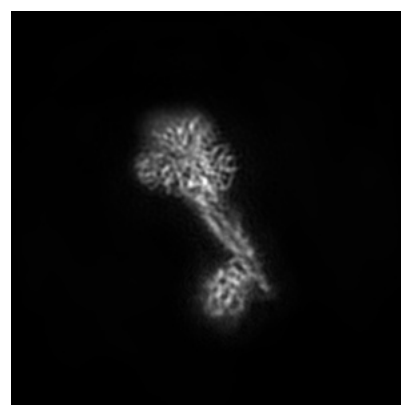
6.1.1 Primary map



X



Y



Z

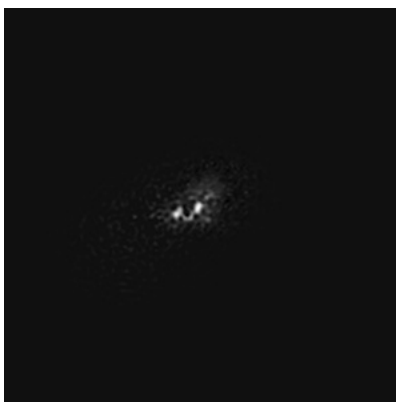
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

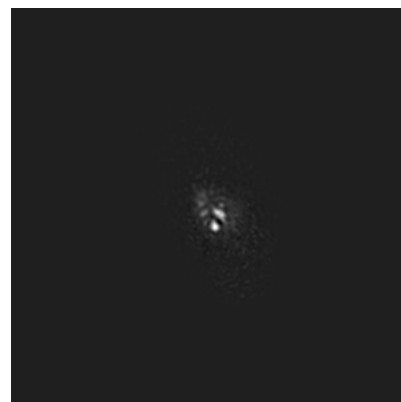
6.2.1 Primary map



X Index: 96



Y Index: 96

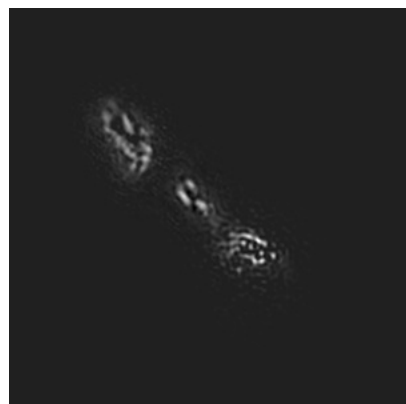


Z Index: 96

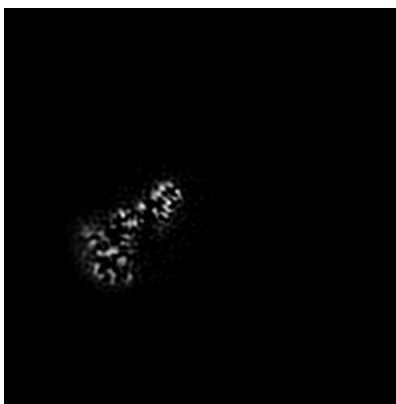
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

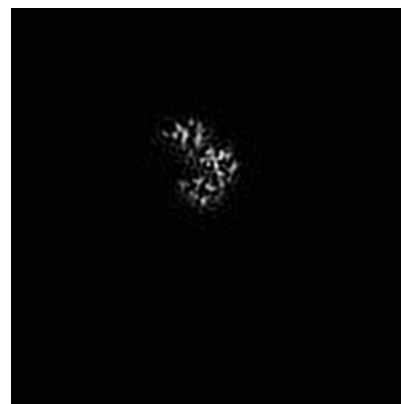
6.3.1 Primary map



X Index: 100



Y Index: 116



Z Index: 79

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

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

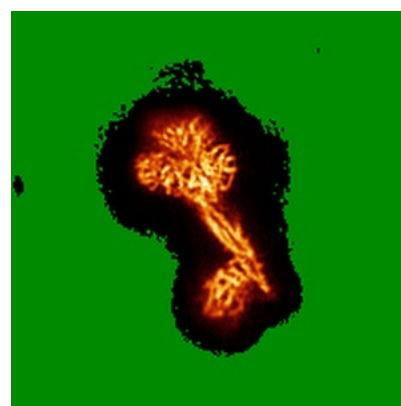
6.4.1 Primary map



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 0.0394. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

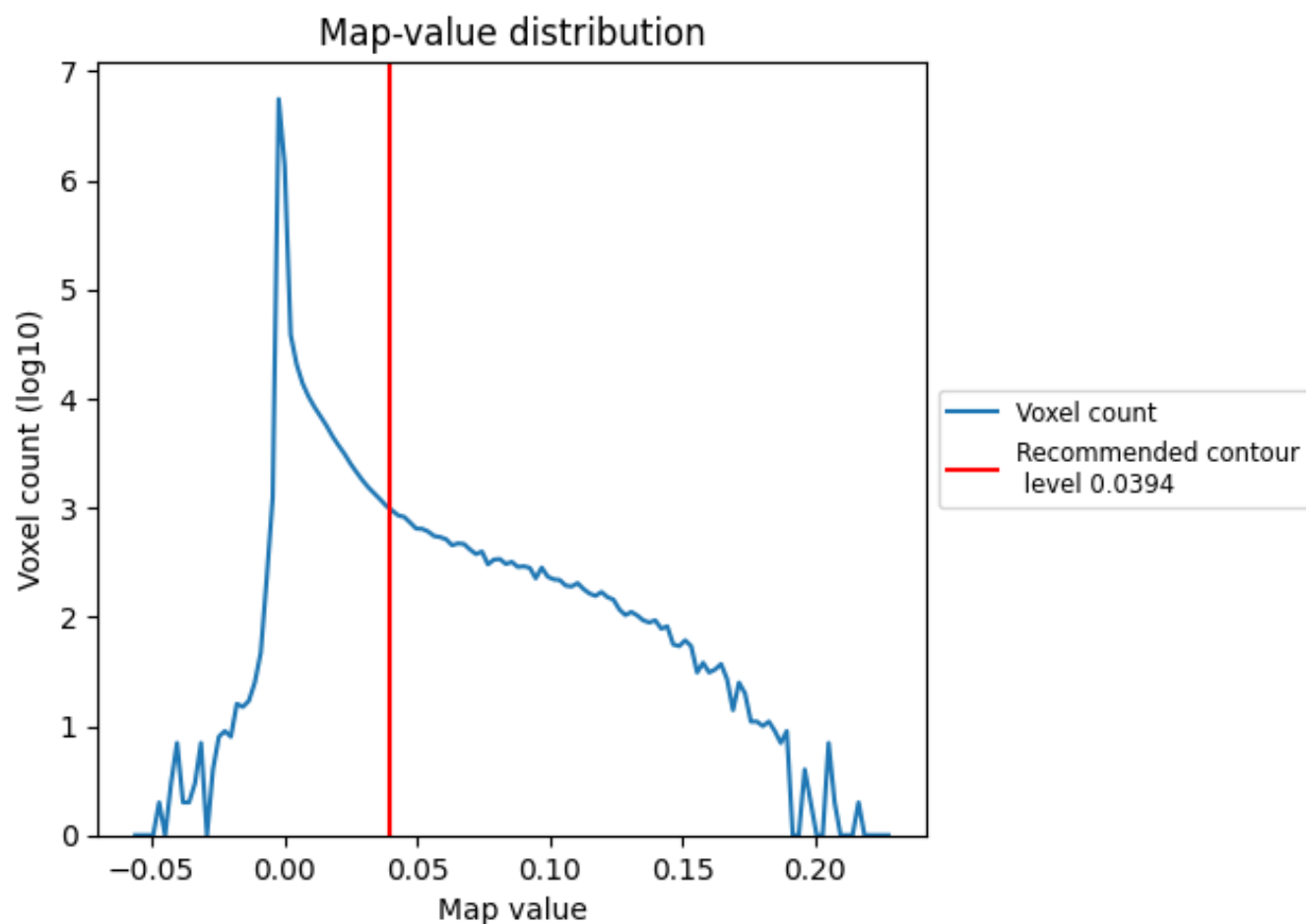
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

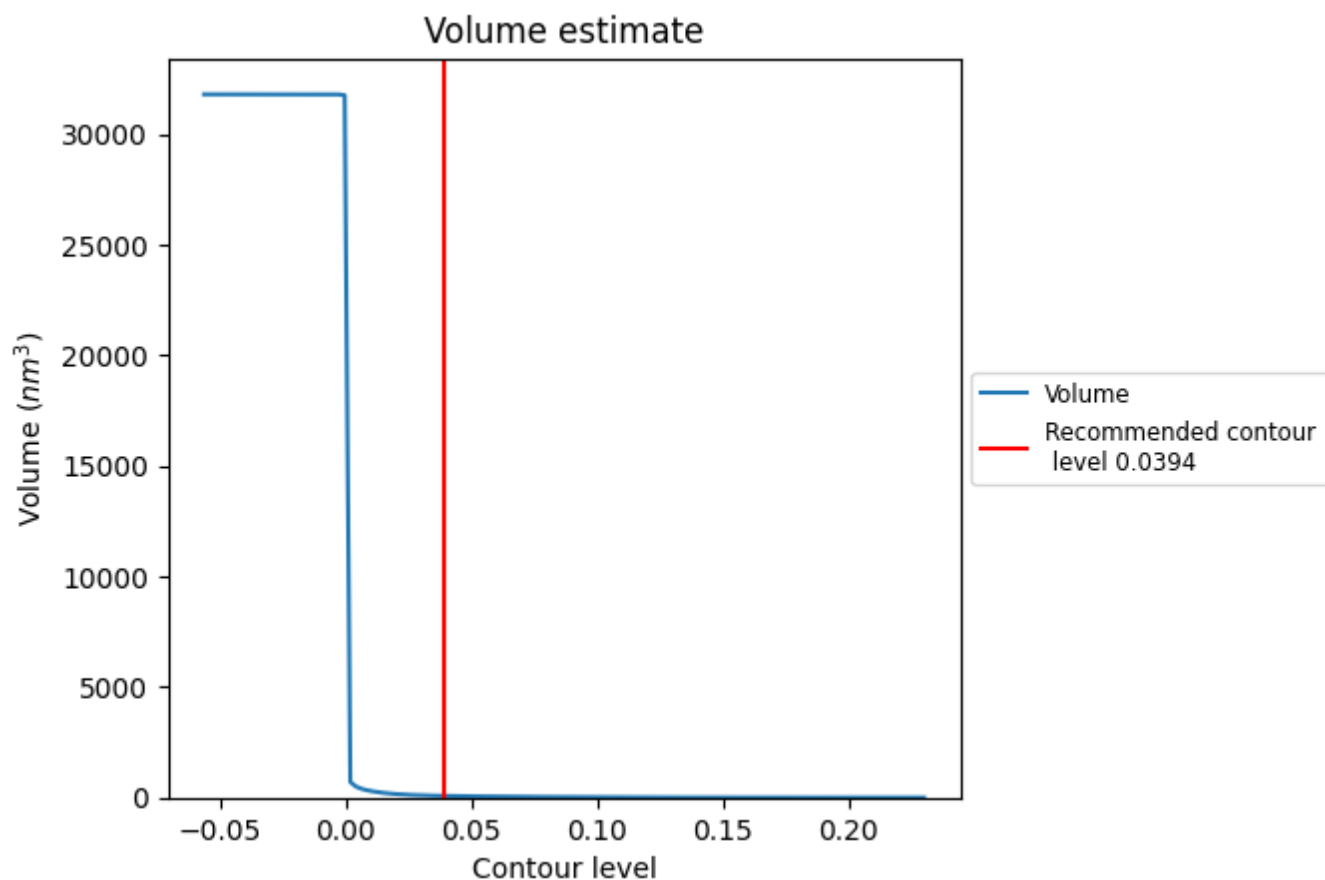
This section contains the results of statistical analysis of the map.

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.

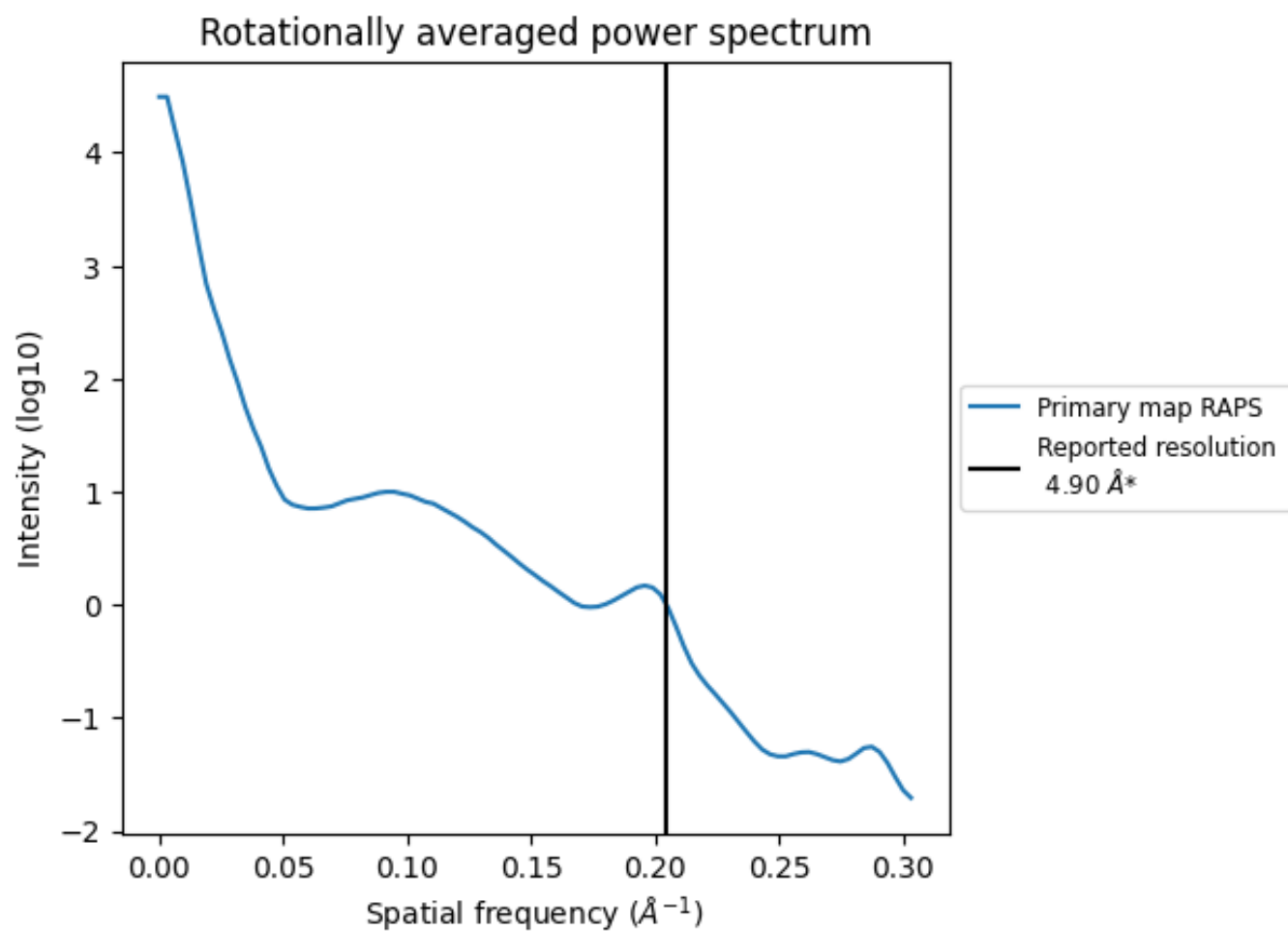
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm³; this corresponds to an approximate mass of 68 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 0.204 Å⁻¹

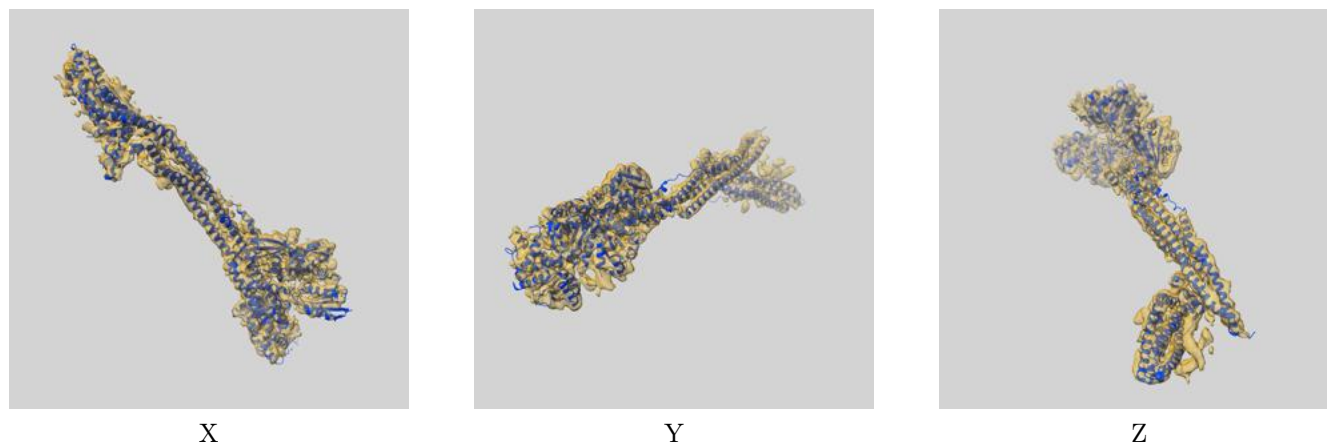
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

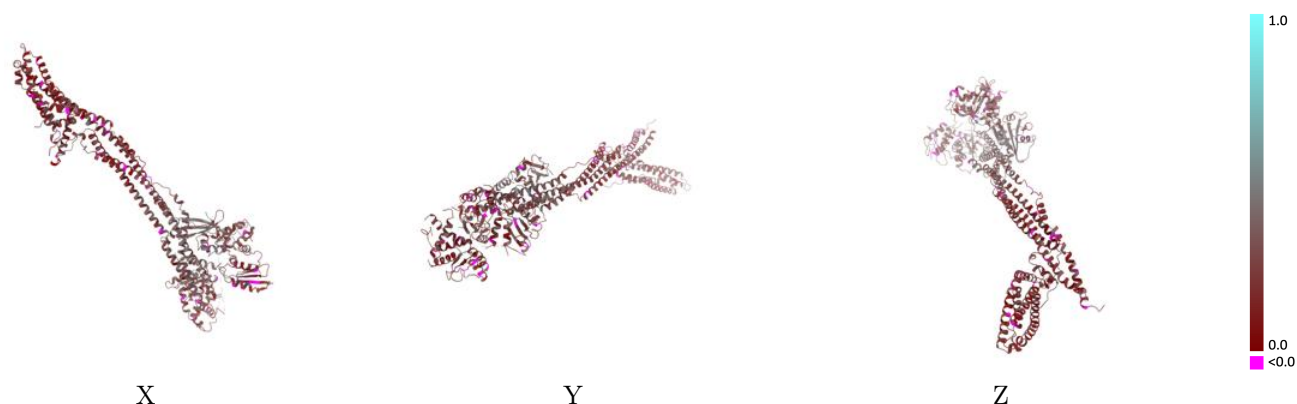
This section contains information regarding the fit between EMDB map EMD-54579 and PDB model 9S4Q. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



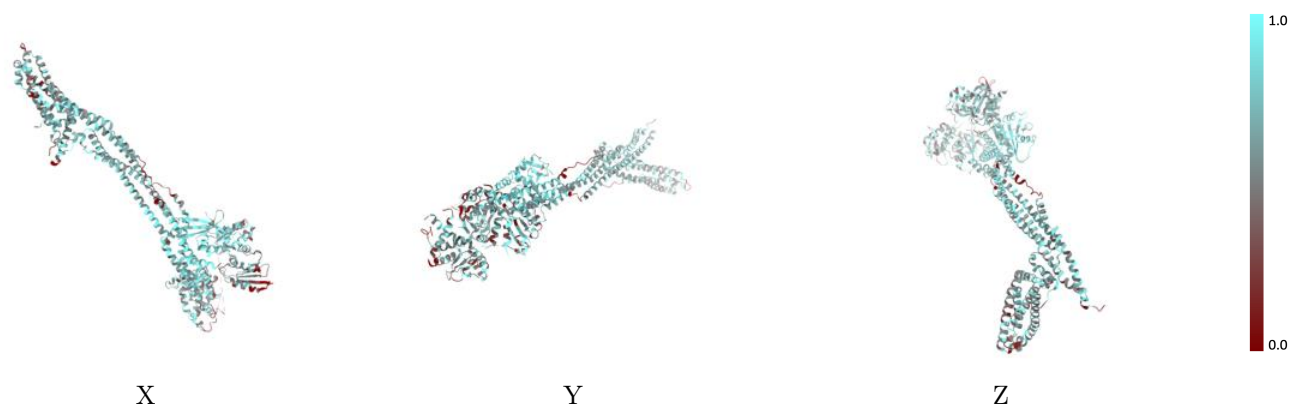
The images above show the 3D surface view of the map at the recommended contour level 0.0394 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



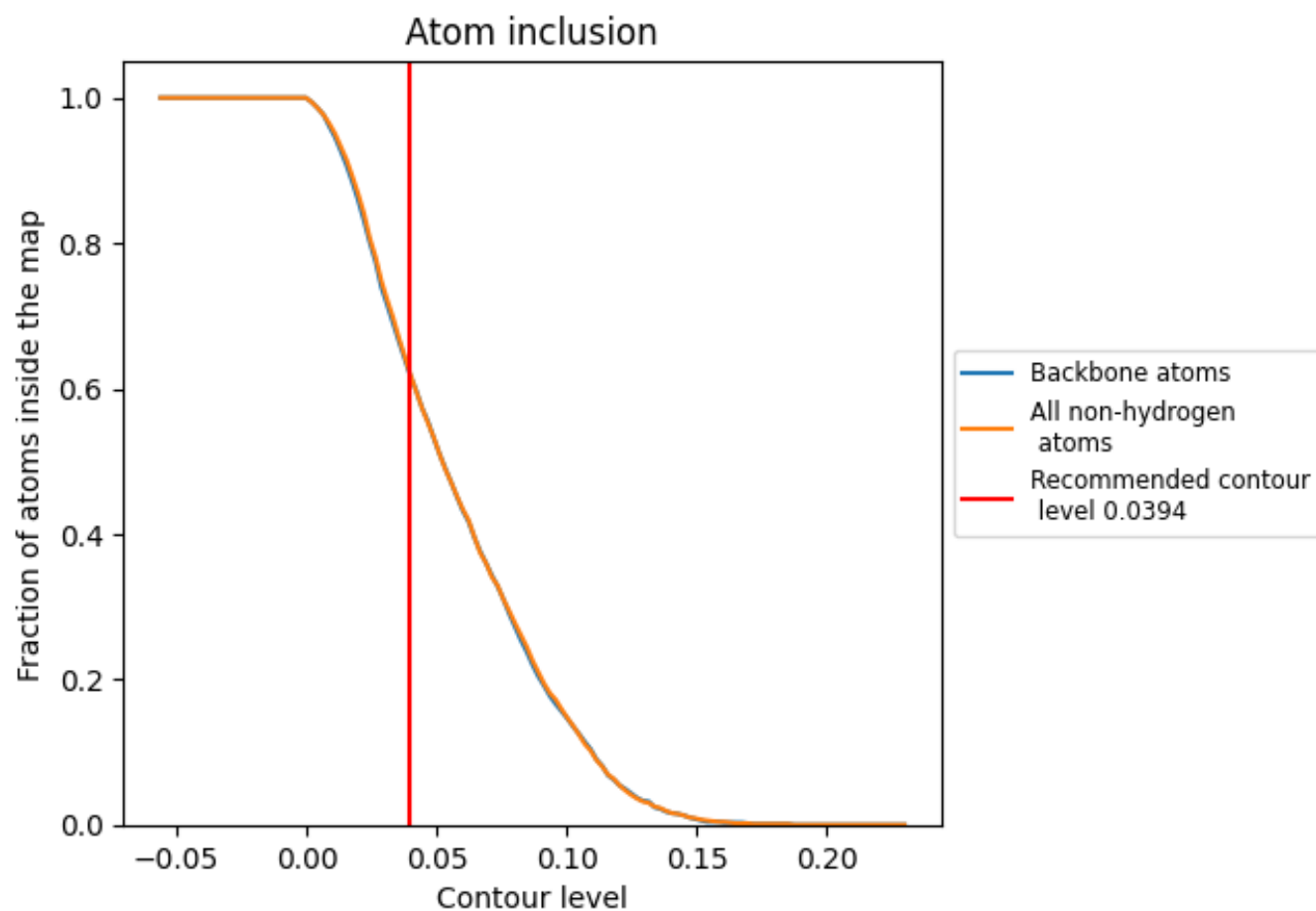
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0394).

9.4 Atom inclusion ⓘ



At the recommended contour level, 62% of all backbone atoms, 62% 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 (0.0394) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6250	<div><div></div></div> 0.2580
24	<div><div></div></div> 0.5830	<div><div></div></div> 0.2650
25	<div><div></div></div> 0.5950	<div><div></div></div> 0.2240
Ds	<div><div></div></div> 0.6150	<div><div></div></div> 0.2720
Kl	<div><div></div></div> 0.6980	<div><div></div></div> 0.3220
Mt	<div><div></div></div> 0.6380	<div><div></div></div> 0.2460
Nn	<div><div></div></div> 0.6340	<div><div></div></div> 0.2370
Ns	<div><div></div></div> 0.6690	<div><div></div></div> 0.2660
Zw	<div><div></div></div> 0.5120	<div><div></div></div> 0.2090

1.0

0.0

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