



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 12:58 AM EST

PDB ID : 7JTS
EMDB ID : EMD-22480
Title : Stalk of radial spoke 1 attached with doublet microtubule from *Chlamydomonas reinhardtii*
Authors : Gui, M.; Ma, M.; Sze-Tu, E.; Wang, X.; Koh, F.; Zhong, E.; Berger, B.; Davis, J.; Dutcher, S.; Zhang, R.; Brown, A.
Deposited on : 2020-08-18
Resolution : 6.10 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

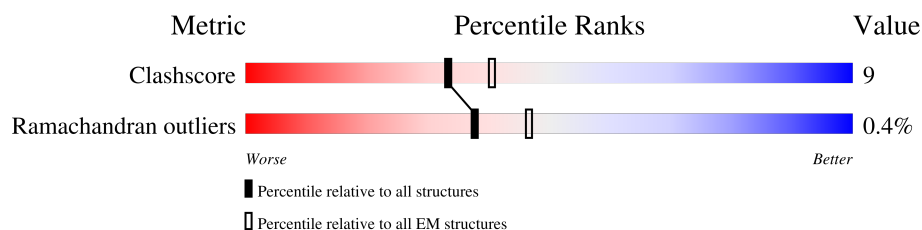
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 6.10 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	E	516	 8% 92%
1	F	516	 9% 91%
2	a	91	 92% 8%
2	b	91	 92% 8%
2	c	91	 92% 8%
2	d	91	 92% 8%
2	e	91	 92% 8%
2	f	91	 91% 8%
2	g	91	 92% 8%

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Mol	Chain	Length	Quality of chain
2	h	91	<div><div></div><div>92%</div><div>8%</div></div>
3	m	256	<div><div>7%</div><div>71%</div><div>28%</div></div>
4	s	682	<div><div>43%</div><div>57%</div></div>
5	t	163	<div><div>86%</div><div>12%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6801 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 Radial spoke protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	E	40	Total	C	N	O	0	0
			197	117	40	40		
1	F	48	Total	C	N	O	0	0
			236	140	48	48		

- Molecule 2 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	a	84	Total	C	N	O	0	0
			417	249	84	84		
2	b	84	Total	C	N	O	0	0
			417	249	84	84		
2	c	84	Total	C	N	O	0	0
			417	249	84	84		
2	d	84	Total	C	N	O	0	0
			417	249	84	84		
2	e	84	Total	C	N	O	0	0
			417	249	84	84		
2	f	84	Total	C	N	O	0	0
			417	249	84	84		
2	g	84	Total	C	N	O	0	0
			417	249	84	84		
2	h	84	Total	C	N	O	0	0
			417	249	84	84		

- Molecule 3 is a protein called FAP207.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	m	184	Total	C	N	O	0	0
			887	519	184	184		

- Molecule 4 is a protein called FAP253.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	s	290	Total 1441	C 861	N 290	O 290	0	0

- Molecule 5 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	t	143	Total 704	C 418	N 143	O 143	0	0

THR	ASP	ALA	PHE	LEU	GLU	ASP	ARG	PRO	PRO	THR	PRO	LEU	PHE	VAL	PRO	GLN	LYS	THR	G139	H196	ARG	ALA	HIS	GLN	GLU	HIS	PHE	GLU	ASN	ILE	ARG	ASN	ALA	GLU	LEU	VAL	ALA	THR	GLN	TYR	ILE	ARG	MET	GLU	ALA	ALA	GLU	ARG	ARG	LYS	LEU	GLU	GLU	LYS	LYS	PHE	ARG	MET	GLN	GLU		
ARG	GLU	ARG	VAL	GLU	VAL	ARG	GLU	ARG	ARG	VAL	VAL	ARG	GLN	LYS	VAL	ALA	LYS	ALA	PHE	ALA	ARG	ALA	TYR	LEU	SER	GLY	ILE	VAL	ASN	THR	VAL	PHE	LEU	ASP	ARG	LEU	VAL	SER	SER	GLY	TYR	ILE	TYR	ASP	PRO	VAL	MET	GLU	VAL	VAL	GLU	THR	THR	ALA	ALA	LYS	PHE	PRO	TRP	LEU	LYS	GLN
ALA	ILE	GLY	TYR	ALA	LEU	ALA	VAL	ARG	GLY	VAL	VAL	ALA	ARG	ARG	VAL	ASP	LYS	LEU	VAL	GLU	ASP	ALA	ALA	ALA	LEU	ALA	ALA	ASN	ALA	SER	THR	LEU	ALA	ASP	LYS	VAL	ALA	ASP	ALA	ALA	THR	ALA	ALA	TRP	ALA	ALA	GLU	GLU	ARG	GLN	ALA	LYS	ALA	GLY								
LYS	GLU	LEU	ALA	ALA	VAL	ARG	ARG	ARG	VAL	ARG	PRO	THR	PHE	VAL	LEU	GLU	ASP	GLU	LEU	PRO	ALA	VAL	ALA	SER	ALA	ASP	ALA	GLU	ALA	ALA	ALA	GLU	THR	LYS	GLN	ALA	ALA	TRP	LYS	ASP	ALA	ALA	ALA	ALA	ALA	TRP	LYS	ASP	ALA	LYS	ALA	GLU	ALA	ARG	ALA	PRO	PRO					
ALA	GLU	ALA	ALA	GLU	GLN	GLY	LYS	ARG	LYS	ALA	LEU	LEU	GLY	GLU	LEU	ALA	ALA	THR	ALA	ALA	ALA	GLU	GLY	ARG	GLY	GLU	GLU	ALA	PRO	ALA	ALA	GLU	PRO	PRO	LEU	PRO	ASP	GLY	VAL	VAL	ASN	GLU	GLY	ALA	ALA	ALA	ALA	VAL	VAL	VAL	VAL	PRO	LYS	ALA	ALA	PRO	PRO					
PRO	VAL	LYS	GLU	VAL	THR	ASP	ILE	ASP	ILE	ILE	LEU	SER	TYR	MET	MET	ASP	LYS	GLY	ALA	ILE	THR	LYS	ASP	ILE	ILE	GLN	ALA	LEU	VAL	HIS	ALA	LEU	GLY	LYS	ALA	TYR	THR	ASN	HIS	PRO	ALA	PHE	ALA	GLU	ALA	GLY	GLY	ALA														

- Molecule 2: Dynein 8 kDa light chain, flagellar outer arm

Chain a:

92%

8%

MET	ALA	SER	GLY	SER	SER	K7	S90	GLY
-----	-----	-----	-----	-----	-----	----	-----	-----

- Molecule 2: Dynein 8 kDa light chain, flagellar outer arm

Chain b:

92%

8%

MET	ALA	SER	GLY	SER	SER	K7	S90	GLY
-----	-----	-----	-----	-----	-----	----	-----	-----

- Molecule 2: Dynein 8 kDa light chain, flagellar outer arm

Chain c:

92%

8%

MET	ALA	SER	GLY	SER	SER	K7	S90	GLY
-----	-----	-----	-----	-----	-----	----	-----	-----

- Molecule 2: Dynein 8 kDa light chain, flagellar outer arm

Chain d:

92%

8%

MET	ALA	SER	GLY	SER	SER	K7	S90	GLY
-----	-----	-----	-----	-----	-----	----	-----	-----

- Molecule 2: Dynein 8 kDa light chain, flagellar outer arm

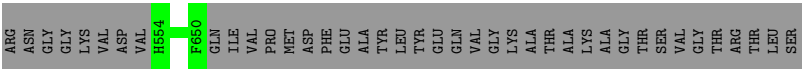
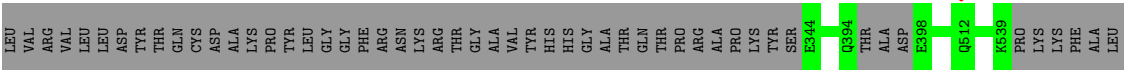
Chain e:

92%

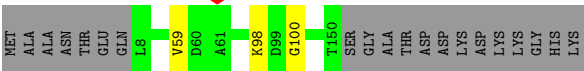
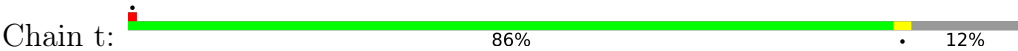
8%

MET	ALA	SER	GLY	SER	SER	K7	S90	GLY
-----	-----	-----	-----	-----	-----	----	-----	-----

- [illegible]



● Molecule 5: Calmodulin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143514	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 ($e^-/\text{\AA}^2$)	38.9	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	0.049	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	1167.296, 1167.296, 1167.296	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.403, 1.403, 1.403	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	E	0.31	0/195	0.58	0/268
1	F	0.32	0/235	0.50	0/325
2	a	0.32	0/416	0.63	0/579
2	b	0.31	0/416	0.64	0/579
2	c	0.28	0/416	0.59	0/579
2	d	0.29	0/416	0.57	0/579
2	e	0.27	0/416	0.50	0/579
2	f	0.30	0/416	0.55	0/579
2	g	0.31	0/416	0.60	0/579
2	h	0.29	0/416	0.53	0/579
3	m	0.37	0/886	0.77	0/1219
4	s	0.35	0/1438	0.48	0/2003
5	t	0.30	0/703	0.57	0/976
All	All	0.32	0/6785	0.58	0/9423

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	E	197	0	83	0	0
1	F	236	0	107	0	0
2	a	417	0	196	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	417	0	196	0	0
2	c	417	0	196	0	0
2	d	417	0	196	0	0
2	e	417	0	196	0	0
2	f	417	0	196	0	0
2	g	417	0	196	0	0
2	h	417	0	196	0	0
3	m	887	0	423	0	0
4	s	1441	0	635	0	0
5	t	704	0	324	0	0
All	All	6801	0	3140	0	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.

There are no clashes within the asymmetric unit.

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	E	36/516 (7%)	35 (97%)	1 (3%)	0	100	100
1	F	46/516 (9%)	45 (98%)	1 (2%)	0	100	100
2	a	82/91 (90%)	78 (95%)	4 (5%)	0	100	100
2	b	82/91 (90%)	76 (93%)	6 (7%)	0	100	100
2	c	82/91 (90%)	73 (89%)	9 (11%)	0	100	100
2	d	82/91 (90%)	79 (96%)	3 (4%)	0	100	100
2	e	82/91 (90%)	77 (94%)	5 (6%)	0	100	100
2	f	82/91 (90%)	72 (88%)	9 (11%)	1 (1%)	13	50
2	g	82/91 (90%)	72 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	82/91 (90%)	75 (92%)	7 (8%)	0	100	100
3	m	182/256 (71%)	158 (87%)	22 (12%)	2 (1%)	14	52
4	s	284/682 (42%)	262 (92%)	22 (8%)	0	100	100
5	t	141/163 (86%)	128 (91%)	10 (7%)	3 (2%)	7	36
All	All	1345/2861 (47%)	1230 (91%)	109 (8%)	6 (0%)	38	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	m	104	ASP
3	m	43	THR
5	t	100	GLY
5	t	98	LYS
5	t	59	VAL
2	f	54	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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-22480. 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](#)

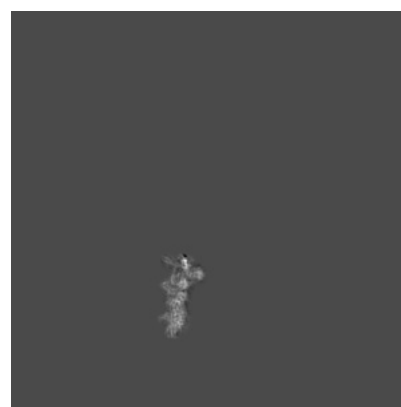
6.1.1 Primary map



X



Y

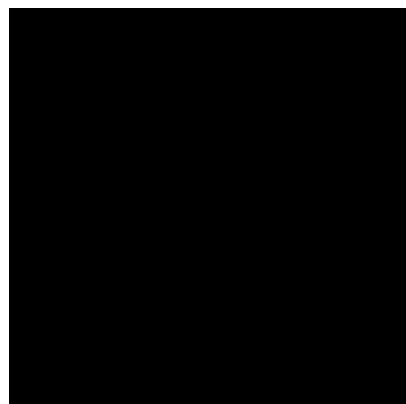


Z

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

6.2 Central slices [i](#)

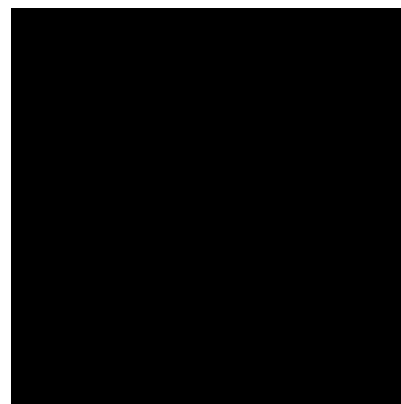
6.2.1 Primary map



X Index: 416



Y Index: 416

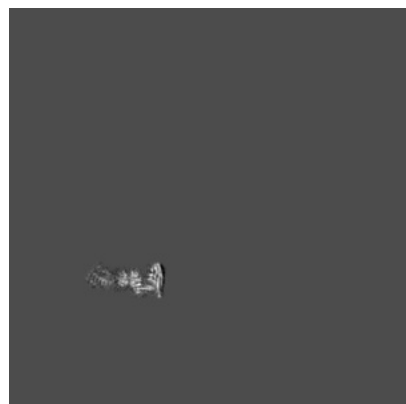


Z Index: 416

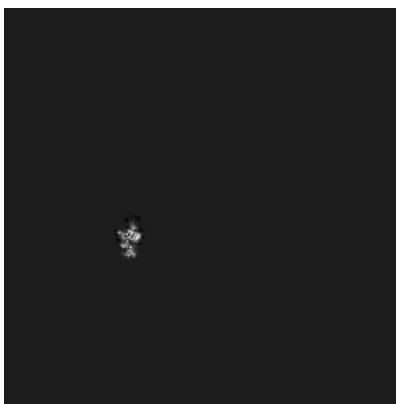
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 362



Y Index: 265



Z Index: 264

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

6.4 Orthogonal surface views [i](#)

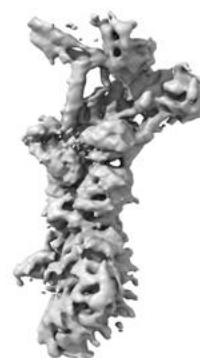
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

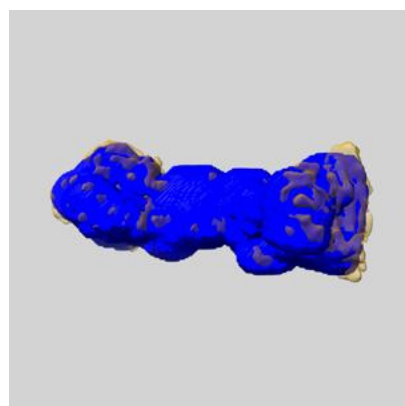
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

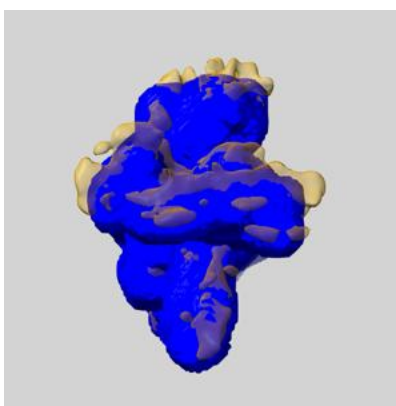
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

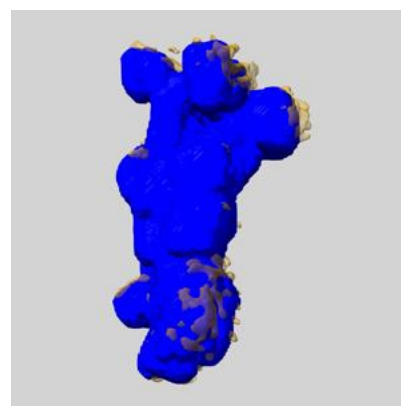
6.5.1 emd_22480_msk_1.map [i](#)



X



Y

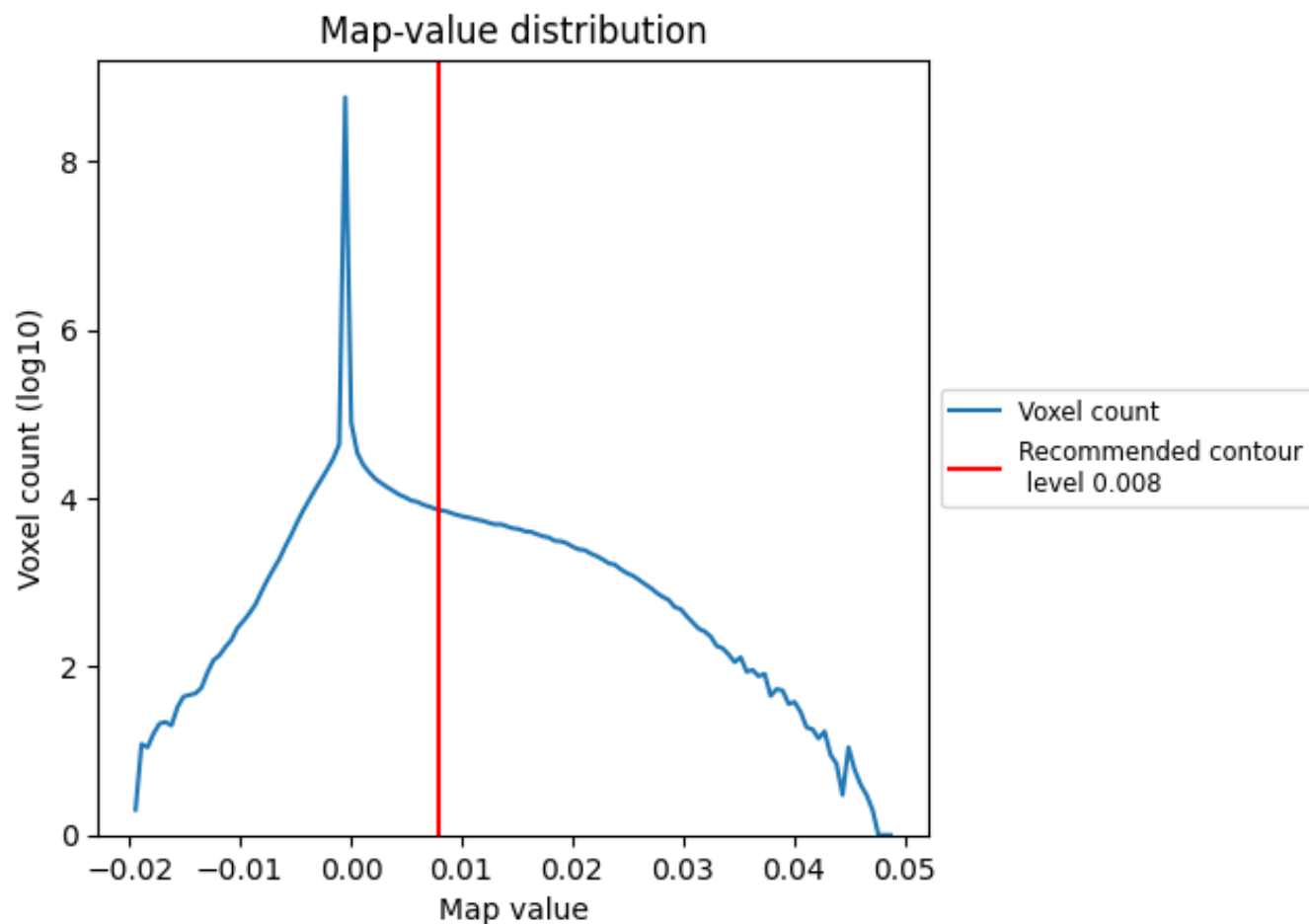


Z

7 Map analysis [i](#)

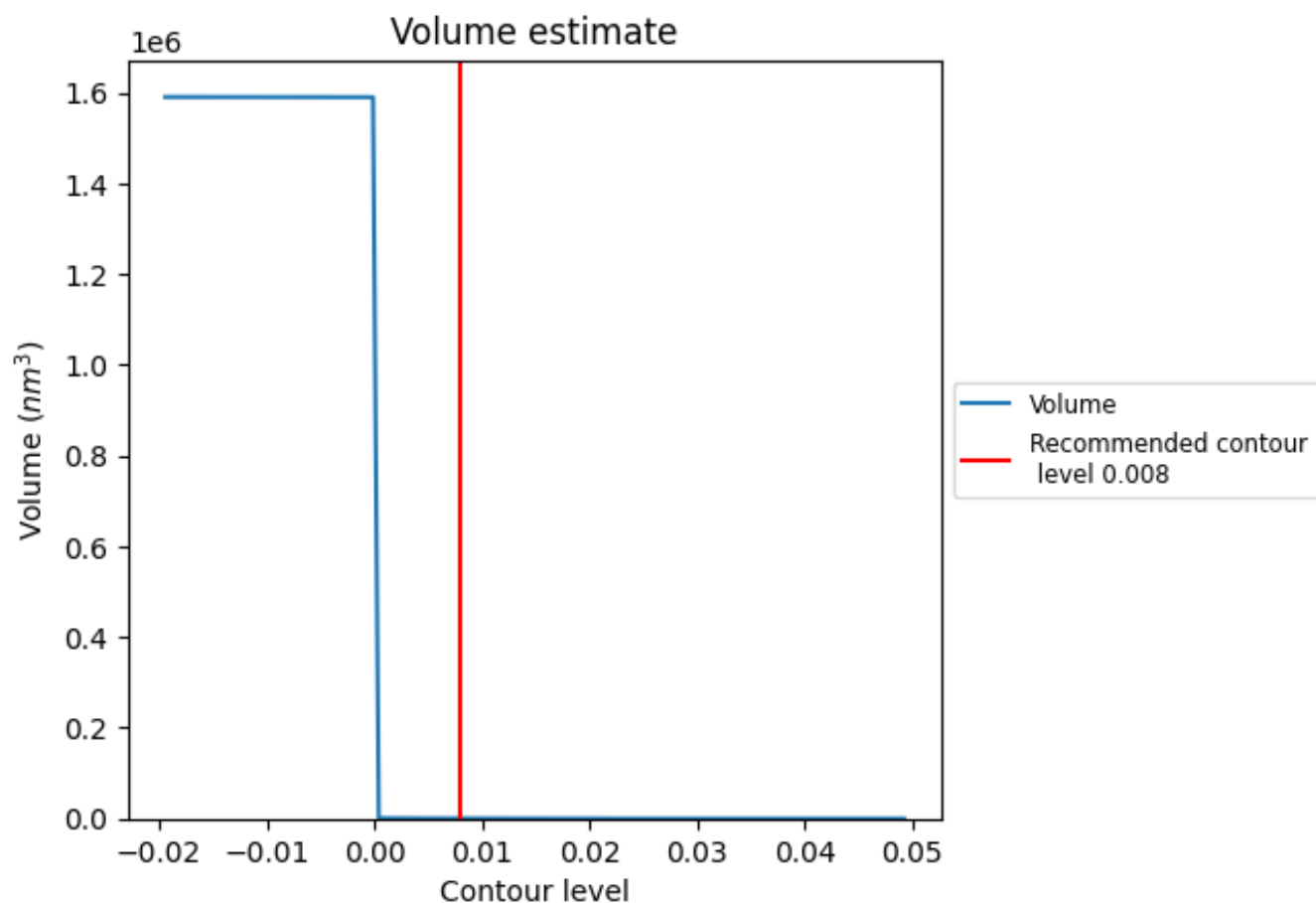
This section contains the results of statistical analysis of the map.

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.

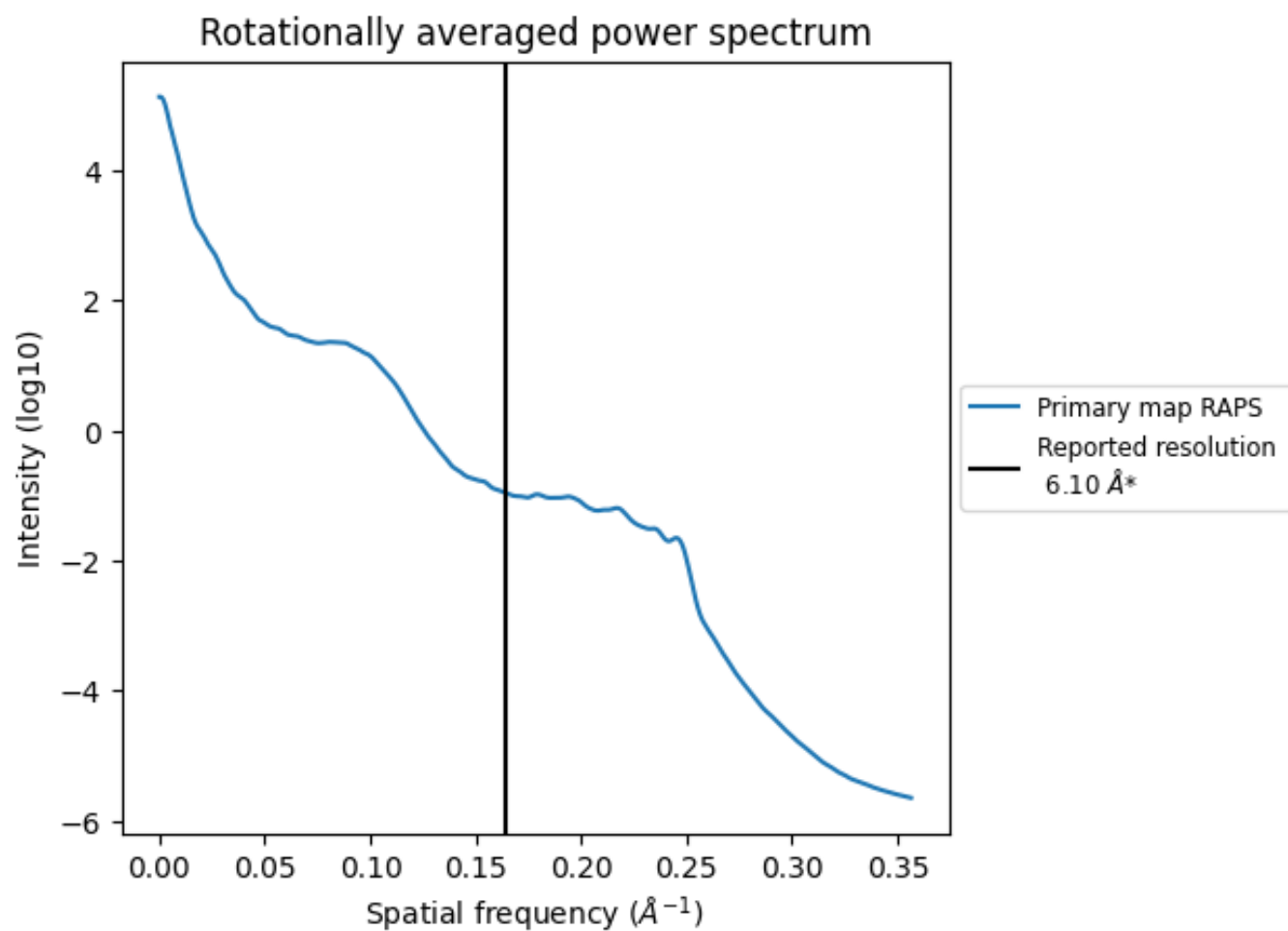
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 379 nm^3 ; this corresponds to an approximate mass of 343 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 0.164 Å⁻¹

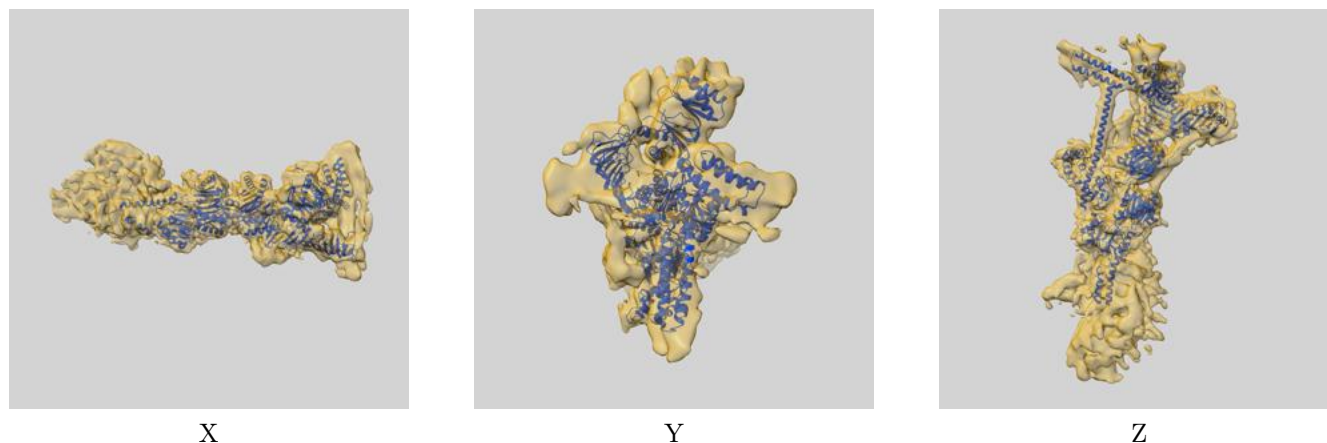
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

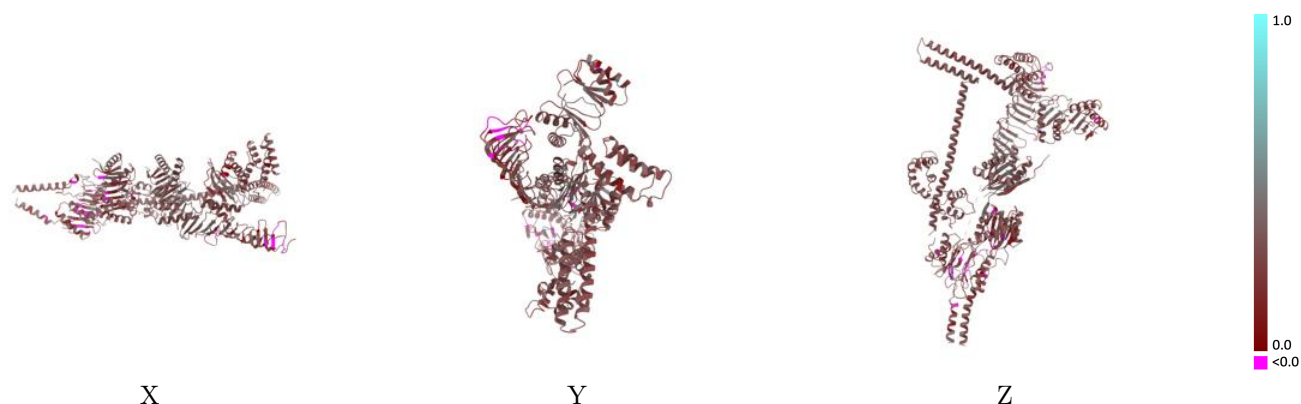
This section contains information regarding the fit between EMDB map EMD-22480 and PDB model 7JTS. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



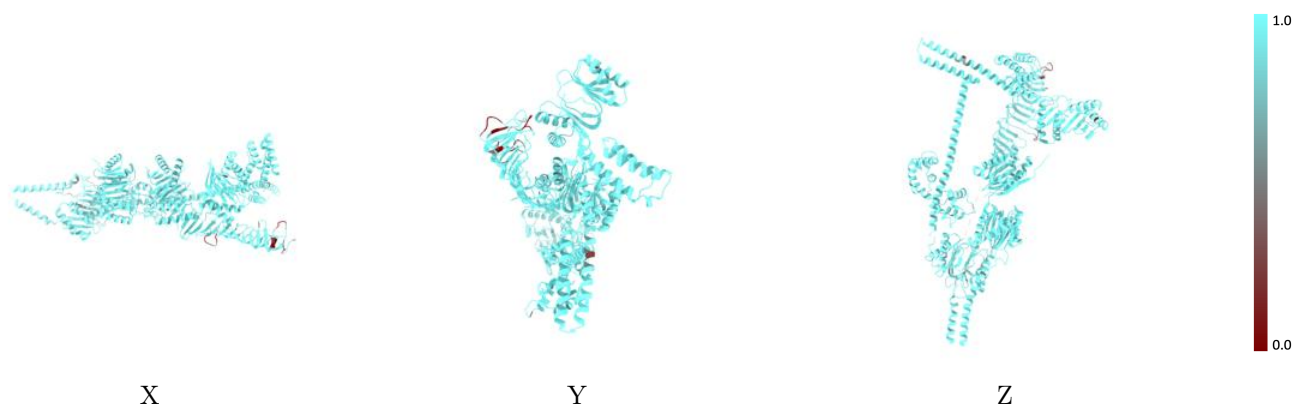
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



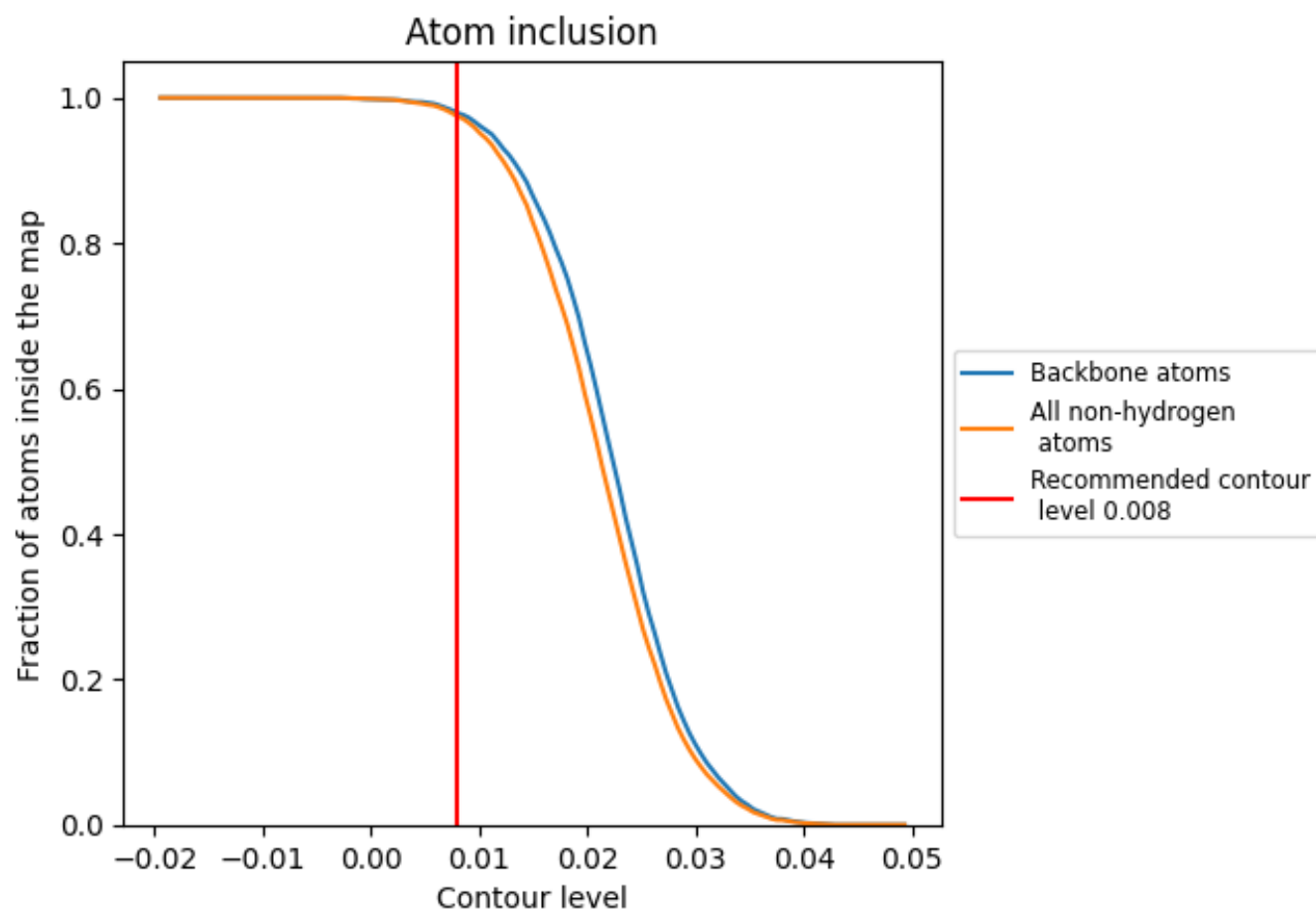
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9743	 0.2680
E	 0.9543	 0.2530
F	 0.9746	 0.2910
a	 0.9760	 0.2230
b	 0.9808	 0.1790
c	 0.9832	 0.2510
d	 0.9928	 0.2280
e	 1.0000	 0.3320
f	 1.0000	 0.3310
g	 0.9832	 0.2610
h	 0.9976	 0.3210
m	 0.8918	 0.2350
s	 0.9868	 0.2910
t	 0.9872	 0.2750

