



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:23 pm GMT

PDB ID : 2BSG  
EMDB ID : EMD-1126  
Title : The modeled structure of fibrin (gpwac) of bacteriophage T4 based on cryo-EM reconstruction of the extended tail of bacteriophage T4  
Authors : Kostyuchenko, V.A.; Chipman, P.R.; Leiman, P.G.; Arisaka, F.; Mesyanzhinov, V.V.; Rossmann, M.G.  
Deposited on : 2005-05-20  
Resolution : 15.00 Å (reported)  
Based on initial model : 1AA0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

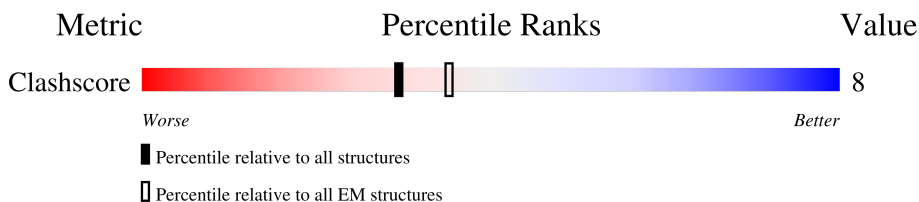
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



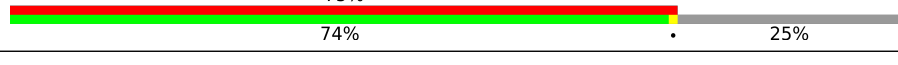
The reported resolution of this entry is 15.00 Å.

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)
Clashscore	158937	4297

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  $\geq 3$ , 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	487	
1	B	487	
1	C	487	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1089 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.

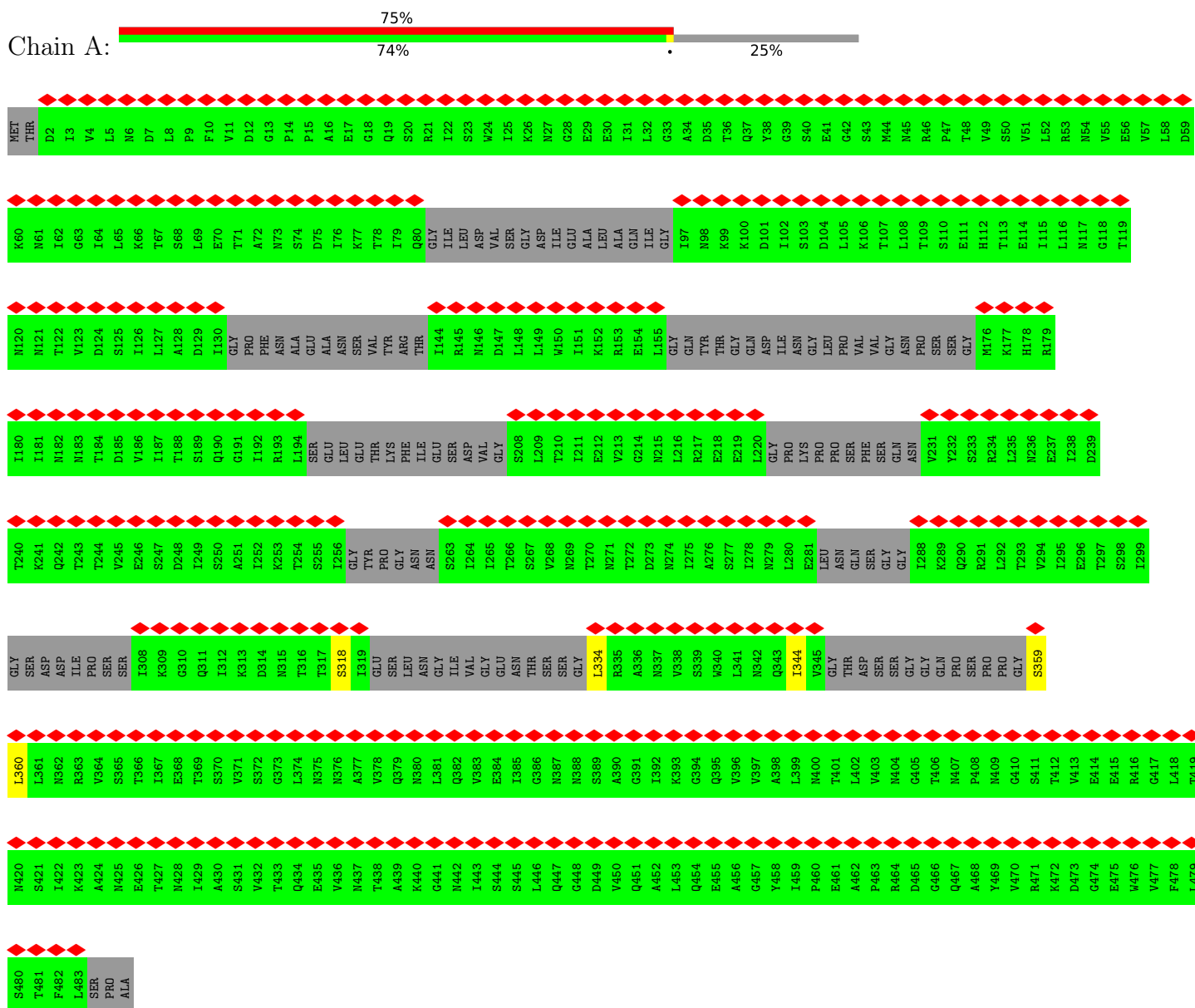
- Molecule 1 is a protein called FIBRITIN.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	363	Total C 363 363	1	363
1	B	363	Total C 363 363	1	363
1	C	363	Total C 363 363	1	363

### 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: FIBRITIN



#### • Molecule 1: FIBRITIN



MET	THR	D2	I3	V4	L5	N6	D7	L8	P9	F10	V11	D12	G13	P14	P15	A16	E17	G18	Q19	S20	R21	I22	S23	W24	I25	K26	N27	G28	E29	E30	I31	L32	G33	A34	D35	T36	Q37	Y38	G39	S40	E41	G42	S43	M44	M45	R46	P47	T48	V49	S50	V51	L52	R53	N54	V55	E56	V57	L58	D59	
K60	N61	G63	I64	L65	K66	T67	S68	L69	E70	T71	A72	N73	S74	D75	I76	K77	T78	I79	Q80	GLY	I144	R145	M146	V147	L148	L149	W150	I151	A152	R153	G154	L155	GLY	I197	N198	K100	D101	I102	S103	D104	L105	K106	V107	M108	T109	S110	E111	H112	T113	E114	I115	L116	N117	G118	T119					
M120	M121	V123	D124	S125	I126	L127	A128	D129	I130	GLY	PHE	ASN	ALA	GLU	ASN	GLU	VAL	TYR	ARG	THR	I144	R145	M146	D147	L148	L149	W150	I151	A152	R153	G154	L155	GLY	GLN	TYR	THR	GLY	GLN	ASP	ASN	GLY	LEU	PRO	PRO	VAL	PHE	VAL	GLY	ASN	PRO	PRO	LYS	Y232	S233	R234	L235	N236	E237	D238	
I180	I181	M183	T184	D185	V186	I187	S188	Q189	G191	I192	R193	L194	SER	LEU	THR	LYS	PHE	ARG	ILE	GLU	S263	I264	L265	T266	S267	W268	N269	T270	N271	T272	D273	N274	L275	A276	S277	I278	N279	L280	E281	LEU	ASN	GLN	THR	ASP	SER	SER	GLY	GLY	T288	K289	Q290	R291	L292	T293	V294	I295	E296	T297	S298	I299
T240	K241	Q242	T243	T244	V245	E246	S247	D248	L249	S250	A251	K253	T254	S255	I256	GLY	TYR	PRO	GLY	ASN	S263	I264	L265	T266	S267	W268	N269	T270	N271	T272	D273	N274	L275	A276	S277	I278	N279	L280	E281	LEU	ASN	GLN	THR	ASP	SER	SER	GLY	GLY	T288	K289	Q290	R291	L292	T293	V294	I295	E296	T297	S298	I299
GLY	SER	ASP	ILE	PRO	SER	SER	I308	K309	G310	Q311	K313	D314	N315	T316	T317	S318	I319	GLU	SER	LEU	ASN	GLY	ILE	VAL	GLY	GLU	ASN	THR	SER	SER	GLY	L334	R335	A336	N337	V338	S339	K340	L341	N342	Q343	I344	V345	GLY	THR	ASP	SER	SER	GLY	GLY	GLN	PRO	PRO	PRO	GLY	S359				
L360	L361	R362	R363	V364	S365	T366	I367	E368	T369	S370	V371	S372	G373	L374	N375	R376	A377	V378	Q379	R380	L381	Q382	V383	E384	L385	G386	N387	R388	S389	A390	G391	I392	K393	G394	Q395	V396	V397	A398	L399	M400	T401	L402	V403	M404	G405	T406	M407	P408	M409	G410	S411	T412	V413	E414	E415	R416	G417	L418	T419	
M420	S421	I422	K423	A424	M425	E426	T427	M428	L429	A430	S431	V432	T433	Q434	E435	V436	M437	T438	A439	K440	G441	M442	L443	S444	S445	L446	Q447	G448	D449	V450	Q451	A452	L453	Q454	E455	A456	A457	Y458	L459	P460	E461	A462	P463	R464	D465	G466	Q467	A468	Y469	V470	R471	K472	D473	G474	E475	W476	V477	F478	L479	
S480	T481	F482	L483	SER	PRO	ALA																																																						

• Molecule 1: FIBRITIN



MET	THR	D2	I3	V4	L5	N6	D7	L8	P9	F10	V11	D12	G13	P14	P15	A16	E17	G18	Q19	S20	R21	I22	S23	W24	I25	K26	N27	G28	E29	E30	I31	L32	G33	A34	D35	T36	Q37	Y38	G39	S40	E41	G42	S43	M44	M45	R46	P47	T48	V49	S50	V51	L52	R53	N54	V55	E56	V57	L58	D59	
K60	N61	I62	G63	I64	L65	K66	T67	S68	L69	E70	T71	A72	N73	S74	D75	I76	K77	T78	I79	Q80	GLY	I144	R145	M146	V147	L148	L149	W150	I151	A152	R153	G154	L155	GLY	I197	N198	K99	K100	D101	I102	S103	D104	L105	K106	V107	M108	T109	S110	E111	H112	T113	E114	I115	L116	N117	G118	T119			
M120	M121	T122	V123	D124	S125	I126	L127	A128	D129	I130	GLY	PRO	PHE	ASN	ALA	GLU	ASN	SER	VAL	TYR	ARG	THR	I144	R145	M146	D147	L148	L149	W150	I151	A152	R153	G154	L155	GLY	GLN	TYR	THR	GLY	GLN	ASP	ASN	ILE	LEU	PRO	PRO	VAL	VAL	GLY	GLY	ASN	PRO	PRO	SER	SER	GLY	M176	K177	H178	R179



## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of segments used	3029	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH IMAGE	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	7.953	Depositor
Minimum map value	-2.953	Depositor
Average map value	0.059	Depositor
Map value standard deviation	0.533	Depositor
Recommended contour level	1.01	Depositor
Map size ( $\text{\AA}$ )	714.6, 714.6, 1508.6	wwPDB
Map dimensions	180, 180, 380	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	3.97, 3.97, 3.97	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	363	0	0	3	0
1	B	363	0	0	3	0
1	C	363	0	0	3	0
All	All	1089	0	0	9	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.

All (9) 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:B:370:SER:CA	1:B:372:SER:CA	1.81	1.56
1:A:344:ILE:CA	1:A:360:LEU:CA	1.84	1.49
1:A:318:SER:CA	1:A:334:LEU:CA	2.33	1.06
1:B:370:SER:CA	1:B:371:VAL:CA	2.54	0.85
1:B:318:SER:CA	1:B:334:LEU:CA	2.71	0.69
1:C:318:SER:CA	1:C:334:LEU:CA	2.76	0.64

*Continued on next page...*



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:CA	1:A:359:SER:CA	2.81	0.59
1:C:344:ILE:CA	1:C:360:LEU:CA	2.84	0.55
1:C:319:ILE:CA	1:C:334:LEU:CA	2.89	0.51

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

#### 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

There are no chain breaks in this entry.

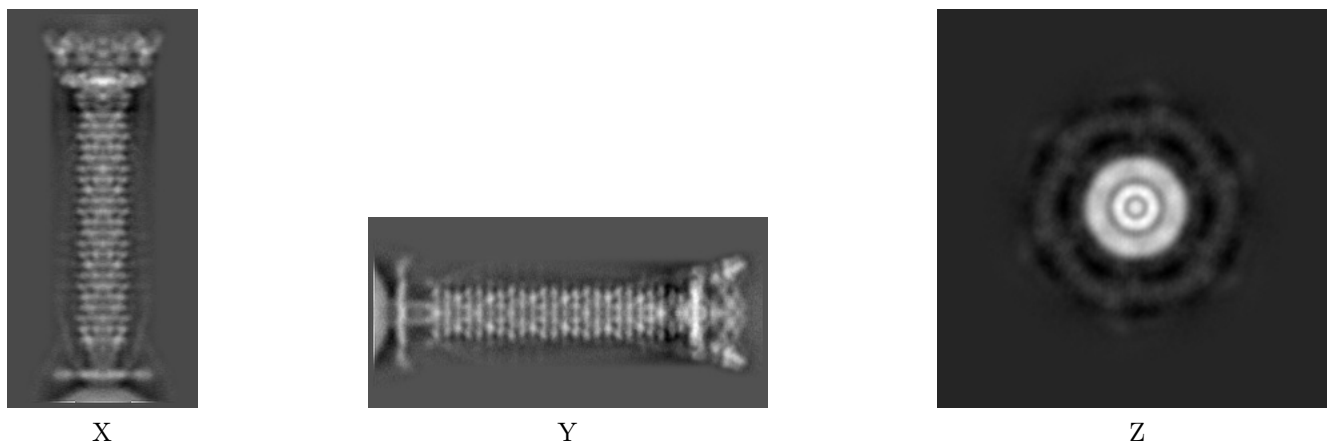
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1126. 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](#)

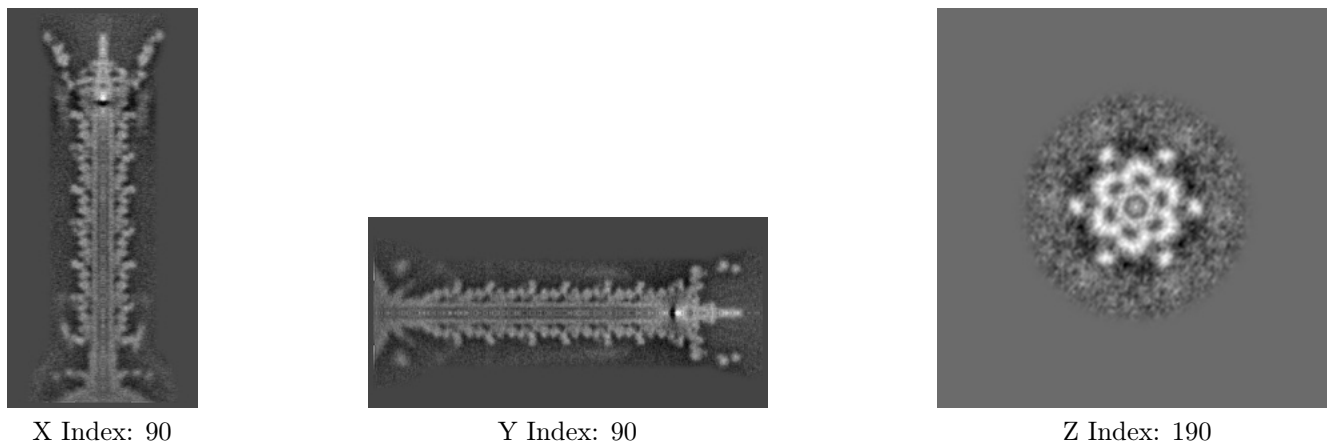
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

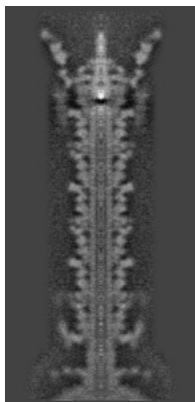
#### 6.2.1 Primary map



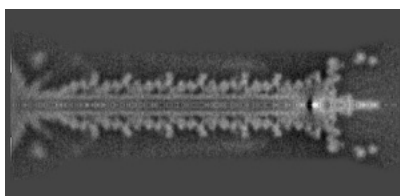
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

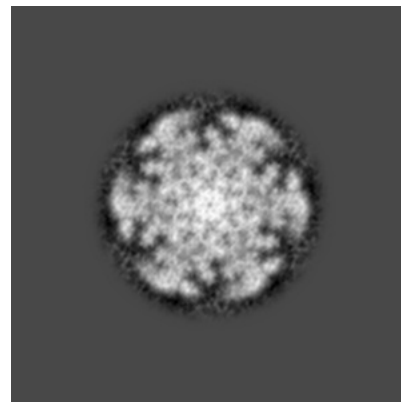
### 6.3.1 Primary map



X Index: 89



Y Index: 90



Z Index: 310

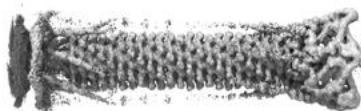
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

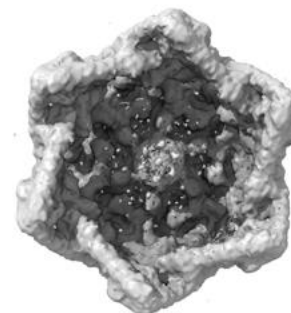
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

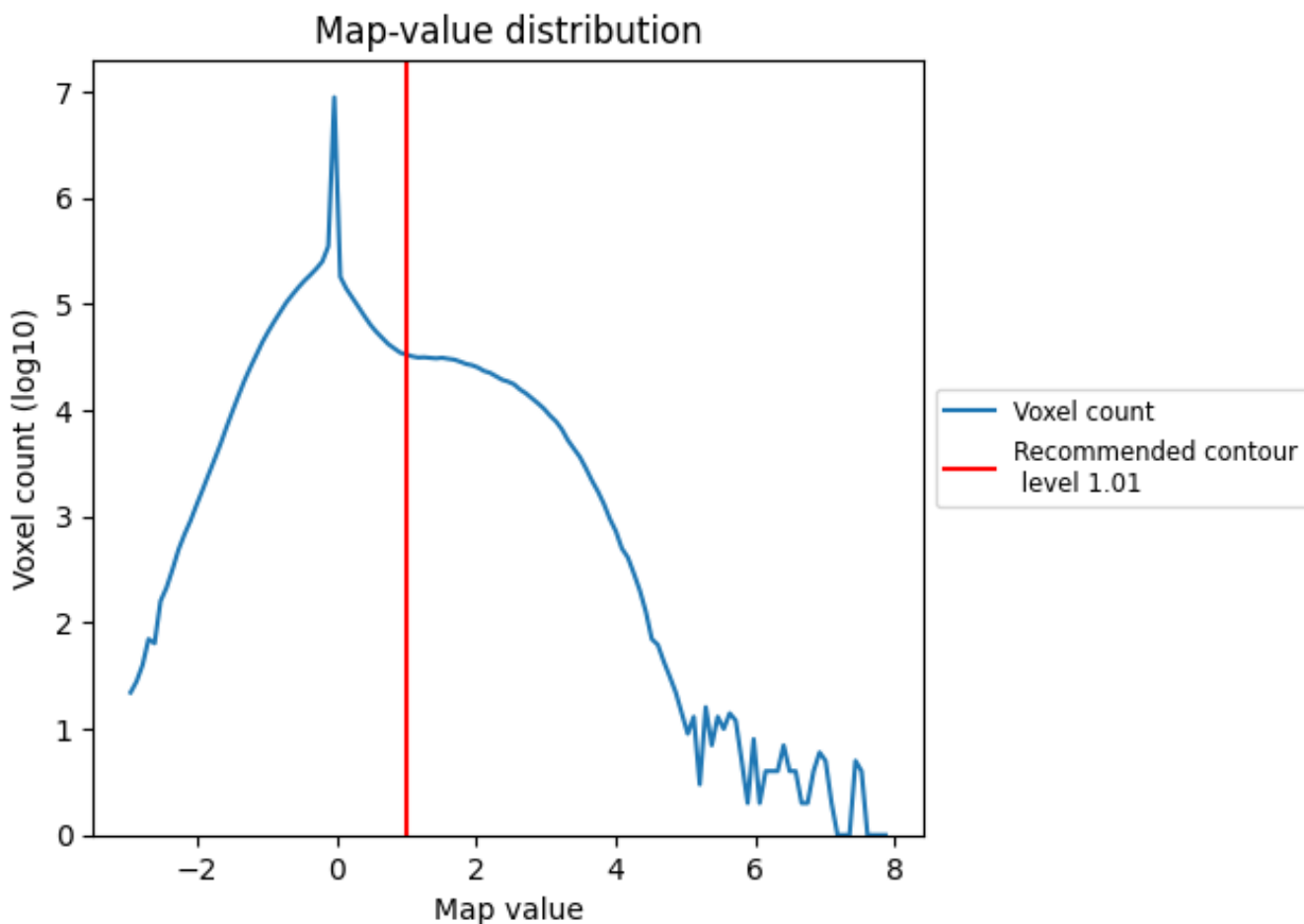
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

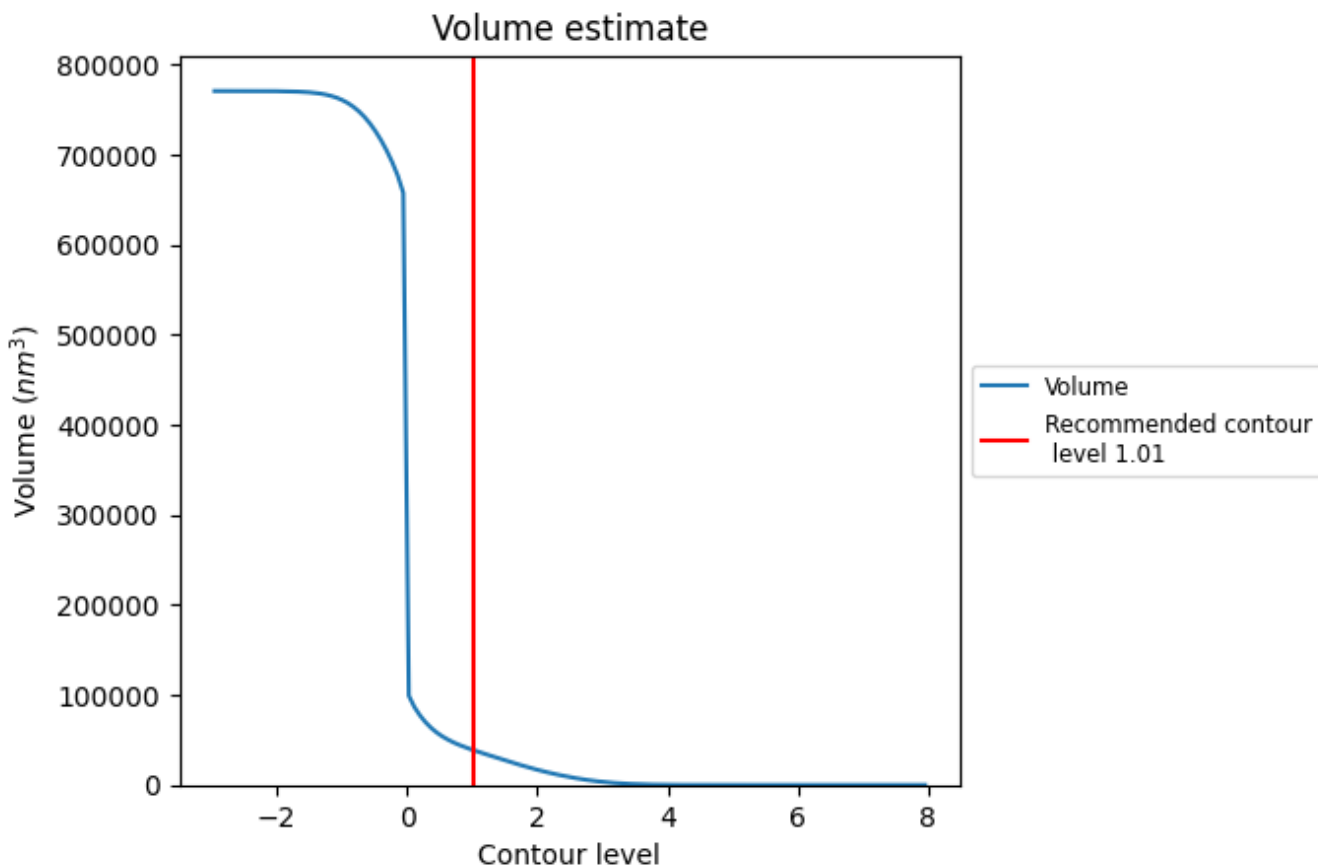
This section contains the results of statistical analysis of the map.

### 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 38892  $\text{nm}^3$ ; this corresponds to an approximate mass of 35132 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 [\(i\)](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation

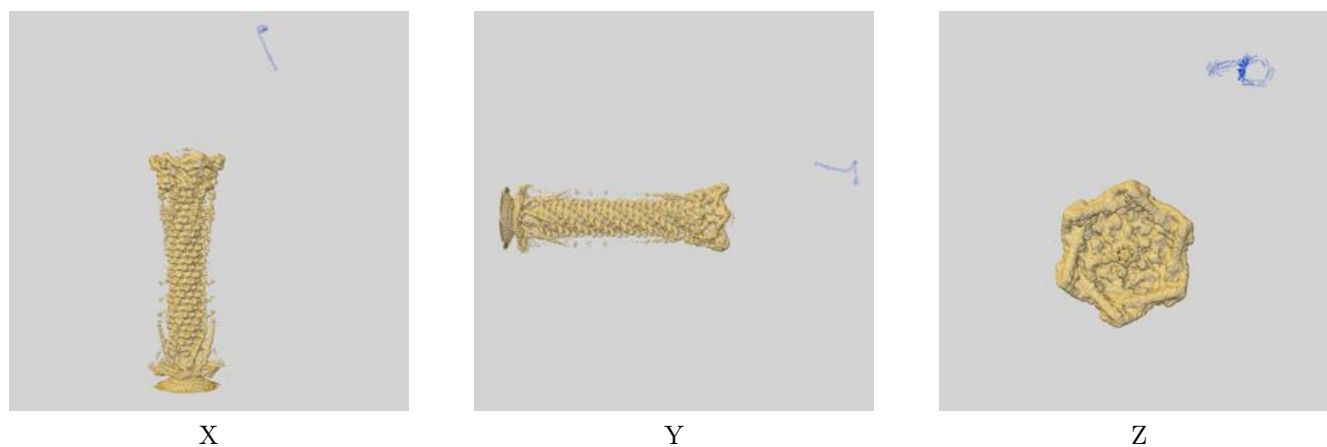
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

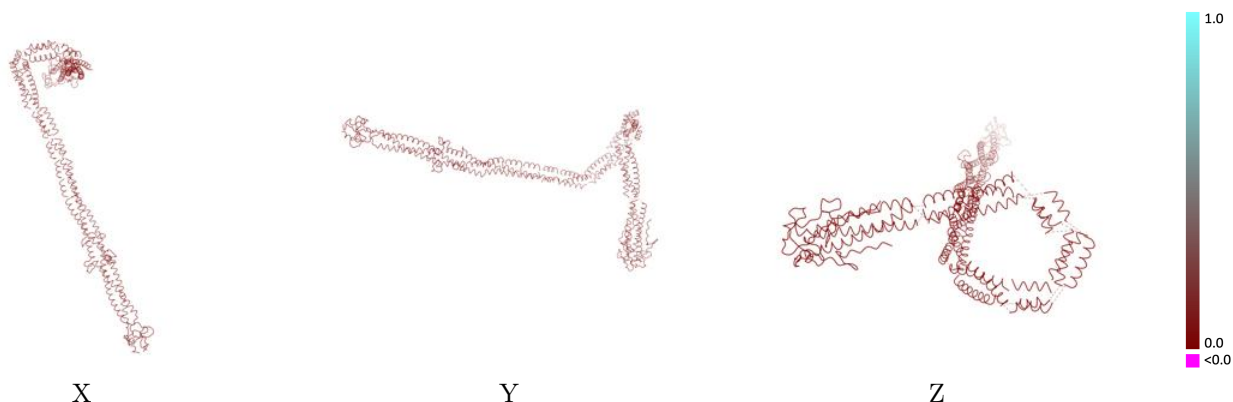
This section contains information regarding the fit between EMDB map EMD-1126 and PDB model 2BSG. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlay [i](#)



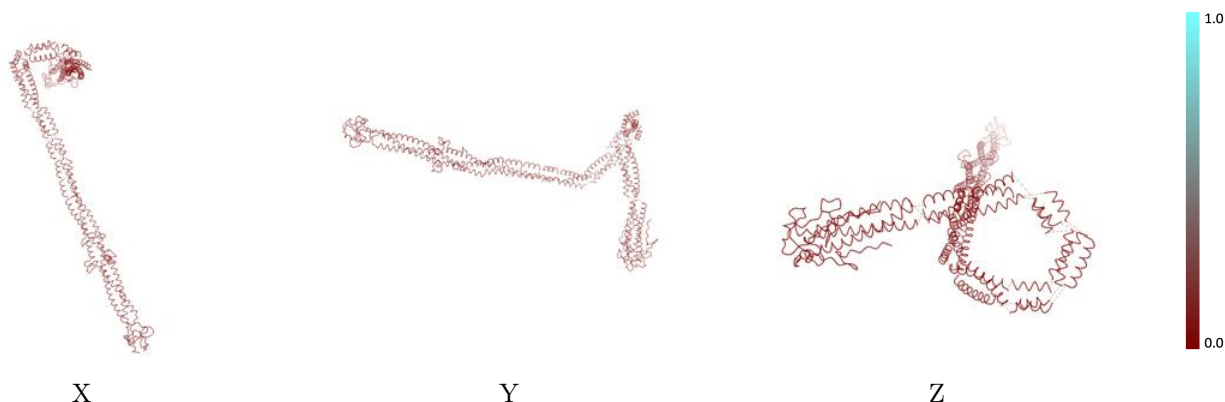
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



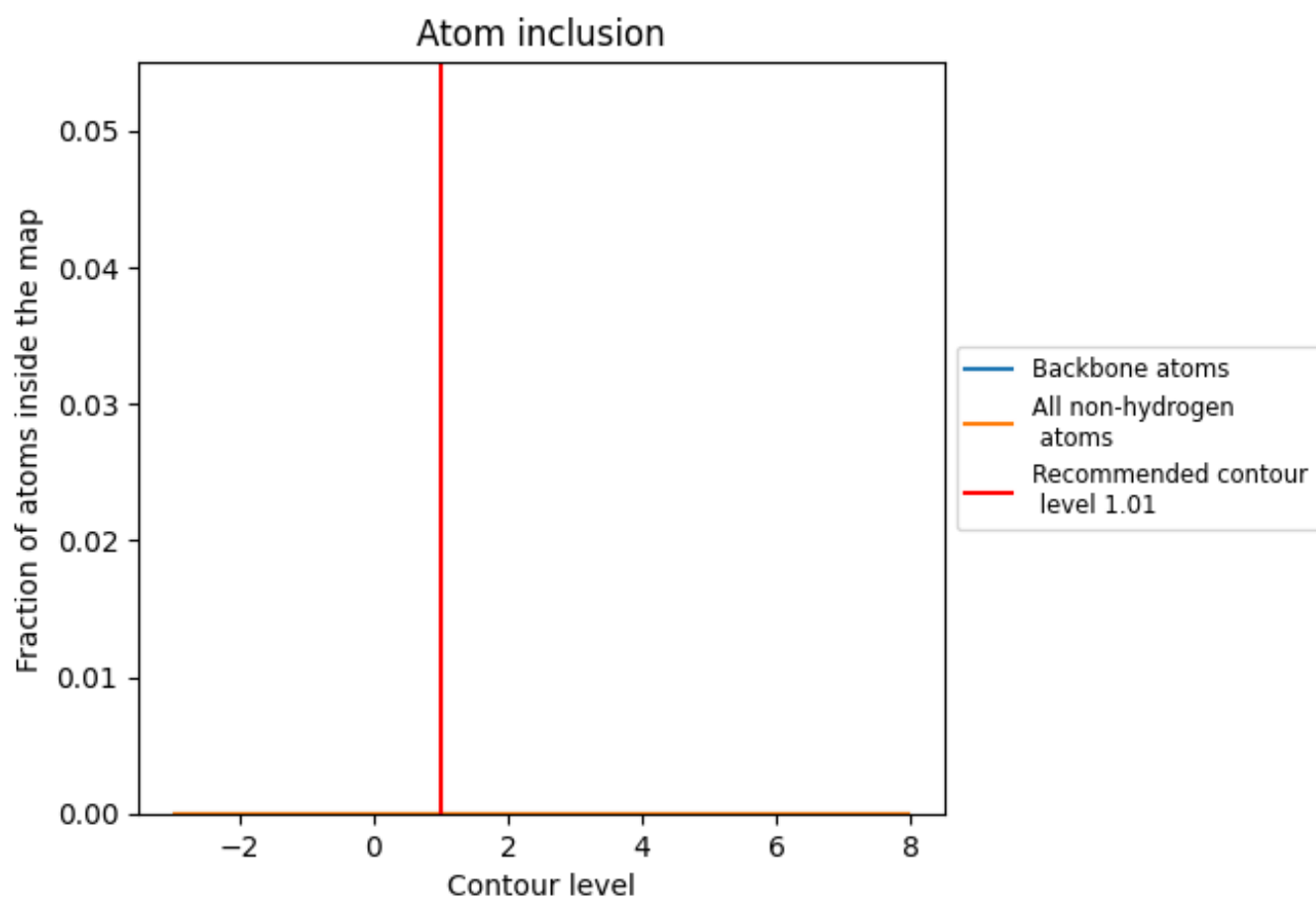
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.01).









## 9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0000	 0.0000
A	 0.0000	 0.0000
B	 0.0000	 0.0000
C	 0.0000	 0.0000

