Full wwPDB EM Validation Report (i)

Apr 29, 2024 – 04:24 pm BST

PDB ID	:	2BSG
EMDB ID	:	EMD-1126
Title	:	The modeled structure of fibritin (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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

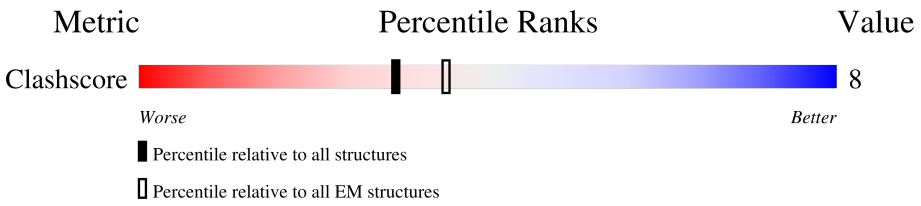
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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 >=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 <=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	75% 74% • 25%
1	B	487	75% 74% • 25%
1	C	487	75% 74% • 25%

2 Entry composition (i)

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.

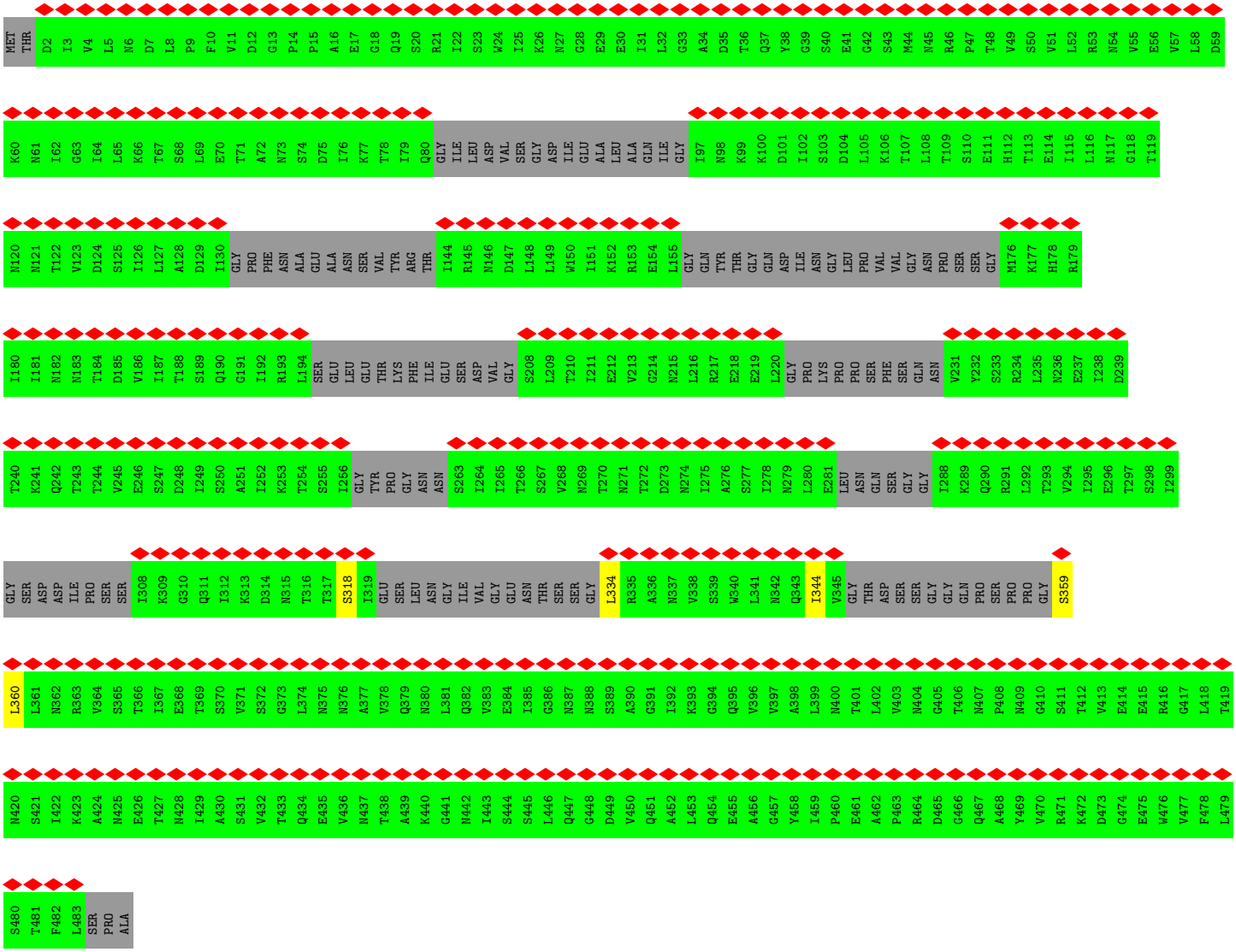
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
1	A	363	363	363	1	363
			Total	C		
1	B	363	363	363	1	363
			Total	C		
1	C	363	363	363	1	363

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.

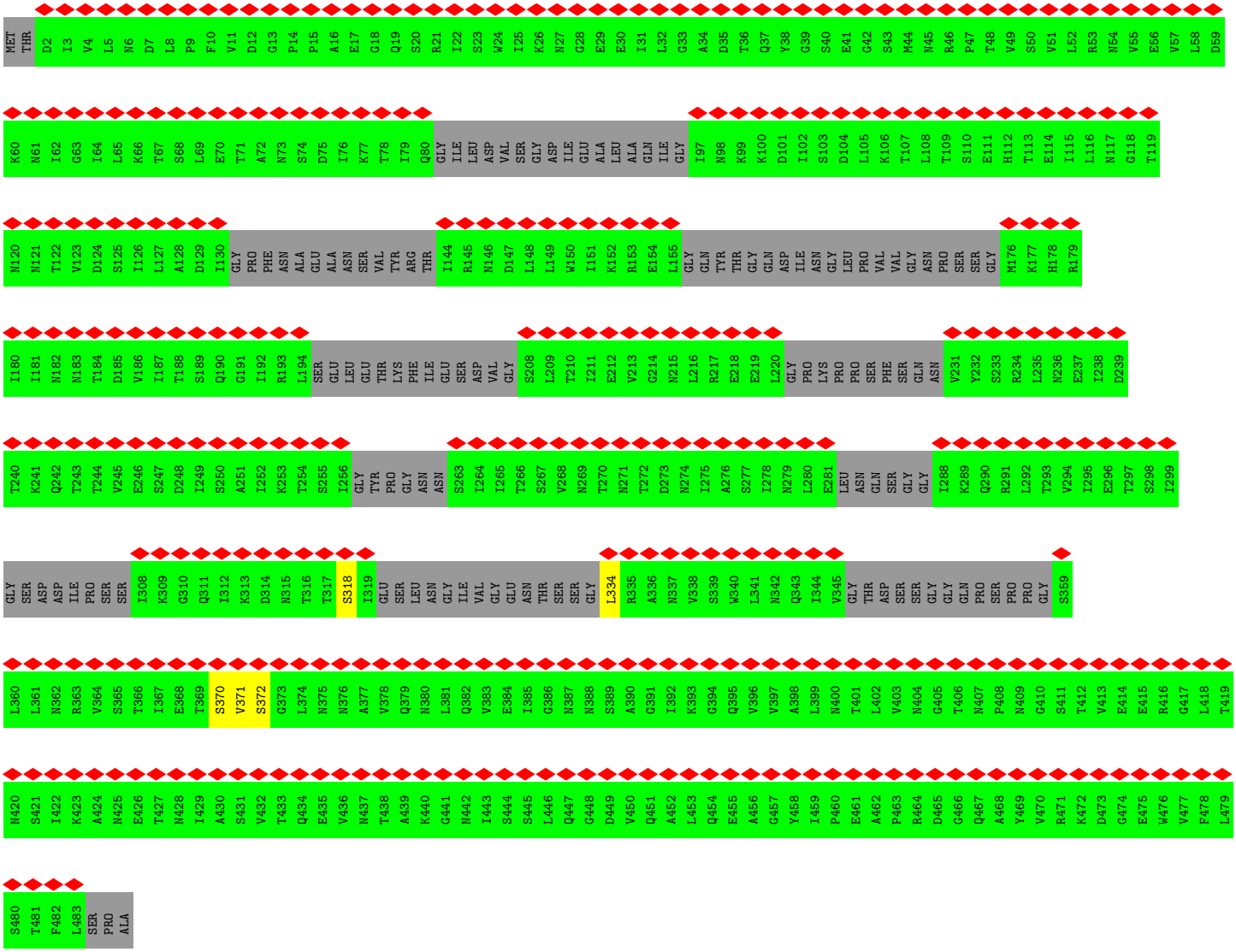
- Molecule 1: FIBRITIN

Chain A: 75% 74% 25%



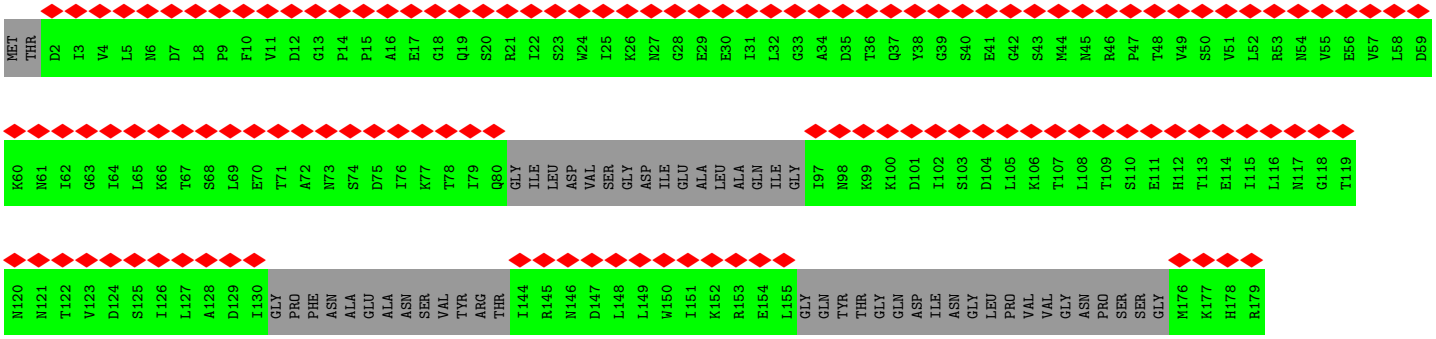
- Molecule 1: FIBRITIN

Chain B:



- Molecule 1: FIBRITIN

Chain C:



I180 I181 N182 N183 T184 D185 V186 I187 T188 S189 Q190 G191 I192 R193 L194 SER GLU LEU GLU THR LYS PHE ILE GLU SER ASP VAL GLY S208 L209 T210 I211 E212 V213 G214 N215 L216 R217 E218 E219 L220 GLY PRO LYS PRO PRO SER PHE SER GLN ASN V231 Y232 S233 R234 L235 N236 E237 I238 D239

T240 K241 Q242 T243 T244 V245 E246 S247 D248 I249 S250 A251 I252 K253 T254 S255 T256 GLY TYR PRO GLY ASN ASN S263 I264 I265 T266 S267 V268 N269 T270 N271 T272 D273 N274 I275 A276 S277 I278 N279 L280 E281 LEU ASN GLN SER GLY GLY I288 K289 Q290 R291 L292 T293 V294 I295 E296 T297 S298 I299

GLY SER ASP ASP ILE PRO SER SER I308 K309 G310 Q311 I312 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 W340 L341 N342 Q343 I344 V345 GLY THR ASP SER SER GLY GLY GLN PRO SER PRO PRO GLY S359

L360 L361 N362 R363 V364 S365 T366 I367 E368 T369 S370 V371 S372 G373 L374 N375 N376 A377 V378 Q379 N380 L381 Q382 V383 E384 I385 G386 N387 N388 S389 A390 G391 I392 K393 G394 Q395 V396 V397 A398 L399 N400 T401 L402 V403 N404 G405 T406 M407 P408 M409 G410 S411 T412 V413 E414 E415 R416 G417 L418 T419

N420 S421 I422 K423 A424 M425 E426 T427 M428 I429 A430 S431 V432 T433 Q434 E435 V436 N437 T438 A439 K440 G441 M442 I443 S444 S445 L446 Q447 G448 D449 V450 Q451 A452 L453 Q454 E455 A456 G457 Y458 I459 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

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	714.6, 714.6, 1508.6	wwPDB
Map dimensions	180, 180, 380	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	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

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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 (i)

There are no chain breaks in this entry.

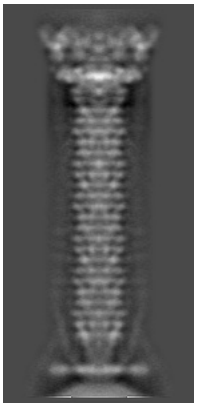
6 Map visualisation (i)

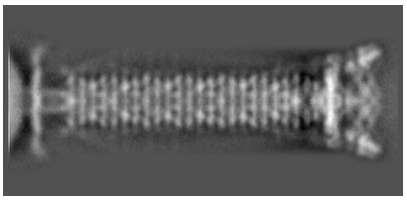
This section contains visualisations of the EMDB entry EMD-1126. These allow visual inspection of the internal detail of the map and identification of artifacts.

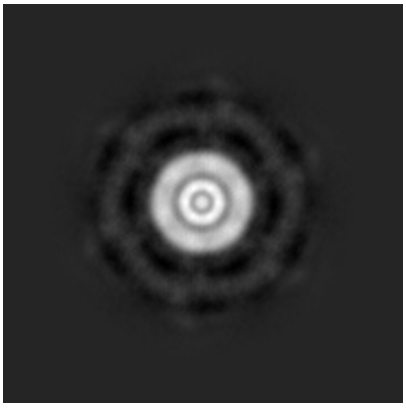
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

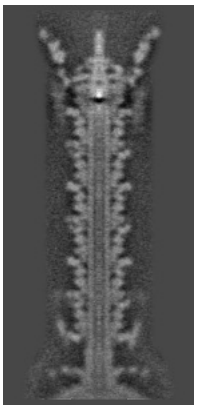

Y

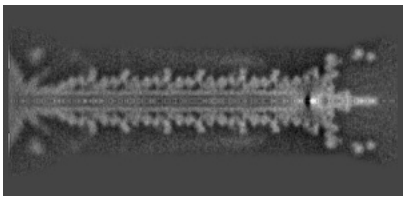

Z

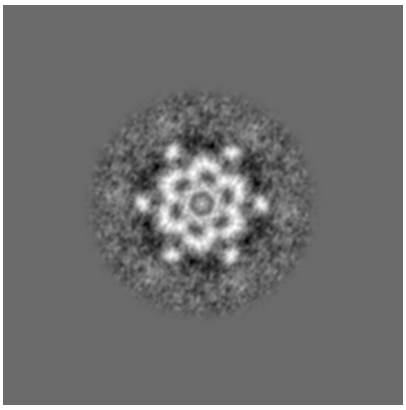
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 90

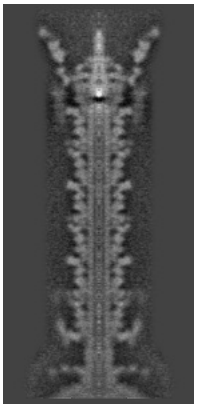

Y Index: 90

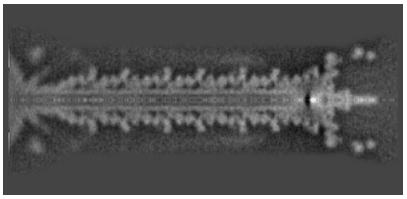

Z Index: 190

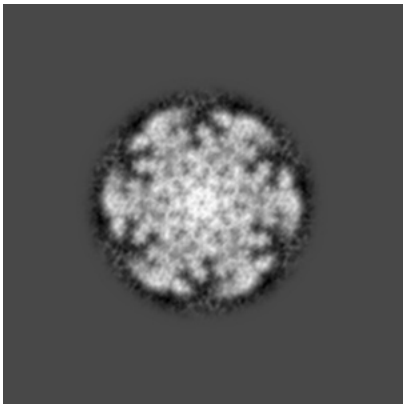
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 89

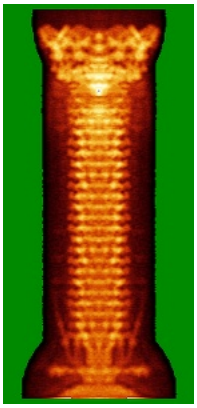

Y Index: 90

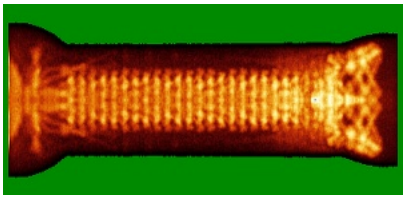

Z Index: 310

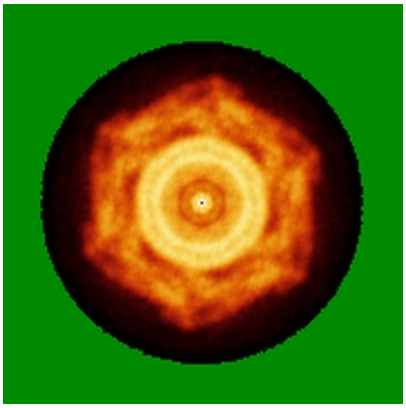
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

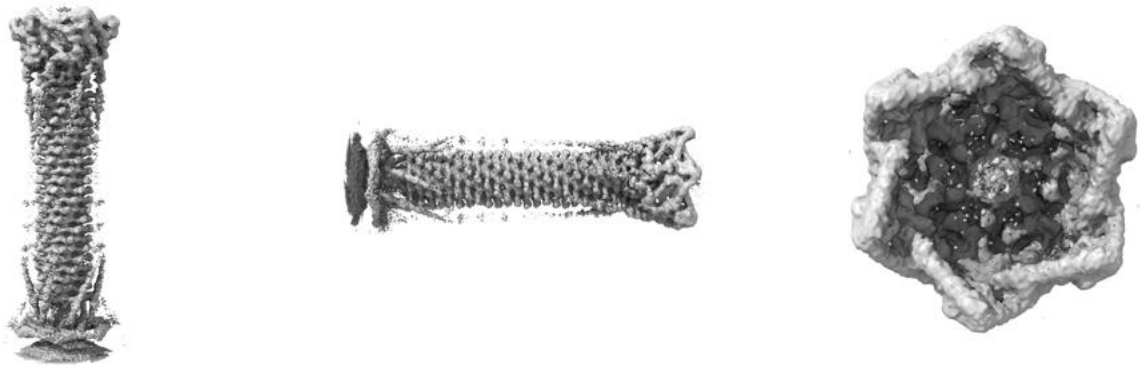

Y


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

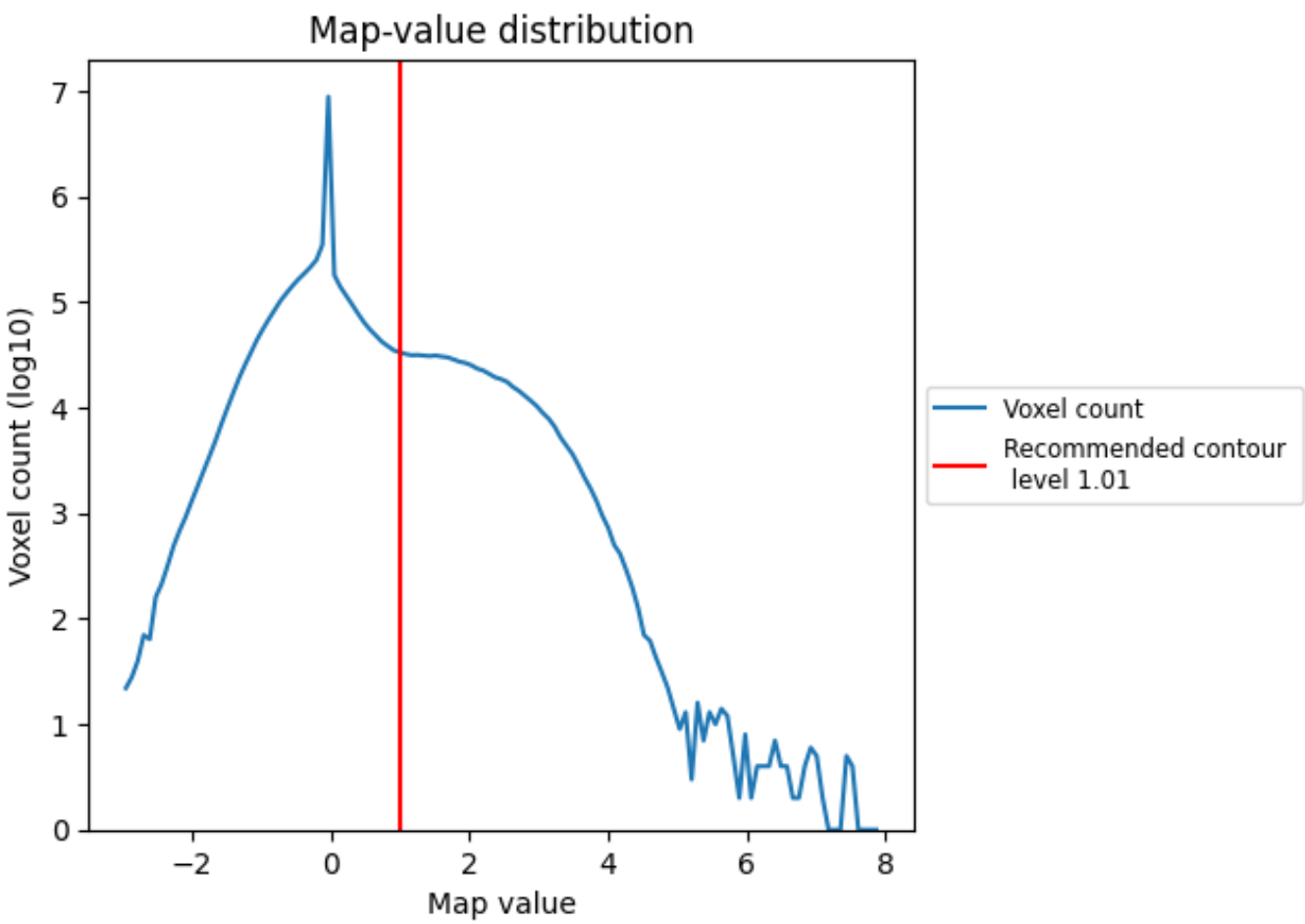
6.6 Mask visualisation (i)

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

7 Map analysis (i)

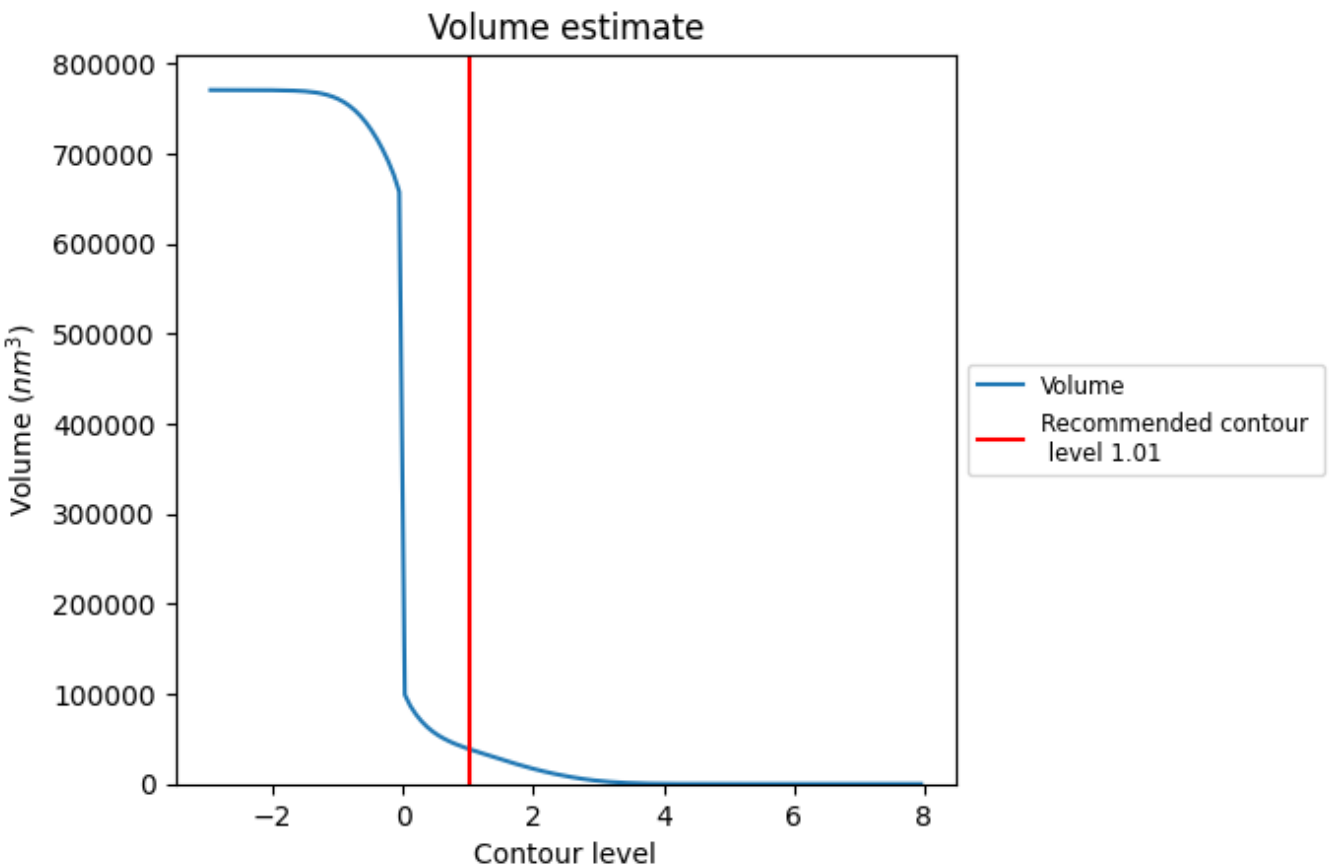
This section contains the results of statistical analysis of the map.

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 38892 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 (i)

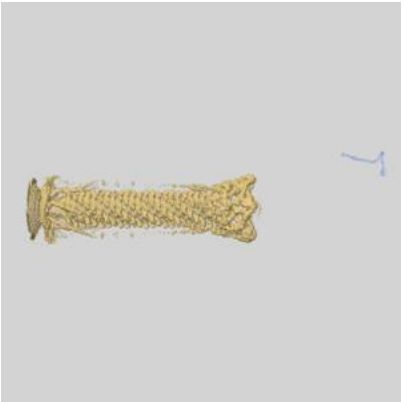
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

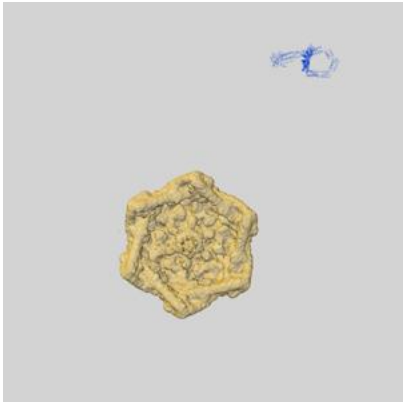
This section contains information regarding the fit between EMDB map EMD-1126 and PDB model 2BSG. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)

X



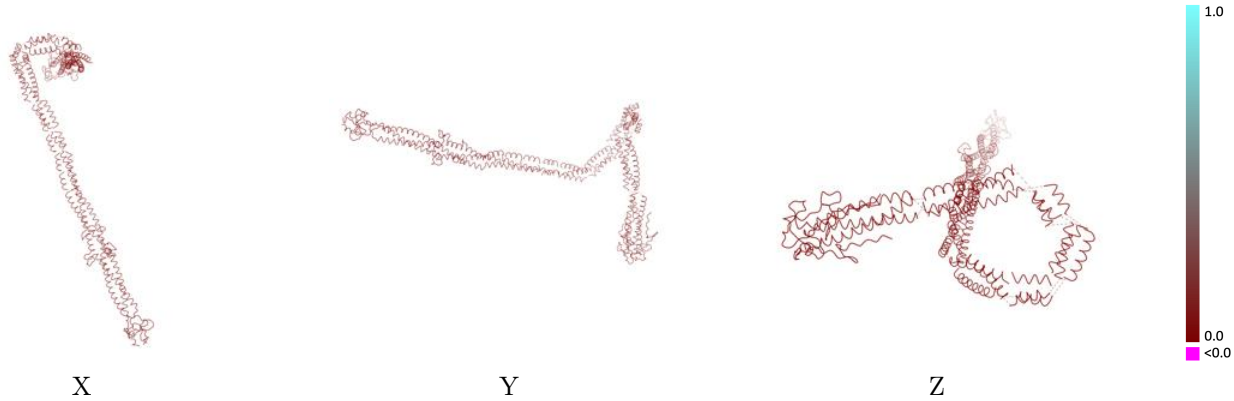
Y



Z

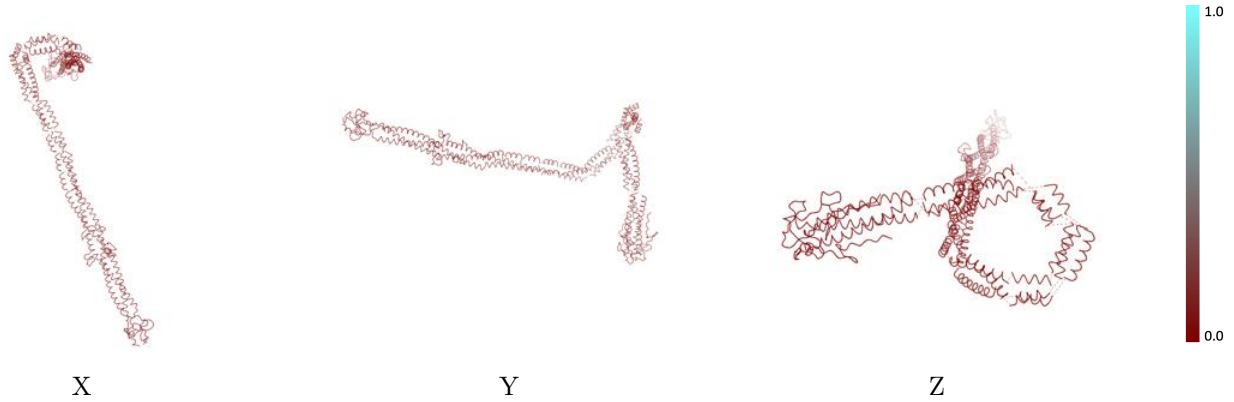
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



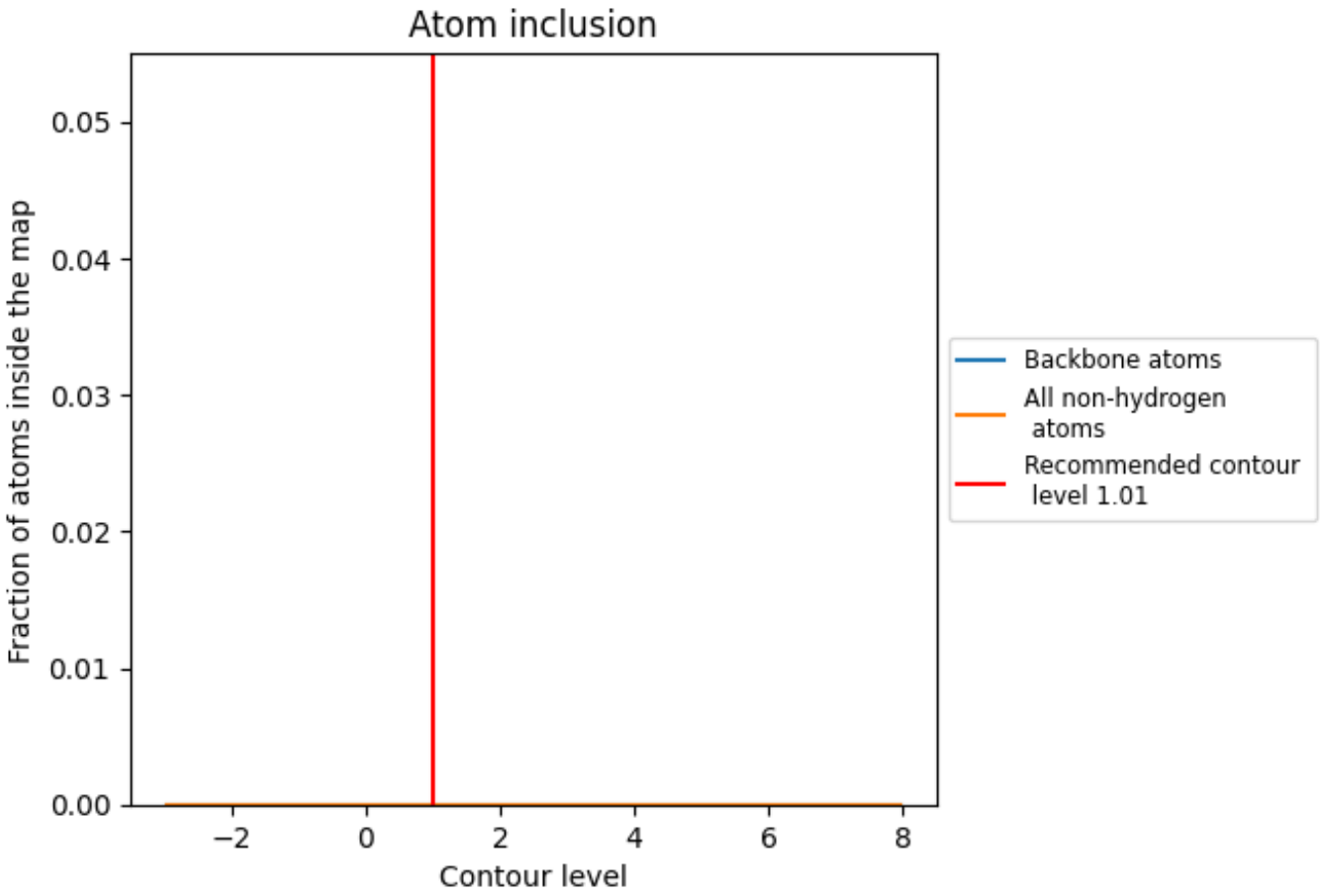
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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