

Integrative Structure Validation Report ?

October 15, 2026 - 03:11 PM PDT

The following software was used in the production of this report:

IHMValidation Version 3.2

Python-IHM Version 2.9

MolProbity Version 4.5.2

EMDB validation analysis Version 0.0.1.dev132

ChimeraX Version 1.11.1

Chimera Version 1.19

MapQ Version 1.8.1

PDB ID	9AAQ pdb_00009aaq
Structure Title	Fibrillar adhesin CdrA from Pseudomonas aeruginosa Downfield
Structure Authors	Fazio, N.T.; Moss, E.; Reichhardt, C.; Di Trani, J.; Barrington, M.J. ; BoClair, M.L.
Deposited on	2026-04-22

This is a PDB-IHM Structure Validation Report.

We welcome your comments at helpdesk@pdb-ihm.org

A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available [here](#).

1. Overview ?

1.1. Summary ?

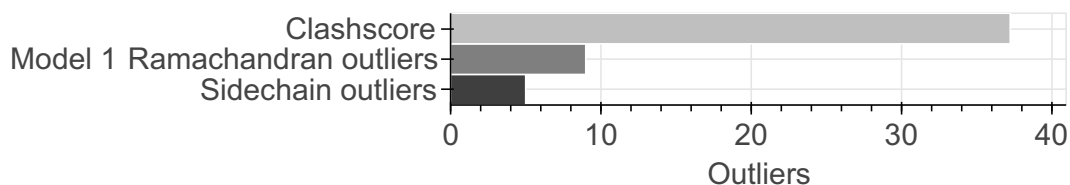
This entry consists of 1 model(s). A total of 9 dataset(s) were used to build this entry.

Name	Type	Count
3DEM volume	Experimental data	2
NMR data	Experimental data	6
De Novo model	Starting model	1

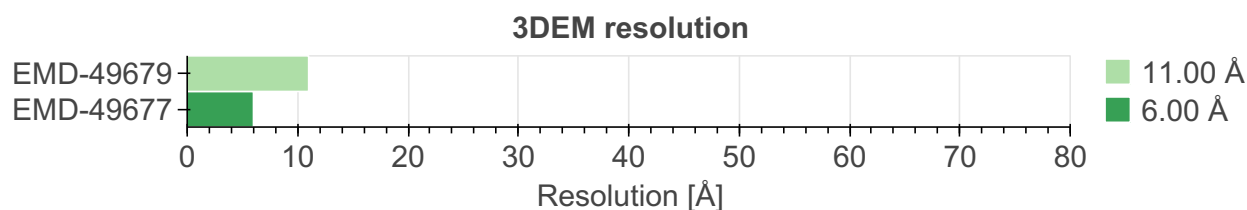
1.2. Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

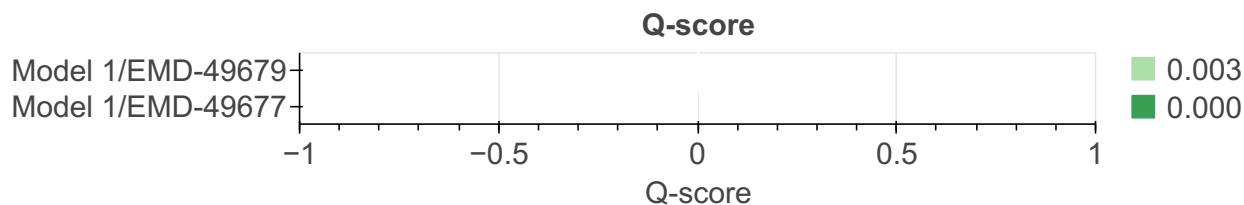
Model Quality: MolProbity Analysis ?



Data Quality ?



Fit to Data Used for Modeling ?



2. Model Details ?

2.1. Ensemble information ?

This entry consists of 0 distinct ensemble(s).

2.2. Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Filamentous haemagglutinin FhaB/tRNA nuclease CdiA-like TPS domain-containing protein	A	1668	-	1-1668	100.00 / 100.00	Atomic

2.3. Datasets used for modeling ?

There are 9 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	3DEM volume	EMDB	EMD-49677
2	NMR data	Other	10.5281/zenodo.14994263
3	De Novo model	AlphaFoldDB	AF-Q9HVG6-F1
4	3DEM volume	EMDB	EMD-49679
5	NMR data	Zenodo	10.5281/zenodo.14994263
6	NMR data	Zenodo	10.5281/zenodo.14994263
7	NMR data	Zenodo	10.5281/zenodo.14994263
8	NMR data	Zenodo	10.5281/zenodo.14994263
9	NMR data	Zenodo	10.5281/zenodo.14994263

2.4. Methodology and software ?

This entry is a result of 5 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Initial Modeling	Not available	N*-terminal domain and each repeat module were modeled individually	Not available	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	2	Energy Minimization with Tinker 8	Energy minimization	All simulations were performed in the gas phase at a dielectric of 80 and without charges. We performed energy minimization in Cartesian coordinate space using limited memory BFGS quasi-Newton nonlinear optimization with the Amber99sb force field to an RMS gradient convergence of 1 kcal mol ⁻¹ Å ⁻¹ . We restrained the phi and psi angles +/- 5 degrees relative to the TALOS-N value for the identified residues with a force constant of 125 kcal Å ⁻² . For repeat modules where the residue identity varied, we did not include a restraint. We additionally included longer-distance restraints between V14-G16 (6.6 Å), R46-A48 (6.7 Å) and L29-Y69 (6.2 Å) +/- 1 Å with a force constant of 100 kcal Å ⁻² . As the sequence is not identical between all residues, the residue location varied slightly, but distances were maintained. All other values were maintained from the AlphaFold model.	Not available	False	False
1	3	TALOS-N to determine torsion angles	Not available	Determination of torsion (phi/psi) angles from chemical shift information from solid-state NMR.	Not available	False	False
1	4	Geometry Minimization in Phenix	Not available	Phenix geometry-minimization to fix rotamers and Ramachandran angles	Not available	False	False
1	5	Model Validation	Validation:	MolProbity to compare torsion angles from chemical shift data and final PDB file	Not available	False	False

There are 7 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	AlphaFold 3	Not available	Initial Model	https://alphafold.ebi.ac.uk/
6	TALOS-N	Not available	Restraint Development from solid state NMR chemical shifts and long-distance restraints	https://spin.niddk.nih.gov/bax/software/TALOS-N/
4	Tinker 8	Not available	Energy minimization of elongation domain	https://dasher.wustl.edu/tinker/
5	Phenix	1.21.2	Geometry Minimization	https://phenix-online.org/
7	MolProbity	4.5.2	Model Validation	http://molprobity.biochem.duke.edu/
2	UCSF ChimeraX	1.10.1	Model Building	https://www.rbvi.ucsf.edu/chimerax/

ID	Software name	Software version	Software classification	Software location
3	cryoSPARC	4.7.1	experimental determination of cryoEM maps	https://guide.cryosparc.com/

3. Data quality ?

3.3. 3DEM ?

This section describes quality of the 3DEM datasets

[EMD-49677](#)

[3.3.1. Experimental information](#) ?

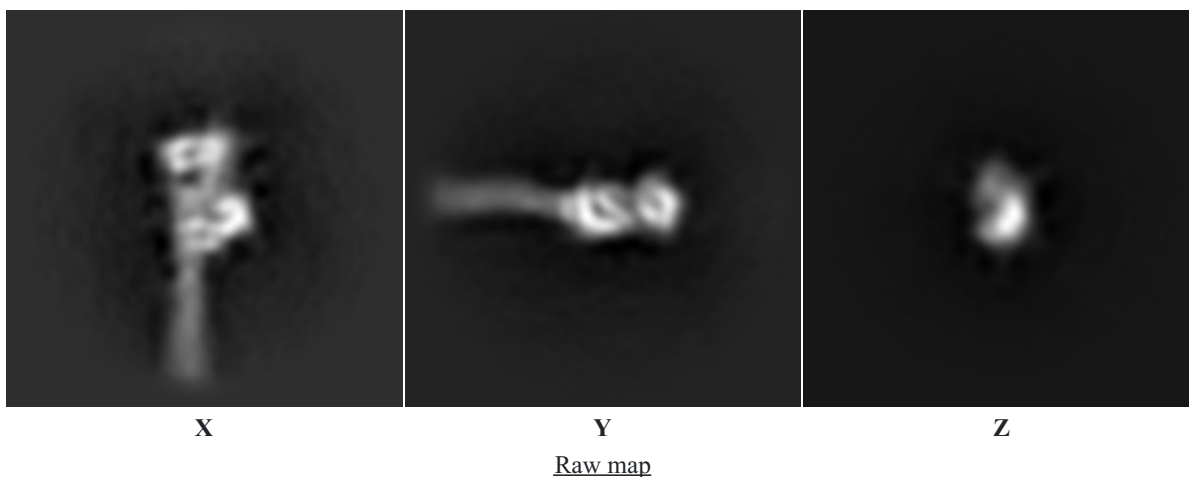
EM reconstruction method:	SINGLE PARTICLE
Resolution:	6.00 Å
Recommended level:	0.160
Estimated volume:	171.20 nm ³
Specimen preparation:	Preparation ID 1 Vitrification
Map-only validation report:	wwPDB validation report

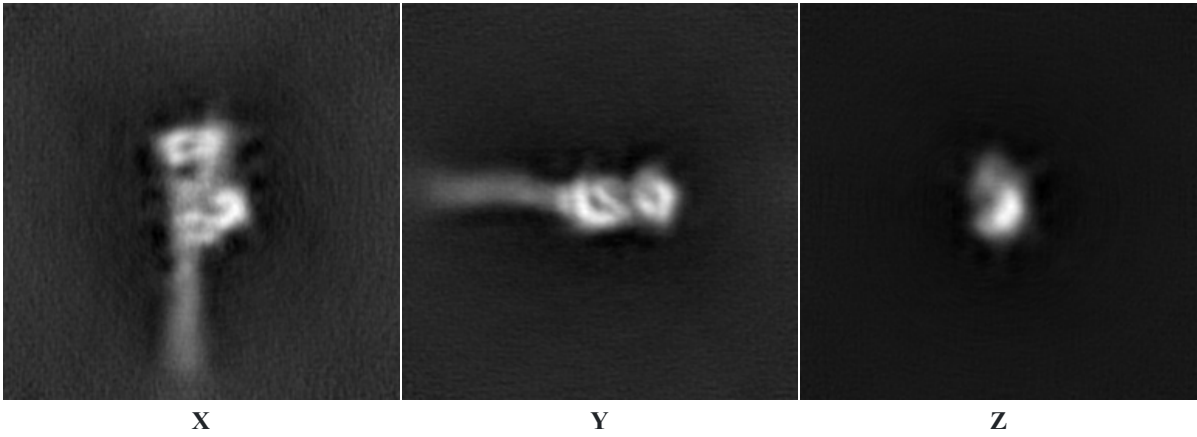
[3.3.2. Map visualisation](#) ?

This section contains visualisations of the EMDB entry EMD-49677. These allow visual inspection of the internal detail of the map and identification of artifacts. Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

[3.3.2.1. Orthogonal projections](#) ?

[Primary map](#)

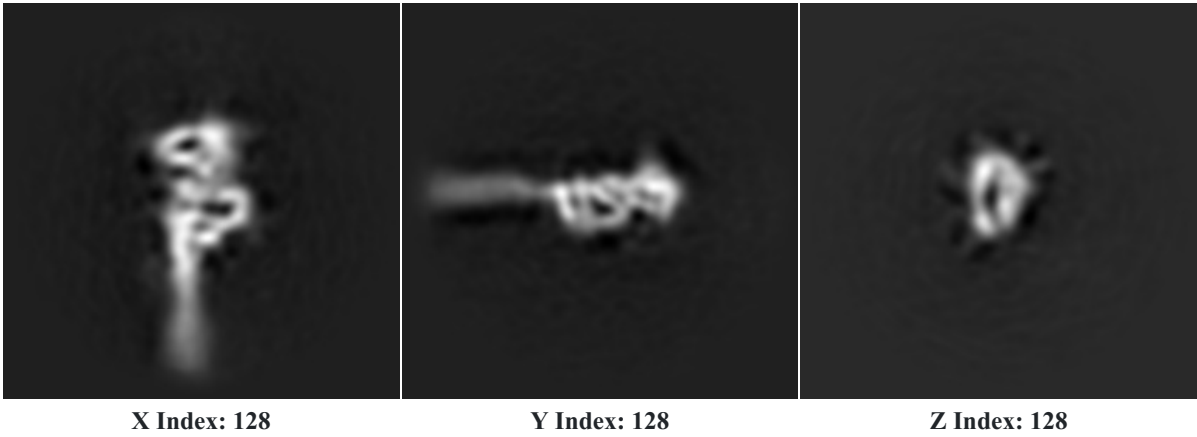




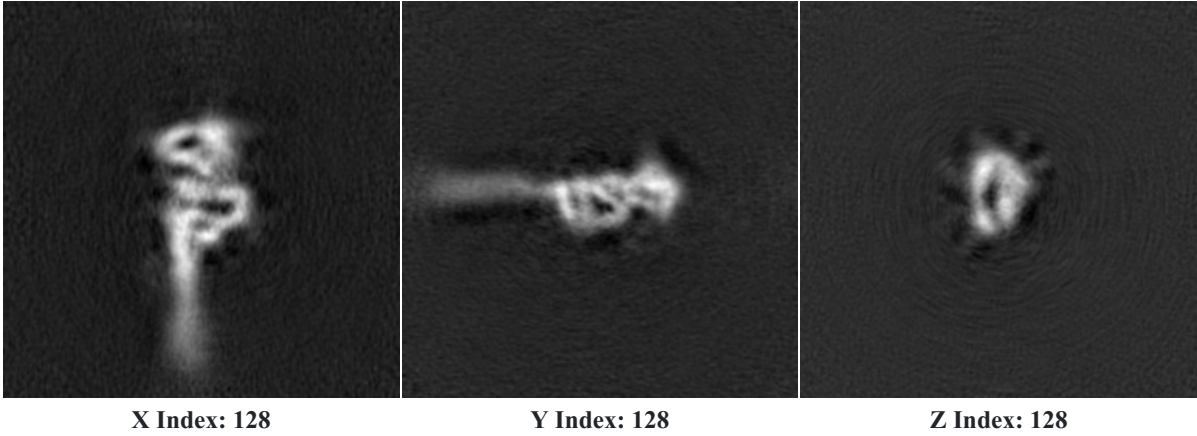
The images above show the map projected in three orthogonal directions.

3.3.2.2. Central slices ?

Primary map



Raw map



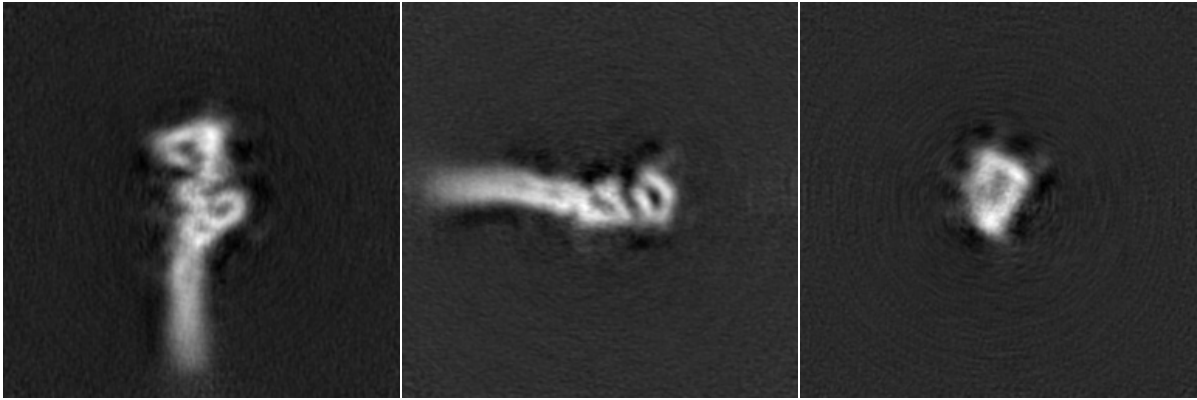
The images above show central slices of the map in three orthogonal directions.

3.3.2.3. Largest variance slices ?

Primary map



X Index: 134 Y Index: 117 Z Index: 117
Raw map

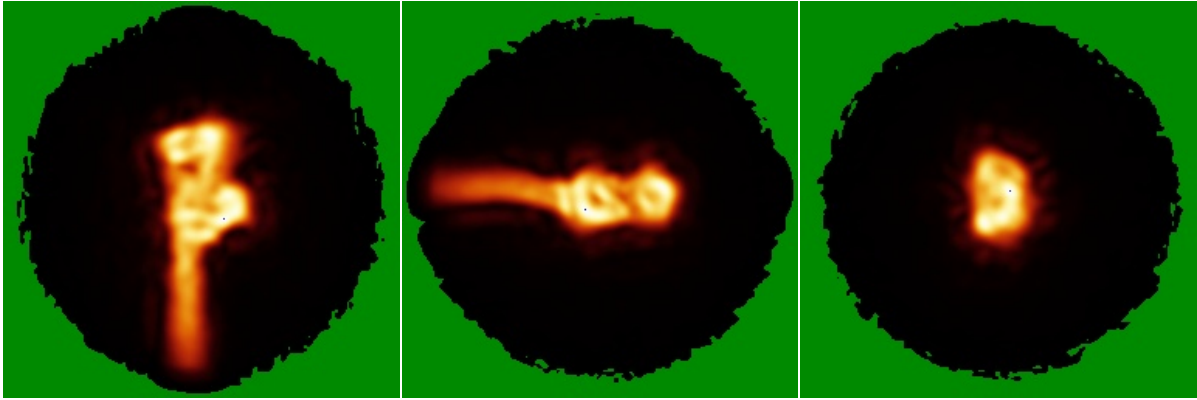


X Index: 134 Y Index: 117 Z Index: 117

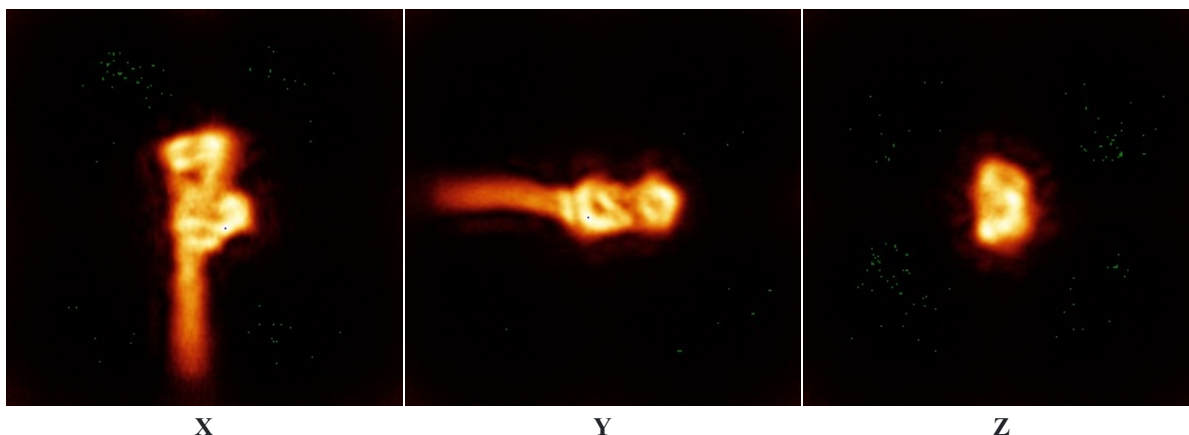
The images above show the largest variance slices of the map in three orthogonal directions.

3.3.2.4 Orthogonal standard-deviation projections (false-color) ?

Primary map



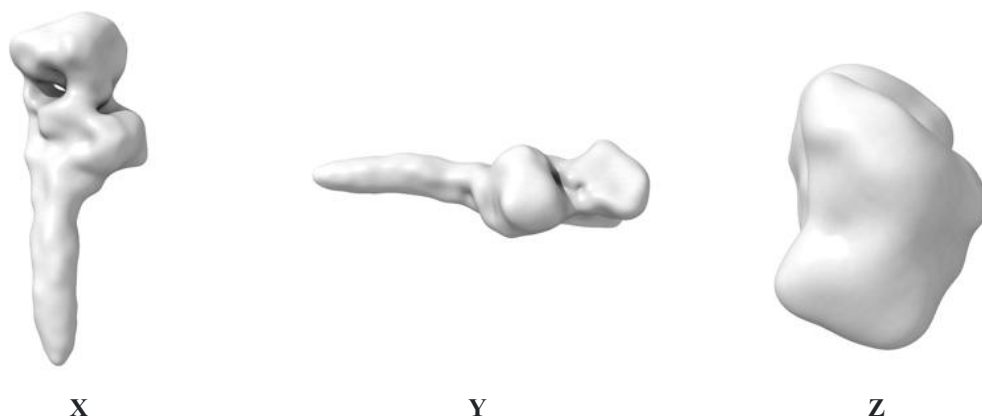
X Y Z
Raw map



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.

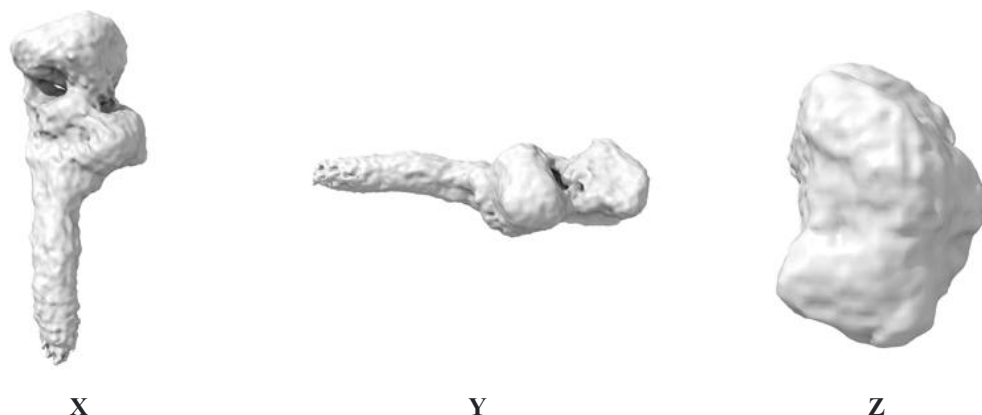
3.3.2.5. Orthogonal surface views ?

Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.160 . These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

Raw map

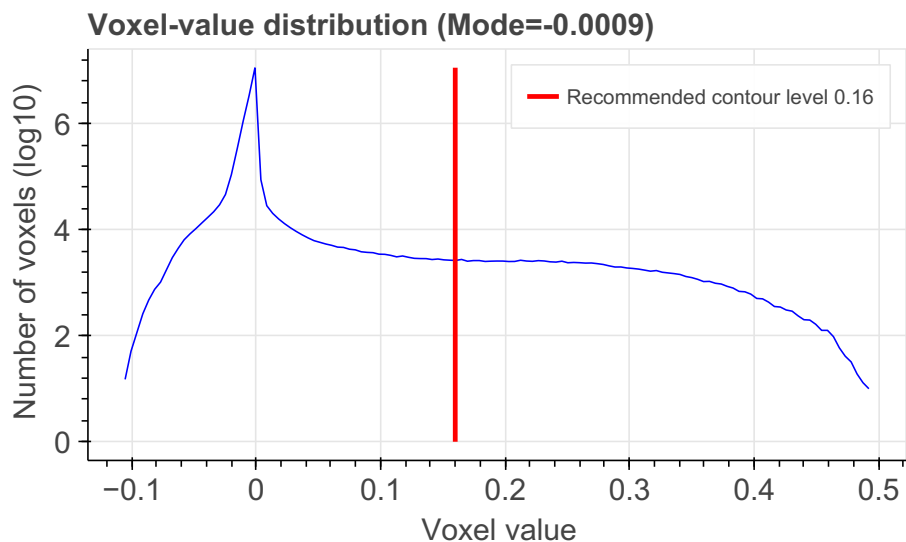


These images show the 3D surface of the raw map. The raw map's contour level 0.150 was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

3.3.3. Map analysis ?

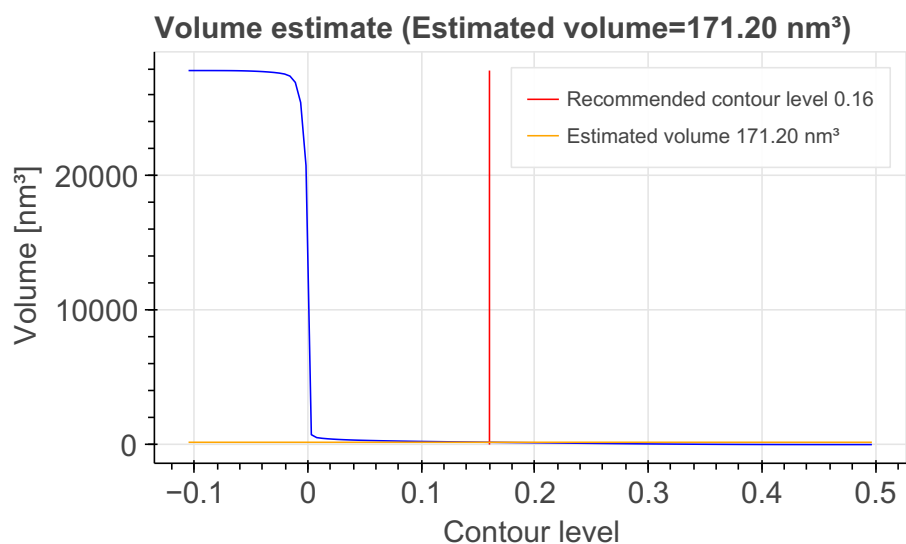
This section contains the results of statistical analysis of the map.

3.3.3.1. Map-value distribution ?



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.

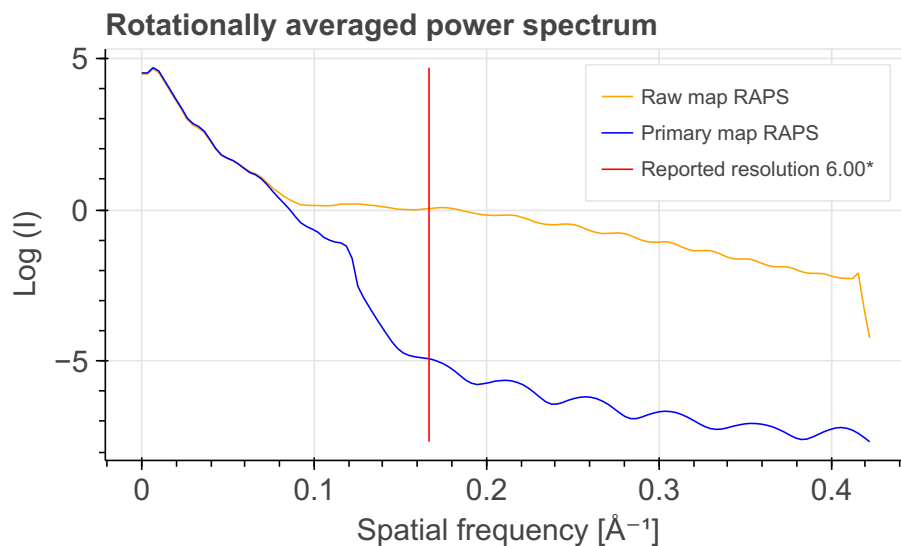
3.3.3.2. Volume estimate ?



The volume at the recommended contour level is 171.20 nm³.

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.

3.3.3.3. Rotationally averaged power spectrum ?

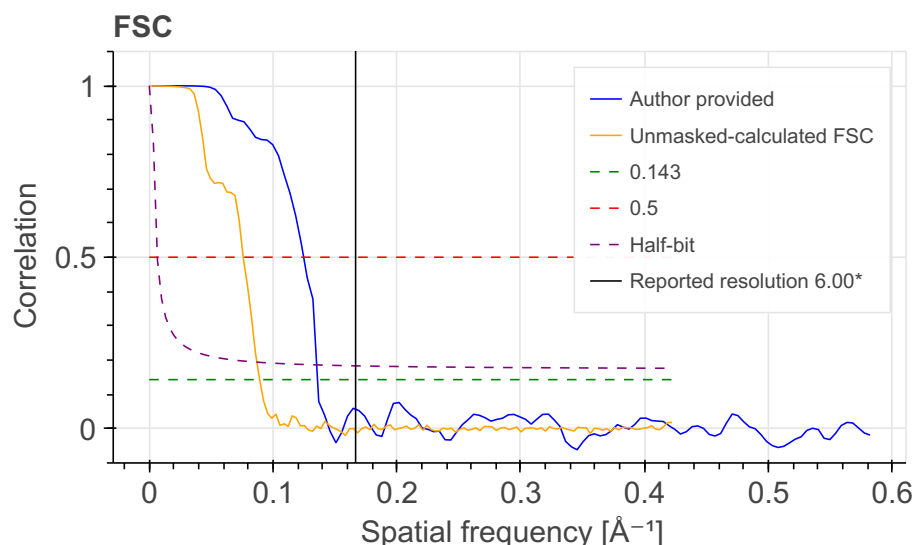


*Reported resolution corresponds to spatial frequency of $0.167 \text{ \AA}^{-1}$

3.3.4. Fourier-Shell correlation ?

3.3.4.1. FSC ?

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.



*Reported resolution corresponds to spatial frequency of $0.167 \text{ \AA}^{-1}$

3.3.4.2. Resolution estimates ?

Resolution estimate ($\text{\AA}$)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	7.36	8.02	7.40
Unmasked-calculated*	11.22	13.18	11.51

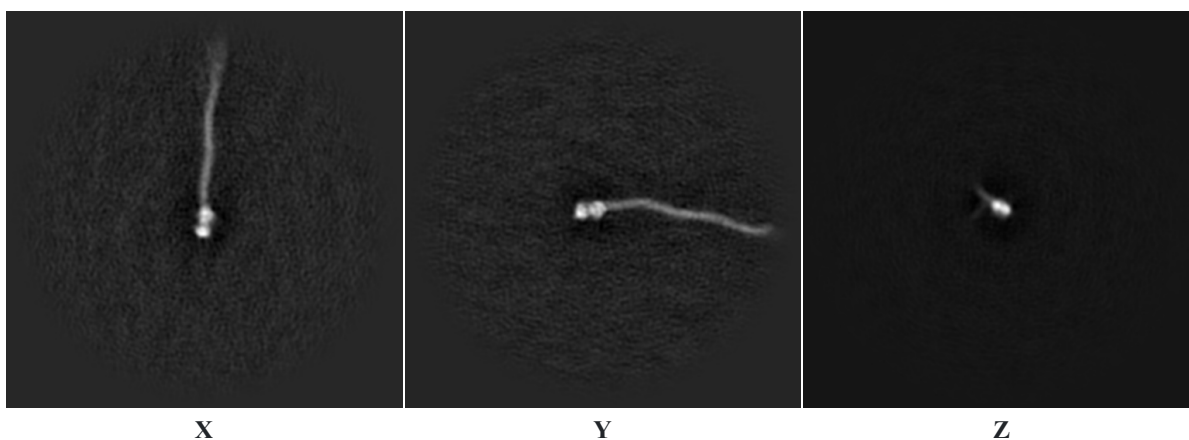
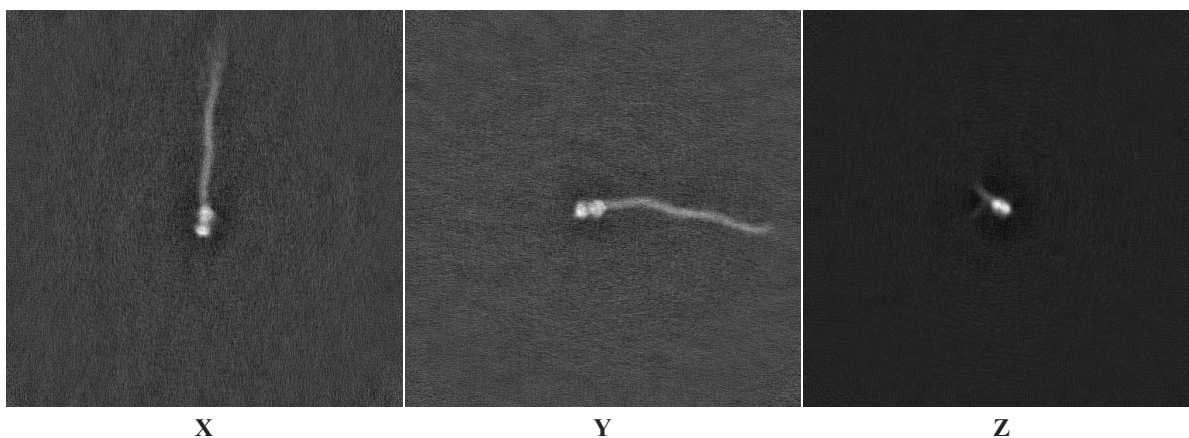
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 11.22 differs from the reported value 6.00 by more than 10%.

[EMD-49679](#)[3.3.1. Experimental information](#)

EM reconstruction method:	SINGLE PARTICLE		
Resolution:	11.00 Å		
Recommended level:	0.750		
Estimated volume:	47.69 nm ³		
Specimen preparation:	Preparation ID	1	Vitrification
Map-only validation report:	wwPDB validation report		

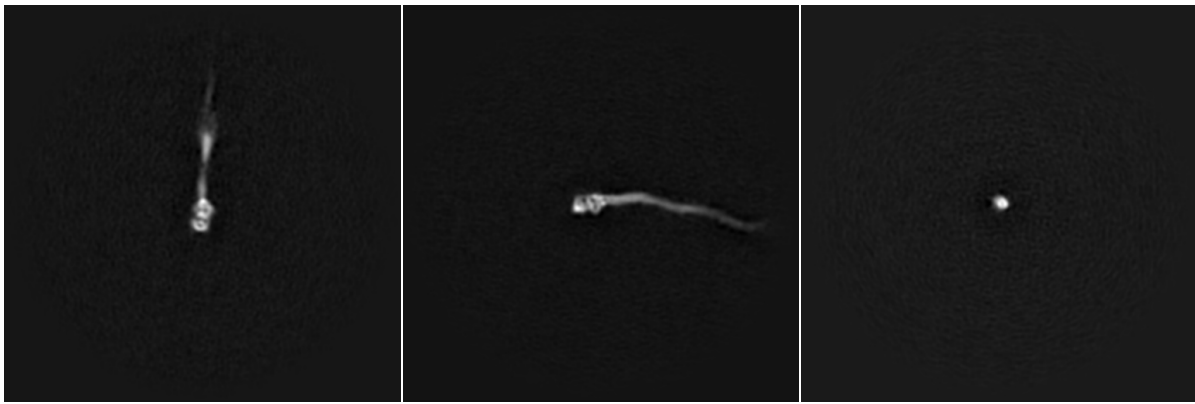
[3.3.2. Map visualisation](#)

This section contains visualisations of the EMDB entry EMD-49679. These allow visual inspection of the internal detail of the map and identification of artifacts. Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

[3.3.2.1. Orthogonal projections](#)[Primary map](#)[Raw map](#)

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

[3.3.2.2. Central slices](#)[Primary map](#)

**X Index: 256****Y Index: 256****Z Index: 256**

Raw map

**X Index: 256****Y Index: 256****Z Index: 256**

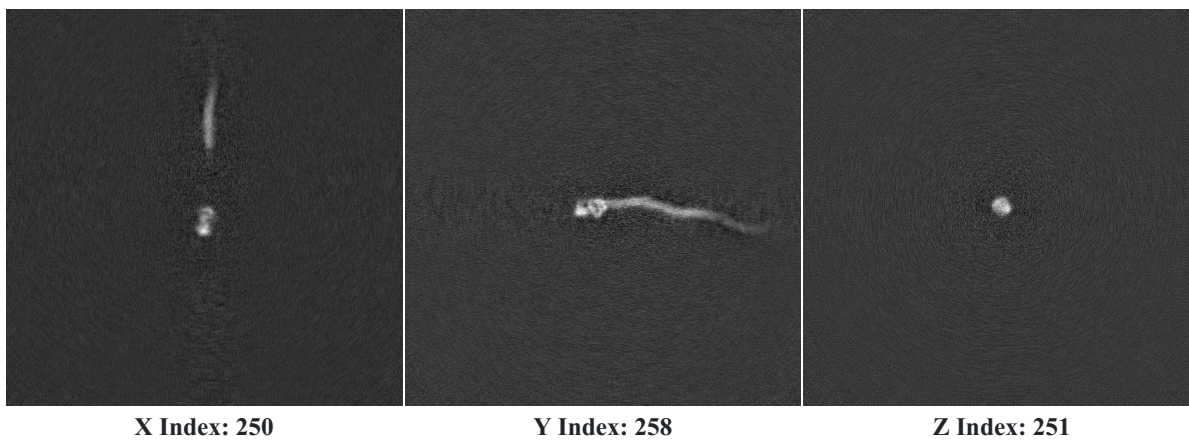
The images above show central slices of the map in three orthogonal directions.

3.3.2.3. Largest variance slices ?

Primary map

**X Index: 250****Y Index: 258****Z Index: 225**

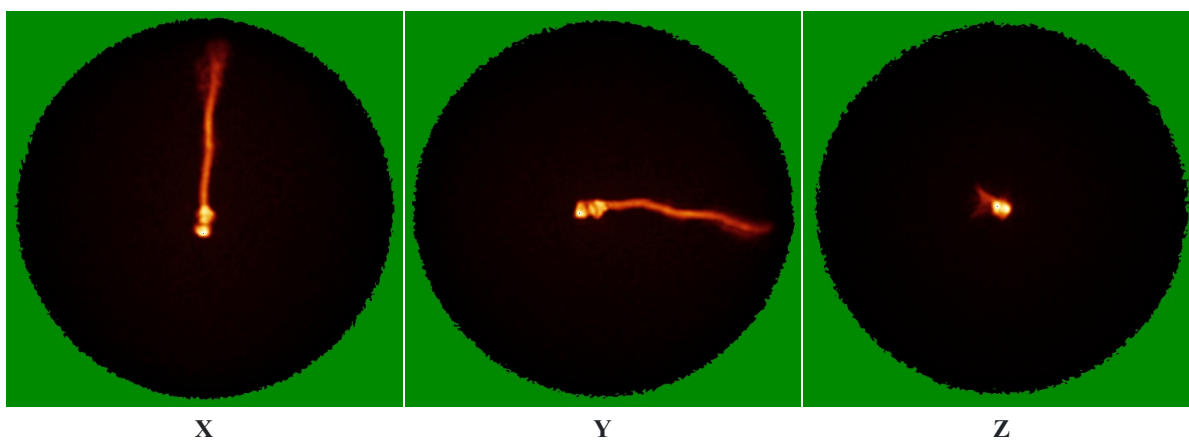
Raw map



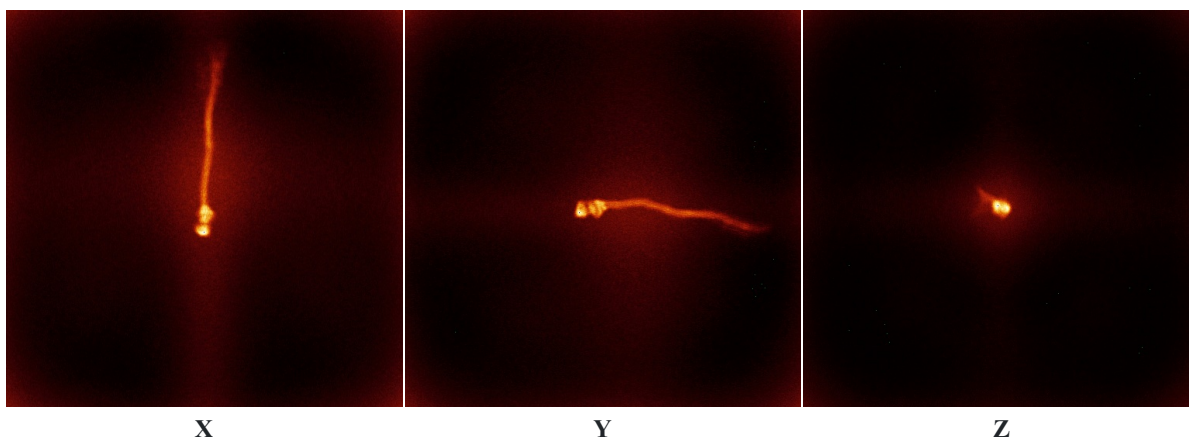
The images above show the largest variance slices of the map in three orthogonal directions.

3.3.2.4 Orthogonal standard-deviation projections (false-color) ?

Primary map



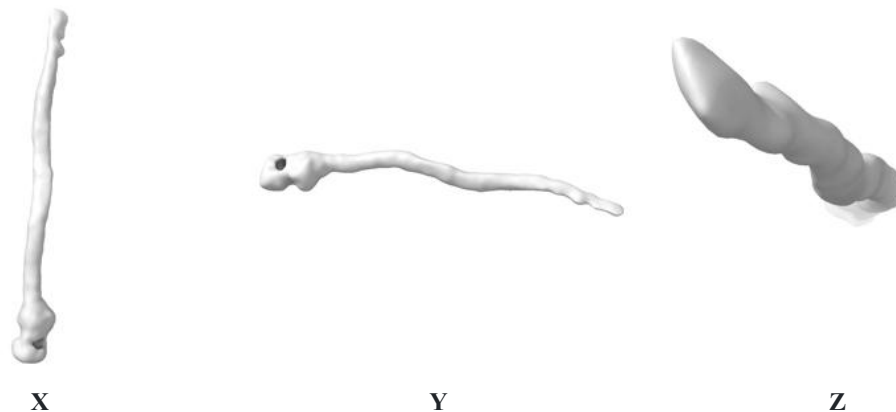
Raw map



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.

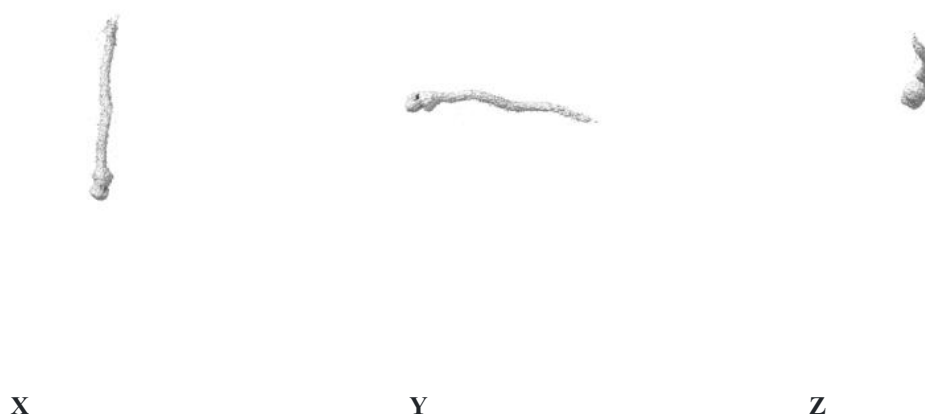
3.3.2.5. Orthogonal surface views ?

Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.750 . These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

Raw map

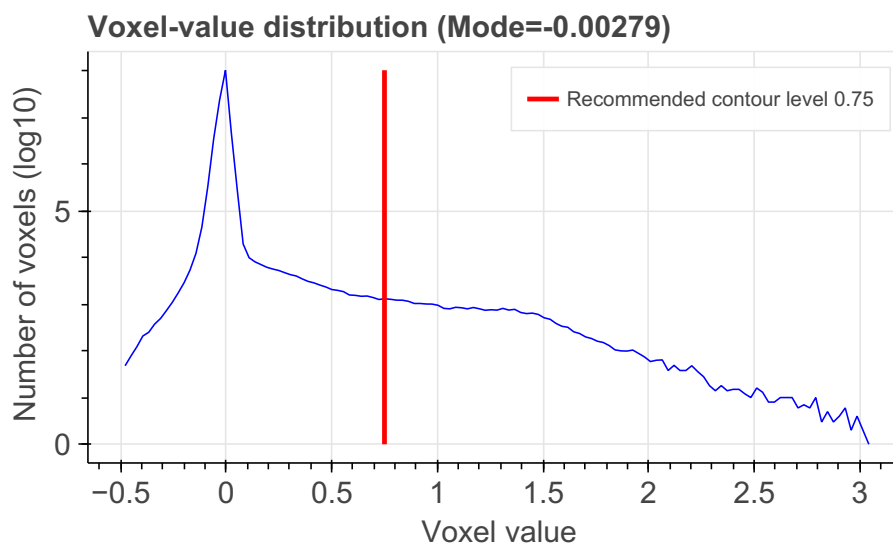


These images show the 3D surface of the raw map. The raw map's contour level 0.190 was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

3.3.3. Map analysis ?

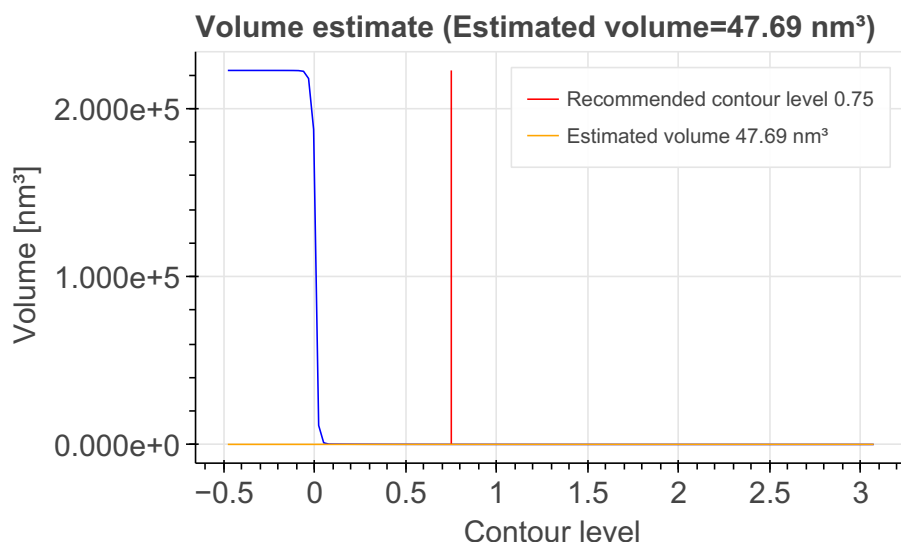
This section contains the results of statistical analysis of the map.

3.3.3.1. Map-value distribution ?



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.

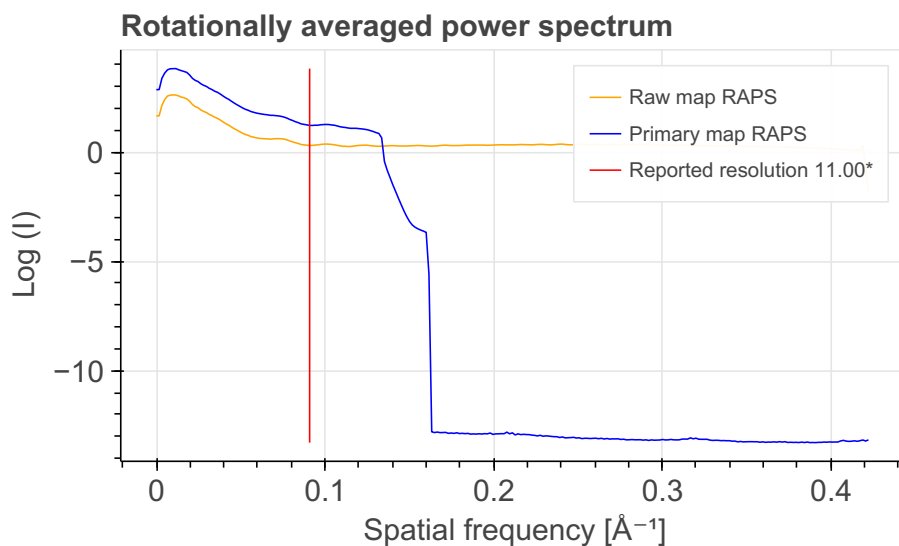
3.3.3.2. Volume estimate ?



The volume at the recommended contour level is 47.69 nm³.

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.

3.3.3.3. Rotationally averaged power spectrum ?

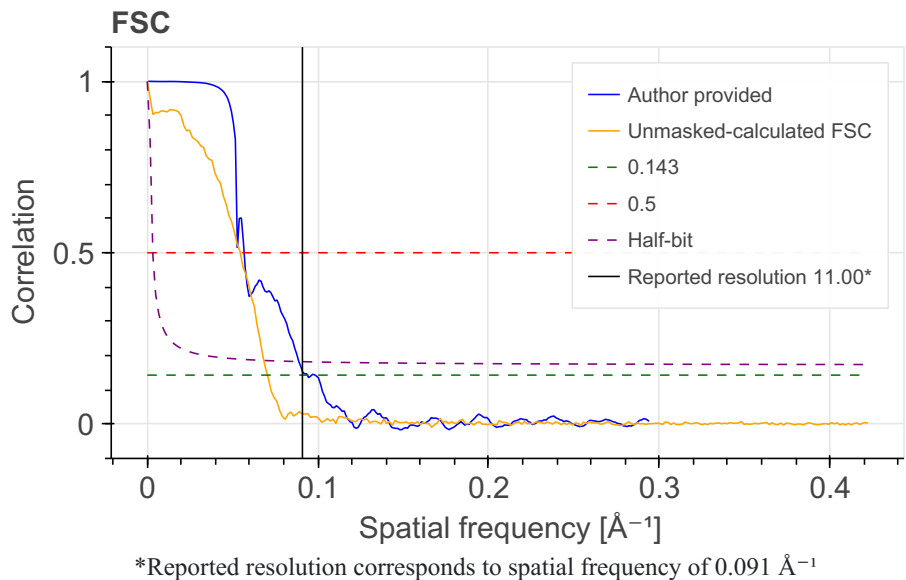


*Reported resolution corresponds to spatial frequency of 0.091 Å⁻¹

3.3.4. Fourier-Shell correlation ?

3.3.4.1. FSC ?

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.



3.3.4.2. Resolution estimates ?

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.00	-	-
Author-provided FSC curve	10.66	17.64	11.22
Unmasked-calculated*	14.20	18.32	14.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 14.20 differs from the reported value 11.00 by more than 10%.

3.4. NMR ?

Validation for this section is under development.

4. Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

4.1b. MolProbity Analysis ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-partice or particle-atom pairs for which excluded volume was analysed.

Standard geometry: bond outliers ?

There are 15 bond length outliers in this entry (0.12% of 12167 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	1358	THR	C-N	99.46	2.72	1.33	1	1
A	1519	THR	C-N	94.16	2.65	1.33	1	1
A	793	THR	C-N	93.66	2.64	1.33	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	954	THR	C-N	86.08	2.53	1.33	1	1
A	1439	THR	C-N	83.88	2.50	1.33	1	1
A	874	THR	C-N	79.19	2.44	1.33	1	1
A	1116	THR	C-N	76.34	2.40	1.33	1	1
A	471	THR	C-N	60.26	2.31	1.34	1	1
A	713	THR	C-N	56.31	2.12	1.33	1	1
A	632	THR	C-N	42.29	1.92	1.33	1	1
A	1197	THR	C-N	33.34	1.80	1.33	1	1
A	1035	THR	C-N	32.57	1.79	1.33	1	1
A	1599	LEU	C-N	30.13	0.86	1.34	1	1
A	1277	THR	C-N	26.96	1.71	1.33	1	1
A	551	THR	C-N	14.37	1.57	1.34	1	1

Standard geometry: angle outliers ?

There are 42 bond angle outliers in this entry (0.25% of 16540 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	1197	THR	C-N-CA	53.21	25.92	121.70	1	1
A	632	THR	O-C-N	48.79	44.93	123.00	1	1
A	1116	THR	C-N-CA	47.95	35.39	121.70	1	1
A	874	THR	C-N-CA	44.63	41.37	121.70	1	1
A	1358	THR	C-N-CA	42.24	45.67	121.70	1	1
A	1439	THR	C-N-CA	42.03	46.05	121.70	1	1
A	713	THR	C-N-CA	41.82	46.42	121.70	1	1
A	954	THR	O-C-N	41.70	56.29	123.00	1	1
A	471	THR	CA-C-N	39.89	57.07	116.90	1	1
A	1197	THR	O-C-N	39.69	59.49	123.00	1	1
A	1519	THR	C-N-CA	39.67	50.29	121.70	1	1
A	1599	LEU	O-C-N	38.37	61.60	123.00	1	1
A	1599	LEU	CA-C-N	38.02	59.87	116.90	1	1
A	793	THR	CA-C-N	37.43	41.34	116.20	1	1
A	1439	THR	CA-C-N	34.13	47.94	116.20	1	1
A	1519	THR	CA-C-N	33.75	48.70	116.20	1	1
A	1116	THR	CA-C-N	33.52	49.16	116.20	1	1
A	874	THR	CA-C-N	33.33	49.54	116.20	1	1
A	1035	THR	C-N-CA	30.22	67.31	121.70	1	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	1358	THR	CA-C-N	29.66	56.89	116.20	1	1
A	793	THR	C-N-CA	29.46	68.66	121.70	1	1
A	1277	THR	CA-C-N	28.58	59.03	116.20	1	1
A	632	THR	C-N-CA	28.04	71.23	121.70	1	1
A	1197	THR	CA-C-N	27.41	61.38	116.20	1	1
A	1035	THR	CA-C-N	26.34	63.52	116.20	1	1
A	551	THR	CA-C-N	26.16	77.66	116.90	1	1
A	1277	THR	C-N-CA	25.00	76.70	121.70	1	1
A	551	THR	O-C-N	23.67	85.13	123.00	1	1
A	713	THR	CA-C-N	23.22	69.75	116.20	1	1
A	954	THR	C-N-CA	20.60	84.62	121.70	1	1
A	954	THR	CA-C-N	20.07	76.07	116.20	1	1
A	471	THR	O-C-N	17.35	150.76	123.00	1	1
A	1599	LEU	C-N-CD	17.07	55.02	125.00	1	1
A	471	THR	C-N-CA	16.94	37.89	122.60	1	1
A	551	THR	C-N-CA	14.77	48.77	122.60	1	1
A	1599	LEU	C-N-CA	12.94	57.88	122.60	1	1
A	1277	THR	O-C-N	10.49	106.22	123.00	1	1
A	1035	THR	O-C-N	9.62	107.61	123.00	1	1
A	632	THR	CA-C-N	9.43	97.34	116.20	1	1
A	1358	THR	O-C-N	7.20	134.52	123.00	1	1
A	551	THR	C-N-CD	6.14	99.82	125.00	1	1
A	1519	THR	O-C-N	4.55	130.27	123.00	1	1

Too-close contacts ?

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all atomic models in this entry.

Model ID	Clash score	Number of clashes
1	37.27	250

There are 250 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:6:ILE:HB	A:52:VAL:HG13	0.97	1	1
A:322:LEU:HD11	A:334:LEU:HD13	0.94	1	1
A:259:SER:HB2	A:363:GLU:HG2	0.92	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:221:THR:HA	A:349:LEU:O	0.90	1	1
A:294:GLY:HA2	A:337:GLY:O	0.88	1	1
A:404:LEU:HD13	A:430:ALA:HB3	0.88	1	1
A:71:ILE:HG23	A:95:ARG:HB2	0.87	1	1
A:208:VAL:HG23	A:369:MET:HE2	0.85	1	1
A:389:THR:HG23	A:464:GLN:HB3	0.82	1	1
A:219:GLY:HA2	A:351:LEU:HD12	0.81	1	1
A:71:ILE:HG12	A:95:ARG:HG3	0.81	1	1
A:46:ALA:HB2	A:50:LEU:HD12	0.81	1	1
A:40:GLY:HA2	A:66:ARG:HG2	0.78	1	1
A:262:LEU:HB2	A:321:GLU:HB3	0.77	1	1
A:61:LEU:HD12	A:67:GLY:HA2	0.77	1	1
A:4:LEU:HD21	A:44:LEU:HD22	0.76	1	1
A:85:ILE:HB	A:114:VAL:HB	0.73	1	1
A:113:ILE:HG12	A:138:ALA:H	0.73	1	1
A:179:ALA:HB1	A:460:GLN:HB2	0.72	1	1
A:144:LEU:HD12	A:160:ALA:HB2	0.72	1	1
A:264:THR:HG22	A:265:ASN:H	0.71	1	1
A:284:PRO:HA	A:320:ASP:HA	0.71	1	1
A:104:SER:HB2	A:134:GLN:HE21	0.70	1	1
A:116:LEU:HD12	A:121:LEU:HB2	0.70	1	1
A:397:TYR:HB2	A:470:VAL:HG11	0.69	1	1
A:189:PHE:HE1	A:194:ASN:HA	0.69	1	1
A:44:LEU:HB2	A:70:LEU:HD12	0.68	1	1
A:37:LEU:HB3	A:61:LEU:HD13	0.68	1	1
A:211:ARG:HH21	A:226:LEU:HD13	0.67	1	1
A:239:PHE:HD1	A:367:VAL:HG12	0.67	1	1
A:385:THR:HG22	A:460:GLN:HB3	0.67	1	1
A:82:SER:HB3	A:103:LEU:HB2	0.66	1	1
A:434:ALA:HB1	A:438:SER:OG	0.66	1	1
A:159:TYR:CE2	A:458:ARG:HG2	0.65	1	1
A:102:PHE:HZ	A:133:GLN:HG3	0.64	1	1
A:46:ALA:HB2	A:50:LEU:HB2	0.64	1	1
A:390:ALA:HB3	A:466:GLY:N	0.64	1	1
A:87:PHE:HB3	A:116:LEU:HD23	0.64	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:264:THR:HG23	A:279:PRO:HG3	0.63	1	1
A:300:THR:HG22	A:332:GLU:HB3	0.63	1	1
A:92:LEU:HB2	A:116:LEU:HD11	0.63	1	1
A:207:SER:HA	A:370:PHE:HD1	0.62	1	1
A:440:VAL:HG13	A:470:VAL:O	0.62	1	1
A:55:PRO:HB3	A:84:PRO:HD2	0.62	1	1
A:284:PRO:HG2	A:298:THR:HG21	0.62	1	1
A:303:TRP:CG	A:330:LEU:HD13	0.61	1	1
A:151:ILE:HG13	A:165:LEU:HD12	0.61	1	1
A:221:THR:HB	A:350:ASP:OD1	0.61	1	1
A:404:LEU:CD1	A:430:ALA:HB3	0.61	1	1
A:178:ASN:O	A:383:GLN:HA	0.60	1	1
A:8:ALA:HA	A:30:ALA:HB2	0.60	1	1
A:217:SER:HB3	A:362:ALA:HB2	0.60	1	1
A:71:ILE:HG23	A:95:ARG:CB	0.59	1	1
A:167:THR:HG21	A:172:LEU:HB2	0.59	1	1
A:116:LEU:CD1	A:121:LEU:HB2	0.59	1	1
A:307:TRP:CZ2	A:330:LEU:HD12	0.59	1	1
A:388:LEU:HD13	A:408:MET:HE2	0.59	1	1
A:419:ASN:HB2	A:425:LEU:CD2	0.59	1	1
A:390:ALA:HB3	A:466:GLY:CA	0.59	1	1
A:57:ILE:HG23	A:86:LEU:HD12	0.58	1	1
A:432:THR:HB	A:445:ILE:HG12	0.58	1	1
A:390:ALA:HB3	A:466:GLY:HA3	0.58	1	1
A:227:THR:HG22	A:344:ARG:CB	0.58	1	1
A:46:ALA:CB	A:50:LEU:HB2	0.58	1	1
A:228:ALA:HB2	A:369:MET:HE1	0.58	1	1
A:277:ALA:HB2	A:289:VAL:HG22	0.58	1	1
A:303:TRP:CE2	A:330:LEU:HD22	0.58	1	1
A:60:ASN:O	A:61:LEU:HD23	0.58	1	1
A:147:ARG:HG3	A:166:GLN:HB3	0.58	1	1
A:388:LEU:HB2	A:408:MET:CE	0.58	1	1
A:92:LEU:HB3	A:121:LEU:HD13	0.57	1	1
A:55:PRO:HG3	A:84:PRO:HD2	0.57	1	1
A:227:THR:HG22	A:344:ARG:HB2	0.57	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:92:LEU:CB	A:116:LEU:HD11	0.57	1	1
A:244:TYR:HB3	A:361:PHE:HD1	0.57	1	1
A:261:TYR:CE1	A:322:LEU:HB2	0.57	1	1
A:221:THR:HG22	A:350:ASP:HA	0.57	1	1
A:236:ARG:HB2	A:370:PHE:O	0.57	1	1
A:268:TYR:CE2	A:275:VAL:HB	0.56	1	1
A:287:PHE:HB2	A:296:VAL:HG21	0.56	1	1
A:37:LEU:CD2	A:68:LEU:HB2	0.56	1	1
A:5:ARG:HA	A:51:SER:O	0.56	1	1
A:358:PHE:HB3	A:361:PHE:CD2	0.56	1	1
A:113:ILE:HG23	A:138:ALA:O	0.56	1	1
A:217:SER:CB	A:362:ALA:HB2	0.56	1	1
A:163:LEU:HG	A:165:LEU:HD23	0.56	1	1
A:397:TYR:OH	A:437:ALA:HA	0.56	1	1
A:162:ASN:ND2	A:188:VAL:HG22	0.56	1	1
A:442:GLN:HG3	A:469:THR:HG23	0.56	1	1
A:267:ARG:HD2	A:346:ASP:HB2	0.56	1	1
A:164:ALA:HA	A:200:THR:HG22	0.55	1	1
A:264:THR:HG22	A:265:ASN:N	0.55	1	1
A:443:TYR:O	A:467:ARG:HD3	0.55	1	1
A:143:ASN:OD1	A:162:ASN:HB3	0.55	1	1
A:79:VAL:HB	A:100:ILE:CD1	0.55	1	1
A:90:GLY:O	A:119:GLY:HA3	0.55	1	1
A:201:ALA:HB1	A:375:THR:O	0.55	1	1
A:449:ALA:HB3	A:461:LEU:HD21	0.55	1	1
A:37:LEU:HB3	A:61:LEU:CD1	0.55	1	1
A:37:LEU:HD23	A:42:VAL:CG2	0.55	1	1

Torsion angles: Protein backbone ?

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	1648	1621	18	9

There are 9 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	551	THR	1
A	552	PRO	1
A	633	LYS	1
A	1035	THR	1
A	1036	LYS	1
A	1277	THR	1
A	1278	LYS	1
A	1599	LEU	1
A	1600	PRO	1

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	1246	1119	122	5

There are 5 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	240	THR	1
A	267	ARG	1
A	471	THR	1
A	807	VAL	1
A	1508	ASP	1

5. Fit to Data Used for Modeling Assessment ?

5.3. 3DEM

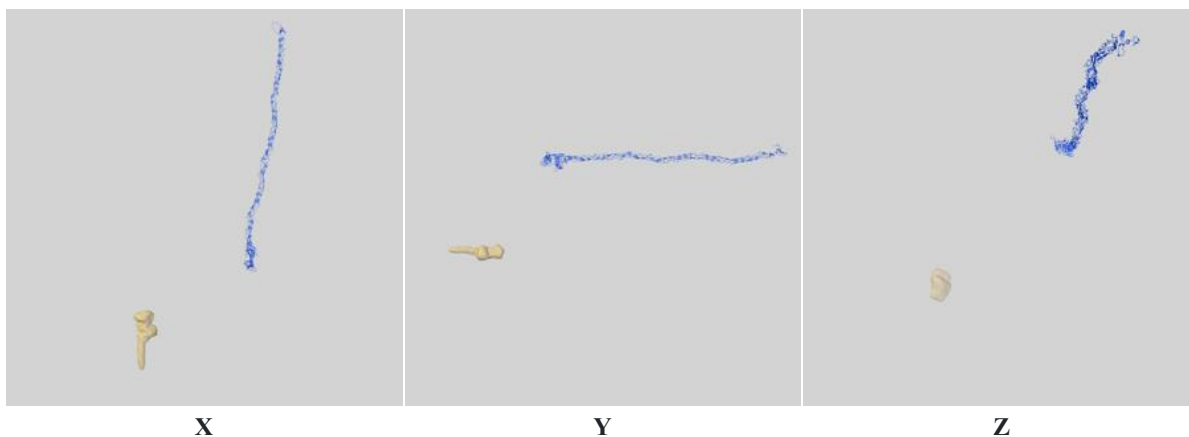
This section describes fit of models to the 3DEM data. Only results for the representative model, selected as a first model with the largest number of asymmetric units.

[EMD-49677](#)

5.3.1. Map-model fit ?

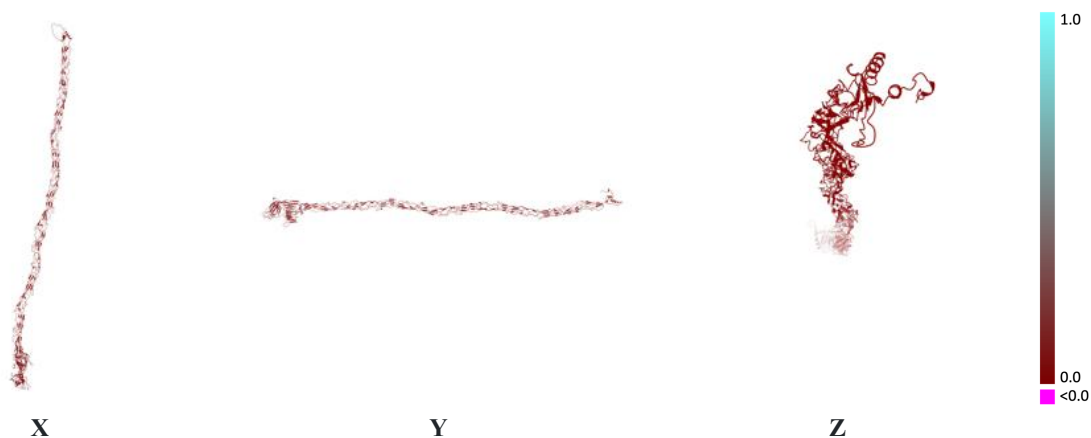
Only results for the representative Model 1 are shown.

5.3.1.1 Map-model overlay ?



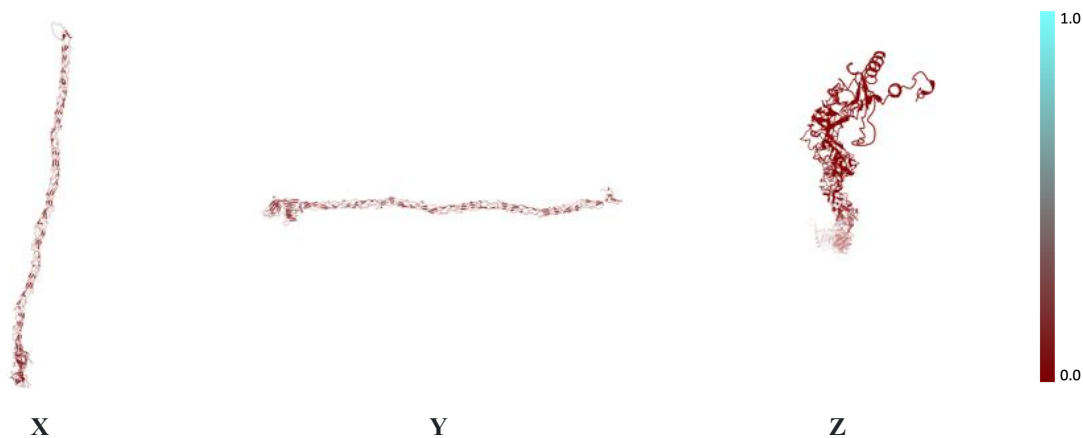
The images above show the 3D surface view of the map at the recommended contour level 0.160 at 50% transparency in yellow overlaid with a ribbon representation of the model colored in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

5.3.1.2. Q-score mapped to coordinate model ?



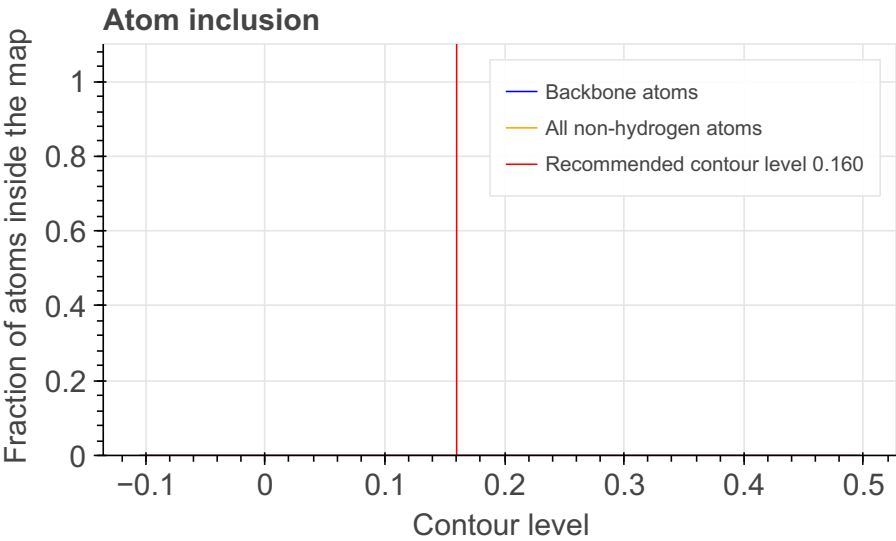
The images above show the model with each residue colored according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

5.3.1.3. Atom inclusion mapped to coordinate model ?



The images above show the model with each residue colored according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level 0.160 .

5.3.1.4. Atom inclusion ?



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

5.3.1.5. Map-model fit summary ?

The table lists the average atom inclusion at the recommended contour level (0.160) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.000	0.000
A	0.000	0.000

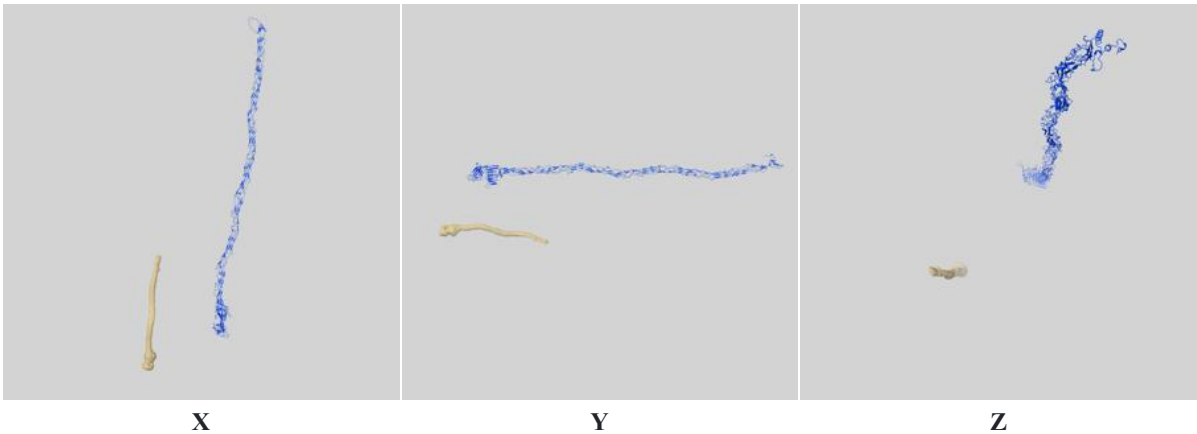


EMD-49679

5.3.1. Map-model fit ?

Only results for the representative Model 1 are shown.

5.3.1.1 Map-model overlay ?



The images above show the 3D surface view of the map at the recommended contour level 0.750 at 50% transparency in yellow overlaid with a ribbon representation of the model colored in blue. These images allow for the visual assessment of the quality of fit

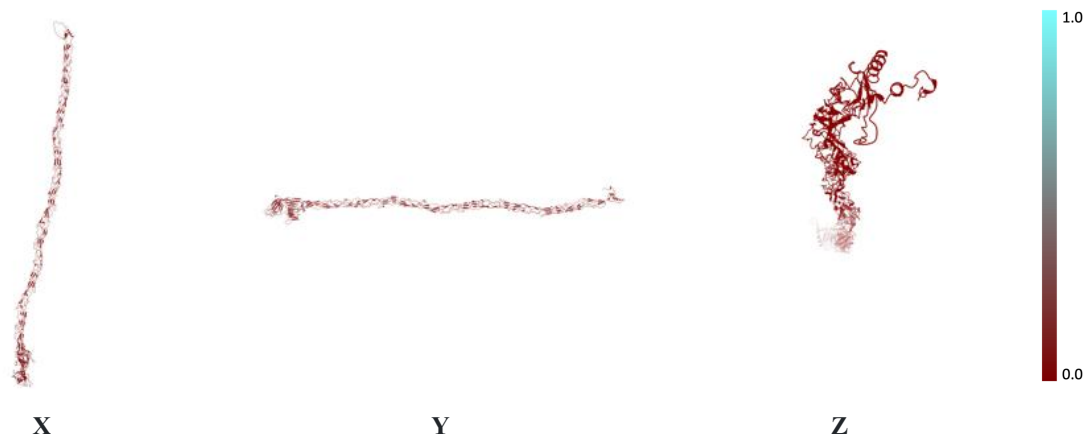
between the atomic model and the map.

5.3.1.2. Q-score mapped to coordinate model ?



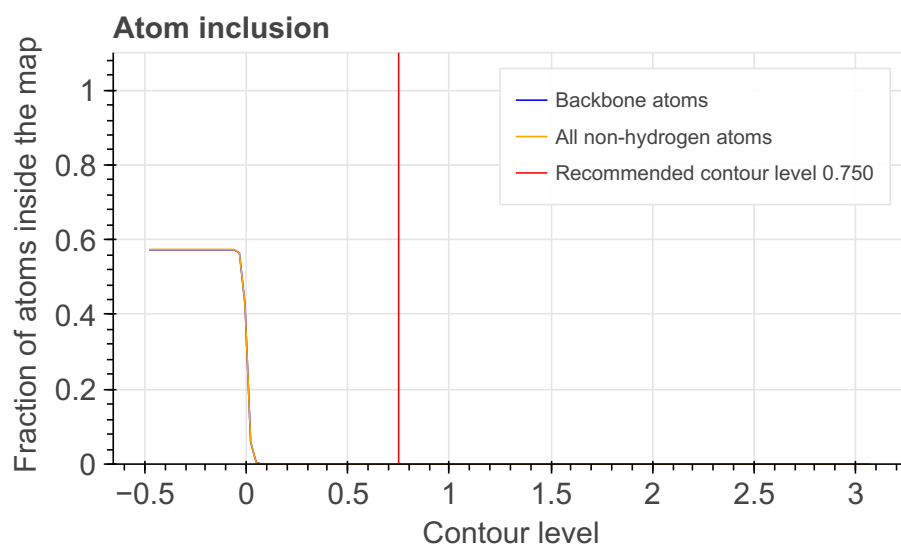
The images above show the model with each residue colored according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

5.3.1.3. Atom inclusion mapped to coordinate model ?



The images above show the model with each residue colored according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level 0.750 .

5.3.1.4. Atom inclusion ?



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

5.3.1.5. Map-model fit summary ?

The table lists the average atom inclusion at the recommended contour level (0.750) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.000	0.003
A	0.000	0.003



5.4. NMR ?

Validation for this section is under development.

6. Fit to Data Used for Validation Assessment ?

Validation for this section is under development.

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