WORLDWIDE wwPDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Nov 19, 2024 – 01:15 pm GMT

PDB ID	:	9EZM
EMDB ID	:	EMD-50089
Title	:	CryoEM structure of the contracted sheath in H. borinquense
Authors	:	Zachs, T.; Malit, J.J.; Xu, J.; Schuerch, A.; Sivabalasarma, S.; Nussbaum, P.; Albers, S.V.; Pilhofer, M.
Deposited on	:	2024-04-12
Resolution	:	2.90 Å(reported)

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 2.90 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.
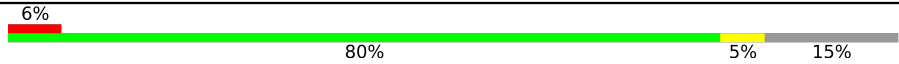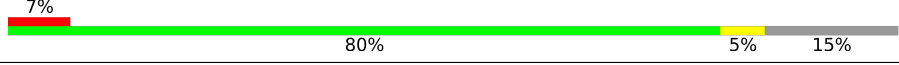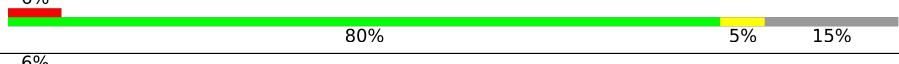
Metric	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▌Percentile relative to all structures

▯Percentile relative to all EM structures
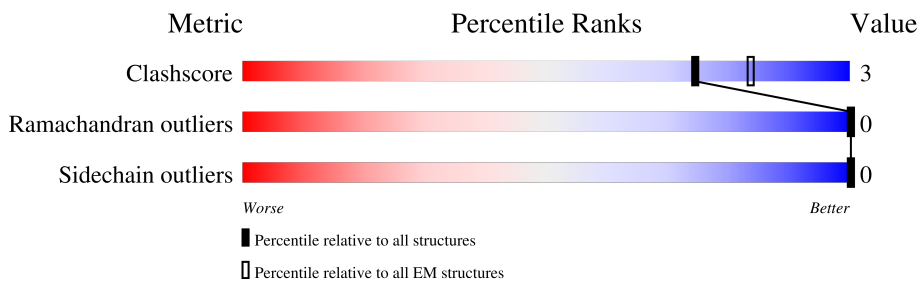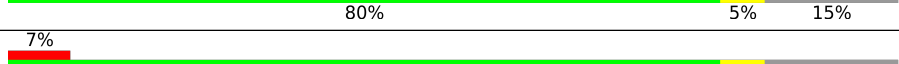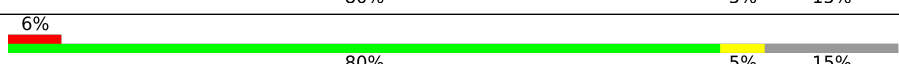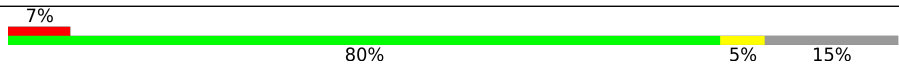
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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.
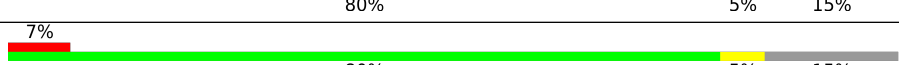
Mol	Chain	Length	Quality of chain
1	A	574	6% / 80% / 5% / 15%
1	B	574	6% / 80% / 5% / 15%
1	C	574	6% / 80% / 5% / 15%
1	D	574	6% / 80% / 5% / 15%
1	E	574	6% / 80% / 5% / 15%
1	F	574	6% / 80% / 5% / 15%
1	G	574	6% / 80% / 5% / 15%
1	H	574	6% / 80% / 5% / 15%

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WORLDWIDE
wwPDB
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Mol	Chain	Length	Quality of chain
1	I	574	6% 80% 5% 15%
1	J	574	7% 80% 5% 15%
1	K	574	6% 80% 5% 15%
1	L	574	6% 80% 5% 15%
1	M	574	6% 80% 5% 15%
1	N	574	6% 80% 5% 15%
1	O	574	7% 80% 5% 15%
1	P	574	7% 80% 5% 15%
1	Q	574	6% 80% 5% 15%
1	R	574	7% 80% 5% 15%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 68022 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.

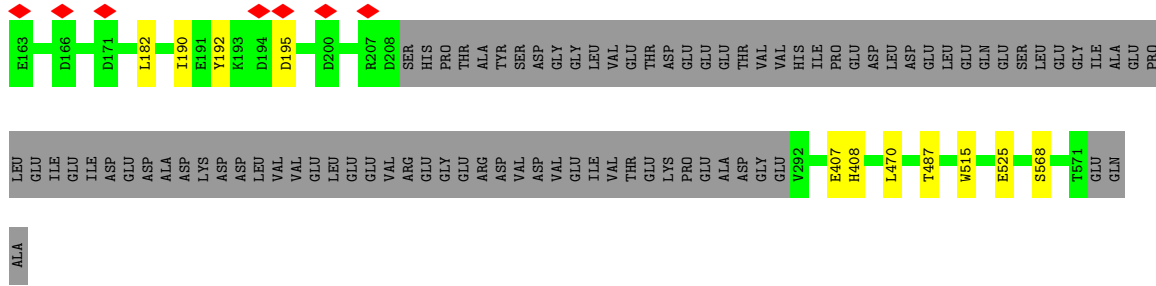- Molecule 1 is a protein called Phage tail sheath protein FI.

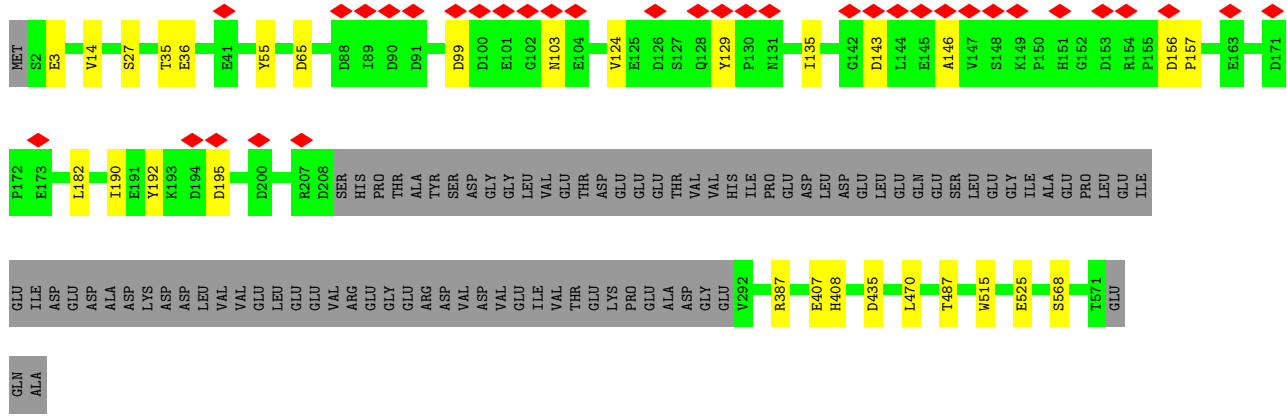| Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	B	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	C	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	D	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	E	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	F	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	G	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	H	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	I	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	J	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	K	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	L	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	M	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	N	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	O	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	P	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		
1	Q	487	Total	C	N	O	S	0	0
			3779	2357	643	770	9		

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wwPDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	487	3779	2357	643	770	9	0	0

3 Residue-property plots ⓘ

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.
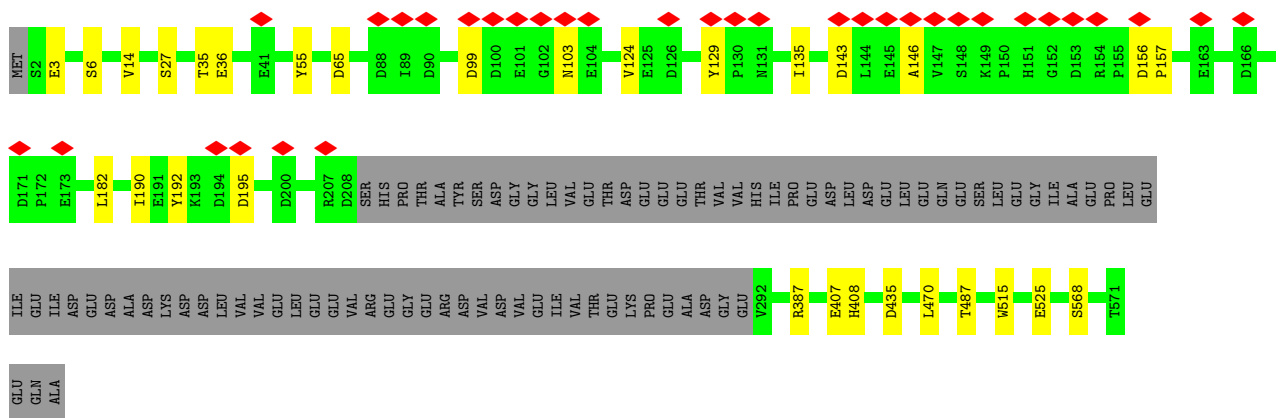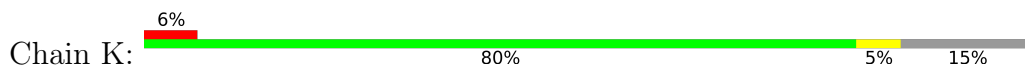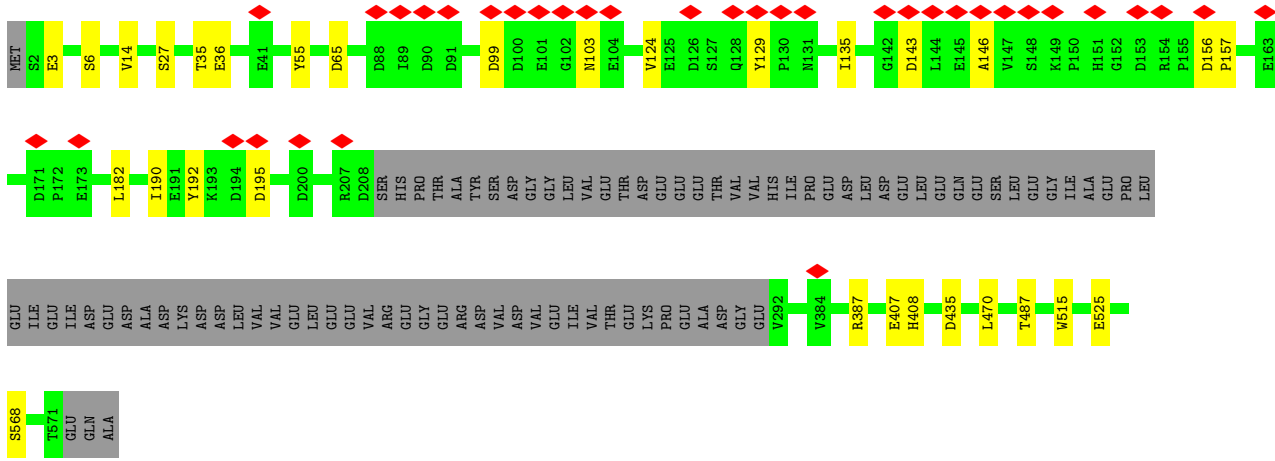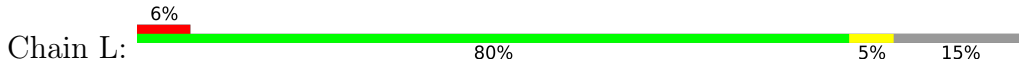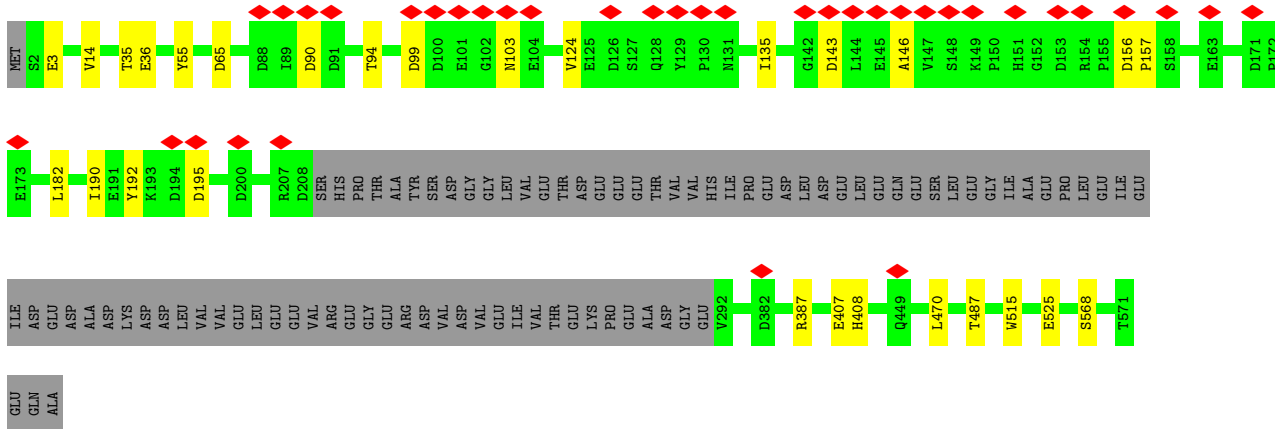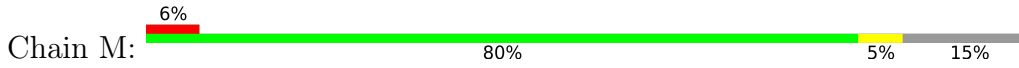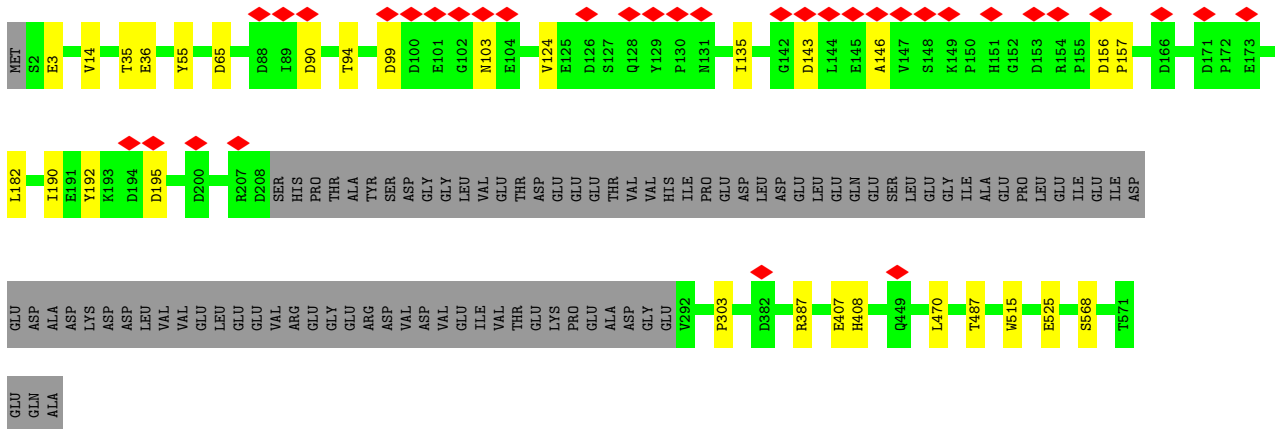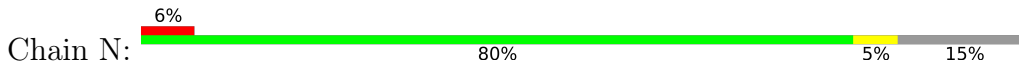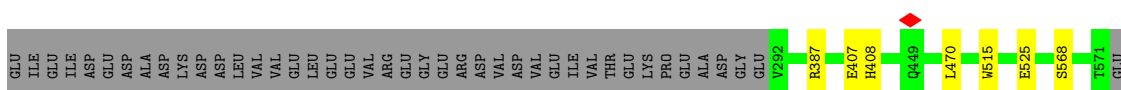
• Molecule 1: Phage tail sheath protein FI

Chain A:

• Molecule 1: Phage tail sheath protein FI

Chain B:

• Molecule 1: Phage tail sheath protein FI

Chain C:

E163 D166 D171 L182 I190 E191 Y192 K193 D194 D195 D200 R207 D208 SER HIS PRO THR ALA TYR SER ASP GLY LEU VAL GLU THR ASP GLU GLU THR VAL VAL HIS ILE PRO GLU ASP LEU ASP GLU LEU GLU GLN SER LEU GLU GLY ILE ALA GLU PRO

LEU GLU ILE ILE ASP ASP ALA ASP LYS ASP ASP LEU VAL VAL GLU LEU GLU GLU VAL ARG GLU GLY GLU ARG ASP VAL ASP VAL ILE VAL GLU ILE VAL THR GLU LYS PRO GLU ALA ASP GLY GLU V292 E407 H408 L470 T487 W515 E525 S568 T571 GLU GLN

ALA

• Molecule 1: Phage tail sheath protein FI

Chain D:

6%

80%   5%   15%

MET S2 V14 S27 T35 E36 Y55 D65 D88 I89 D90 D91 D99 D100 E101 G102 N103 V124 E125 D126 S127 Q128 Y129 P130 N131 I135 G142 D143 L144 E145 A146 V147 S148 K149 P150 H151 G152 D153 R154 P155 D156 P157 S158 E163 D171 P172 E173

L182 I190 E191 Y192 K193 D194 D195 D200 R207 D208 SER HIS PRO THR ALA TYR SER ASP GLY LEU VAL GLU THR ASP GLU GLU THR VAL VAL HIS ILE PRO GLU ASP LEU ASP GLU LEU GLU GLN SER LEU GLU GLY ILE ALA GLU PRO LEU GLU ILE GLU ILE ASP

GLU ASP ALA ASP LYS ASP ASP LEU VAL VAL GLU LEU GLU GLU VAL ARG GLU GLY GLU ARG ASP VAL ASP VAL ILE VAL THR GLU LYS PRO GLU ALA ASP GLY GLU V292 P303 D382 R387 E407 H408 D435 L470 W515 E525 S568 T571 GLU GLN

ALA

• Molecule 1: Phage tail sheath protein FI

Chain E:

6%

80%   5%   15%

MET S2 S6 V14 S27 T35 E36 Y55 D65 D88 I89 D90 D91 D99 D100 E101 G102 N103 E104 V124 E125 D126 S127 Q128 Y129 P130 N131 I135 G142 D143 L144 E145 A146 V147 S148 K149 P150 H151 G152 D153 R154 P155 D156 P157 S158 D166 D171

P172 E173 L182 I190 E191 Y192 K193 D194 D195 D200 R207 D208 SER HIS PRO THR ALA TYR SER ASP GLY LEU VAL GLU THR ASP GLU GLU THR VAL VAL HIS ILE PRO GLU ASP LEU ASP GLU LEU GLU GLN GLU GLU SER LEU GLU GLY ILE ALA GLU PRO LEU GLU GLU ILE

GLU ILE ASP GLU ASP ALA ASP LYS ASP ASP LEU VAL VAL GLU LEU GLU GLU VAL ARG GLU GLY GLU ARG ASP VAL ASP VAL ILE VAL THR GLU LYS PRO GLU ALA ASP GLY GLU V292 D325 D382 E407 H408 D435 L470 T487 W515 E525 S568

T571 GLU GLN ALA

• Molecule 1: Phage tail sheath protein FI

Chain F:

6%

80%   5%   15%

• Molecule 1: Phage tail sheath protein FI

Chain G:

• Molecule 1: Phage tail sheath protein FI

Chain H:

• Molecule 1: Phage tail sheath protein FI

Chain I:

• Molecule 1: Phage tail sheath protein FI

Chain J:

• Molecule 1: Phage tail sheath protein FI

Chain K:

• Molecule 1: Phage tail sheath protein FI

Chain L:

• Molecule 1: Phage tail sheath protein FI

Chain M:

• Molecule 1: Phage tail sheath protein FI

Chain N:

• Molecule 1: Phage tail sheath protein FI

Chain O:

• Molecule 1: Phage tail sheath protein FI

Chain P:

• Molecule 1: Phage tail sheath protein FI

Chain Q:

GLU
GLN
ALA

• Molecule 1: Phage tail sheath protein FI

Chain R:

7%

80%   5%   15%

MET S2 E3 S6 V14 T35 E36 Y55 D65 A87 D88 I89 D90 D91 T94 D99 D100 E101 G102 N103 E104 V124 E125 D126 S127 Q128 Y129 P130 N131 I135 D143 L144 E145 A146 V147 S148 K149 P150 H151 G152 D153 R154 P155 D156 P157 E163 D171

P172 E173 E179 L182 I190 E191 Y192 K193 D194 D195 D200 R207 D208 SER HIS PRO THR ALA TYR SER ASP GLY LEU VAL GLU THR ASP GLU GLU GLU THR VAL VAL HIS ILE PRO GLU ASP LEU ASP GLU LEU GLU GLN GLU SER LEU GLY ILE ALA GLU PRO LEU

GLU ILE GLU ILE ASP GLU ASP ALA ASP LYS ASP ASP LEU VAL VAL GLU LEU GLU GLU VAL ARG GLU GLY GLU ARG ASP VAL ASP VAL GLU ILE VAL THR GLU LYS PRO GLU ALA ASP GLY GLU V292 R387 E407 H408 Q449 L470 W515 E525 S568 T571 GLU

GLN
ALA

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=33.24°, rise=17.09 Å, axial sym=C6	Depositor
Number of segments used	127891	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 $(e^-/\text{Å}^2)$	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	A	0.28	0/3864	0.49	1/5257 (0.0%)
1	B	0.28	0/3864	0.49	1/5257 (0.0%)
1	C	0.28	0/3864	0.49	1/5257 (0.0%)
1	D	0.29	0/3864	0.49	1/5257 (0.0%)
1	E	0.28	0/3864	0.49	1/5257 (0.0%)
1	F	0.28	0/3864	0.49	1/5257 (0.0%)
1	G	0.28	0/3864	0.49	1/5257 (0.0%)
1	H	0.28	0/3864	0.49	1/5257 (0.0%)
1	I	0.28	0/3864	0.49	1/5257 (0.0%)
1	J	0.29	0/3864	0.49	1/5257 (0.0%)
1	K	0.28	0/3864	0.49	1/5257 (0.0%)
1	L	0.29	0/3864	0.49	1/5257 (0.0%)
1	M	0.28	0/3864	0.49	1/5257 (0.0%)
1	N	0.28	0/3864	0.49	1/5257 (0.0%)
1	O	0.28	0/3864	0.49	1/5257 (0.0%)
1	P	0.29	0/3864	0.49	1/5257 (0.0%)
1	Q	0.29	0/3864	0.49	1/5257 (0.0%)
1	R	0.29	0/3864	0.49	1/5257 (0.0%)
All	All	0.28	0/69552	0.49	18/94626 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	470	LEU	CA-CB-CG	7.28	132.04	115.30
1	Q	470	LEU	CA-CB-CG	7.28	132.04	115.30
1	I	470	LEU	CA-CB-CG	7.27	132.03	115.30
1	M	470	LEU	CA-CB-CG	7.27	132.02	115.30
1	G	470	LEU	CA-CB-CG	7.27	132.02	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts   ⓘ

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	3779	0	3564	29	0
1	B	3779	0	3564	29	0
1	C	3779	0	3564	30	0
1	D	3779	0	3564	28	0
1	E	3779	0	3564	31	0
1	F	3779	0	3564	30	0
1	G	3779	0	3564	34	0
1	H	3779	0	3564	31	0
1	I	3779	0	3564	34	0
1	J	3779	0	3564	35	0
1	K	3779	0	3564	35	0
1	L	3779	0	3564	35	0
1	M	3779	0	3564	29	0
1	N	3779	0	3564	30	0
1	O	3779	0	3564	30	0
1	P	3779	0	3564	27	0
1	Q	3779	0	3564	30	0
1	R	3779	0	3564	29	0
All	All	68022	0	64152	392	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 3.

The worst 5 of 392 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:I:129:TYR:CE2	1:O:387:ARG:NE	2.06	1.22
1:B:129:TYR:CE2	1:G:387:ARG:NE	2.07	1.22
1:H:129:TYR:CZ	1:N:387:ARG:NH2	2.08	1.21
1:J:129:TYR:CE2	1:P:387:ARG:NE	2.05	1.21
1:K:129:TYR:CE2	1:Q:387:ARG:NE	2.06	1.21

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	B	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	C	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	D	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	E	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	F	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	G	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	H	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	I	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	J	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	K	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	L	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	M	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	N	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	O	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	P	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	Q	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
1	R	483/574 (84%)	475 (98%)	8 (2%)	0	100	100
All	All	8694/10332 (84%)	8550 (98%)	144 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	410/487 (84%)	410 (100%)	0	100	100
1	B	410/487 (84%)	410 (100%)	0	100	100
1	C	410/487 (84%)	410 (100%)	0	100	100
1	D	410/487 (84%)	410 (100%)	0	100	100
1	E	410/487 (84%)	410 (100%)	0	100	100
1	F	410/487 (84%)	410 (100%)	0	100	100
1	G	410/487 (84%)	410 (100%)	0	100	100
1	H	410/487 (84%)	410 (100%)	0	100	100
1	I	410/487 (84%)	410 (100%)	0	100	100
1	J	410/487 (84%)	410 (100%)	0	100	100
1	K	410/487 (84%)	410 (100%)	0	100	100
1	L	410/487 (84%)	410 (100%)	0	100	100
1	M	410/487 (84%)	410 (100%)	0	100	100
1	N	410/487 (84%)	410 (100%)	0	100	100
1	O	410/487 (84%)	410 (100%)	0	100	100
1	P	410/487 (84%)	410 (100%)	0	100	100
1	Q	410/487 (84%)	410 (100%)	0	100	100
1	R	410/487 (84%)	410 (100%)	0	100	100
All	All	7380/8766 (84%)	7380 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	408	HIS
1	R	408	HIS
1	Q	408	HIS
1	I	408	HIS
1	N	408	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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-50089. 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.

6.1   Orthogonal projections (i)

6.1.1   Primary map
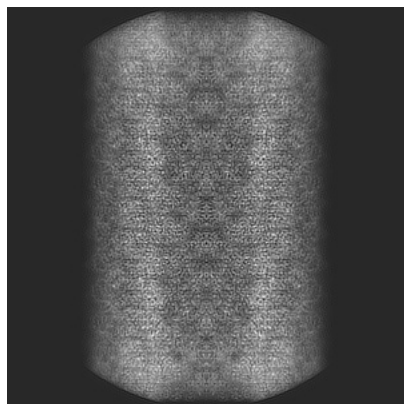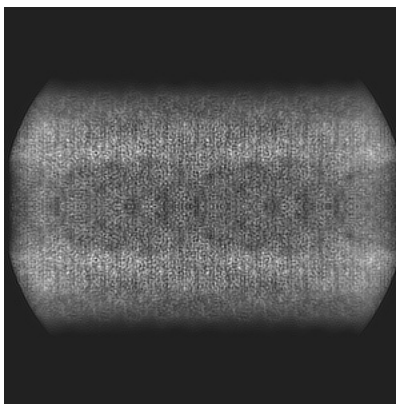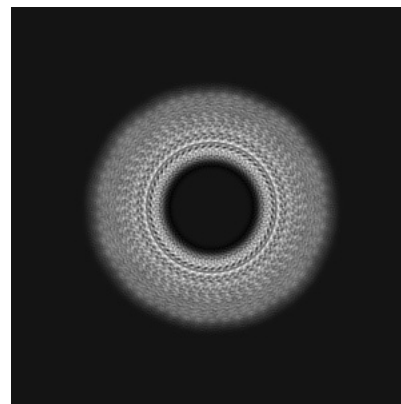
X   Y   Z

6.1.2   Raw map

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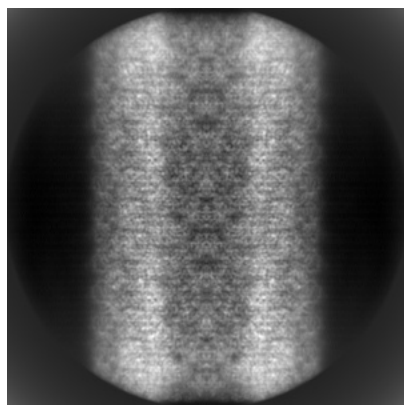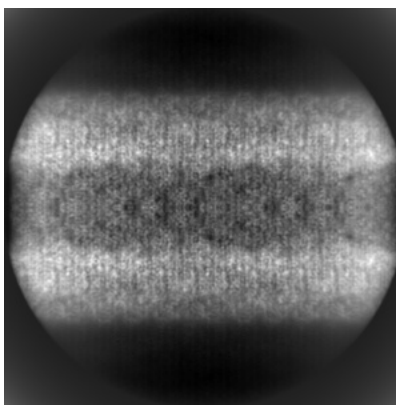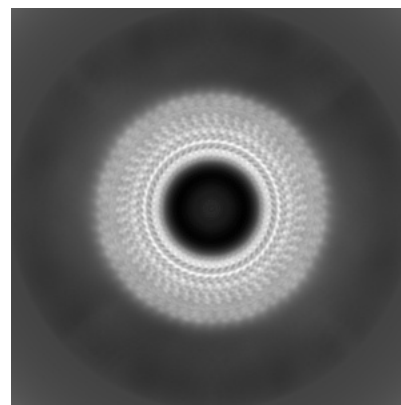
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
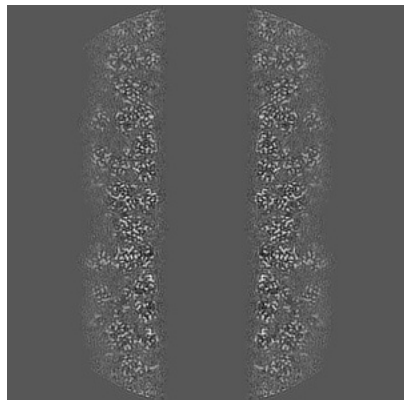
6.2.1 Primary map
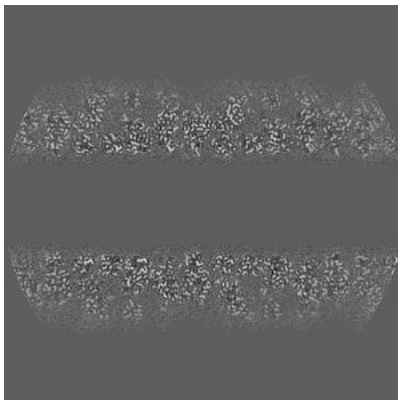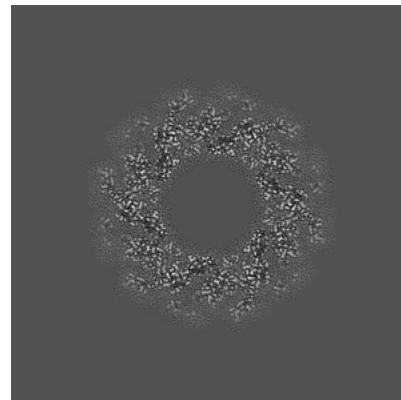
| X Index: 200 | Y Index: 200 | Z Index: 200 |

6.2.2 Raw map
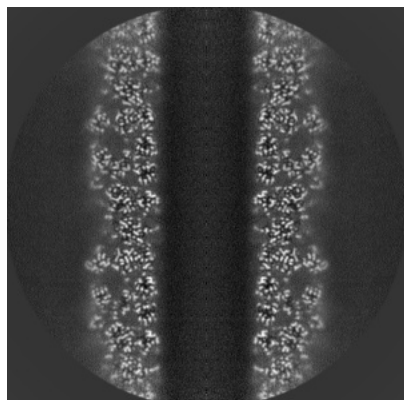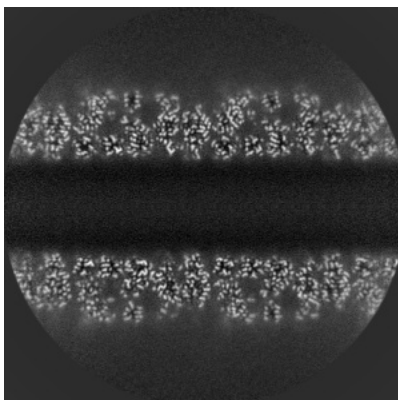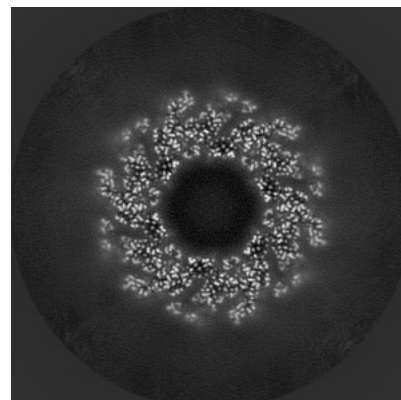
| X Index: 200 | Y Index: 200 | Z Index: 200 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
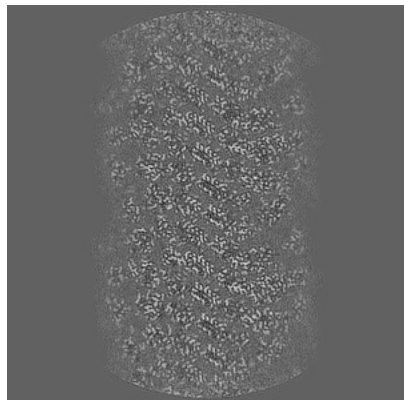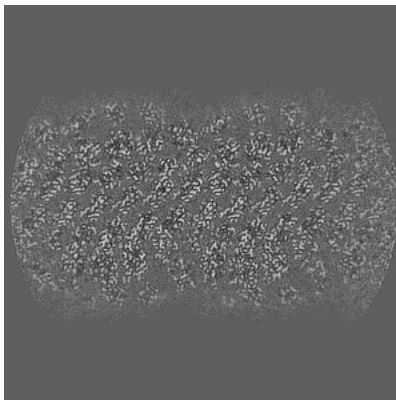
X Index: 144	Y Index: 145	Z Index: 172
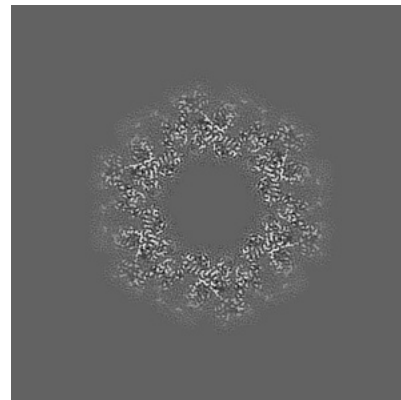
6.3.2 Raw map
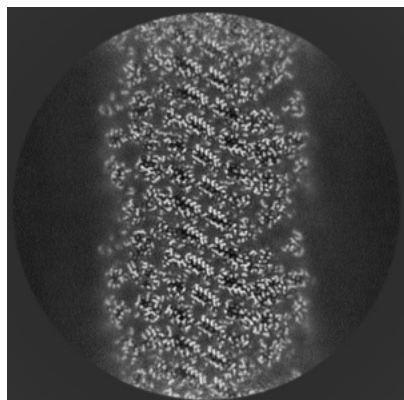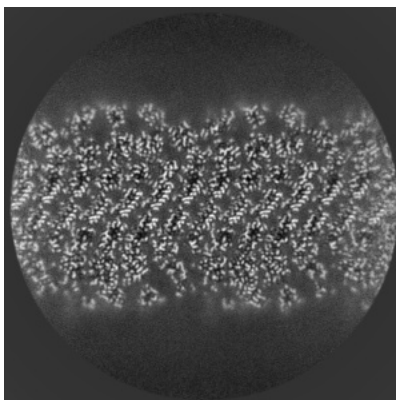
X Index: 144	Y Index: 144	Z Index: 41
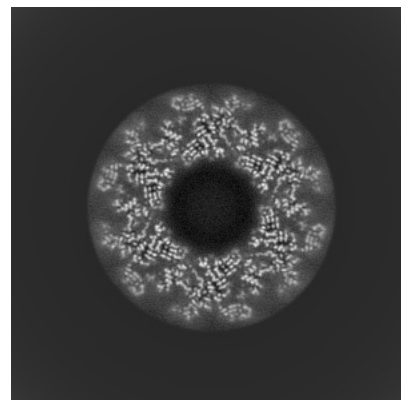
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1   Primary map
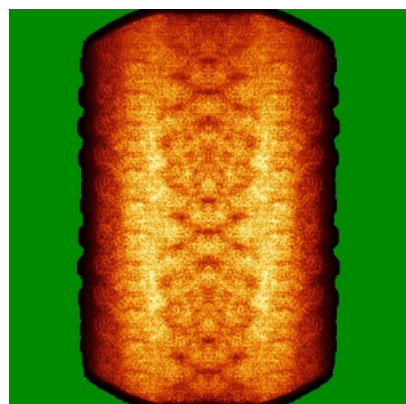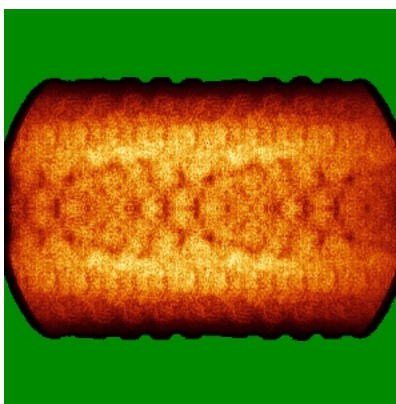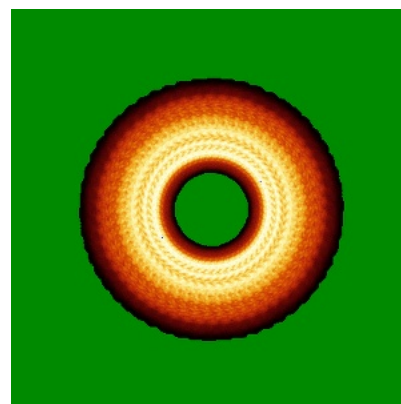
| X | Y | Z |

6.4.2   Raw map

| X | Y | Z |
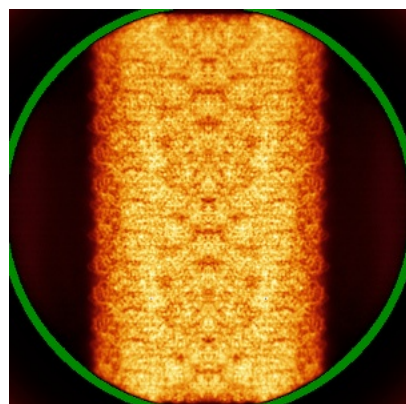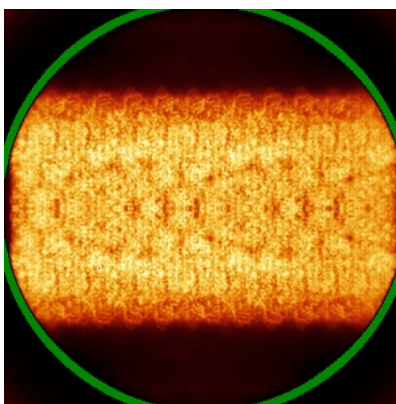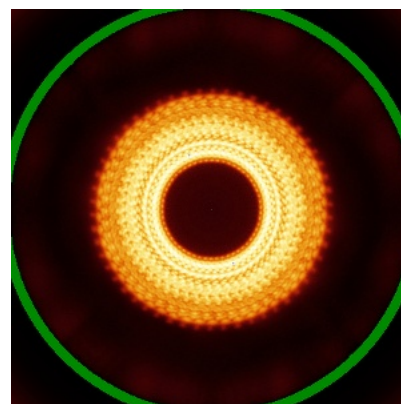
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map
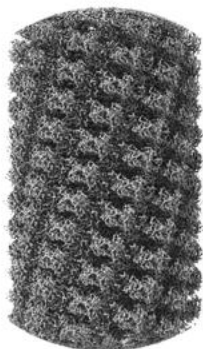
X   Y   Z
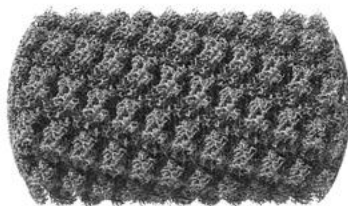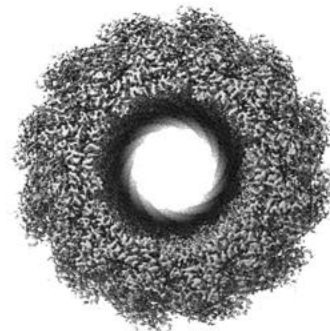
The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map
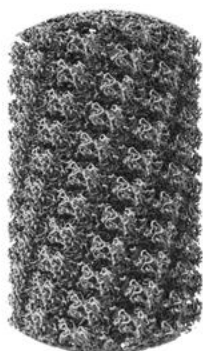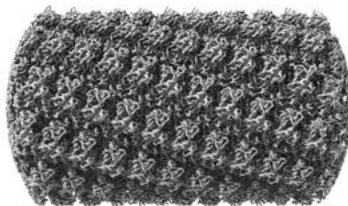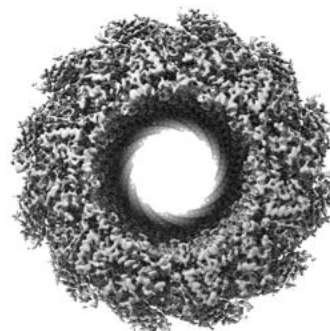
X   Y   Z

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

6.6 Mask visualisation ⓘ

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

6.6.1 emd_50089_msk_1.map ⓘ

X   Y   Z
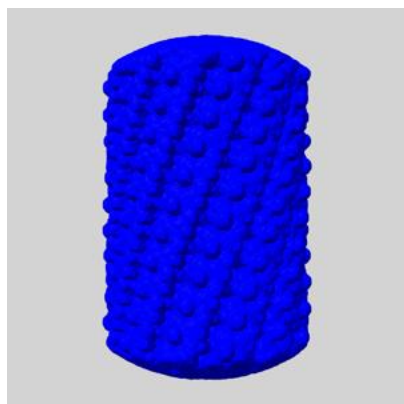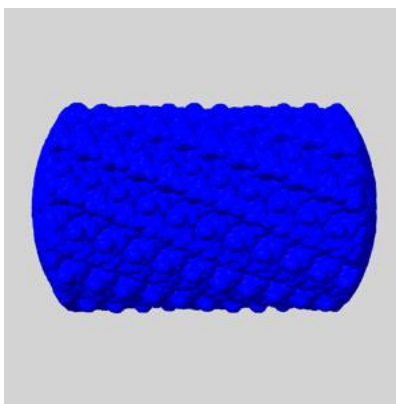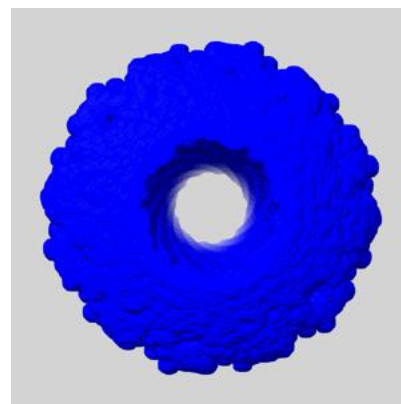
7 Map analysis ⓘ

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

7.1 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.

7.2 Volume estimate ⓘ
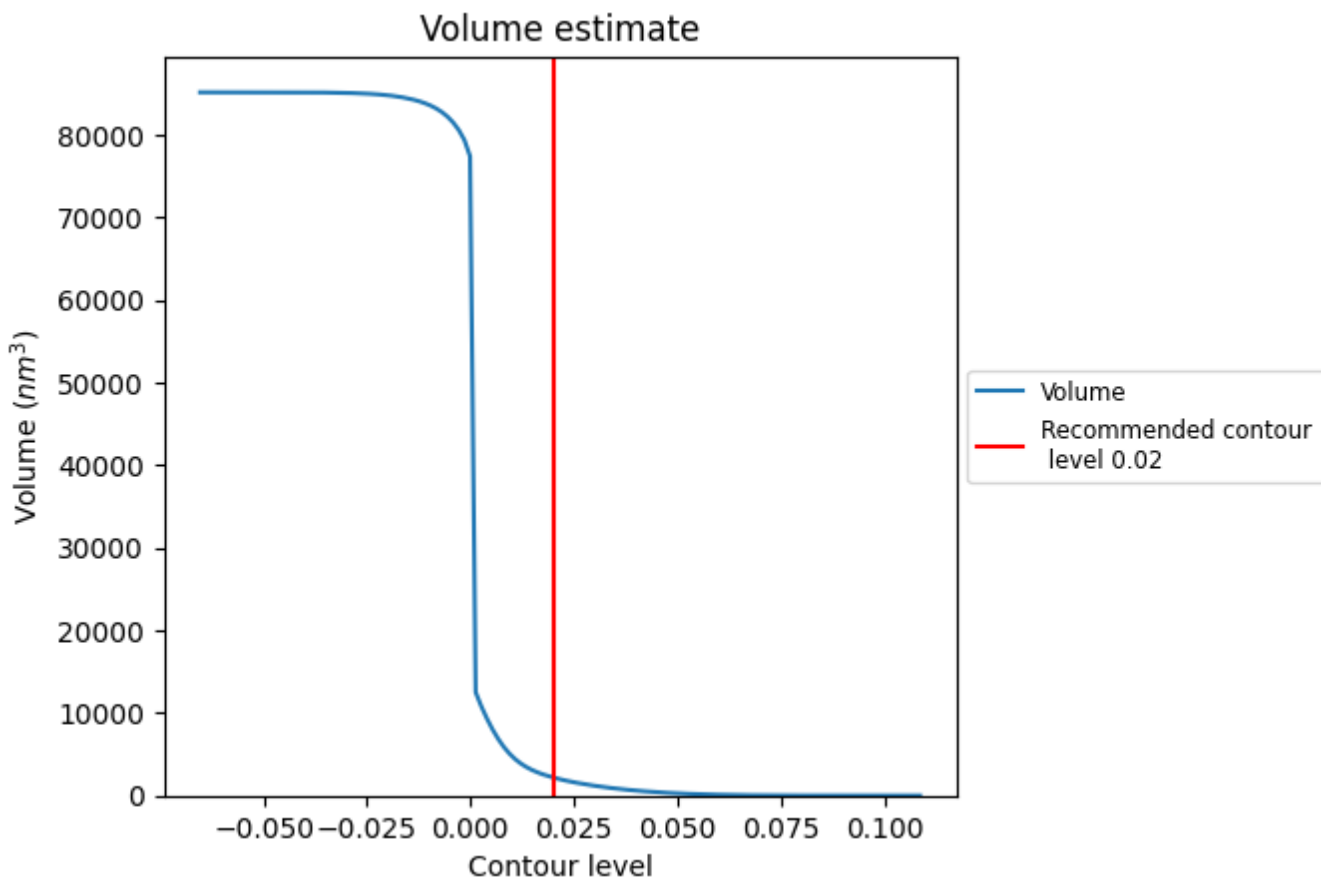
The volume at the recommended contour level is 2188 nm^3; this corresponds to an approximate mass of 1976 kDa.

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   ⓘ
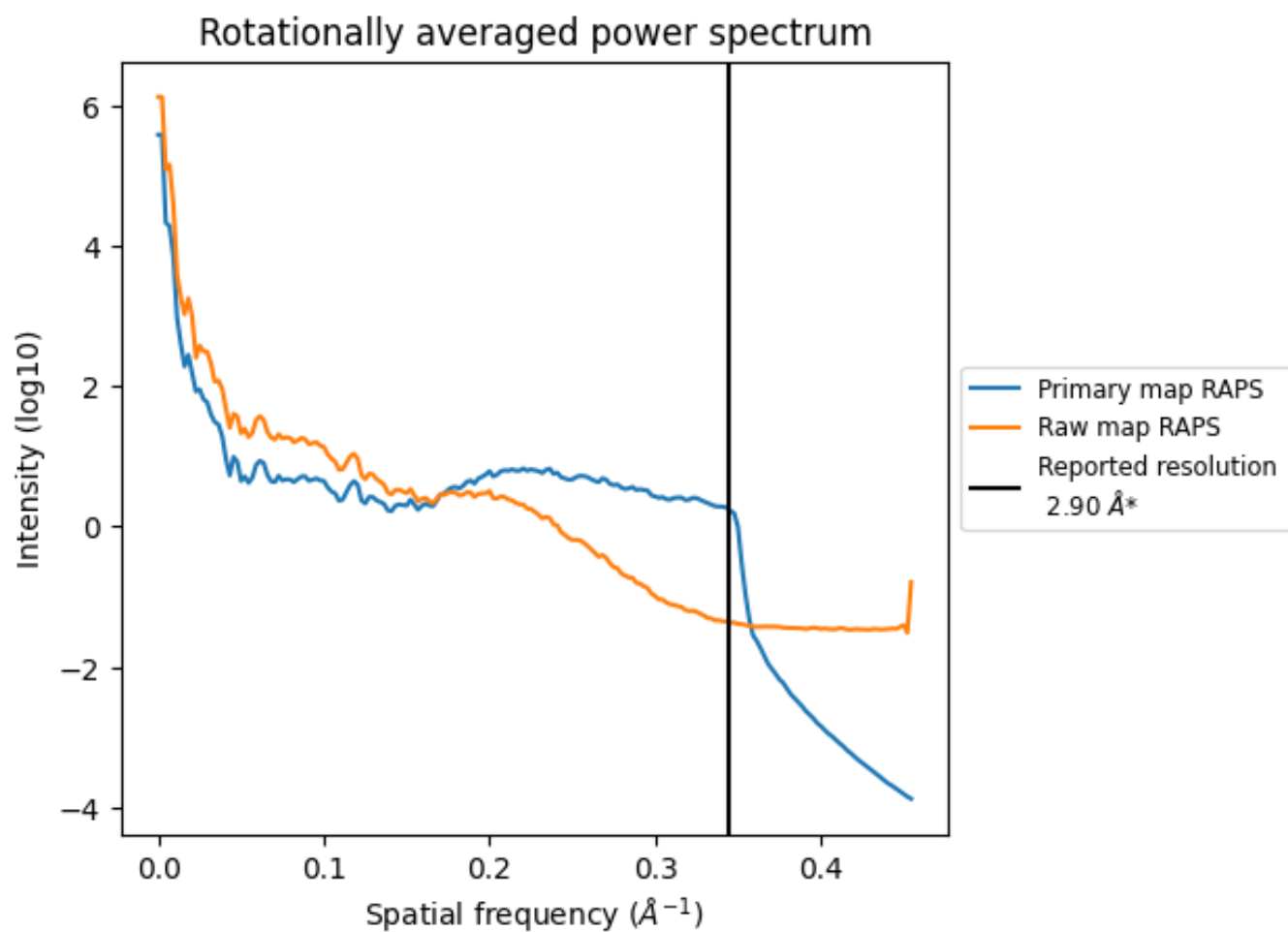
*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8   Fourier-Shell correlation ⓘ

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.

8.1   FSC ⓘ
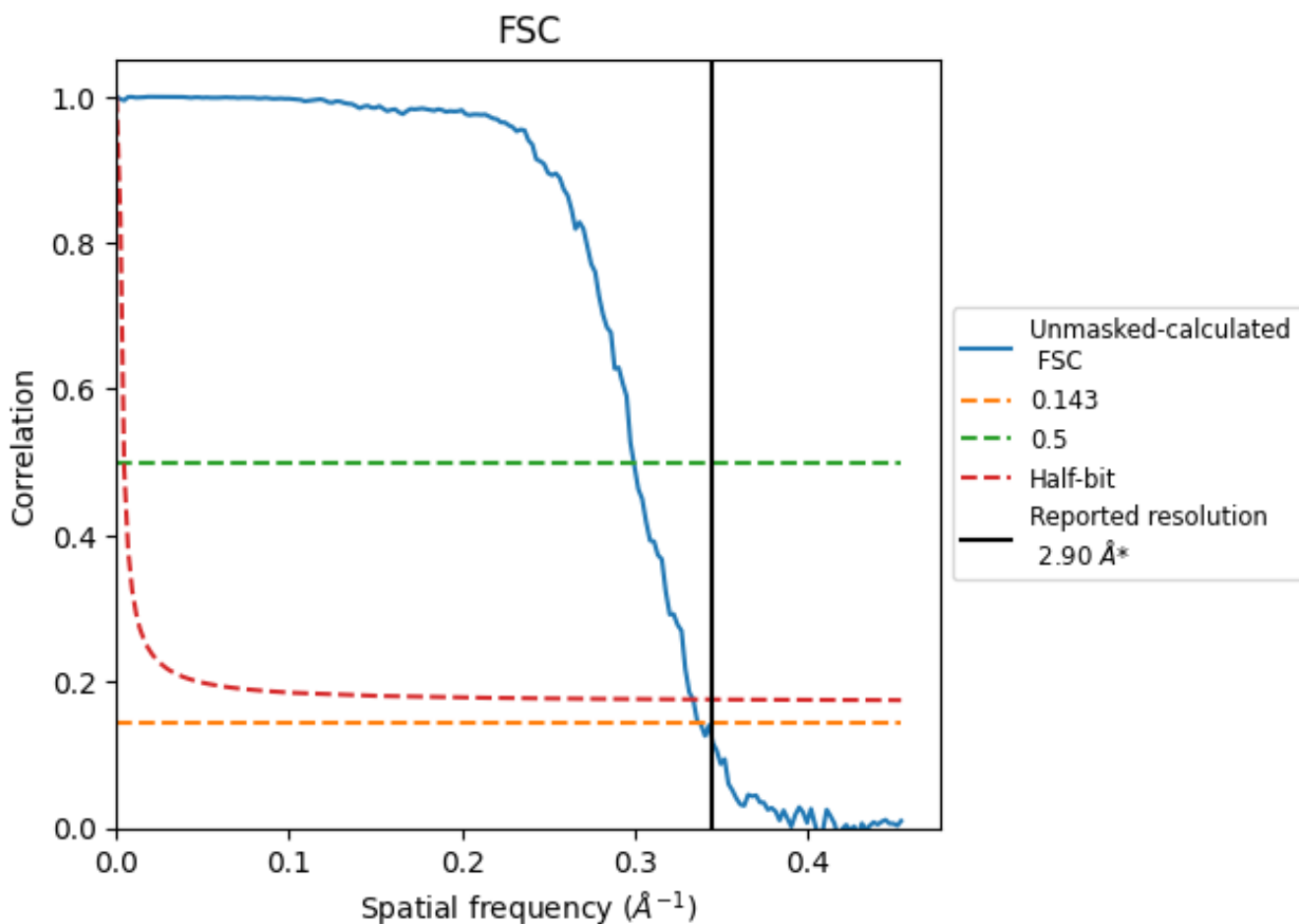
*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.96	3.34	2.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-50089 and PDB model 9EZM. Per-residue inclusion information can be found in section 3 on page 6.

9.1   Map-model overlay ⓘ

<div align="center">X   Y   Z</div>
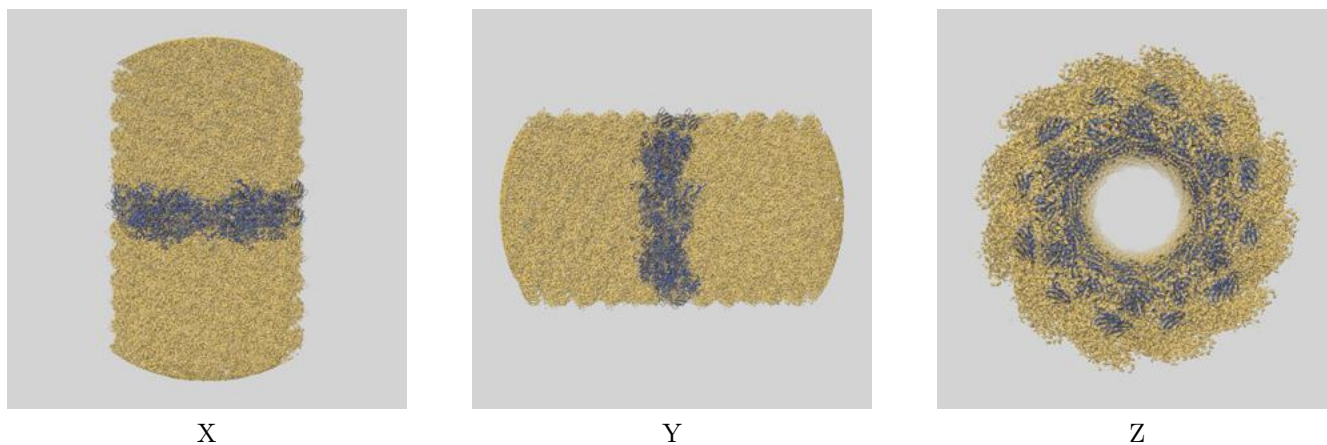
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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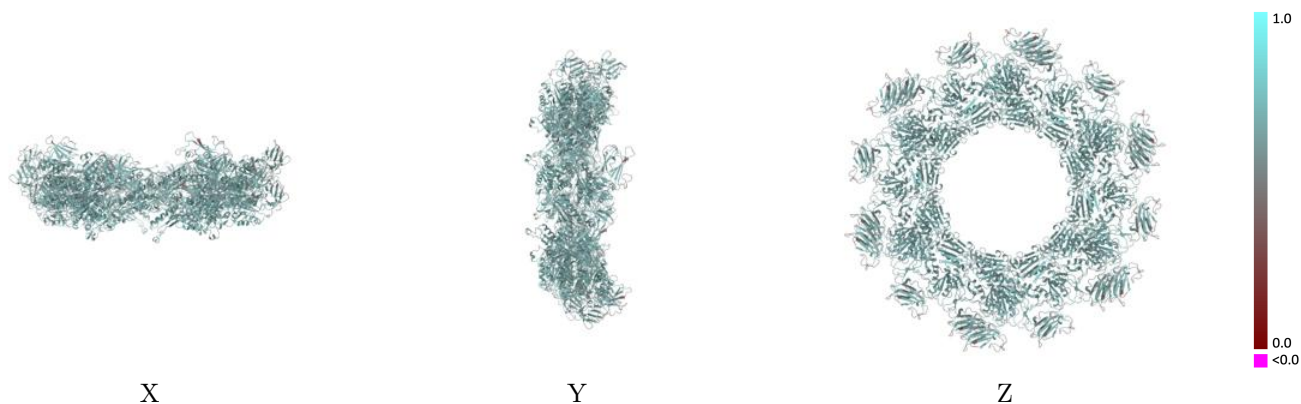
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
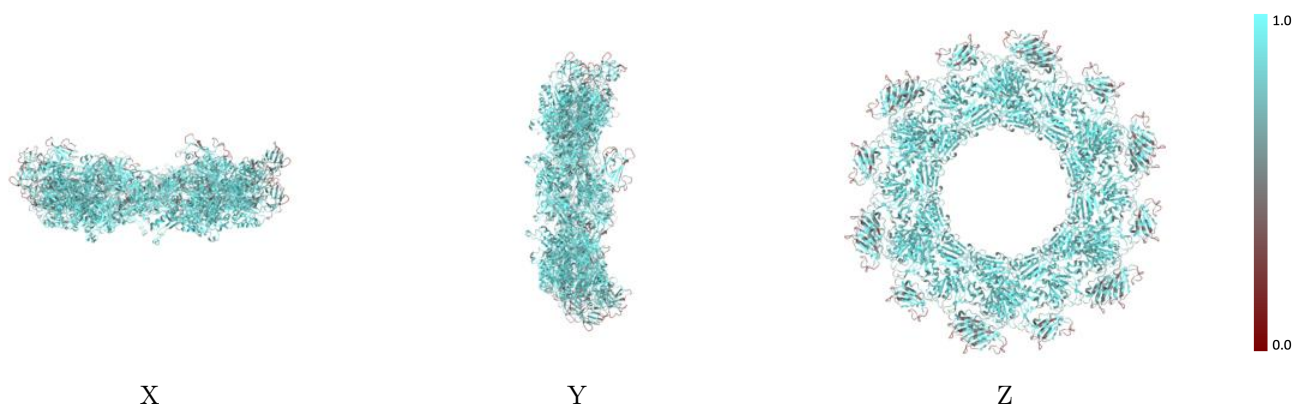
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4   Atom inclusion ⓘ
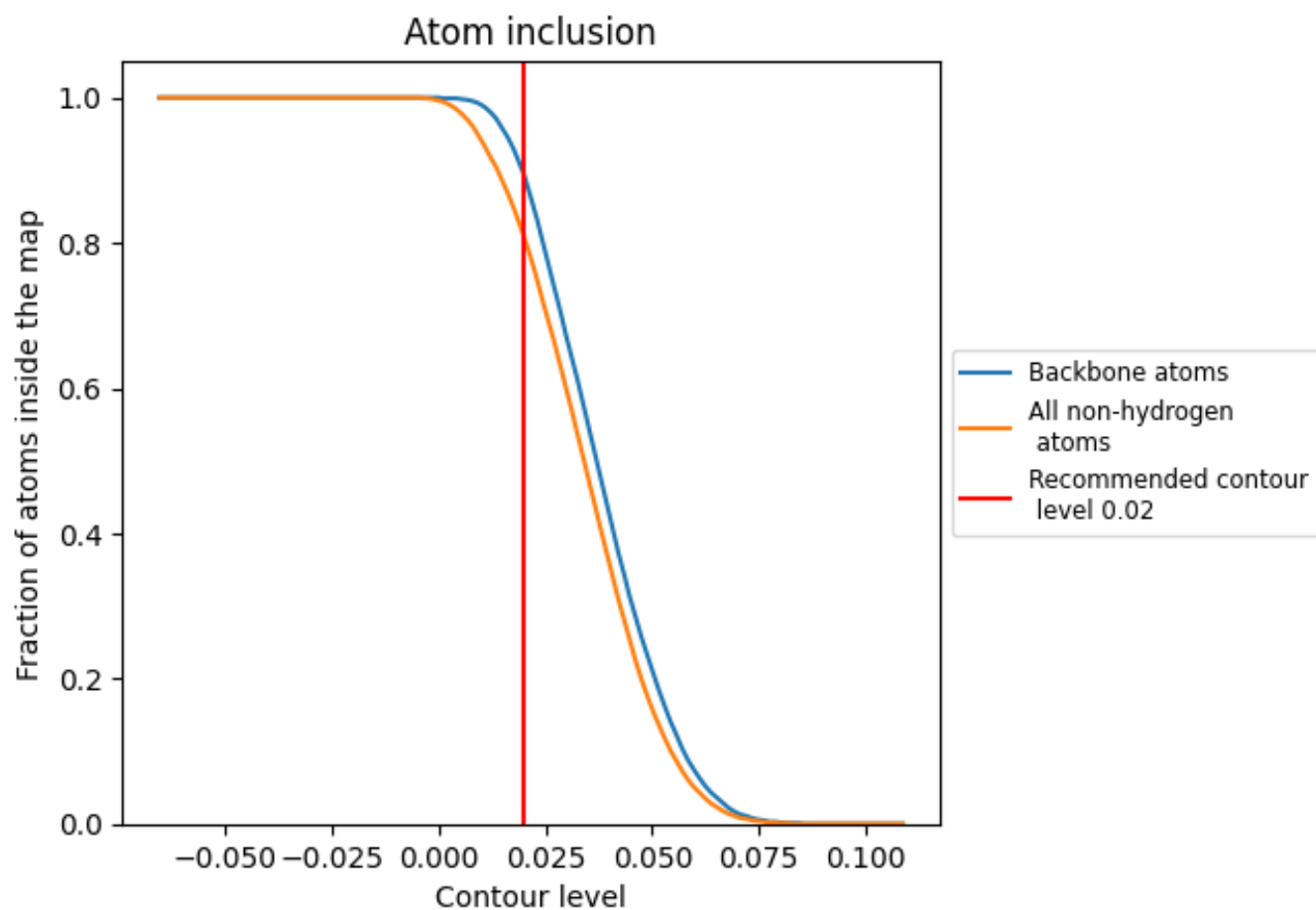
At the recommended contour level, 89% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.6210
A	0.8200	0.6280
B	0.8120	0.6250
C	0.8130	0.6240
D	0.8160	0.6280
E	0.8120	0.6250
F	0.8130	0.6250
G	0.8060	0.6150
H	0.8040	0.6160
I	0.8040	0.6160
J	0.8050	0.6170
K	0.8030	0.6170
L	0.8040	0.6160
M	0.8100	0.6190
N	0.8090	0.6210
O	0.8060	0.6200
P	0.8080	0.6200
Q	0.8100	0.6210
R	0.8060	0.6210

1.0

0.0
<0.0