



# wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 12:20 PM UTC

PDB ID : 9C8E / pdb\_00009c8e  
EMDB ID : EMD-45302  
Title : mouse Seipin complex  
Authors : Li, C.; Han, Y.; Wynn, R.M.; Chen, Z.; Scherer, P.E.  
Deposited on : 2024-06-12  
Resolution : 3.19 Å(reported)

This is a wwPDB EM Validation Summary 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.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

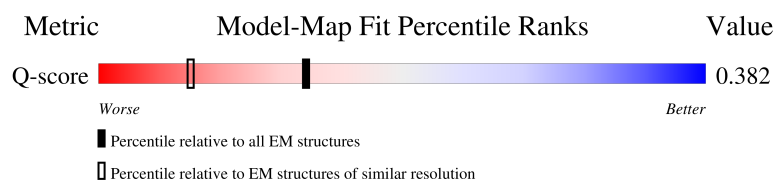
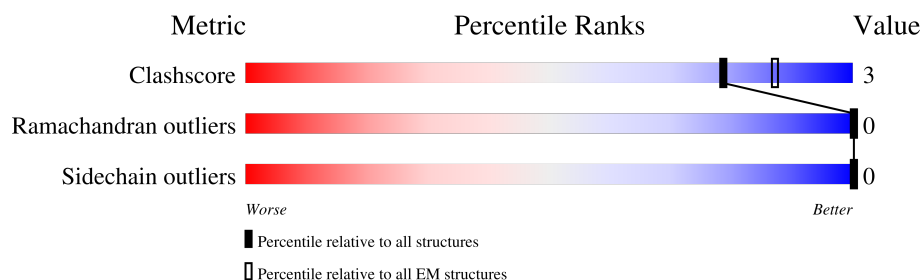
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.19 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14455 ( 2.69 - 3.69 )

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	454	 35% 63%
1	B	454	 33% 63%
1	C	454	 33% 63%
1	D	454	 34% 63%

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Mol	Chain	Length	Quality of chain
1	E	454	
1	F	454	
1	G	454	
1	H	454	
1	I	454	
1	J	454	
1	K	454	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29465 atoms, of which 14714 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 Seipin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	167	Total 2677	C 861	H 1336	N 227	O 246	S 7	0	0
1	B	167	Total 2677	C 861	H 1336	N 227	O 246	S 7	0	0
1	C	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	D	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	E	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	F	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	G	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	H	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	I	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	J	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0
1	K	167	Total 2679	C 861	H 1338	N 227	O 246	S 7	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-70	MET	-	initiating methionine	UNP A0A0R4J225
A	-69	SER	-	expression tag	UNP A0A0R4J225
A	-68	GLY	-	expression tag	UNP A0A0R4J225
A	-67	ARG	-	expression tag	UNP A0A0R4J225
A	-66	TRP	-	expression tag	UNP A0A0R4J225
A	-65	SER	-	expression tag	UNP A0A0R4J225
A	-64	HIS	-	expression tag	UNP A0A0R4J225
A	-63	PRO	-	expression tag	UNP A0A0R4J225

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-62	GLN	-	expression tag	UNP A0A0R4J225
A	-61	PHE	-	expression tag	UNP A0A0R4J225
A	-60	GLU	-	expression tag	UNP A0A0R4J225
A	-59	LYS	-	expression tag	UNP A0A0R4J225
B	-70	MET	-	initiating methionine	UNP A0A0R4J225
B	-69	SER	-	expression tag	UNP A0A0R4J225
B	-68	GLY	-	expression tag	UNP A0A0R4J225
B	-67	ARG	-	expression tag	UNP A0A0R4J225
B	-66	TRP	-	expression tag	UNP A0A0R4J225
B	-65	SER	-	expression tag	UNP A0A0R4J225
B	-64	HIS	-	expression tag	UNP A0A0R4J225
B	-63	PRO	-	expression tag	UNP A0A0R4J225
B	-62	GLN	-	expression tag	UNP A0A0R4J225
B	-61	PHE	-	expression tag	UNP A0A0R4J225
B	-60	GLU	-	expression tag	UNP A0A0R4J225
B	-59	LYS	-	expression tag	UNP A0A0R4J225
C	-70	MET	-	initiating methionine	UNP A0A0R4J225
C	-69	SER	-	expression tag	UNP A0A0R4J225
C	-68	GLY	-	expression tag	UNP A0A0R4J225
C	-67	ARG	-	expression tag	UNP A0A0R4J225
C	-66	TRP	-	expression tag	UNP A0A0R4J225
C	-65	SER	-	expression tag	UNP A0A0R4J225
C	-64	HIS	-	expression tag	UNP A0A0R4J225
C	-63	PRO	-	expression tag	UNP A0A0R4J225
C	-62	GLN	-	expression tag	UNP A0A0R4J225
C	-61	PHE	-	expression tag	UNP A0A0R4J225
C	-60	GLU	-	expression tag	UNP A0A0R4J225
C	-59	LYS	-	expression tag	UNP A0A0R4J225
D	-70	MET	-	initiating methionine	UNP A0A0R4J225
D	-69	SER	-	expression tag	UNP A0A0R4J225
D	-68	GLY	-	expression tag	UNP A0A0R4J225
D	-67	ARG	-	expression tag	UNP A0A0R4J225
D	-66	TRP	-	expression tag	UNP A0A0R4J225
D	-65	SER	-	expression tag	UNP A0A0R4J225
D	-64	HIS	-	expression tag	UNP A0A0R4J225
D	-63	PRO	-	expression tag	UNP A0A0R4J225
D	-62	GLN	-	expression tag	UNP A0A0R4J225
D	-61	PHE	-	expression tag	UNP A0A0R4J225
D	-60	GLU	-	expression tag	UNP A0A0R4J225
D	-59	LYS	-	expression tag	UNP A0A0R4J225
E	-70	MET	-	initiating methionine	UNP A0A0R4J225
E	-69	SER	-	expression tag	UNP A0A0R4J225

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-68	GLY	-	expression tag	UNP A0A0R4J225
E	-67	ARG	-	expression tag	UNP A0A0R4J225
E	-66	TRP	-	expression tag	UNP A0A0R4J225
E	-65	SER	-	expression tag	UNP A0A0R4J225
E	-64	HIS	-	expression tag	UNP A0A0R4J225
E	-63	PRO	-	expression tag	UNP A0A0R4J225
E	-62	GLN	-	expression tag	UNP A0A0R4J225
E	-61	PHE	-	expression tag	UNP A0A0R4J225
E	-60	GLU	-	expression tag	UNP A0A0R4J225
E	-59	LYS	-	expression tag	UNP A0A0R4J225
F	-70	MET	-	initiating methionine	UNP A0A0R4J225
F	-69	SER	-	expression tag	UNP A0A0R4J225
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F	-61	PHE	-	expression tag	UNP A0A0R4J225
F	-60	GLU	-	expression tag	UNP A0A0R4J225
F	-59	LYS	-	expression tag	UNP A0A0R4J225
G	-70	MET	-	initiating methionine	UNP A0A0R4J225
G	-69	SER	-	expression tag	UNP A0A0R4J225
G	-68	GLY	-	expression tag	UNP A0A0R4J225
G	-67	ARG	-	expression tag	UNP A0A0R4J225
G	-66	TRP	-	expression tag	UNP A0A0R4J225
G	-65	SER	-	expression tag	UNP A0A0R4J225
G	-64	HIS	-	expression tag	UNP A0A0R4J225
G	-63	PRO	-	expression tag	UNP A0A0R4J225
G	-62	GLN	-	expression tag	UNP A0A0R4J225
G	-61	PHE	-	expression tag	UNP A0A0R4J225
G	-60	GLU	-	expression tag	UNP A0A0R4J225
G	-59	LYS	-	expression tag	UNP A0A0R4J225
H	-70	MET	-	initiating methionine	UNP A0A0R4J225
H	-69	SER	-	expression tag	UNP A0A0R4J225
H	-68	GLY	-	expression tag	UNP A0A0R4J225
H	-67	ARG	-	expression tag	UNP A0A0R4J225
H	-66	TRP	-	expression tag	UNP A0A0R4J225
H	-65	SER	-	expression tag	UNP A0A0R4J225
H	-64	HIS	-	expression tag	UNP A0A0R4J225
H	-63	PRO	-	expression tag	UNP A0A0R4J225

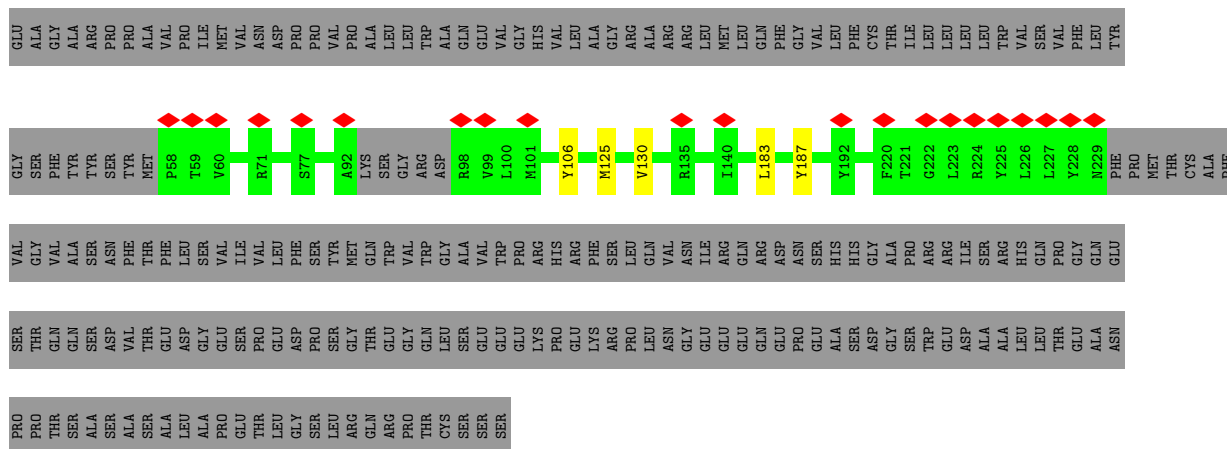
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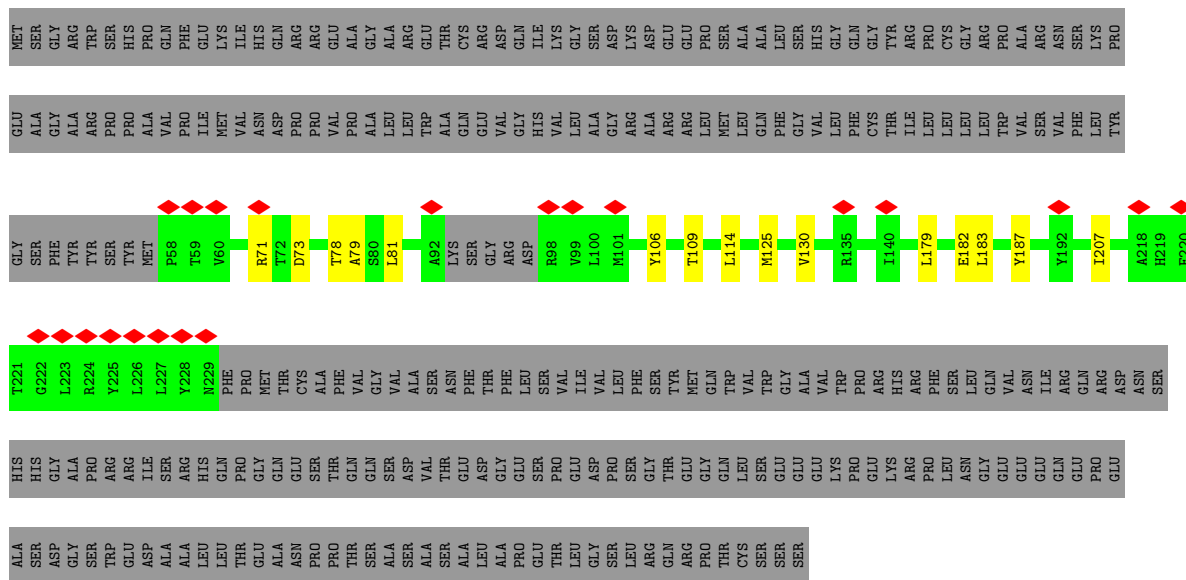
Chain	Residue	Modelled	Actual	Comment	Reference
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H	-61	PHE	-	expression tag	UNP A0A0R4J225
H	-60	GLU	-	expression tag	UNP A0A0R4J225
H	-59	LYS	-	expression tag	UNP A0A0R4J225
I	-70	MET	-	initiating methionine	UNP A0A0R4J225
I	-69	SER	-	expression tag	UNP A0A0R4J225
I	-68	GLY	-	expression tag	UNP A0A0R4J225
I	-67	ARG	-	expression tag	UNP A0A0R4J225
I	-66	TRP	-	expression tag	UNP A0A0R4J225
I	-65	SER	-	expression tag	UNP A0A0R4J225
I	-64	HIS	-	expression tag	UNP A0A0R4J225
I	-63	PRO	-	expression tag	UNP A0A0R4J225
I	-62	GLN	-	expression tag	UNP A0A0R4J225
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I	-59	LYS	-	expression tag	UNP A0A0R4J225
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J	-69	SER	-	expression tag	UNP A0A0R4J225
J	-68	GLY	-	expression tag	UNP A0A0R4J225
J	-67	ARG	-	expression tag	UNP A0A0R4J225
J	-66	TRP	-	expression tag	UNP A0A0R4J225
J	-65	SER	-	expression tag	UNP A0A0R4J225
J	-64	HIS	-	expression tag	UNP A0A0R4J225
J	-63	PRO	-	expression tag	UNP A0A0R4J225
J	-62	GLN	-	expression tag	UNP A0A0R4J225
J	-61	PHE	-	expression tag	UNP A0A0R4J225
J	-60	GLU	-	expression tag	UNP A0A0R4J225
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K	-65	SER	-	expression tag	UNP A0A0R4J225
K	-64	HIS	-	expression tag	UNP A0A0R4J225
K	-63	PRO	-	expression tag	UNP A0A0R4J225
K	-62	GLN	-	expression tag	UNP A0A0R4J225
K	-61	PHE	-	expression tag	UNP A0A0R4J225
K	-60	GLU	-	expression tag	UNP A0A0R4J225
K	-59	LYS	-	expression tag	UNP A0A0R4J225



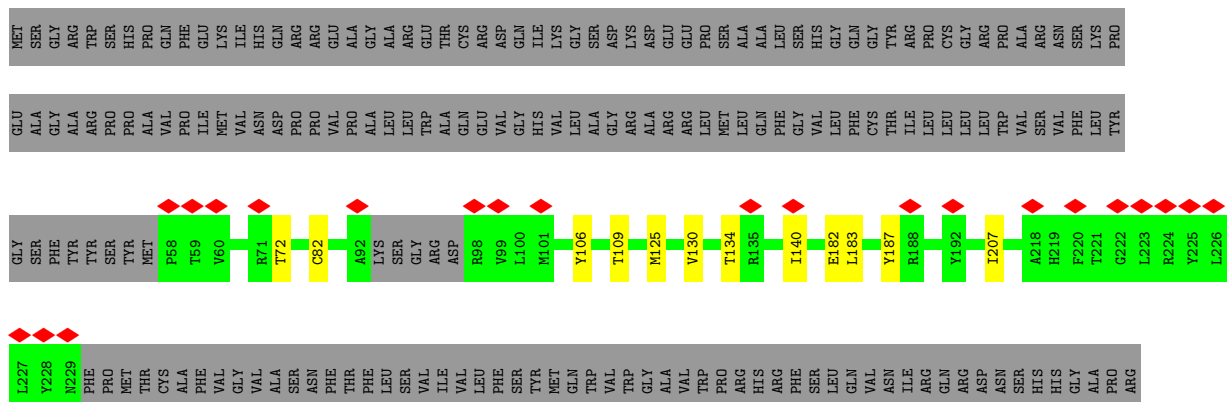
NET	SER	GLY	TRP	SER	HIS	PRO	PHE	GLU	LYS	ILE	HIS	GLN	ARG	ARG	GLU	ALA	GLY	ALA	ALA	GLU	THR	CYS	GLY	SER	ASP	ASP	GLN	ILE	LYS	GLY	SER	ASP	LYS	ASP	GLU	GLU	PRO	SER	ALA	ALA	LEU	SER	HIS	GLY	GLN	GLY	TYR	ARG	PRO	CYS	GLY	ARG	PRO	ASN	ARG	LYS	PRO
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- Molecule 1: Seipin



- Molecule 1: Seipin



GLU	ASP	ARG	TLE	ARG
ALA	ALA	ALA	ARG	ALA
LEU	LEU	LEU	HIS	GLN
LEU	THR	GLN	PRO	PRO
THR	THR	GLY	GLY	GLY
GLU	GLU	GLN	GLN	GLN
ALA	ALA	GLU	GLU	GLU
ASN	ASN	THR	THR	THR
PRO	PRO	THR	THR	THR
PRO	THR	GLN	GLN	GLN
THR	THR	GLN	GLN	GLN
SER	SER	ASP	ASP	ASP
ALA	ALA	VAL	VAL	VAL
ALA	ALA	THR	THR	THR
ALA	ALA	GLU	GLU	GLU
LEU	LEU	ASP	ASP	ASP
ALA	ALA	GLY	GLY	GLY
ALA	ALA	GLU	GLU	GLU
PRO	PRO	SER	SER	SER
GLU	GLU	SER	SER	SER
THR	THR	PRO	PRO	PRO
LEU	LEU	GLU	GLU	GLU
GLY	GLY	ASP	ASP	ASP
SER	SER	PRO	PRO	PRO
SER	SER	ASP	ASP	ASP
LEU	LEU	SER	SER	SER
ARG	ARG	GLY	GLY	GLY
GLN	GLN	THR	THR	THR
ARG	ARG	GLU	GLU	GLU
PRO	PRO	GLY	GLY	GLY
THR	THR	GLN	GLN	GLN
CYS	CYS	LEU	LEU	LEU
SER	SER	SER	SER	SER
SER	SER	GLU	GLU	GLU
SER	SER	GLU	GLU	GLU
SER	SER	LYS	LYS	LYS
LYS	LYS	GLY	GLY	GLY
PRO	PRO	PRO	PRO	PRO
GLU	GLU	GLU	GLU	GLU
LYS	LYS	ARG	ARG	ARG
LEU	LEU	ASN	ASN	ASN
ALA	ALA	LEU	LEU	LEU
GLY	GLY	GLY	GLY	GLY
GLU	GLU	GLU	GLU	GLU
GLN	GLN	GLN	GLN	GLN
GLU	GLU	GLU	GLU	GLU
PRO	PRO	PRO	PRO	PRO
GLU	GLU	ALA	ALA	ALA
ALA	ALA	SER	SER	SER
ASP	ASP	GLY	GLY	GLY
SER	SER	SER	SER	SER
SER	SER	THR	THR	THR

- Molecule 1: Seipin

[illegible]

GLY SER PHE TYR TYR SER TYR MET P58 P59 V60 R71 T78 A79 S80 L81 A92 LYS SER ARG GLY ASP R98 V99 L100 M101 Y106 T109 V130 T134 R135 I140 M148 E182 L183 Y187 Y192 I207 A218 H219 F220 T221 G222 L223 R224

L226	PHE	PRO	MET	THR	CYS	ALA	PHE	VAL	GLY	VAL	ALA	SER	ASN	PHE	THR	PHE	LEU	SER	VAL	ILE	VAL	LEU	PHE	SER	TYR	MET	GLN	TRP	VAL	TRP	GLY	ALA	VAL	TRP	PRO	ARG	HIS	ARG	PHE	SER	LEU	GLN	VAL	ASN	SER	HIS	HIS	GLY	ALA	PRO
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TRP	GLU	ASP	GLY	ARG
GLU	ASP	GLY	ILE	ARG
ALA	ALA	ALA	SER	SER
ALA	ALA	LEU	HIS	ARG
LEU	LEU	LEU	GLN	GLN
THR	THR	GLY	GLN	PRO
GLU	GLU	ALA	GLY	GLN
ALA	ALA	ASN	GLU	GLY
ASN	PRO	PRO	SER	SER
PRO	PRO	THR	THR	THR
THR	SER	SER	GLN	GLN
SER	SER	ALA	SER	GLY
ALA	ALA	ALA	ASP	ASP
ALA	LEU	ALA	GLY	VAL
ALA	ALA	PRO	GLU	GLU
PRO	PRO	THR	SER	GLU
GLY	THR	GLY	GLY	PRO
GLY	LEU	GLY	GLU	GLU
LEU	GLY	ASP	SER	ASP
SER	SER	PRO	SER	PRO
LEU	LEU	SER	GLY	SER
ARG	GLN	ARG	THR	THR
GLN	ARG	GLU	GLU	GLY
ARG	PRO	PRO	GLY	GLY
PRO	THR	THR	GLN	GLN
CYS	CYS	LEU	LEU	LEU
SER	SER	SER	SER	SER
SER	SER	SER	LYS	GLY
SER	GLU	GLU	GLU	GLY
GLU	GLU	GLU	GLU	GLU
LYS	LYS	GLU	GLU	GLU
GLY	GLY	GLY	GLY	GLY
ASN	ASN	LEU	LEU	ASN
ARG	ARG	PRO	PRO	ARG
ALA	ALA	ALA	ALA	ALA
SER	SER	SER	SER	SER
GLY	GLY	GLY	GLY	GLY
SER	SER	SER	SER	SER

- Molecule 1: Seipin

[illegible]

GLY SER PHE TYR TYR SER TYR MET P58 P59 V60 R71 T72 D75 C82 A92 LYS SER GLY ASP R98 V99 L100 M101 Y106 M125 V130 R135 I140 M148 L183 Y187 R188 Y192 Y210 F220 T221 G222 L223 R224 Y225 L226 L227 Y228

**N239** PHE PRO MET THR CYS PHE VAL VAL VAL ASN ASN PHE THR PHE LEU LEU SER VAL ILE VAL LEU PHE SER TYR MET GLN TRP VAL VAL TRP TRP PRO ARG ARG HIS ARG PHE SER LEU LEU GLN VAL ASN ILE ARG GLN ARG ASP ASN SER HIS HTS GLY ALA PRO ARG ARG

[illegible]

- Molecule 1: Seipin





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C11	Depositor
Number of particles used	17212	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.081	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	320.4096, 320.4096, 320.4096	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8344, 0.8344, 0.8344	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.16	0/1372	0.31	0/1862
1	B	0.16	0/1372	0.30	0/1862
1	C	0.15	0/1372	0.29	0/1862
1	D	0.15	0/1372	0.30	0/1862
1	E	0.15	0/1372	0.31	0/1862
1	F	0.16	0/1372	0.31	0/1862
1	G	0.16	0/1372	0.31	0/1862
1	H	0.15	0/1372	0.30	0/1862
1	I	0.16	0/1372	0.29	0/1862
1	J	0.15	0/1372	0.32	0/1862
1	K	0.15	0/1372	0.30	0/1862
All	All	0.15	0/15092	0.30	0/20482

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	1341	1336	1334	6	0
1	B	1341	1336	1334	9	0
1	C	1341	1338	1336	10	0
1	D	1341	1338	1336	9	0
1	E	1341	1338	1336	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1341	1338	1336	12	0
1	G	1341	1338	1336	8	0
1	H	1341	1338	1336	9	0
1	I	1341	1338	1336	9	0
1	J	1341	1338	1336	12	0
1	K	1341	1338	1336	3	0
All	All	14751	14714	14692	82	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 82 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:K:130:VAL:HB	1:K:183:LEU:HD13	1.67	0.75
1:J:130:VAL:HB	1:J:183:LEU:HD13	1.70	0.74
1:E:130:VAL:HB	1:E:183:LEU:HD13	1.69	0.74
1:D:130:VAL:HB	1:D:183:LEU:HD13	1.69	0.73
1:A:130:VAL:HB	1:A:183:LEU:HD13	1.70	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/454 (36%)	155 (95%)	8 (5%)	0	100	100
1	B	163/454 (36%)	156 (96%)	7 (4%)	0	100	100
1	C	163/454 (36%)	155 (95%)	8 (5%)	0	100	100
1	D	163/454 (36%)	157 (96%)	6 (4%)	0	100	100
1	E	163/454 (36%)	155 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	163/454 (36%)	157 (96%)	6 (4%)	0	100	100
1	G	163/454 (36%)	156 (96%)	7 (4%)	0	100	100
1	H	163/454 (36%)	156 (96%)	7 (4%)	0	100	100
1	I	163/454 (36%)	155 (95%)	8 (5%)	0	100	100
1	J	163/454 (36%)	155 (95%)	8 (5%)	0	100	100
1	K	163/454 (36%)	155 (95%)	8 (5%)	0	100	100
All	All	1793/4994 (36%)	1712 (96%)	81 (4%)	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	152/393 (39%)	152 (100%)	0	100	100
1	B	152/393 (39%)	152 (100%)	0	100	100
1	C	152/393 (39%)	152 (100%)	0	100	100
1	D	152/393 (39%)	152 (100%)	0	100	100
1	E	152/393 (39%)	152 (100%)	0	100	100
1	F	152/393 (39%)	152 (100%)	0	100	100
1	G	152/393 (39%)	152 (100%)	0	100	100
1	H	152/393 (39%)	152 (100%)	0	100	100
1	I	152/393 (39%)	152 (100%)	0	100	100
1	J	152/393 (39%)	152 (100%)	0	100	100
1	K	152/393 (39%)	152 (100%)	0	100	100
All	All	1672/4323 (39%)	1672 (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 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	217	HIS
1	H	62	HIS
1	K	88	ASN
1	I	150	HIS
1	C	229	ASN

### 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 oligosaccharides 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-45302. These allow visual inspection of the internal detail of the map and identification of artifacts.

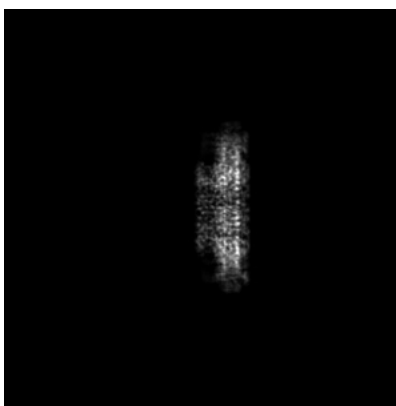
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

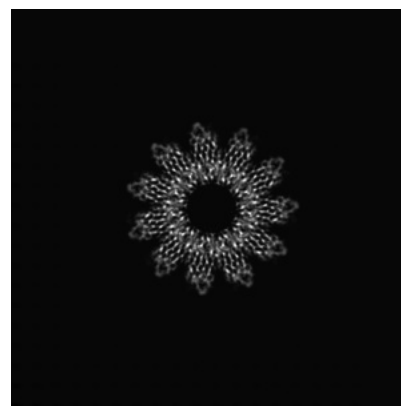
#### 6.1.1 Primary map



X

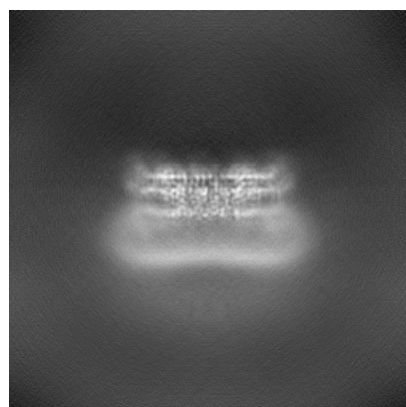


Y

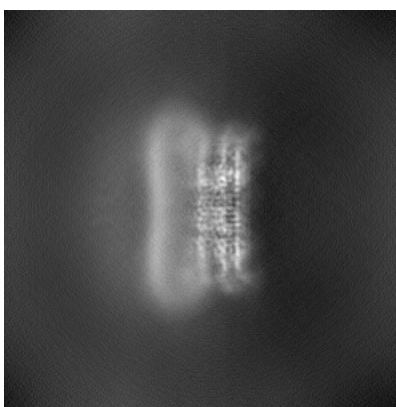


Z

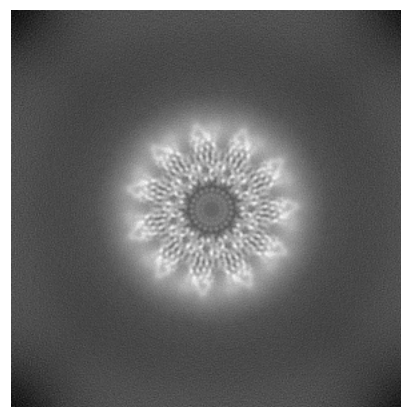
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

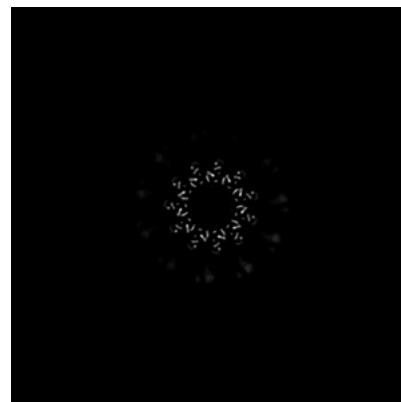
### 6.2.1 Primary map



X Index: 192

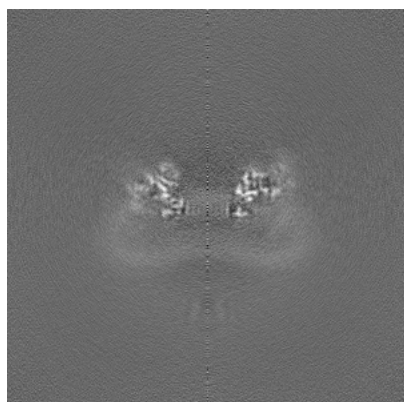


Y Index: 192

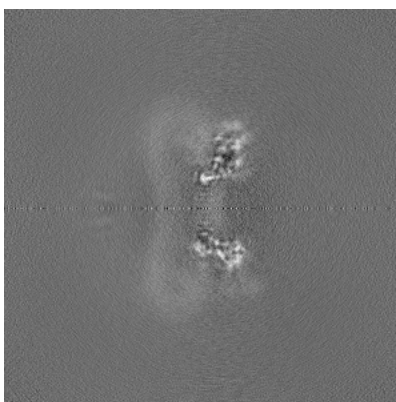


Z Index: 192

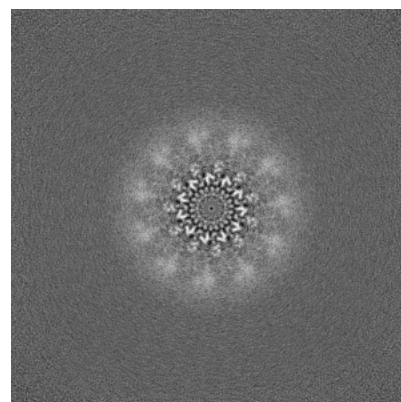
### 6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

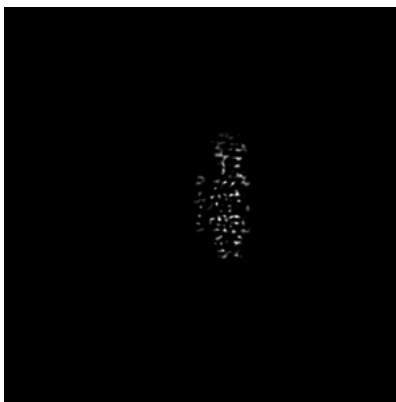
The images above show central slices of the map in three orthogonal directions.

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

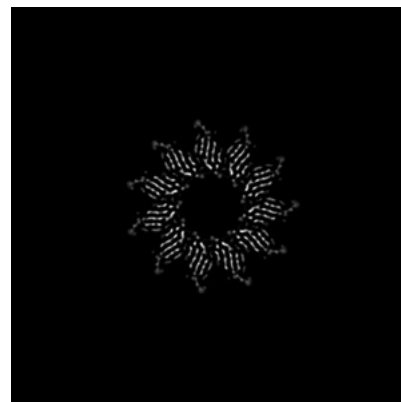
### 6.3.1 Primary map



X Index: 221

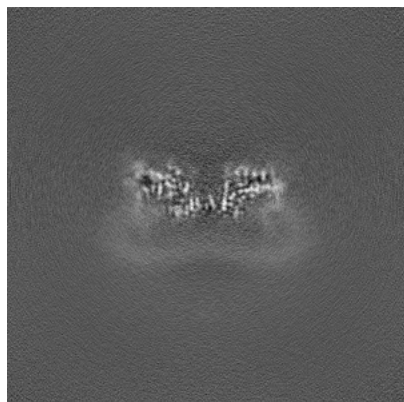


Y Index: 156

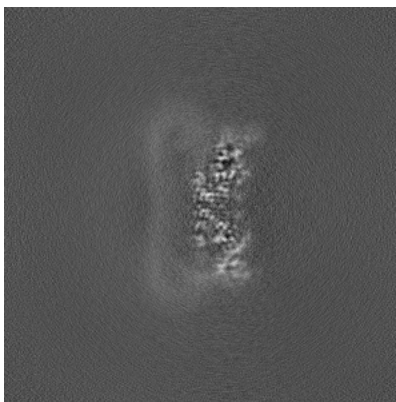


Z Index: 223

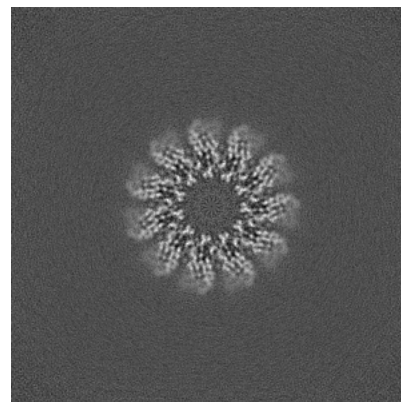
### 6.3.2 Raw map



X Index: 216



Y Index: 219

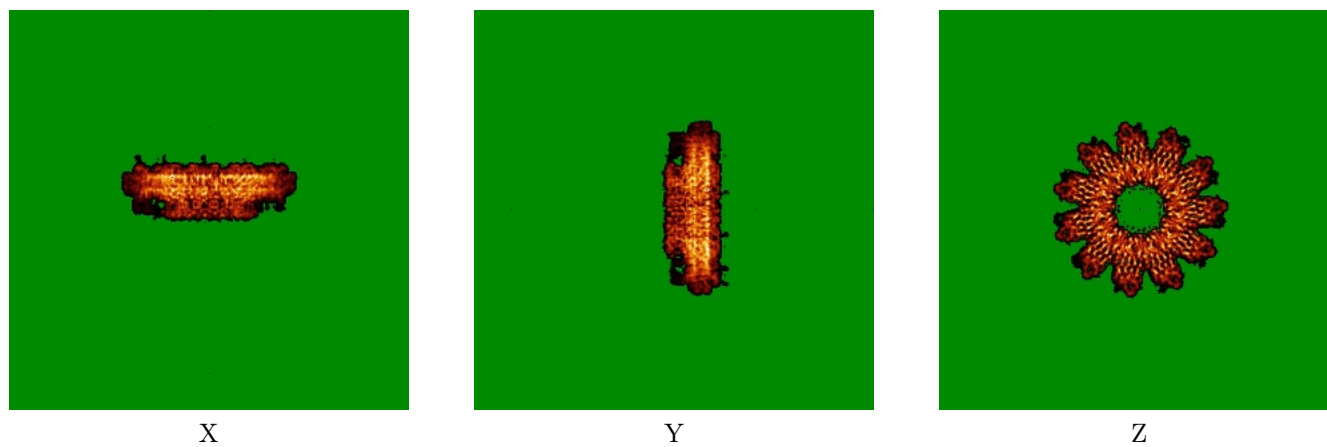


Z Index: 211

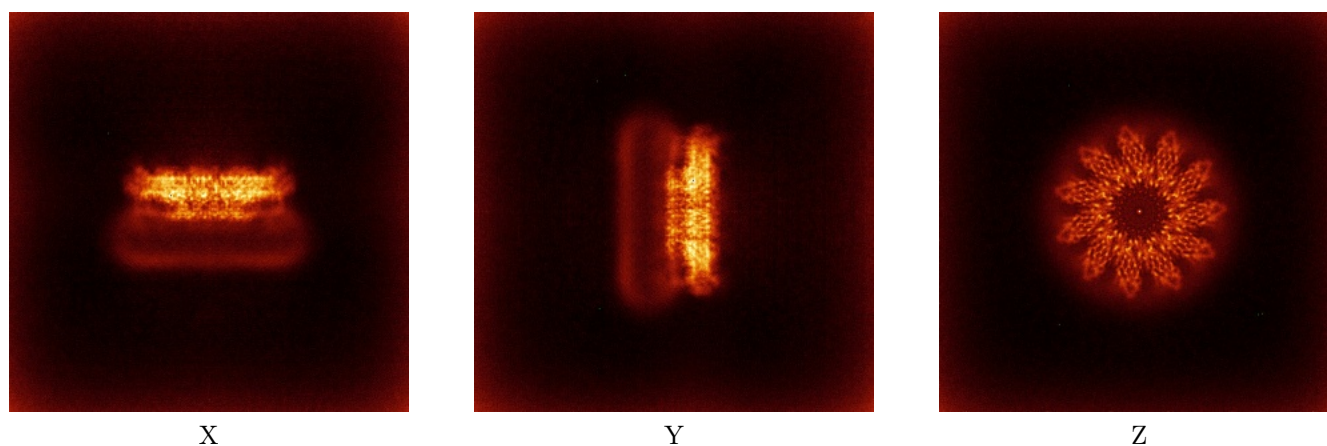
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 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.

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

This section was not generated.

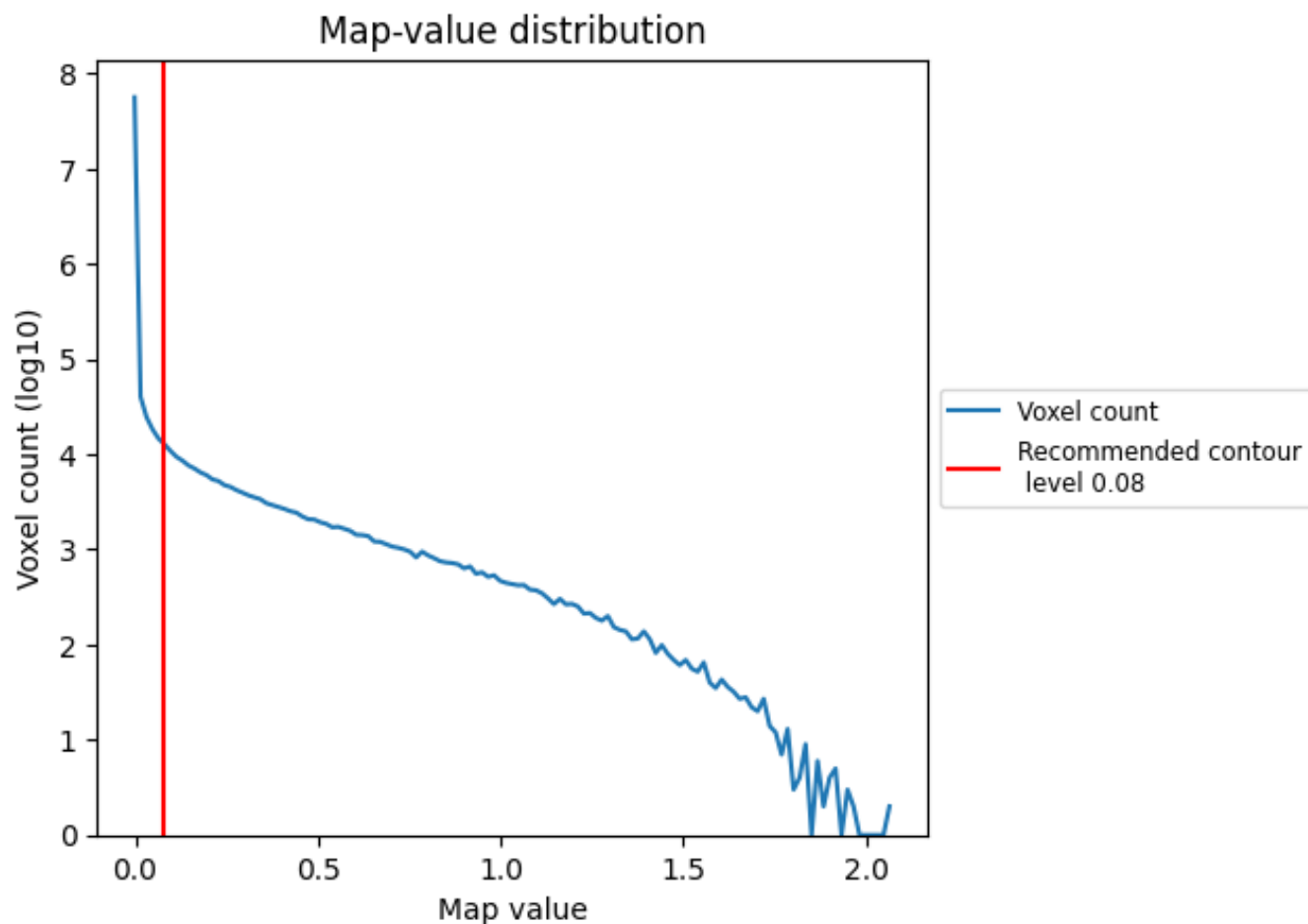
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

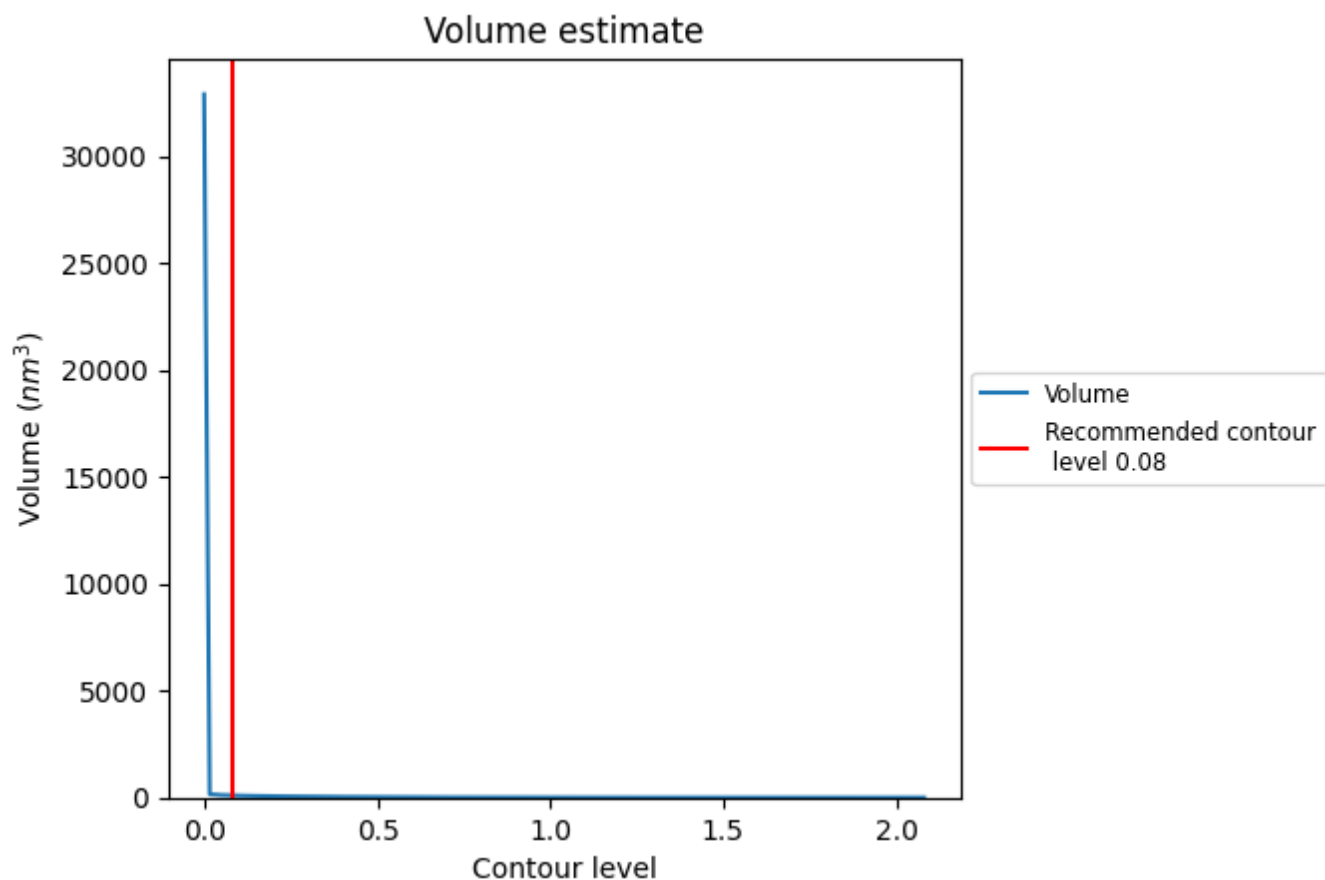
This section contains the results of statistical analysis of the map.

### 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.

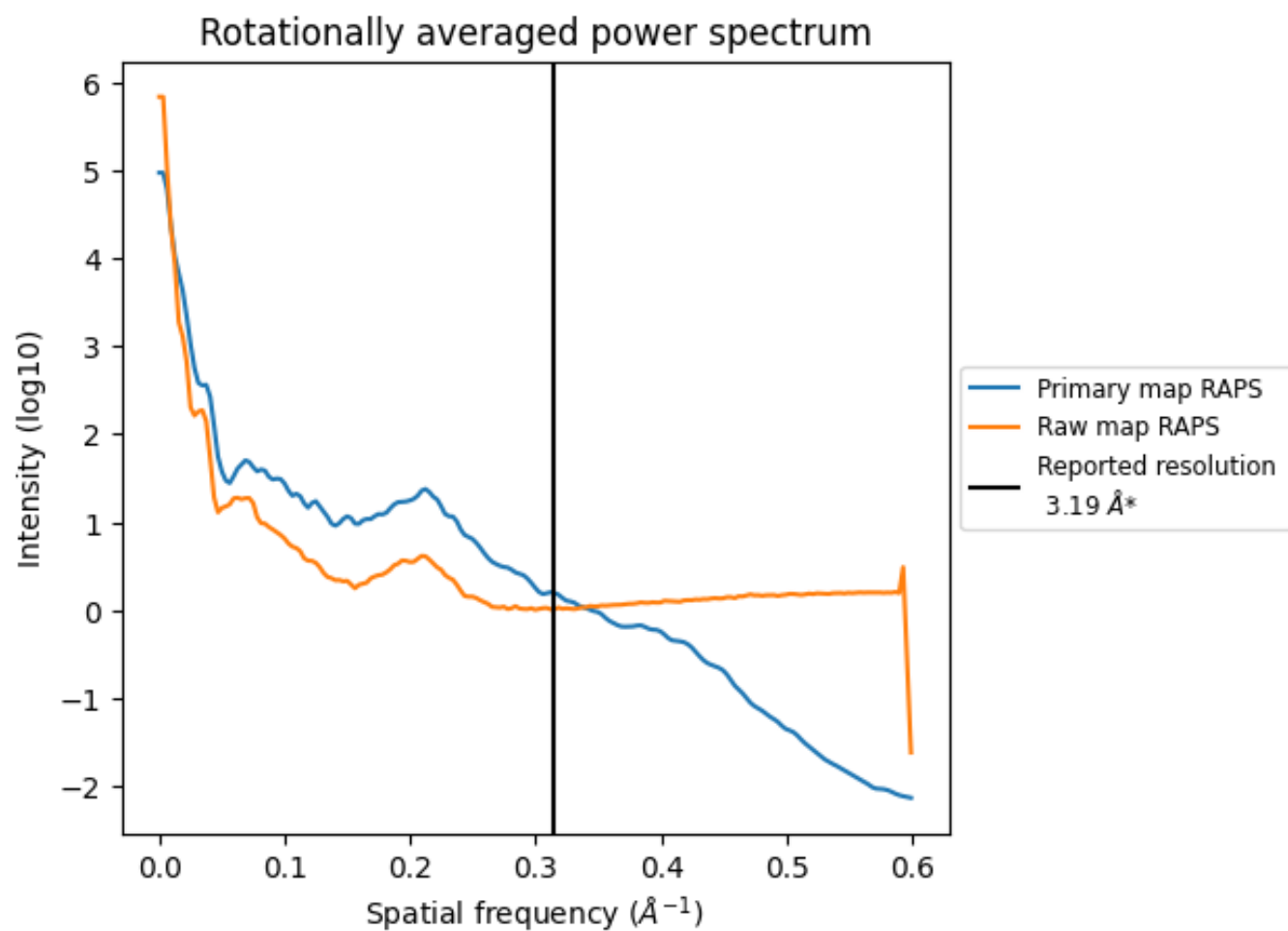
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99  $\text{nm}^3$ ; this corresponds to an approximate mass of 89 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 ⓘ

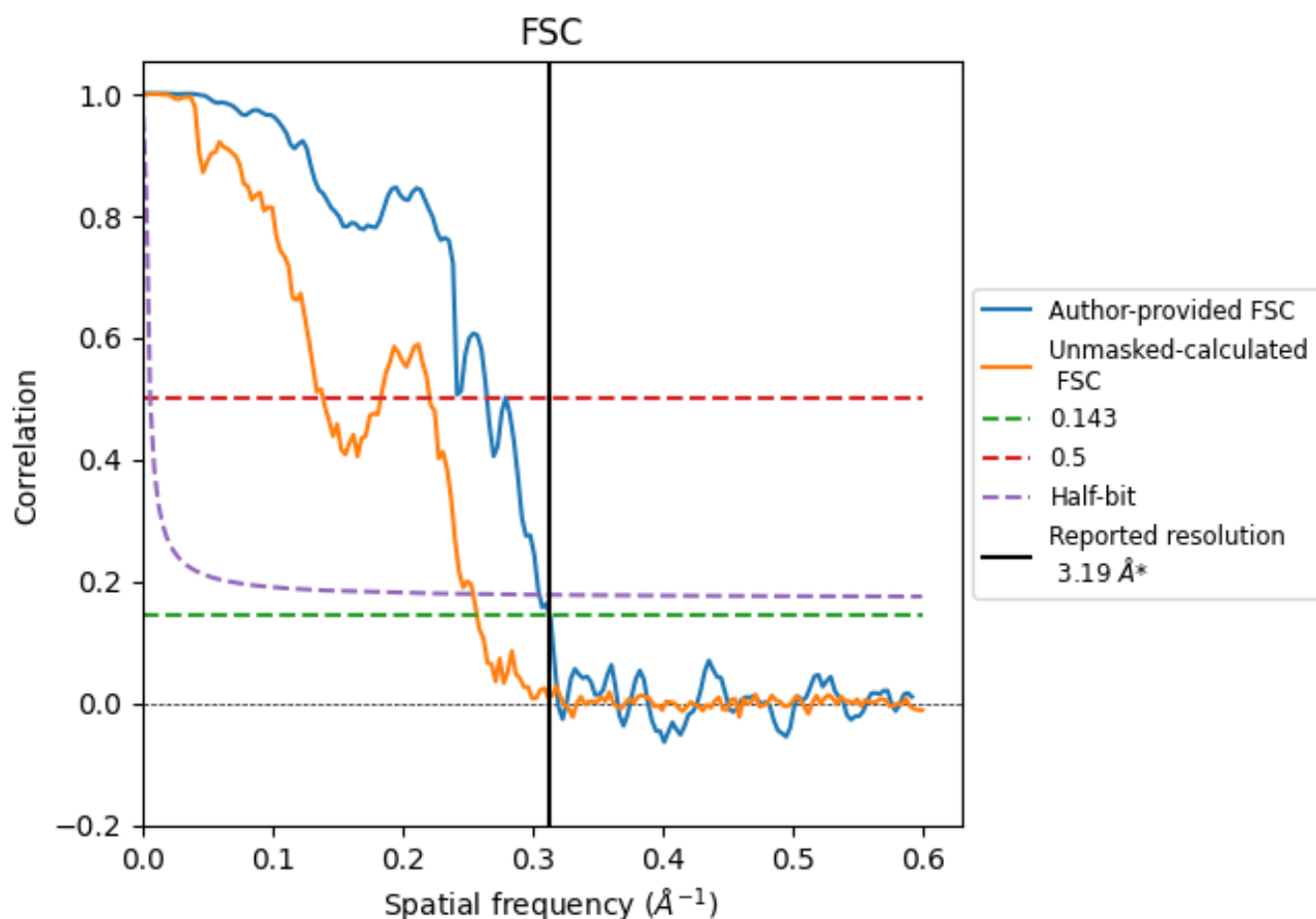


\*Reported resolution corresponds to spatial frequency of  $0.313 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.313  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

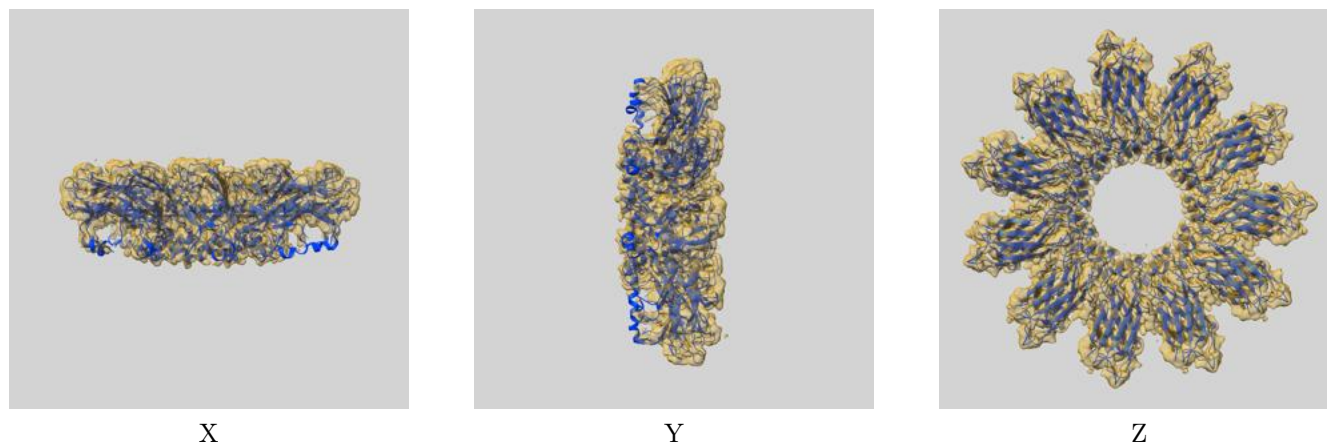
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.19	3.78	3.28
Unmasked-calculated*	3.89	7.20	3.93

\*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 3.89 differs from the reported value 3.19 by more than 10 %

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

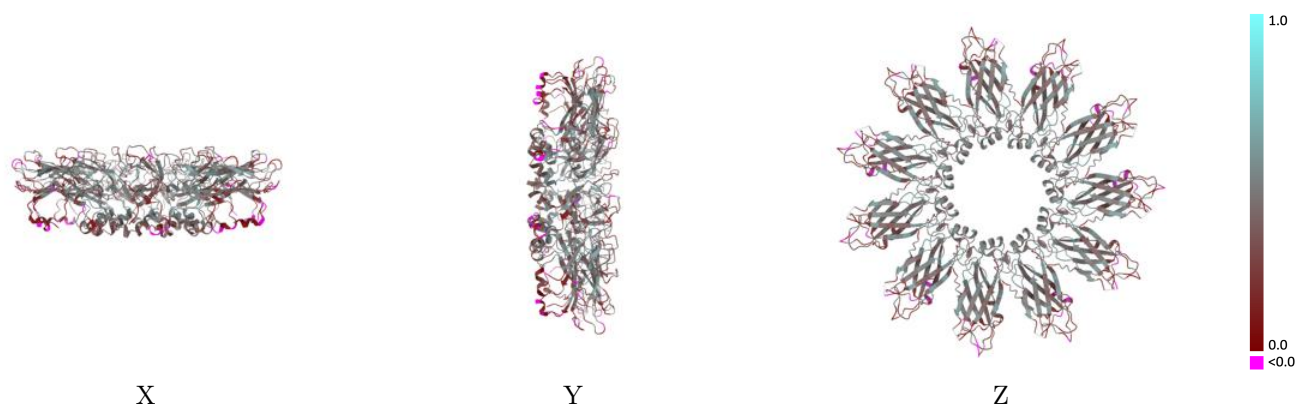
This section contains information regarding the fit between EMDB map EMD-45302 and PDB model 9C8E. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



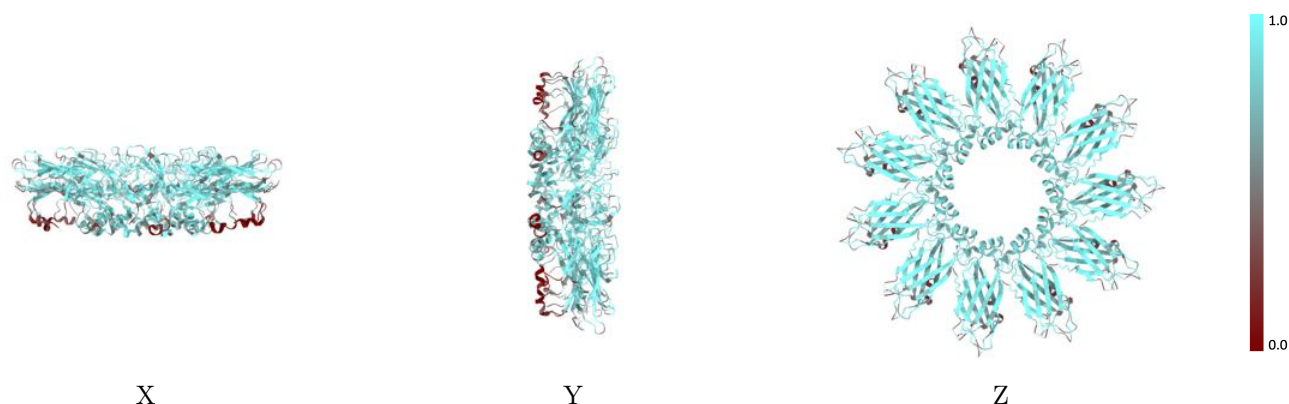
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



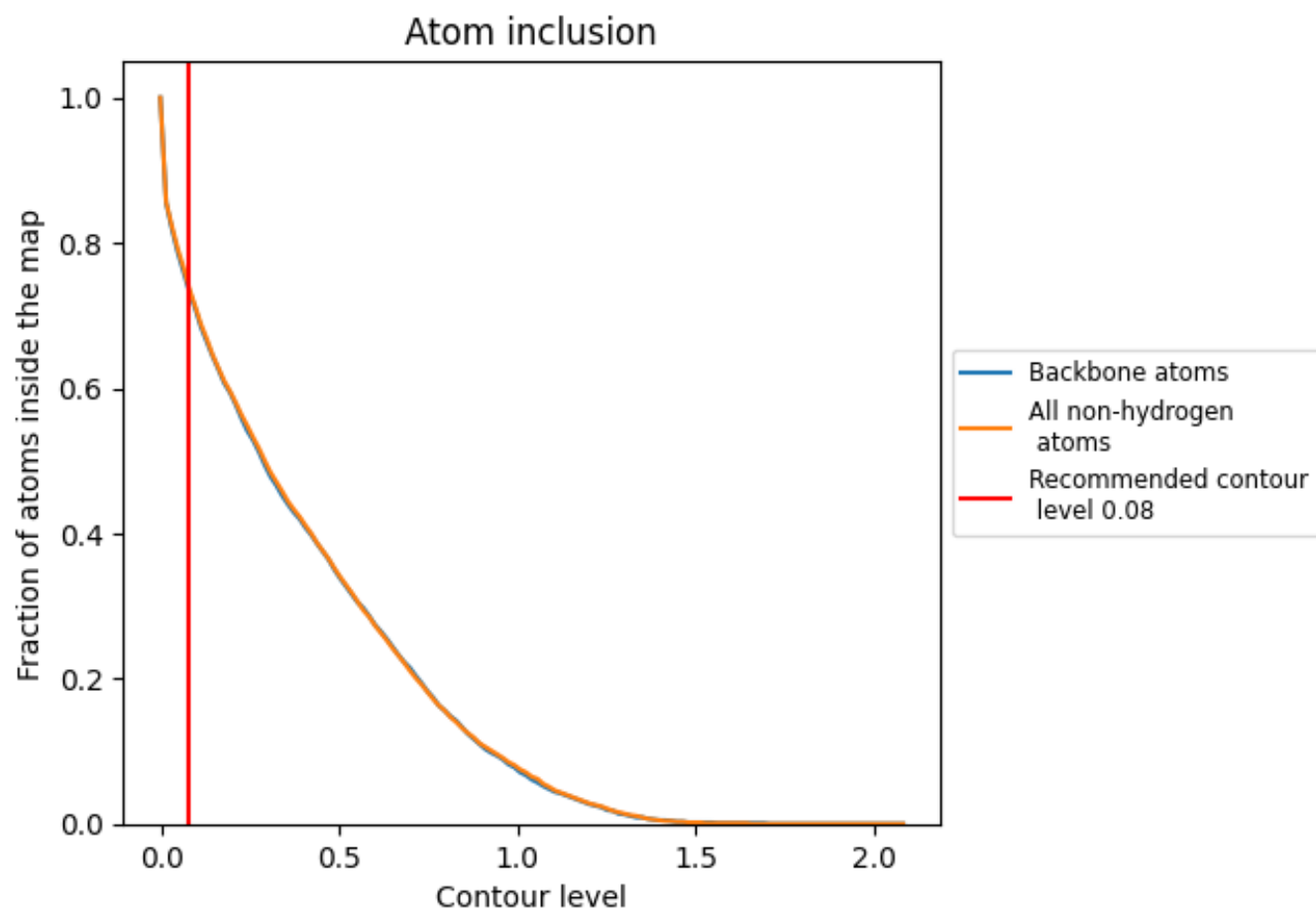
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 74% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7360	<div><div></div></div> 0.3820
A	<div><div></div></div> 0.7550	<div><div></div></div> 0.3850
B	<div><div></div></div> 0.7630	<div><div></div></div> 0.3930
C	<div><div></div></div> 0.7600	<div><div></div></div> 0.3830
D	<div><div></div></div> 0.7550	<div><div></div></div> 0.3810
E	<div><div></div></div> 0.7410	<div><div></div></div> 0.3820
F	<div><div></div></div> 0.7370	<div><div></div></div> 0.3760
G	<div><div></div></div> 0.7400	<div><div></div></div> 0.3850
H	<div><div></div></div> 0.7530	<div><div></div></div> 0.3770
I	<div><div></div></div> 0.7540	<div><div></div></div> 0.3840
J	<div><div></div></div> 0.7500	<div><div></div></div> 0.3760
K	<div><div></div></div> 0.7550	<div><div></div></div> 0.3830

1.0

0.0

<0.0