



wwPDB EM Validation Summary Report ⓘ

Jul 26, 2022 – 10:24 am BST

PDB ID : 7OFQ
EMDB ID : EMD-12875
Title : The archaellum of Methanocaldococcus villosus
Authors : Isupov, M.; Gambelli, L.; Daum, B.
Deposited on : 2021-05-05
Resolution : 3.08 Å (reported)
Based on initial model : 5O4U

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

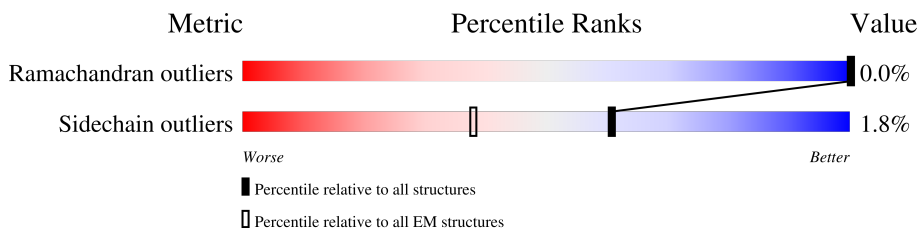
EMDB validation analysis : 0.0.1.dev8
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	209	13% 100%
1	C	209	11% 100%
1	E	209	13% 100%
1	G	209	11% 100%
1	I	209	14% 100%
1	K	209	17% 99% .
1	M	209	25% 99% .
1	O	209	40% 99% .
1	Q	209	12% 99% .

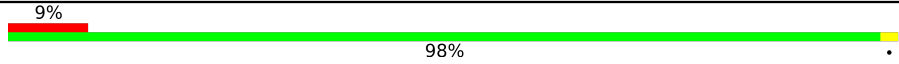
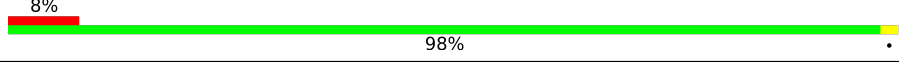
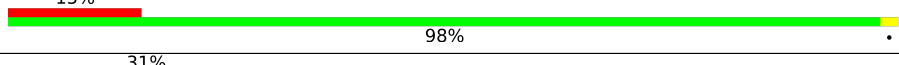
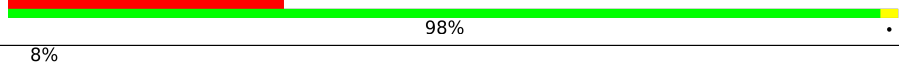
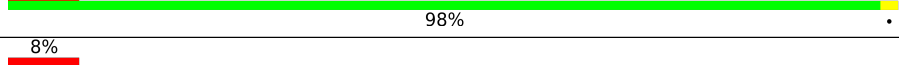
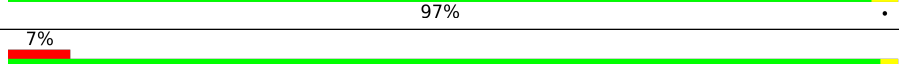
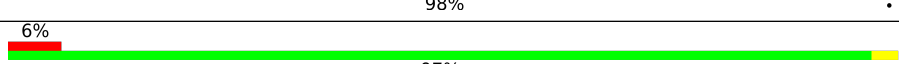
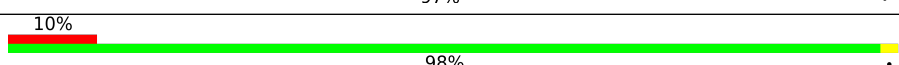
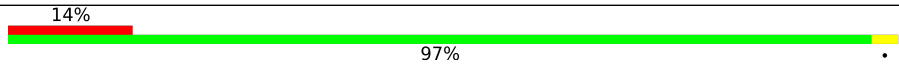
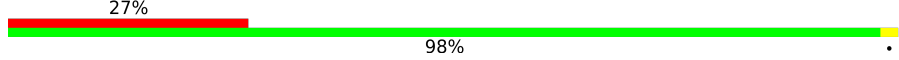

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Mol	Chain	Length	Quality of chain
1	S	209	11% 100%
1	U	209	12% 100%
1	W	209	12% 100%
1	Y	209	11% 100%
1	a	209	15% 100%
1	c	209	20% 99%
1	e	209	14% 99%
1	g	209	11% 100%
1	i	209	9% 100%
1	k	209	10% 100%
1	m	209	12% 99%
1	o	209	11% 100%
1	q	209	19% 100%
1	s	209	49% 100%
2	B	213	10% 98%
2	D	213	9% 98%
2	F	213	10% 97%
2	H	213	9% 98%
2	J	213	12% 98%
2	L	213	17% 98%
2	N	213	26% 98%
2	P	213	10% 98%
2	R	213	8% 98%
2	T	213	10% 98%
2	V	213	8% 98%

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Mol	Chain	Length	Quality of chain
2	X	213	 9% 98%
2	Z	213	 8% 98%
2	b	213	 15% 98%
2	d	213	 31% 98%
2	f	213	 8% 98%
2	h	213	 8% 97%
2	j	213	 7% 98%
2	l	213	 6% 97%
2	n	213	 10% 98%
2	p	213	 14% 97%
2	r	213	 27% 98%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 80691 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 Archaeollin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	209	1554	995	255	299	5	0	0
1	C	209	1554	995	255	299	5	0	0
1	E	209	1554	995	255	299	5	0	0
1	G	209	1554	995	255	299	5	0	0
1	I	209	1554	995	255	299	5	0	0
1	K	209	1554	995	255	299	5	0	0
1	M	209	1554	995	255	299	5	0	0
1	O	209	1554	995	255	299	5	0	0
1	Q	209	1554	995	255	299	5	0	0
1	S	209	1554	995	255	299	5	0	0
1	U	209	1554	995	255	299	5	0	0
1	W	209	1554	995	255	299	5	0	0
1	Y	209	1554	995	255	299	5	0	0
1	a	209	1554	995	255	299	5	0	0
1	c	209	1554	995	255	299	5	0	0
1	e	209	1554	995	255	299	5	0	0
1	g	209	1554	995	255	299	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	k	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	m	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	o	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	q	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		
1	s	209	Total	C	N	O	S	0	0
			1554	995	255	299	5		

- Molecule 2 is a protein called Archaeollin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	D	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	F	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	H	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	J	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	L	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	N	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	P	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	R	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	T	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	V	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	X	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	Z	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	d	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	f	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	h	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	j	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	l	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	n	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	p	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		
2	r	213	Total	C	N	O	S	0	0
			1566	1002	259	300	5		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	
3	E	1	Total	Ca	0
			1	1	
3	F	1	Total	Ca	0
			1	1	
3	G	1	Total	Ca	0
			1	1	
3	H	1	Total	Ca	0
			1	1	
3	I	1	Total	Ca	0
			1	1	
3	J	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
3	K	1	Total 1	Ca 1	0
3	L	1	Total 1	Ca 1	0
3	M	1	Total 1	Ca 1	0
3	N	1	Total 1	Ca 1	0
3	O	1	Total 1	Ca 1	0
3	P	1	Total 1	Ca 1	0
3	Q	1	Total 1	Ca 1	0
3	R	1	Total 1	Ca 1	0
3	S	1	Total 1	Ca 1	0
3	T	1	Total 1	Ca 1	0
3	U	1	Total 1	Ca 1	0
3	V	1	Total 1	Ca 1	0
3	W	1	Total 1	Ca 1	0
3	X	1	Total 1	Ca 1	0
3	Y	1	Total 1	Ca 1	0
3	Z	1	Total 1	Ca 1	0
3	a	1	Total 1	Ca 1	0
3	b	1	Total 1	Ca 1	0
3	c	1	Total 1	Ca 1	0
3	d	1	Total 1	Ca 1	0
3	e	1	Total 1	Ca 1	0

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Mol	Chain	Residues	Atoms		AltConf
3	f	1	Total 1	Ca 1	0
3	g	1	Total 1	Ca 1	0
3	h	1	Total 1	Ca 1	0
3	i	1	Total 1	Ca 1	0
3	j	1	Total 1	Ca 1	0
3	k	1	Total 1	Ca 1	0
3	l	1	Total 1	Ca 1	0
3	m	1	Total 1	Ca 1	0
3	n	1	Total 1	Ca 1	0
3	o	1	Total 1	Ca 1	0
3	p	1	Total 1	Ca 1	0
3	q	1	Total 1	Ca 1	0
3	r	1	Total 1	Ca 1	0
3	s	1	Total 1	Ca 1	0

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms				AltConf
4	A	12	Total 156	C 87	N 6	O 63	0
4	B	24	Total 312	C 174	N 12	O 126	0
4	C	12	Total 156	C 87	N 6	O 63	0
4	D	24	Total 312	C 174	N 12	O 126	0
4	E	12	Total 156	C 87	N 6	O 63	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	F	24	312	174	12	126	0
4	G	12	156	87	6	63	0
4	H	24	312	174	12	126	0
4	I	12	156	87	6	63	0
4	J	24	312	174	12	126	0
4	K	12	156	87	6	63	0
4	L	24	312	174	12	126	0
4	M	12	156	87	6	63	0
4	N	24	312	174	12	126	0
4	O	12	156	87	6	63	0
4	P	24	312	174	12	126	0
4	Q	12	156	87	6	63	0
4	R	24	312	174	12	126	0
4	S	12	156	87	6	63	0
4	T	24	312	174	12	126	0
4	U	12	156	87	6	63	0
4	V	24	312	174	12	126	0
4	W	12	156	87	6	63	0
4	X	24	312	174	12	126	0
4	Y	12	156	87	6	63	0
4	Z	24	312	174	12	126	0

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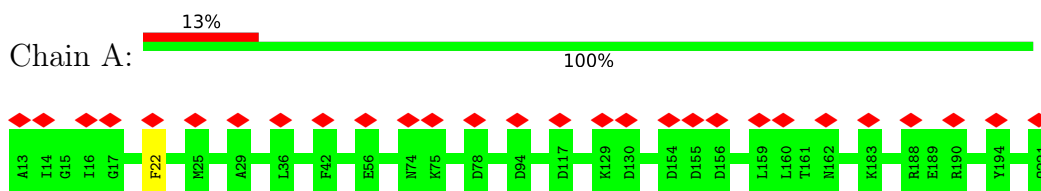
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	a	13	Total 171	C 96	N 6	O 69	0
4	b	23	Total 297	C 165	N 12	O 120	0
4	c	12	Total 156	C 87	N 6	O 63	0
4	d	24	Total 312	C 174	N 12	O 126	0
4	e	12	Total 156	C 87	N 6	O 63	0
4	f	24	Total 312	C 174	N 12	O 126	0
4	g	12	Total 156	C 87	N 6	O 63	0
4	h	24	Total 312	C 174	N 12	O 126	0
4	i	12	Total 156	C 87	N 6	O 63	0
4	j	24	Total 312	C 174	N 12	O 126	0
4	k	12	Total 156	C 87	N 6	O 63	0
4	l	24	Total 312	C 174	N 12	O 126	0
4	m	12	Total 156	C 87	N 6	O 63	0
4	n	24	Total 312	C 174	N 12	O 126	0
4	o	12	Total 156	C 87	N 6	O 63	0
4	p	24	Total 312	C 174	N 12	O 126	0
4	q	12	Total 156	C 87	N 6	O 63	0
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4	s	12	Total 156	C 87	N 6	O 63	0

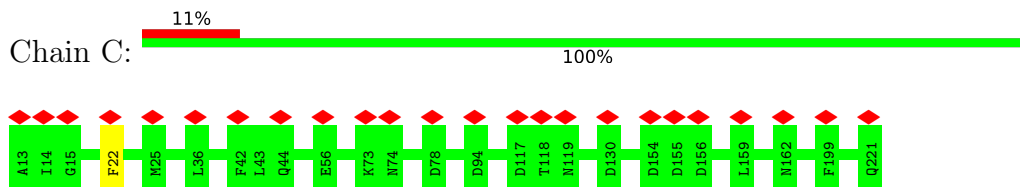
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

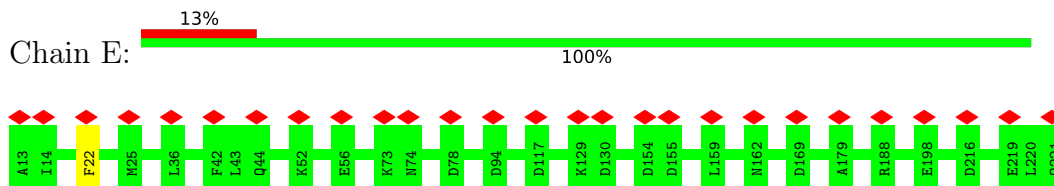
- Molecule 1: Archaeollin



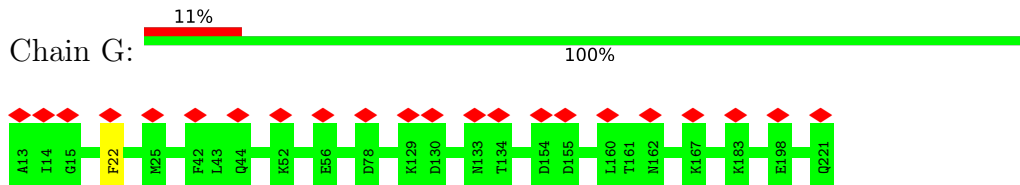
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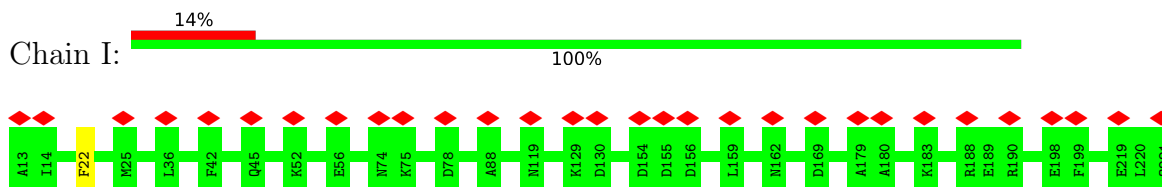
- Molecule 1: Archaeollin



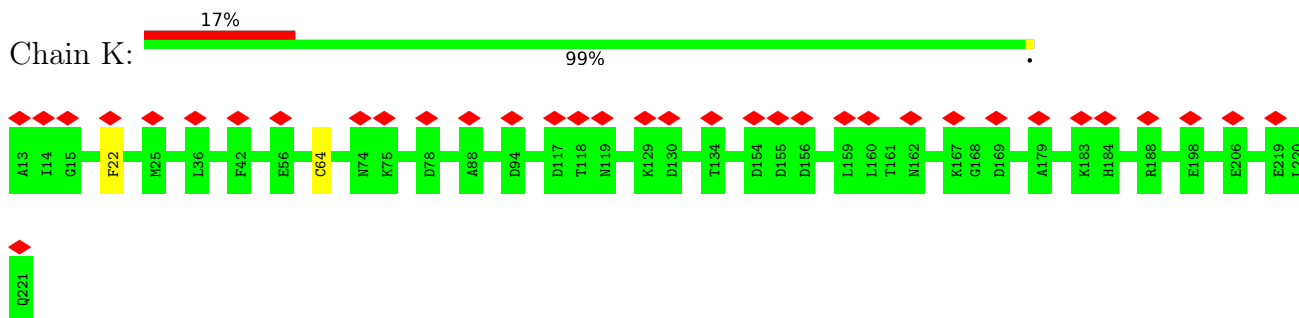
- Molecule 1: Archaeollin



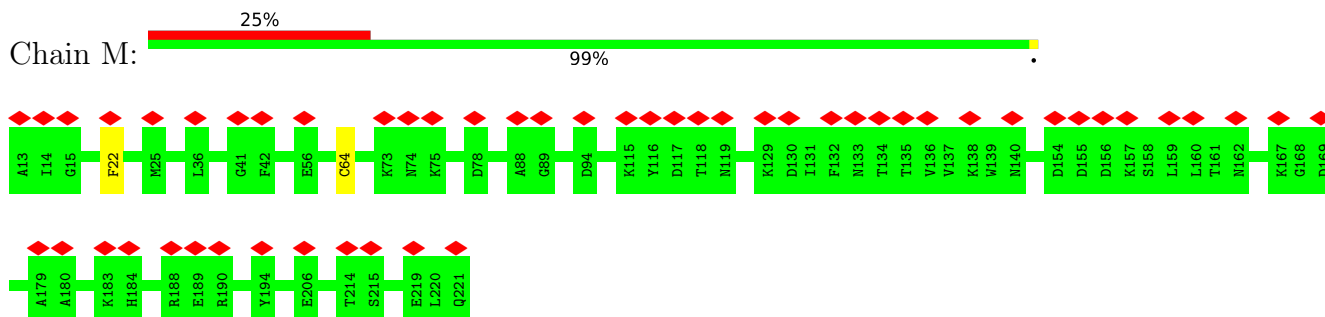
- Molecule 1: Archaeollin



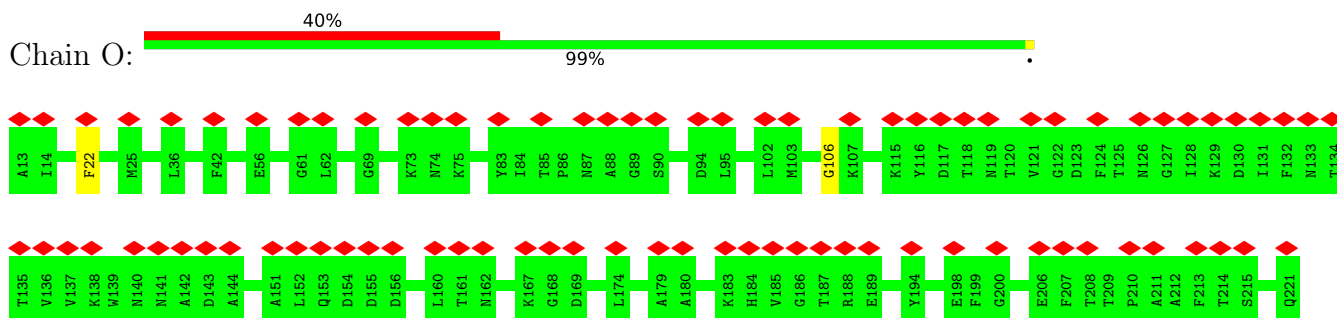
- Molecule 1: Archaeollin



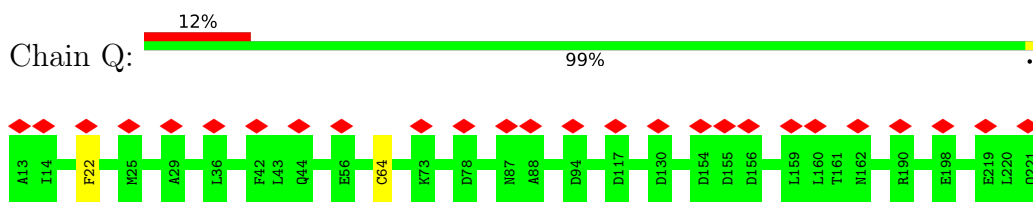
• Molecule 1: Archaeollin



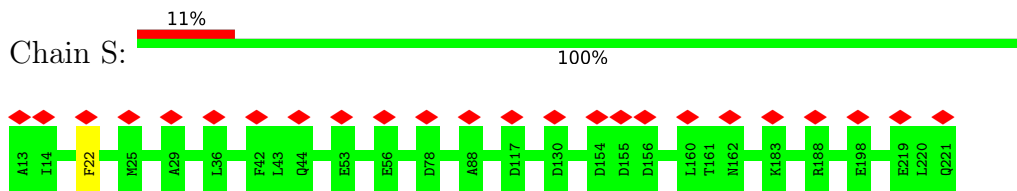
• Molecule 1: Archaeollin



• Molecule 1: Archaeollin

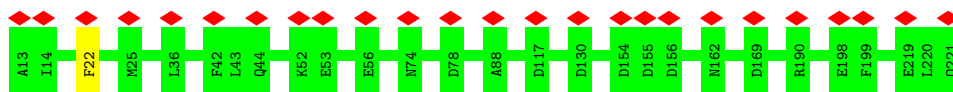


• Molecule 1: Archaeollin

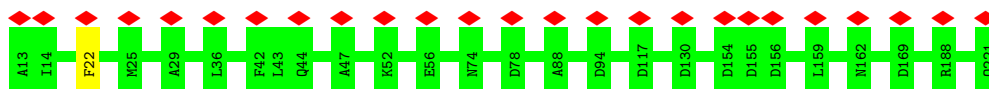


• Molecule 1: Archaeollin

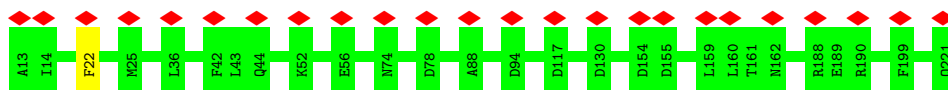




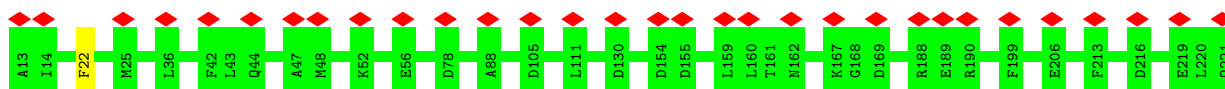
• Molecule 1: Archaeollin



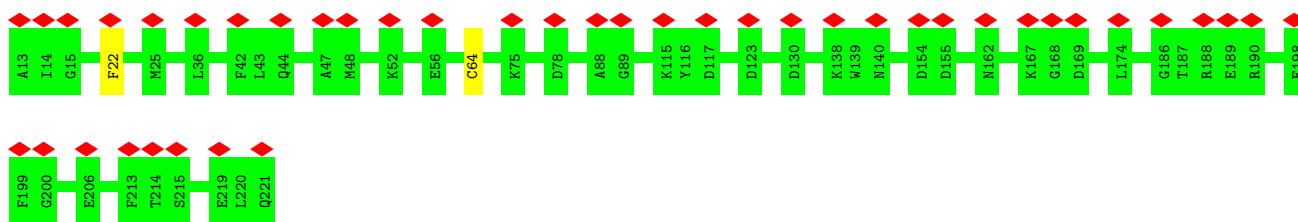
• Molecule 1: Archaeollin



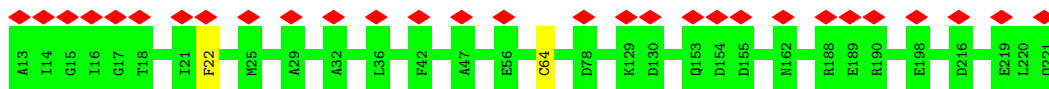
• Molecule 1: Archaeollin



• Molecule 1: Archaeollin

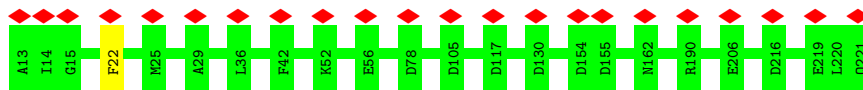


• Molecule 1: Archaeollin

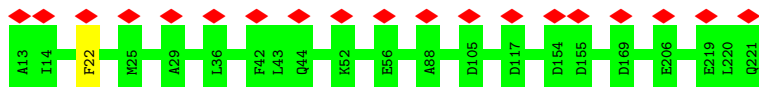


• Molecule 1: Archaeollin

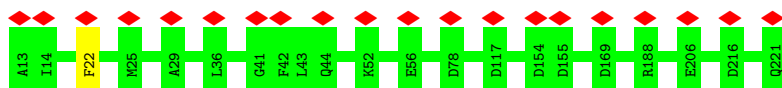




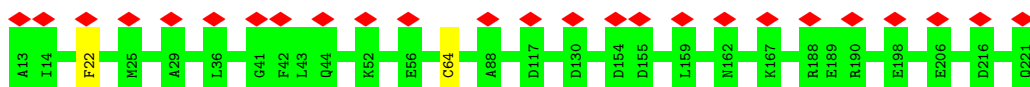
• Molecule 1: Archaeellin



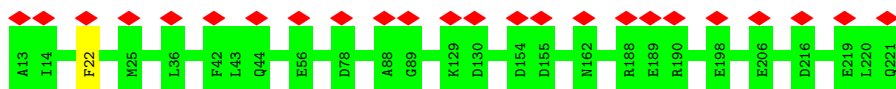
• Molecule 1: Archaeellin



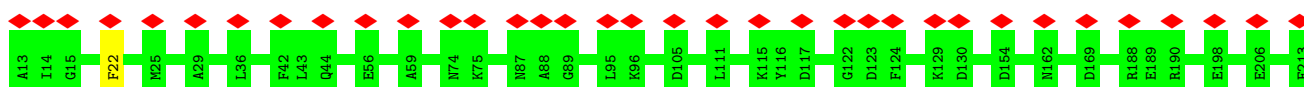
• Molecule 1: Archaeellin



• Molecule 1: Archaeellin

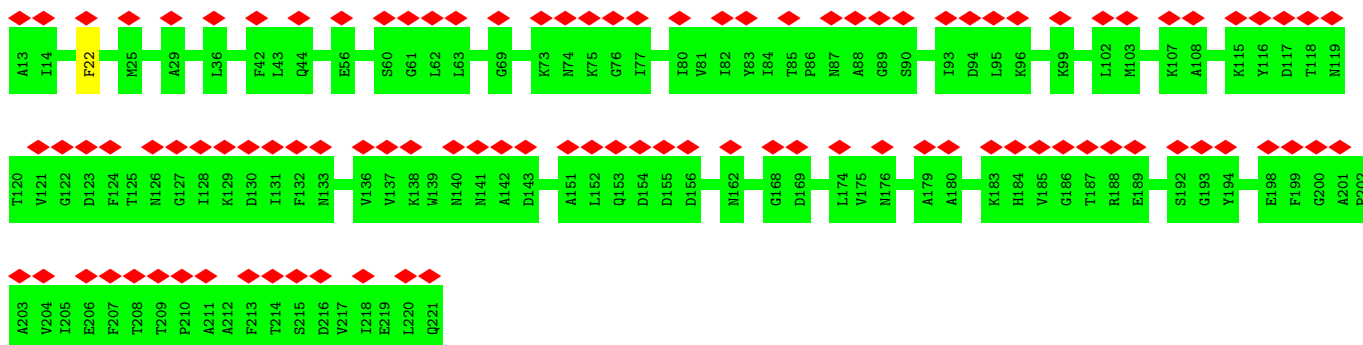


• Molecule 1: Archaeellin

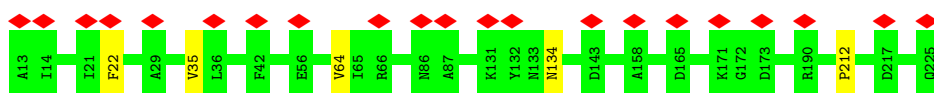


• Molecule 1: Archaeellin

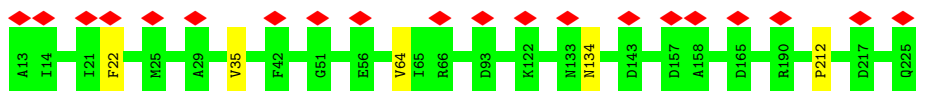




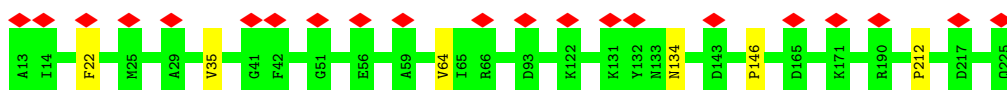
- Molecule 2: Archaelin



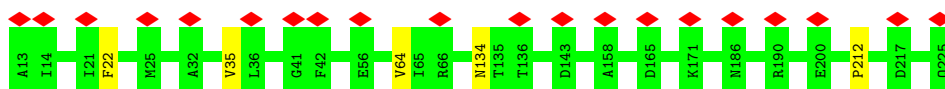
- Molecule 2: Archaelin



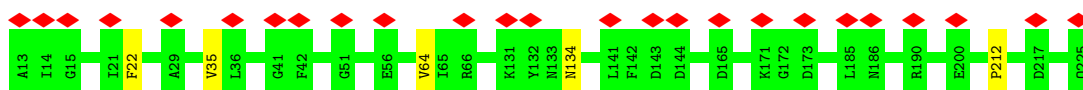
- Molecule 2: Archaelin



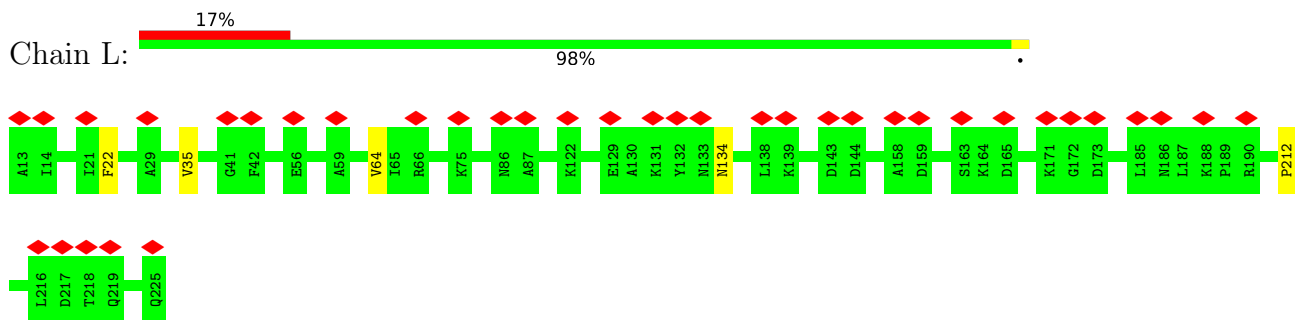
- Molecule 2: Archaelin



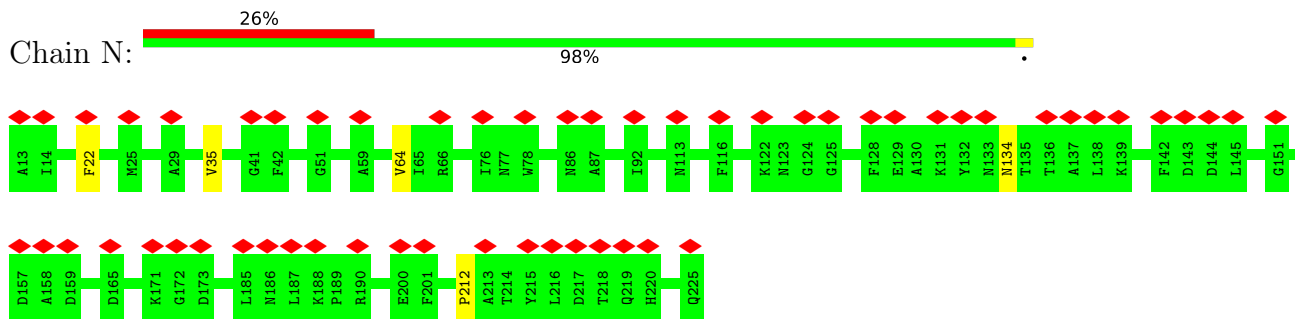
- Molecule 2: Archaelin



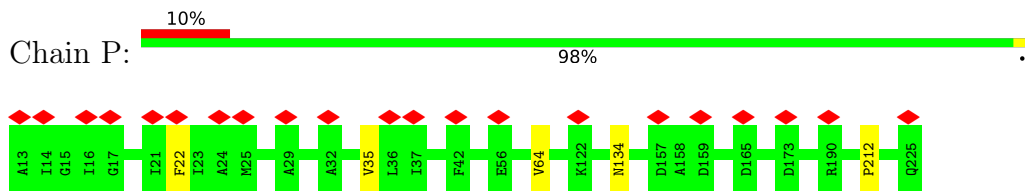
- Molecule 2: Archaelin



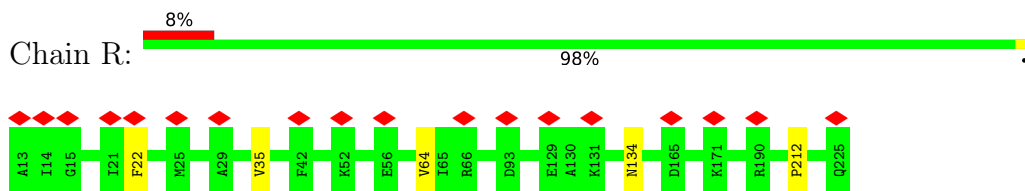
• Molecule 2: Archaeollin



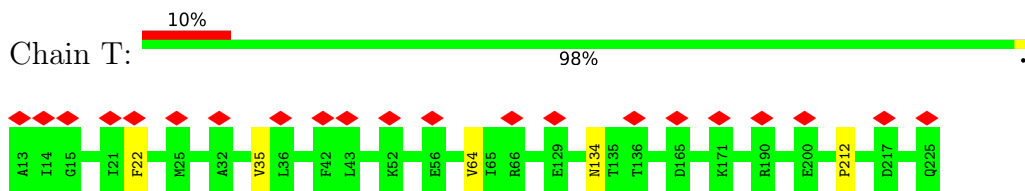
• Molecule 2: Archaeollin



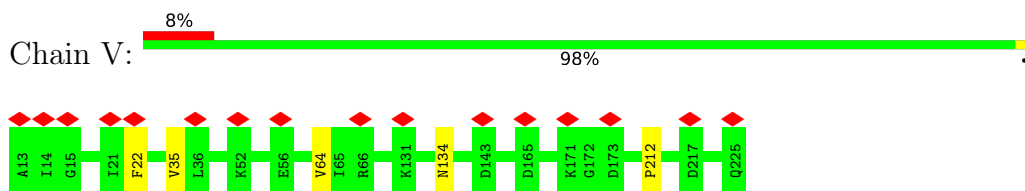
• Molecule 2: Archaeollin



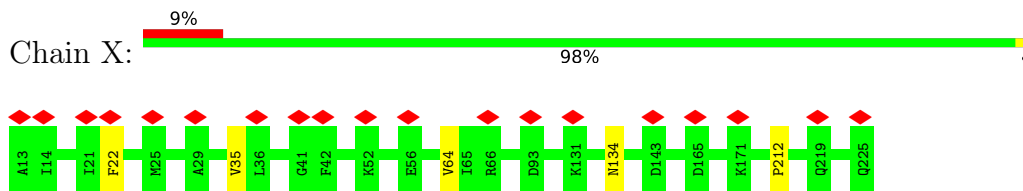
• Molecule 2: Archaeollin



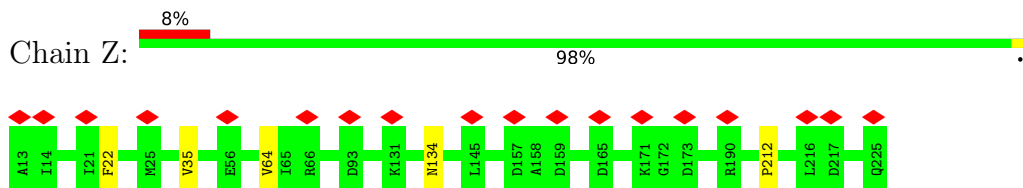
• Molecule 2: Archaeollin



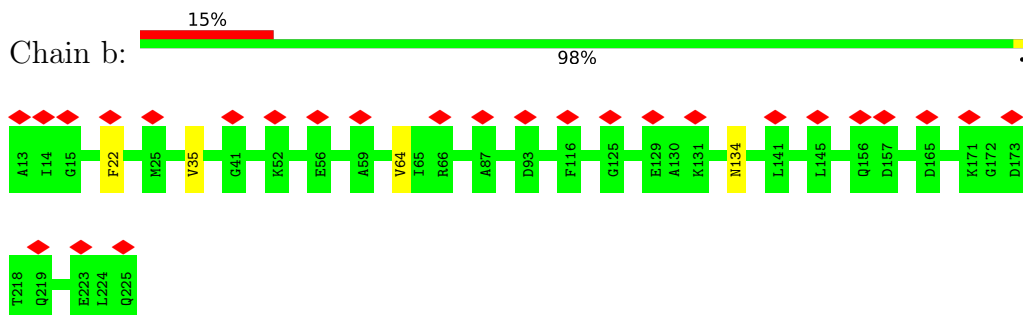
- Molecule 2: Archaeellin



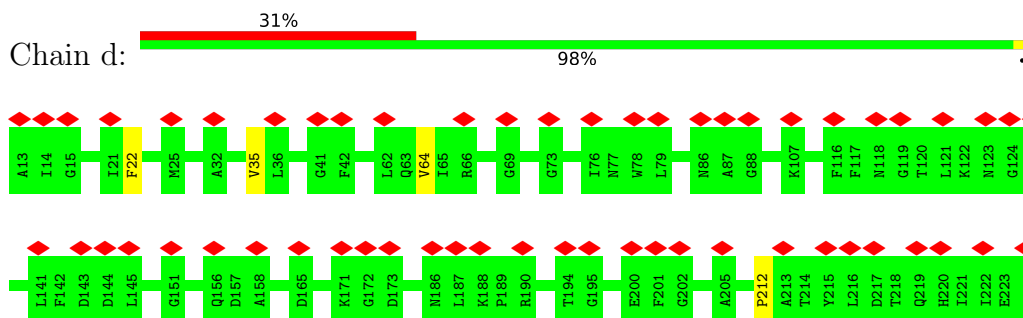
- Molecule 2: Archaeellin



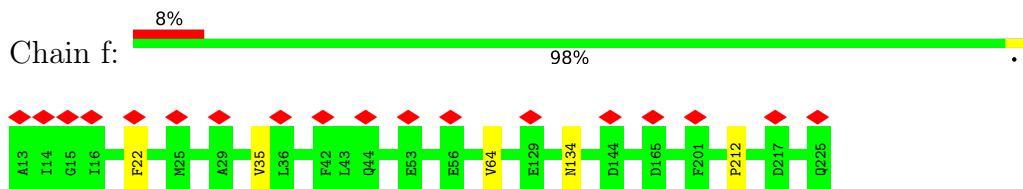
- Molecule 2: Archaeellin



- Molecule 2: Archaeellin

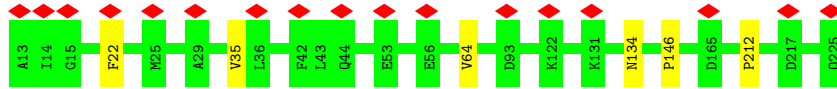


- Molecule 2: Archaeellin

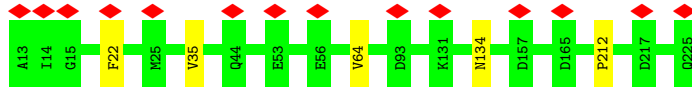


- Molecule 2: Archaeellin

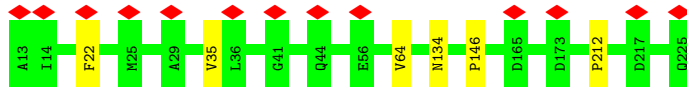




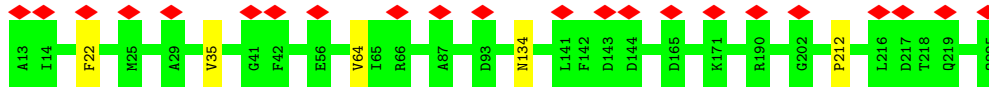
• Molecule 2: Archaeellin



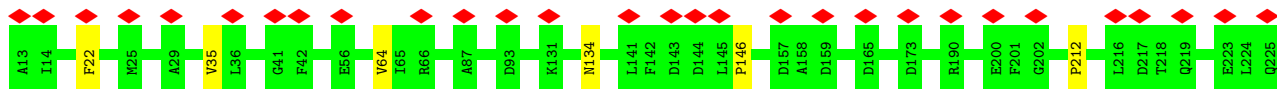
• Molecule 2: Archaeellin



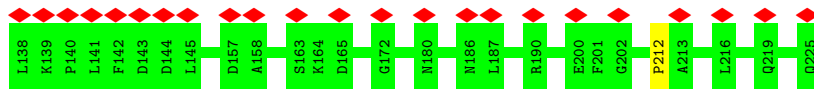
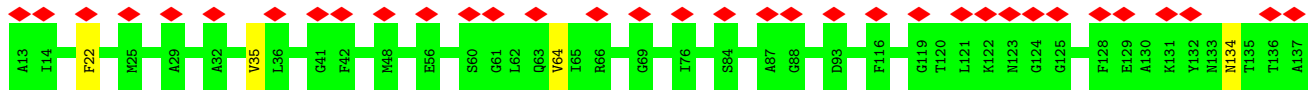
• Molecule 2: Archaeellin



• Molecule 2: Archaeellin



• Molecule 2: Archaeellin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-71.8°, rise=33.4 Å, axial sym=C1	Depositor
Number of segments used	399178	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 ($e^-/\text{Å}^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.073	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.325	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, UNL

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	0.46	0/1578	0.84	0/2144
1	C	0.47	0/1578	0.84	0/2144
1	E	0.47	0/1578	0.85	0/2144
1	G	0.47	0/1578	0.85	0/2144
1	I	0.46	0/1578	0.84	0/2144
1	K	0.47	0/1578	0.85	1/2144 (0.0%)
1	M	0.45	0/1578	0.84	1/2144 (0.0%)
1	O	0.44	0/1578	0.84	0/2144
1	Q	0.47	0/1578	0.85	1/2144 (0.0%)
1	S	0.47	0/1578	0.85	0/2144
1	U	0.47	0/1578	0.85	0/2144
1	W	0.47	0/1578	0.85	0/2144
1	Y	0.47	0/1578	0.85	0/2144
1	a	0.46	0/1578	0.85	0/2144
1	c	0.45	0/1578	0.84	1/2144 (0.0%)
1	e	0.47	0/1578	0.85	1/2144 (0.0%)
1	g	0.47	0/1578	0.85	0/2144
1	i	0.48	0/1578	0.85	0/2144
1	k	0.48	0/1578	0.85	0/2144
1	m	0.47	0/1578	0.85	1/2144 (0.0%)
1	o	0.47	0/1578	0.85	0/2144
1	q	0.45	0/1578	0.84	0/2144
1	s	0.44	0/1578	0.84	0/2144
2	B	0.49	0/1591	0.85	0/2169
2	D	0.50	0/1591	0.85	0/2169
2	F	0.49	0/1591	0.85	0/2169
2	H	0.49	0/1591	0.85	0/2169
2	J	0.49	0/1591	0.85	0/2169
2	L	0.49	0/1591	0.85	0/2169
2	N	0.46	0/1591	0.84	0/2169
2	P	0.49	0/1591	0.85	0/2169
2	R	0.48	0/1591	0.85	0/2169

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	T	0.48	0/1591	0.85	0/2169
2	V	0.48	0/1591	0.85	0/2169
2	X	0.49	0/1591	0.85	0/2169
2	Z	0.48	0/1591	0.85	0/2169
2	b	0.47	0/1591	0.85	0/2169
2	d	0.45	0/1591	0.84	0/2169
2	f	0.48	0/1591	0.85	0/2169
2	h	0.49	0/1591	0.85	0/2169
2	j	0.50	0/1591	0.86	0/2169
2	l	0.50	0/1591	0.85	0/2169
2	n	0.49	0/1591	0.85	0/2169
2	p	0.47	0/1591	0.85	0/2169
2	r	0.46	0/1591	0.84	0/2169
All	All	0.47	0/71296	0.85	6/97030 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	64	CYS	CB-CA-C	-5.06	100.28	110.40
1	c	64	CYS	CB-CA-C	-5.05	100.29	110.40
1	K	64	CYS	CB-CA-C	-5.05	100.30	110.40
1	m	64	CYS	CB-CA-C	-5.04	100.32	110.40
1	e	64	CYS	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	C	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	E	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	G	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	I	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	K	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	M	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	O	207/209 (99%)	199 (96%)	7 (3%)	1 (0%)	29	61
1	Q	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	S	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	U	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	W	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	Y	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	a	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	c	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	e	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	g	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	i	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	k	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	m	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	o	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
1	q	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
1	s	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
2	B	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	D	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	F	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	H	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	J	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	L	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	N	211/213 (99%)	198 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	R	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	T	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	V	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	X	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	Z	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	b	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	d	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	f	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	h	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	j	211/213 (99%)	199 (94%)	12 (6%)	0	100	100
2	l	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	n	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	p	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
2	r	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
All	All	9403/9493 (99%)	8933 (95%)	469 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	106	GLY

5.3.2 Protein sidechains [i](#)

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	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	C	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	E	167/167 (100%)	166 (99%)	1 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	I	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	K	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	M	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	O	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	Q	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	S	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	U	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	W	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	Y	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	a	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	c	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	e	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	g	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	i	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	k	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	m	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	o	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	q	167/167 (100%)	166 (99%)	1 (1%)	86	93
1	s	167/167 (100%)	166 (99%)	1 (1%)	86	93
2	B	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	D	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	F	171/171 (100%)	165 (96%)	6 (4%)	36	67
2	H	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	J	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	L	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	N	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	P	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	R	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	T	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	V	171/171 (100%)	166 (97%)	5 (3%)	42	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	Z	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	b	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	d	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	f	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	h	171/171 (100%)	165 (96%)	6 (4%)	36	67
2	j	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	l	171/171 (100%)	165 (96%)	6 (4%)	36	67
2	n	171/171 (100%)	166 (97%)	5 (3%)	42	70
2	p	171/171 (100%)	165 (96%)	6 (4%)	36	67
2	r	171/171 (100%)	166 (97%)	5 (3%)	42	70
All	All	7603/7603 (100%)	7466 (98%)	137 (2%)	61	80

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	l	146	PRO
2	n	35	VAL
1	q	22	PHE
2	P	212	PRO
2	P	134	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	d	183	ASN
2	j	183	ASN
2	h	183	ASN
2	l	183	ASN
2	N	183	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 849 ligands modelled in this entry, 45 are monoatomic and 804 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

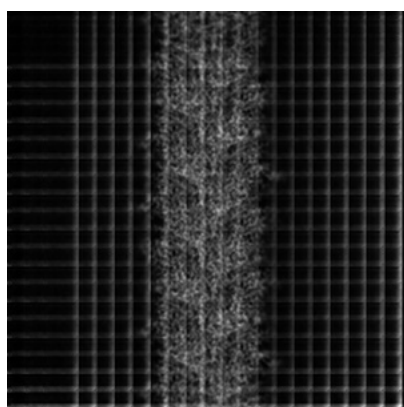
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12875. These allow visual inspection of the internal detail of the map and identification of artifacts.

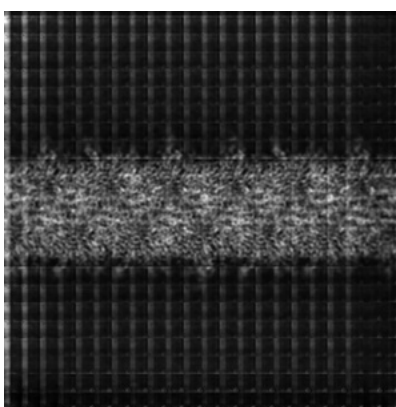
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

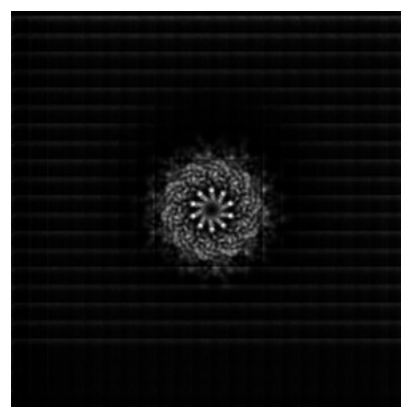
6.1.1 Primary map



X



Y

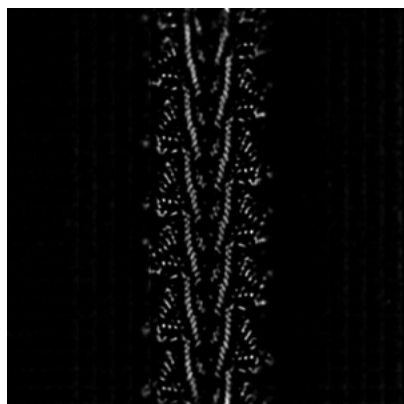


Z

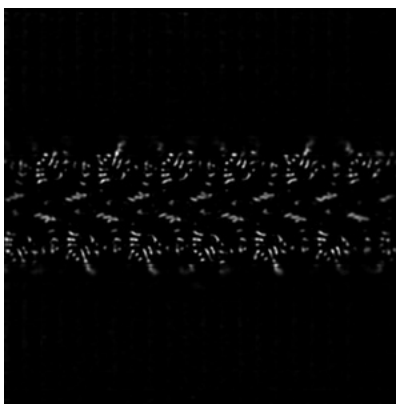
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

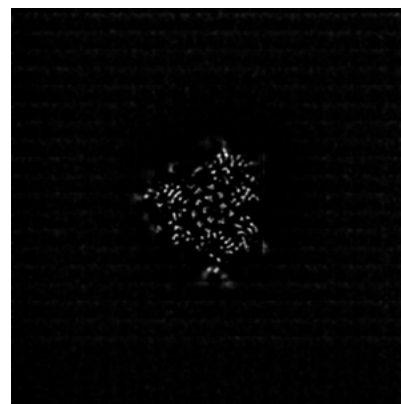
6.2.1 Primary map



X Index: 128



Y Index: 128

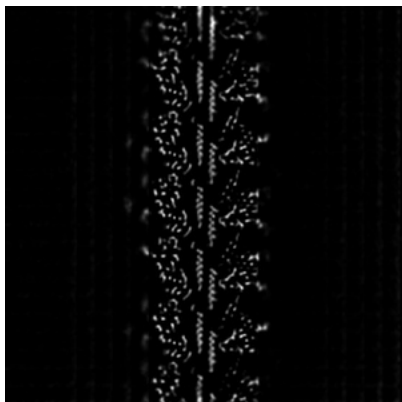


Z Index: 128

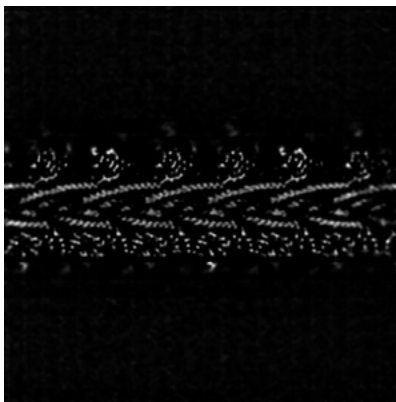
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

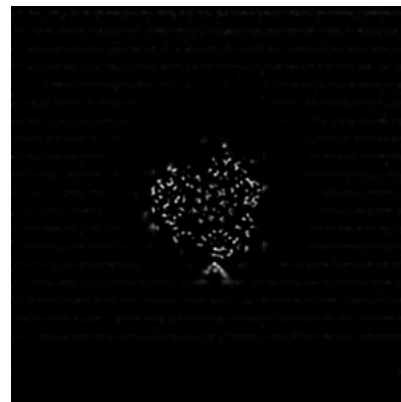
6.3.1 Primary map



X Index: 140



Y Index: 124



Z Index: 130

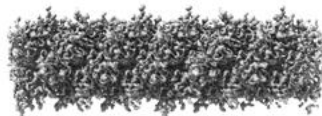
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

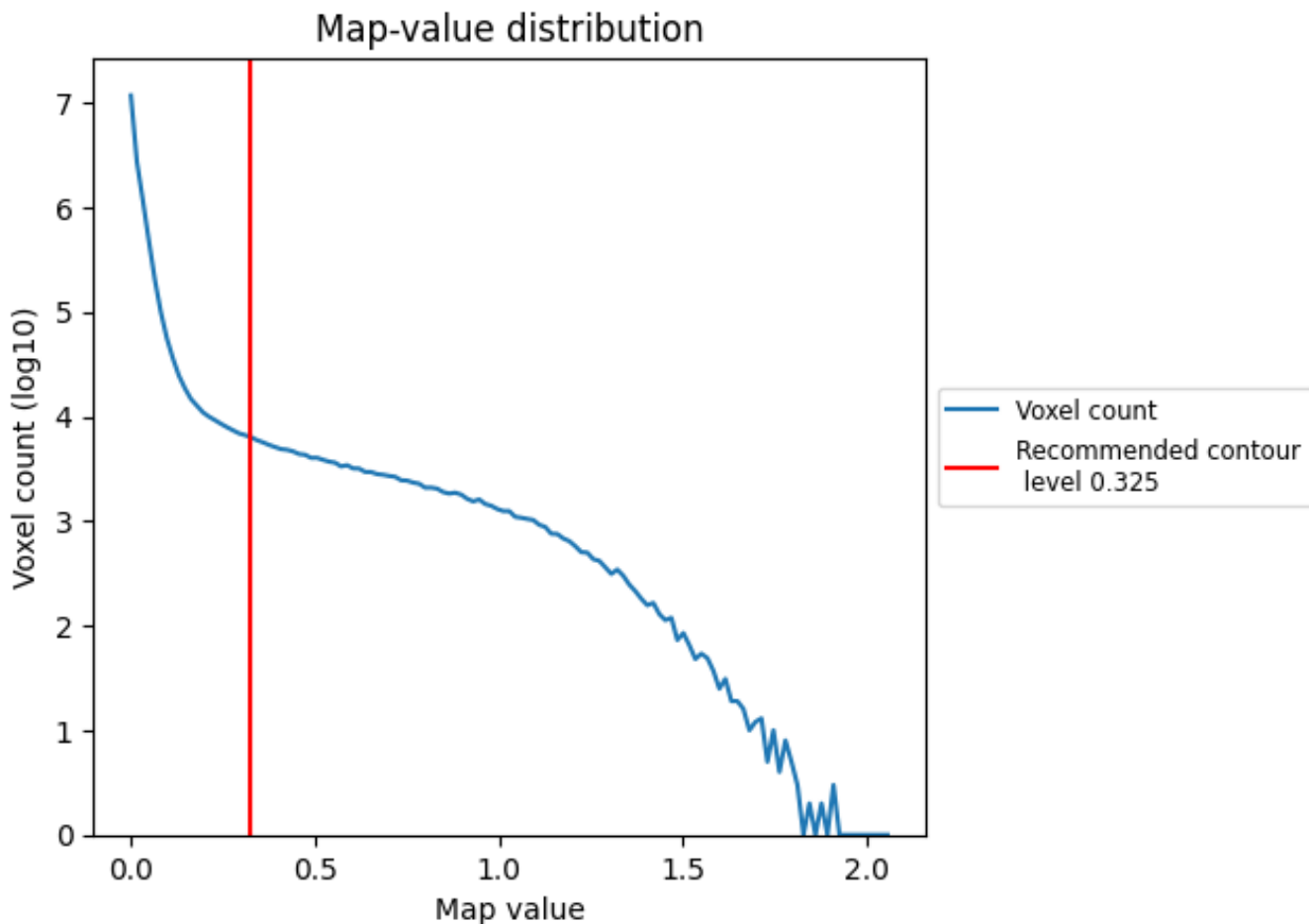
6.5 Mask visualisation

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

7 Map analysis [i](#)

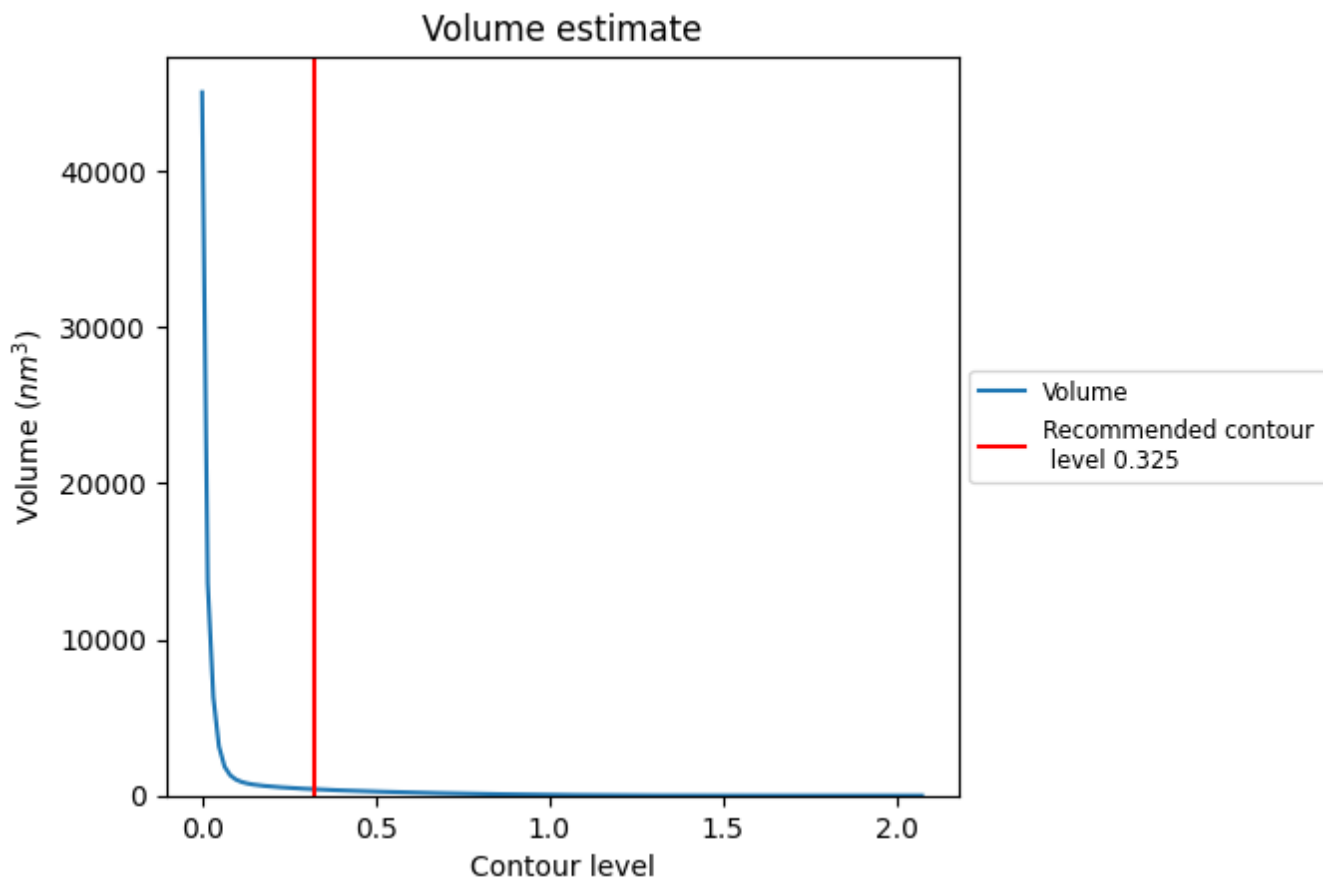
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

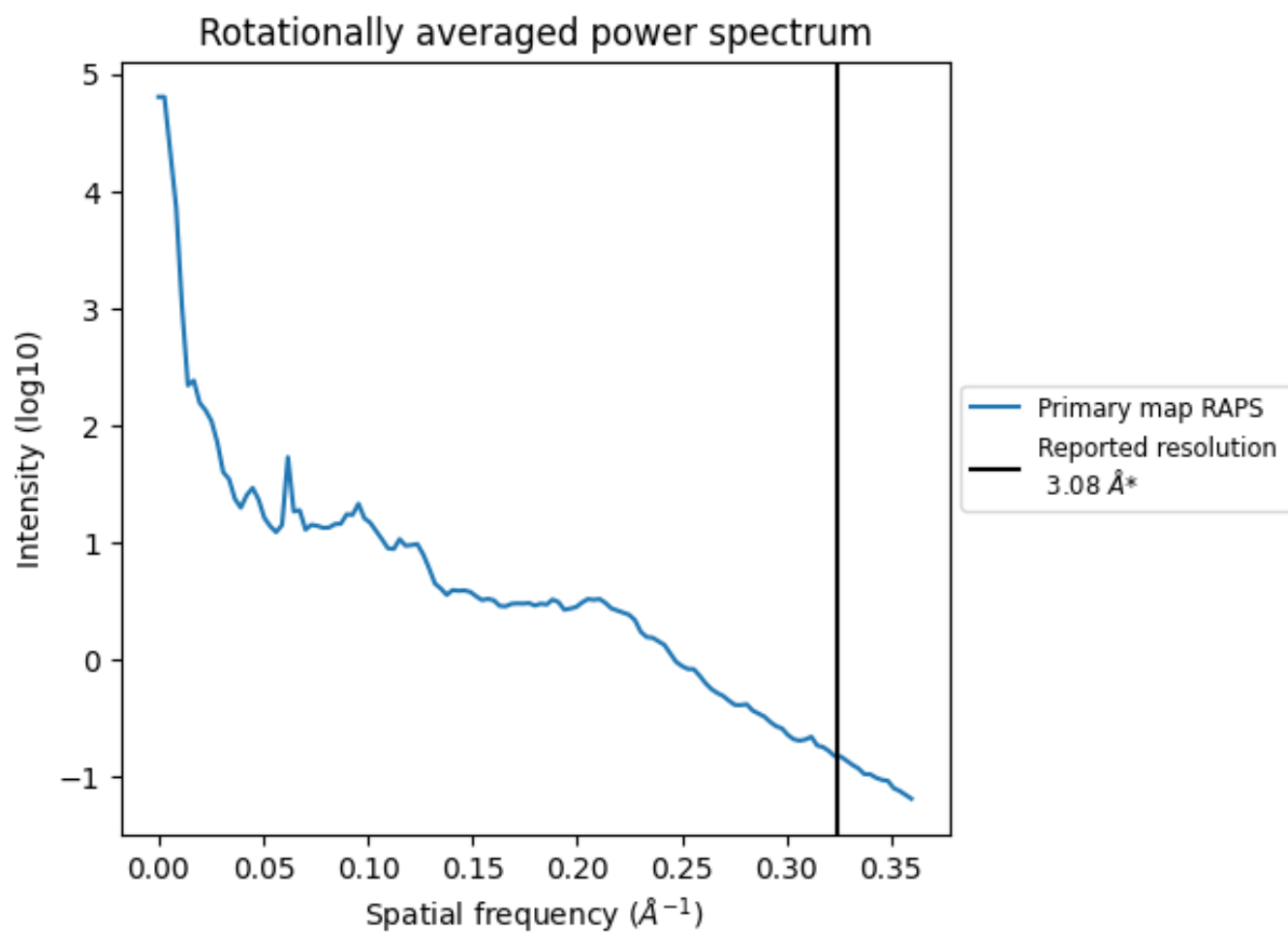
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 403 nm^3 ; this corresponds to an approximate mass of 364 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

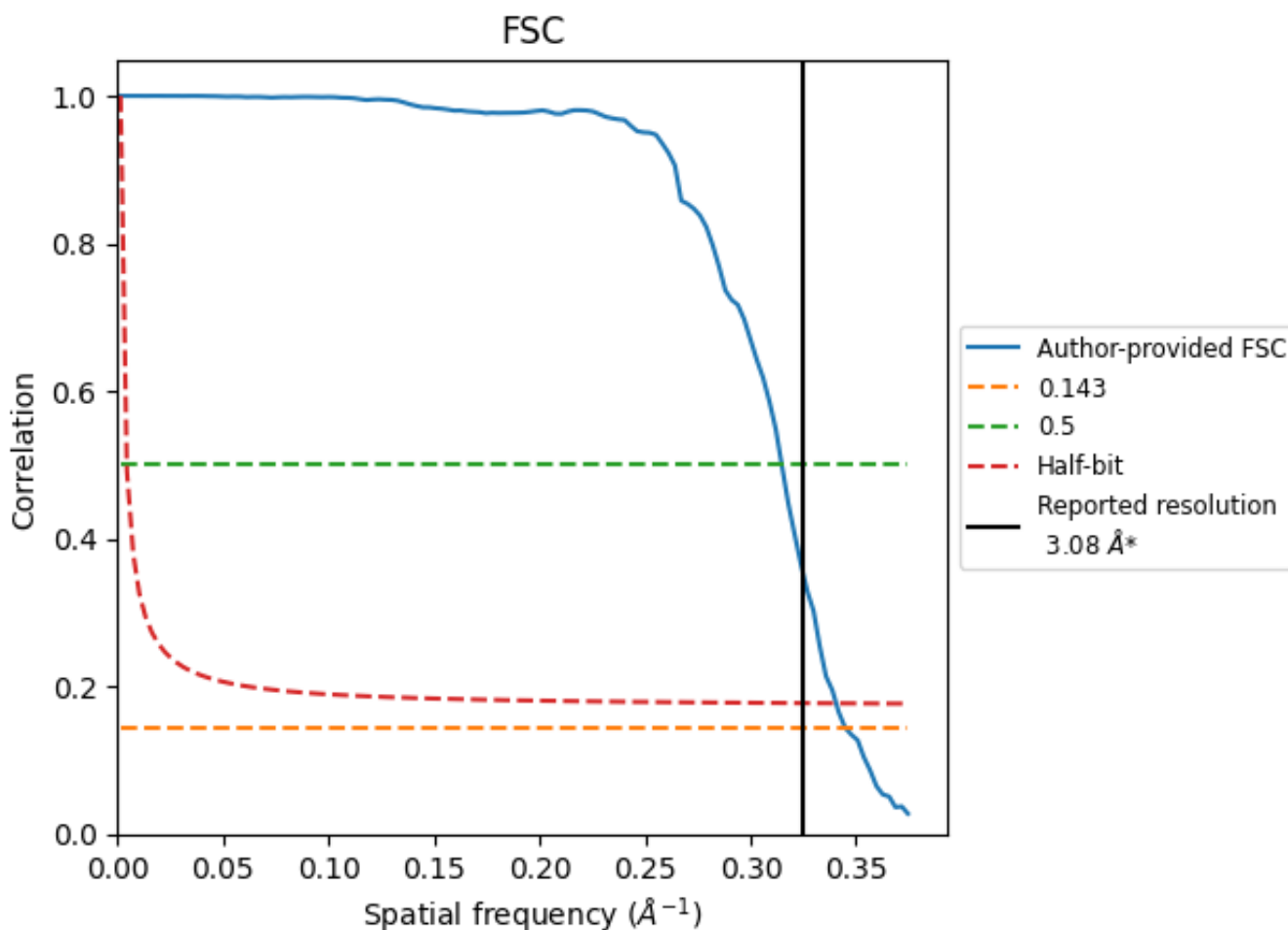


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

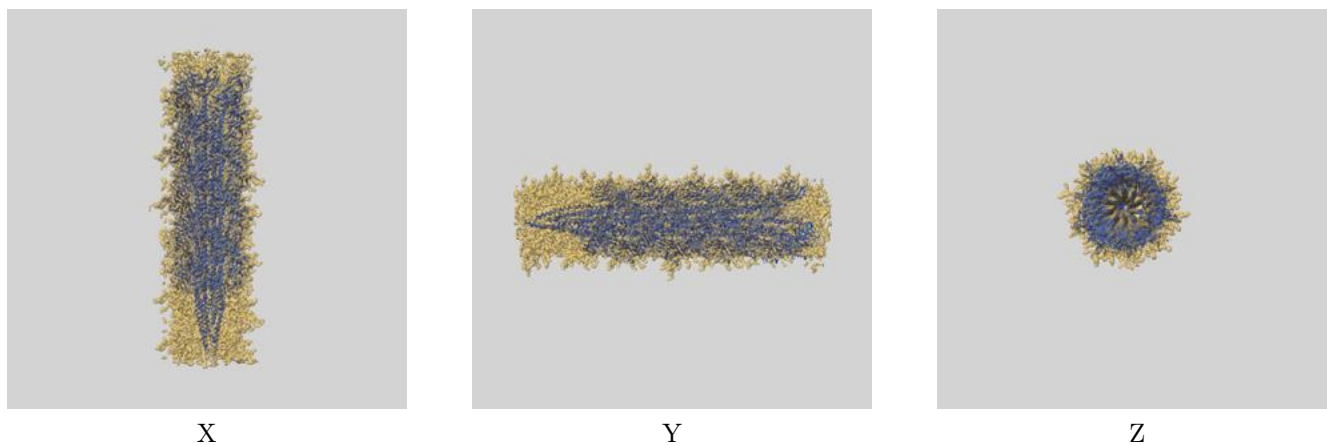
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	2.90	3.18	2.94
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

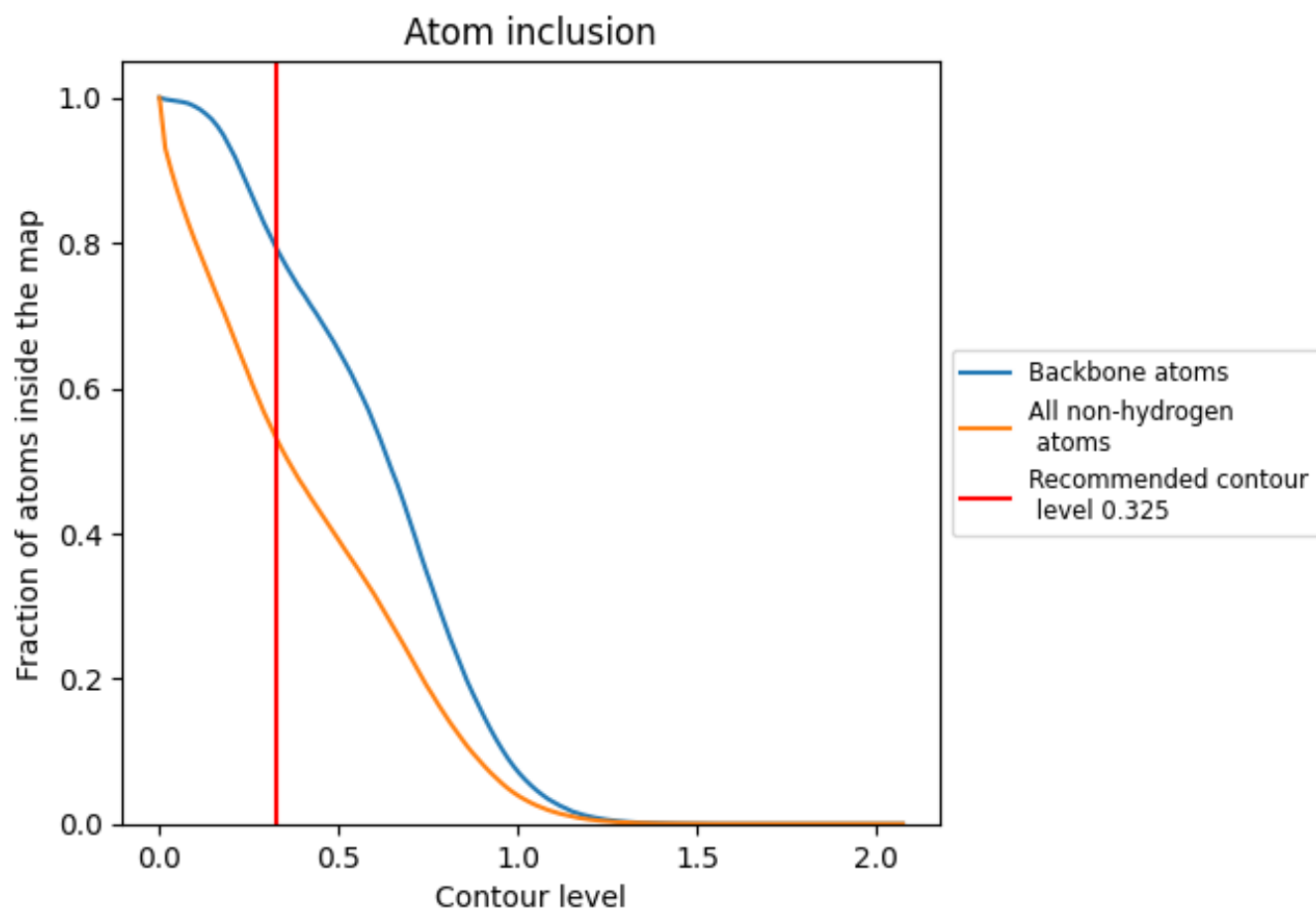
This section contains information regarding the fit between EMDB map EMD-12875 and PDB model 7OFQ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.325 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 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.