wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 10:32 PM EST

PDB ID	:	6X5I
EMDB ID	:	EMD-22051
Title	:	Cryo-EM of peptide-like filament of 1-KMe3
Authors	:	Wang, F.; Feng, Z.; Xu, B.; Egelman, E.H.
Deposited on	:	2020-05-26
Resolution	:	4.30 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 4.30 Å.

There are no overall percentile quality scores available for this entry.

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	0	5	80% 20%
1	AA	5	80% 20%
1	B	5	80% 20%
1	BA	5	80% 20%
1	CA	5	80% 20%
1	D	5	80% 20%
1	DA	5	80% 20%
1	E	5	80% 20%
1	EA	5	80% 20%
1	F	5	80% 20%
1	FA	5	80% 20%
1	G	5	80% 20%
1	GA	5	80% 20%
1	H	5	80% 20%
1	HA	5	80% 20%
1	I	5	80% 20%
1	IA	5	80% 20%
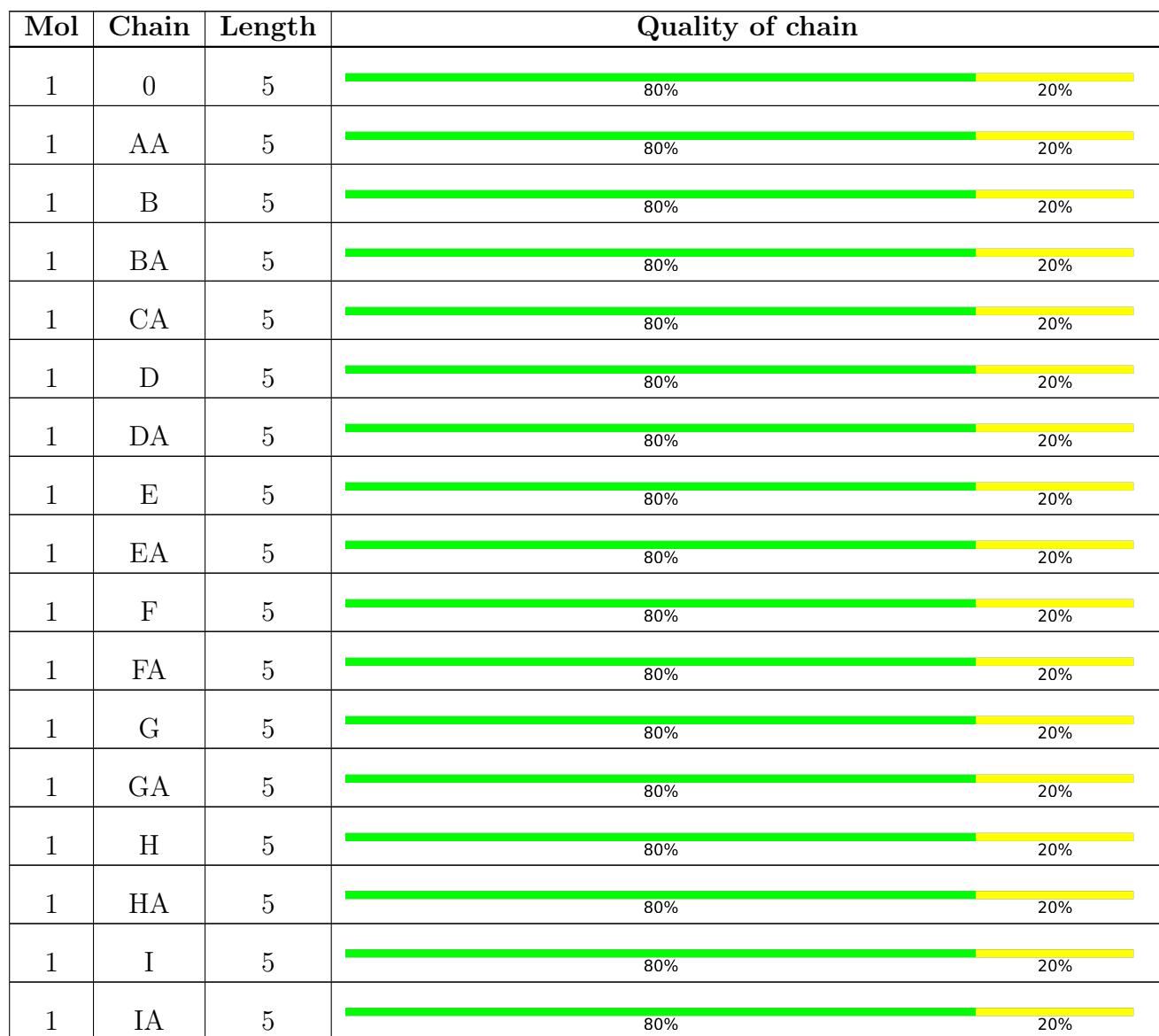
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Mol	Chain	Length	Quality of chain
1	J	5	80% 20%
1	JA	5	80% 20%
1	K	5	80% 20%
1	KA	5	80% 20%
1	L	5	80% 20%
1	LA	5	80% 20%
1	M	5	80% 20%
1	MA	5	80% 20%
1	N	5	80% 20%
1	NA	5	80% 20%
1	O	5	80% 20%
1	OA	5	80% 20%
1	P	5	80% 20%
1	PA	5	80% 20%
1	Q	5	80% 20%
1	QA	5	80% 20%
1	R	5	80% 20%
1	RA	5	80% 20%
1	S	5	80% 20%
1	SA	5	80% 20%
1	T	5	80% 20%
1	U	5	80% 20%
1	V	5	80% 20%
1	W	5	80% 20%
1	X	5	80% 20%

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Mol	Chain	Length	Quality of chain
1	Y	5	80% 20%
1	Z	5	80% 20%
1	a	5	80% 20%
1	b	5	80% 20%
1	c	5	80% 20%
1	d	5	80% 20%
1	e	5	80% 20%
1	f	5	80% 20%
1	g	5	80% 20%
1	h	5	80% 20%
1	i	5	80% 20%
1	j	5	80% 20%
1	k	5	80% 20%
1	l	5	80% 20%
1	m	5	80% 20%
1	n	5	80% 20%
1	o	5	80% 20%
1	p	5	80% 20%
1	q	5	80% 20%
1	r	5	80% 20%
1	s	5	80% 20%
1	t	5	80% 20%
1	u	5	80% 20%
1	v	5	80% 20%
1	w	5	80% 20%

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Mol	Chain	Length	Quality of chain
1	x	5	80% 20%
1	y	5	80% 20%
1	z	5	80% 20%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 8190 atoms, of which 3710 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 (with D amino acids) called 1-KMe3 peptide-like fibril.

| Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	D	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	E	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	F	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	G	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	H	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	I	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	J	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	K	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	L	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	M	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	N	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	O	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	P	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	Q	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	R	5	Total 117	C 45	H 53	N 9	O 10	0	0
1	S	5	Total 117	C 45	H 53	N 9	O 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	U	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	V	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	W	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	X	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	Y	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	Z	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	a	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	b	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	c	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	d	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	e	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	f	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	g	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	h	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	i	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	j	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	k	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	l	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	m	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	n	5	Total	C	H	N	O	0	0
			117	45	53	9	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	p	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	q	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	r	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	s	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	t	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	u	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	v	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	w	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	x	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	y	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	z	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	0	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	AA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	BA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	CA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	DA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	EA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	FA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	GA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	HA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	JA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	KA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	LA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	MA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	NA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	OA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	PA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	QA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	RA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		
1	SA	5	Total	C	H	N	O	0	0
			117	45	53	9	10		

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: 1-KMe3 peptide-like fibril

Chain B:

- Molecule 1: 1-KMe3 peptide-like fibril

Chain D:

- Molecule 1: 1-KMe3 peptide-like fibril

Chain E:

- Molecule 1: 1-KMe3 peptide-like fibril

Chain F:

- Molecule 1: 1-KMe3 peptide-like fibril

Chain G:

- Molecule 1: 1-KMe3 peptide-like fibril

Chain H:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain I:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain J:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain K:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain L:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain M:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain N:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain O:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain P:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain Q:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain R:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain S:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain T:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain U:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain V:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain W:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril
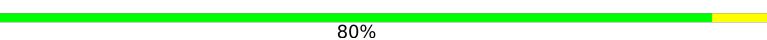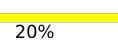
Chain X:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril
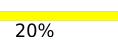
Chain Y:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril
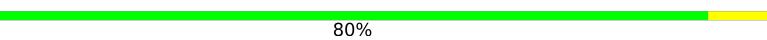
Chain Z:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril
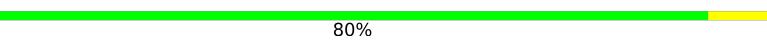
Chain a:

80%   20%
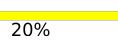
• Molecule 1: 1-KMe3 peptide-like fibril
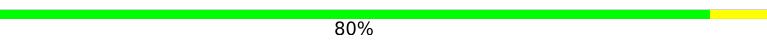
Chain b:

80%   20%
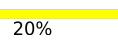
• Molecule 1: 1-KMe3 peptide-like fibril

Chain c:

80%　　　　20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain d:

80%　　　　20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain e:

80%　　　　20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain f:

80%　　　　20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain g:

80%　　　　20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain h:

80%　　　　20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain i:

80%　　　　20%

• Molecule 1: 1-KMe3 peptide-like fibril
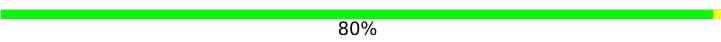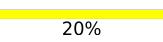
Chain j:

80% 20%

• Molecule 1: 1-KMe3 peptide-like fibril
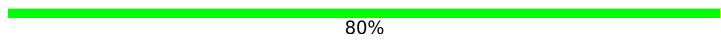
Chain k:

80% 20%

• Molecule 1: 1-KMe3 peptide-like fibril
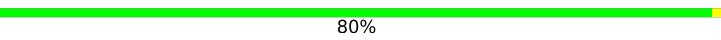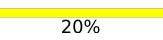
Chain l:

80% 20%

• Molecule 1: 1-KMe3 peptide-like fibril
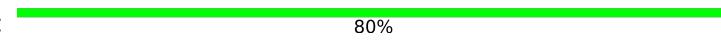
Chain m:

80% 20%

• Molecule 1: 1-KMe3 peptide-like fibril
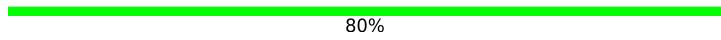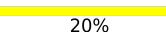
Chain n:

80% 20%

• Molecule 1: 1-KMe3 peptide-like fibril
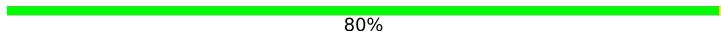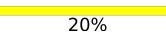
Chain o:

80% 20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain p:

80% 20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain q:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain r:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain s:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain t:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain u:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain v:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain w:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain x:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain y:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain z:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain 0:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain AA:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain BA:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain CA:

80% 20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain DA:
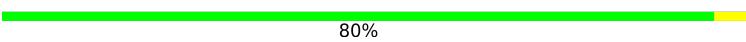
80%   20%
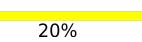
• Molecule 1: 1-KMe3 peptide-like fibril

Chain EA:

80%   20%
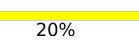
• Molecule 1: 1-KMe3 peptide-like fibril

Chain FA:

80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain GA:
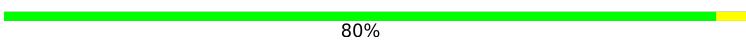
80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain HA:
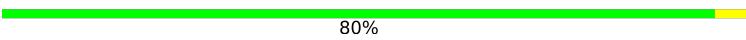
80%   20%
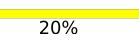
• Molecule 1: 1-KMe3 peptide-like fibril

Chain IA:
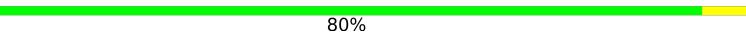
80%   20%
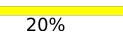
• Molecule 1: 1-KMe3 peptide-like fibril

Chain JA:
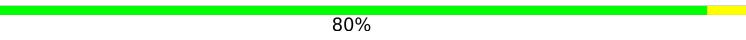
80%   20%

• Molecule 1: 1-KMe3 peptide-like fibril

Chain KA:

80%   20%

UQ41 K5
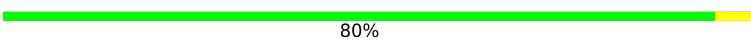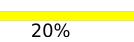
• Molecule 1: 1-KMe3 peptide-like fibril

Chain LA:

80%   20%

UQ41 K5
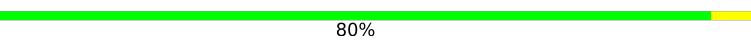
• Molecule 1: 1-KMe3 peptide-like fibril

Chain MA:

80%   20%

UQ41 K5
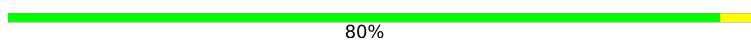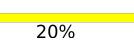
• Molecule 1: 1-KMe3 peptide-like fibril

Chain NA:

80%   20%

UQ41 K5
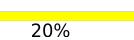
• Molecule 1: 1-KMe3 peptide-like fibril

Chain OA:

80%   20%

UQ41 K5
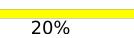
• Molecule 1: 1-KMe3 peptide-like fibril

Chain PA:

80%   20%

UQ41 K5
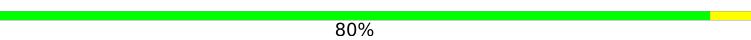
• Molecule 1: 1-KMe3 peptide-like fibril

Chain QA:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain RA:

80%   20%

UQ41 K5

• Molecule 1: 1-KMe3 peptide-like fibril

Chain SA:

80%   20%

UQ41 K5

4   Experimental information   (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=2.3°, rise=4.9 Å, axial sym=C7	Depositor
Number of segments used	108886	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.001	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.000696	Depositor
Map size (Å)	127.2, 127.2, 127.2	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: DPN, DTY, M3L, UQ4

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

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

280 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	M3L	KA	5	1	11,12,12	1.15	0	15,16,16	1.22	2 (13%)
1	M3L	QA	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	DA	5	1	11,12,12	1.16	0	15,16,16	1.23	2 (13%)
1	M3L	BA	5	1	11,12,12	1.17	0	15,16,16	1.22	2 (13%)
1	M3L	HA	5	1	11,12,12	1.16	0	15,16,16	1.18	2 (13%)
1	M3L	G	5	1	11,12,12	1.17	0	15,16,16	1.20	2 (13%)
1	M3L	U	5	1	11,12,12	1.17	0	15,16,16	1.20	2 (13%)
1	M3L	Y	5	1	11,12,12	1.17	0	15,16,16	1.21	2 (13%)
1	M3L	Q	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	m	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	v	5	1	11,12,12	1.16	0	15,16,16	1.22	2 (13%)
1	M3L	V	5	1	11,12,12	1.16	0	15,16,16	1.23	2 (13%)
1	M3L	r	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	O	5	1	11,12,12	1.15	0	15,16,16	1.23	2 (13%)
1	M3L	RA	5	1	11,12,12	1.16	0	15,16,16	1.22	2 (13%)
1	M3L	c	5	1	11,12,12	1.15	0	15,16,16	1.23	2 (13%)
1	M3L	P	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	p	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	u	5	1	11,12,12	1.16	0	15,16,16	1.18	2 (13%)
1	M3L	o	5	1	11,12,12	1.16	0	15,16,16	1.22	2 (13%)
1	M3L	t	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	LA	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	e	5	1	11,12,12	1.15	0	15,16,16	1.19	2 (13%)
1	M3L	g	5	1	11,12,12	1.16	0	15,16,16	1.18	2 (13%)
1	M3L	z	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	s	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	M3L	n	5	1	11,12,12	1.16	0	15,16,16	1.18	2 (13%)
1	M3L	D	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	S	5	1	11,12,12	1.17	0	15,16,16	1.18	2 (13%)
1	M3L	k	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	I	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	b	5	1	11,12,12	1.17	0	15,16,16	1.21	2 (13%)
1	M3L	d	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	q	5	1	11,12,12	1.15	0	15,16,16	1.23	2 (13%)
1	M3L	l	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	y	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	i	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	AA	5	1	11,12,12	1.17	0	15,16,16	1.18	2 (13%)
1	M3L	CA	5	1	11,12,12	1.17	0	15,16,16	1.21	2 (13%)
1	M3L	PA	5	1	11,12,12	1.17	0	15,16,16	1.22	2 (13%)
1	M3L	a	5	1	11,12,12	1.17	0	15,16,16	1.22	2 (13%)
1	M3L	Z	5	1	11,12,12	1.17	0	15,16,16	1.18	2 (13%)
1	M3L	f	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	H	5	1	11,12,12	1.15	0	15,16,16	1.23	2 (13%)
1	M3L	J	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	0	5	1	11,12,12	1.17	0	15,16,16	1.21	2 (13%)
1	M3L	FA	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	M	5	1	11,12,12	1.16	0	15,16,16	1.22	2 (13%)
1	M3L	NA	5	1	11,12,12	1.17	0	15,16,16	1.21	2 (13%)
1	M3L	GA	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	w	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	MA	5	1	11,12,12	1.15	0	15,16,16	1.19	2 (13%)
1	M3L	F	5	1	11,12,12	1.16	0	15,16,16	1.22	2 (13%)
1	M3L	SA	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	T	5	1	11,12,12	1.17	0	15,16,16	1.22	2 (13%)
1	M3L	j	5	1	11,12,12	1.15	0	15,16,16	1.23	2 (13%)
1	M3L	E	5	1	11,12,12	1.17	0	15,16,16	1.18	2 (13%)
1	M3L	L	5	1	11,12,12	1.16	0	15,16,16	1.18	2 (13%)
1	M3L	OA	5	1	11,12,12	1.18	0	15,16,16	1.18	2 (13%)
1	M3L	B	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	JA	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	M3L	X	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	h	5	1	11,12,12	1.16	0	15,16,16	1.22	2 (13%)
1	M3L	K	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)
1	M3L	x	5	1	11,12,12	1.15	0	15,16,16	1.23	2 (13%)
1	M3L	R	5	1	11,12,12	1.17	0	15,16,16	1.21	2 (13%)
1	M3L	EA	5	1	11,12,12	1.16	0	15,16,16	1.21	2 (13%)
1	M3L	IA	5	1	11,12,12	1.17	0	15,16,16	1.22	2 (13%)
1	M3L	N	5	1	11,12,12	1.17	0	15,16,16	1.21	2 (13%)
1	M3L	W	5	1	11,12,12	1.16	0	15,16,16	1.20	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M3L	KA	5	1	-	5/12/12/12	-
1	M3L	QA	5	1	-	5/12/12/12	-
1	M3L	DA	5	1	-	5/12/12/12	-
1	M3L	BA	5	1	-	5/12/12/12	-
1	M3L	HA	5	1	-	5/12/12/12	-
1	M3L	G	5	1	-	5/12/12/12	-
1	M3L	U	5	1	-	5/12/12/12	-
1	M3L	Y	5	1	-	5/12/12/12	-
1	M3L	Q	5	1	-	5/12/12/12	-
1	M3L	m	5	1	-	5/12/12/12	-
1	M3L	v	5	1	-	5/12/12/12	-
1	M3L	V	5	1	-	5/12/12/12	-
1	M3L	r	5	1	-	5/12/12/12	-
1	M3L	O	5	1	-	5/12/12/12	-
1	M3L	RA	5	1	-	5/12/12/12	-
1	M3L	c	5	1	-	5/12/12/12	-
1	M3L	P	5	1	-	5/12/12/12	-
1	M3L	p	5	1	-	5/12/12/12	-
1	M3L	u	5	1	-	5/12/12/12	-
1	M3L	o	5	1	-	5/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M3L	t	5	1	-	5/12/12/12	-
1	M3L	LA	5	1	-	5/12/12/12	-
1	M3L	e	5	1	-	5/12/12/12	-
1	M3L	g	5	1	-	5/12/12/12	-
1	M3L	z	5	1	-	5/12/12/12	-
1	M3L	s	5	1	-	5/12/12/12	-
1	M3L	n	5	1	-	5/12/12/12	-
1	M3L	D	5	1	-	5/12/12/12	-
1	M3L	S	5	1	-	5/12/12/12	-
1	M3L	k	5	1	-	5/12/12/12	-
1	M3L	I	5	1	-	5/12/12/12	-
1	M3L	b	5	1	-	5/12/12/12	-
1	M3L	d	5	1	-	5/12/12/12	-
1	M3L	q	5	1	-	5/12/12/12	-
1	M3L	l	5	1	-	5/12/12/12	-
1	M3L	y	5	1	-	5/12/12/12	-
1	M3L	i	5	1	-	5/12/12/12	-
1	M3L	AA	5	1	-	5/12/12/12	-
1	M3L	CA	5	1	-	5/12/12/12	-
1	M3L	PA	5	1	-	5/12/12/12	-
1	M3L	a	5	1	-	5/12/12/12	-
1	M3L	Z	5	1	-	5/12/12/12	-
1	M3L	f	5	1	-	5/12/12/12	-
1	M3L	H	5	1	-	5/12/12/12	-
1	M3L	J	5	1	-	5/12/12/12	-
1	M3L	0	5	1	-	5/12/12/12	-
1	M3L	FA	5	1	-	5/12/12/12	-
1	M3L	M	5	1	-	5/12/12/12	-
1	M3L	NA	5	1	-	5/12/12/12	-
1	M3L	GA	5	1	-	5/12/12/12	-
1	M3L	w	5	1	-	5/12/12/12	-
1	M3L	MA	5	1	-	5/12/12/12	-
1	M3L	F	5	1	-	5/12/12/12	-
1	M3L	SA	5	1	-	5/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	M3L	T	5	1	-	5/12/12/12	-
1	M3L	j	5	1	-	5/12/12/12	-
1	M3L	E	5	1	-	5/12/12/12	-
1	M3L	L	5	1	-	5/12/12/12	-
1	M3L	OA	5	1	-	5/12/12/12	-
1	M3L	B	5	1	-	5/12/12/12	-
1	M3L	JA	5	1	-	5/12/12/12	-
1	M3L	X	5	1	-	5/12/12/12	-
1	M3L	h	5	1	-	5/12/12/12	-
1	M3L	K	5	1	-	5/12/12/12	-
1	M3L	x	5	1	-	5/12/12/12	-
1	M3L	R	5	1	-	5/12/12/12	-
1	M3L	EA	5	1	-	5/12/12/12	-
1	M3L	IA	5	1	-	5/12/12/12	-
1	M3L	N	5	1	-	5/12/12/12	-
1	M3L	W	5	1	-	5/12/12/12	-

There are no bond length outliers.

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	5	M3L	CB-CA-C	-2.77	103.71	110.30
1	m	5	M3L	CB-CA-C	-2.77	103.71	110.30
1	Y	5	M3L	CB-CA-C	-2.77	103.71	110.30
1	t	5	M3L	CB-CA-C	-2.76	103.73	110.30
1	f	5	M3L	CB-CA-C	-2.76	103.73	110.30

There are no chirality outliers.

5 of 350 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	5	M3L	N-CA-CB-CG
1	B	5	M3L	C-CA-CB-CG
1	B	5	M3L	O-C-CA-N
1	D	5	M3L	N-CA-CB-CG
1	D	5	M3L	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides 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 ⓘ

This section contains visualisations of the EMDB entry EMD-22051. 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 ⓘ

6.1.1   Primary map

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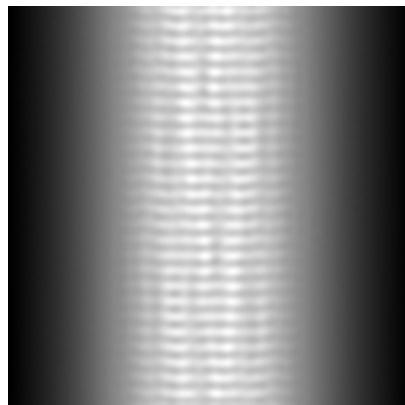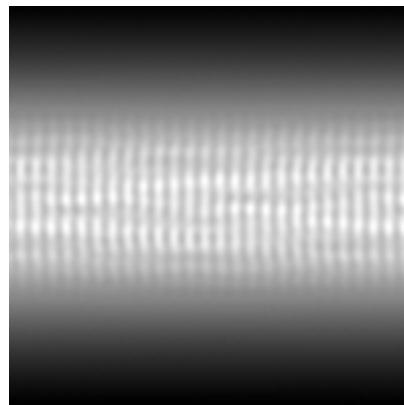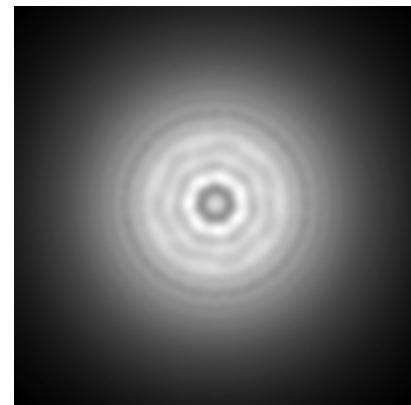
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
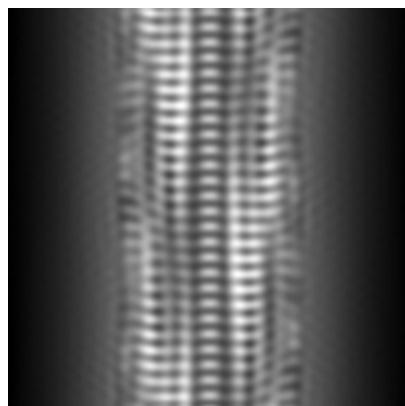
6.2.1   Primary map
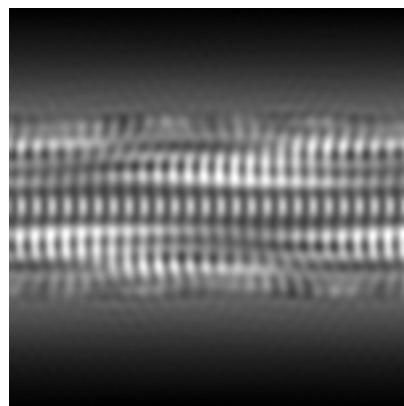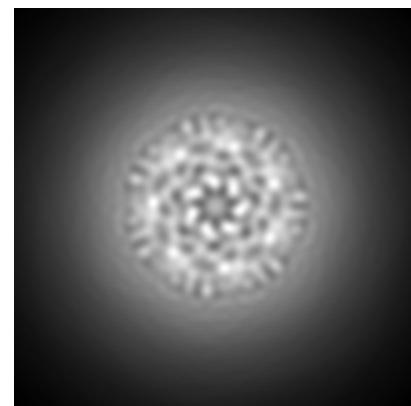
X Index: 60   Y Index: 60   Z Index: 60

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

6.3   Largest variance slices ⓘ
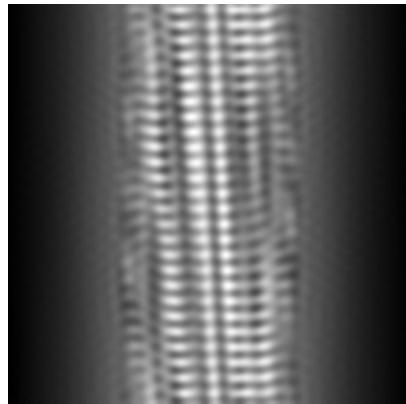
6.3.1   Primary map
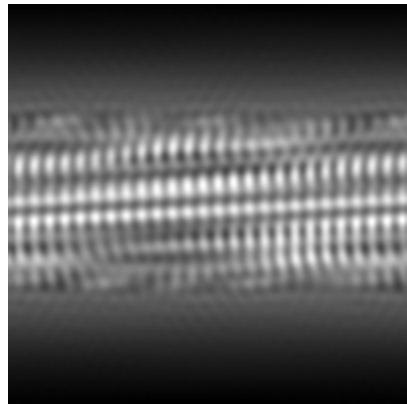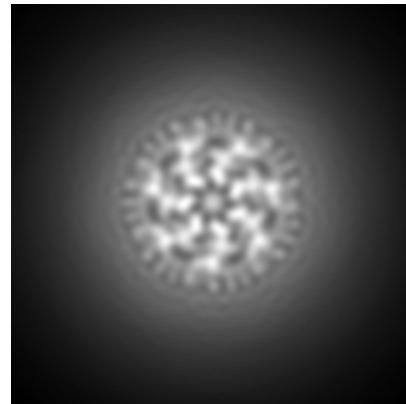
X Index: 53	Y Index: 53	Z Index: 17

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

6.4   Orthogonal surface views ⓘ
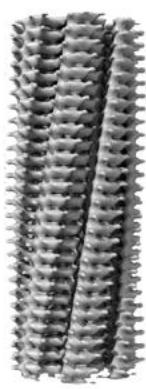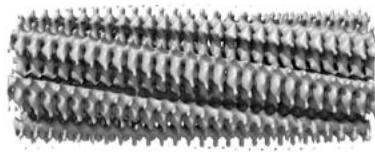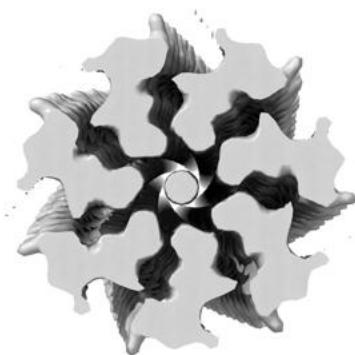
6.4.1   Primary map

X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.000696. 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 ⓘ

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

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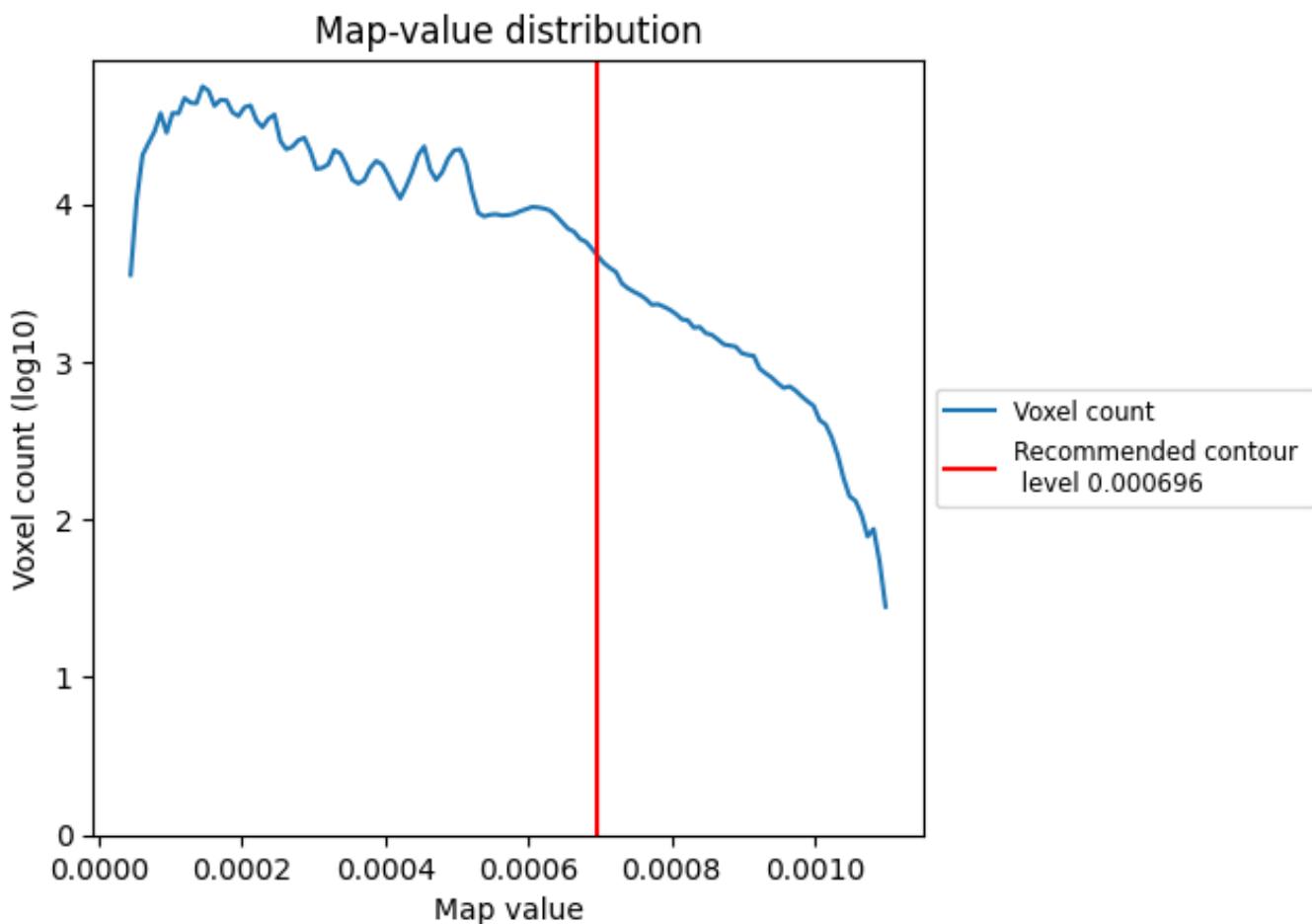
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
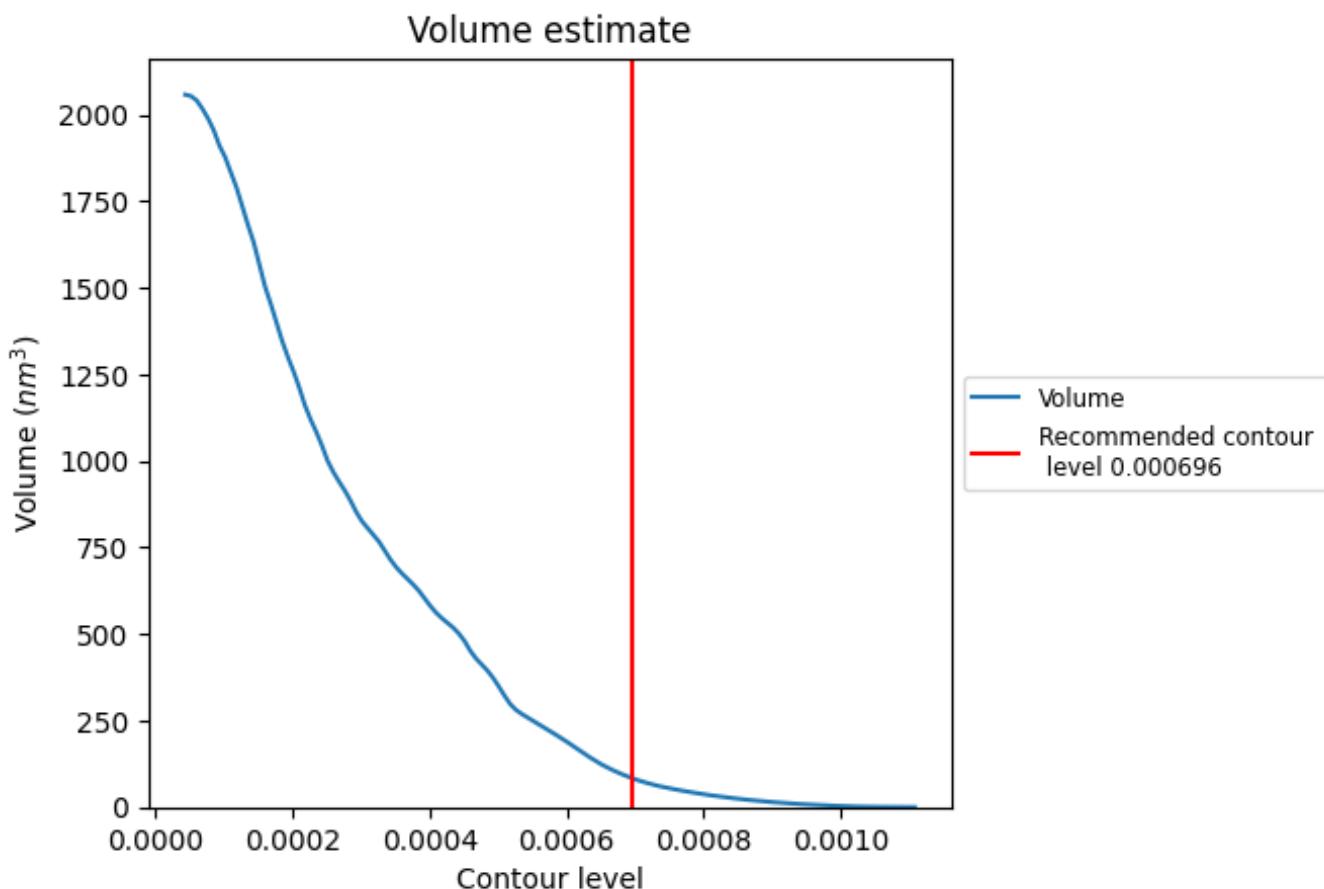
Volume estimate

The volume at the recommended contour level is 83 nm^3; this corresponds to an approximate mass of 75 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 ⓘ
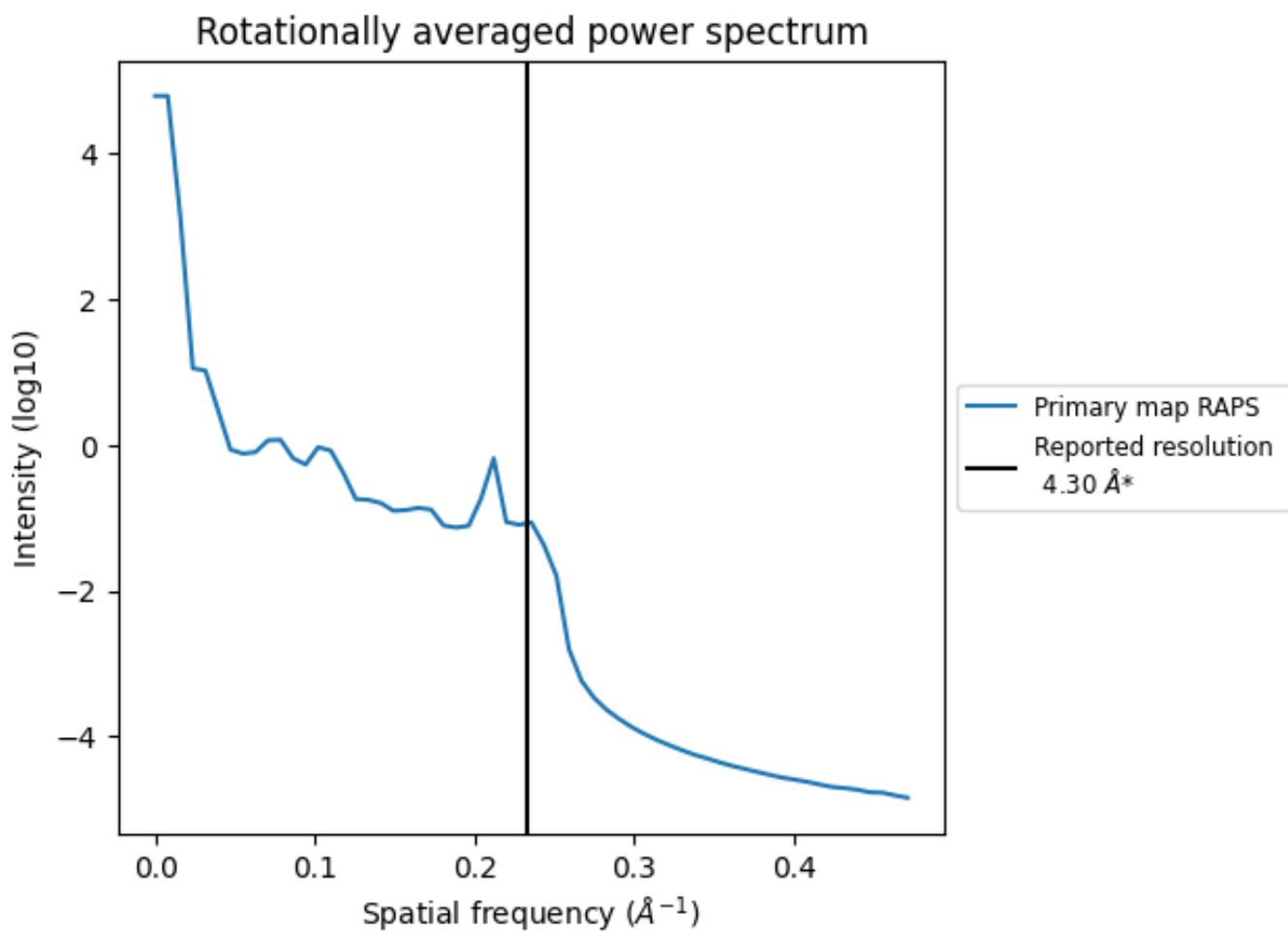
*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8 Fourier-Shell correlation (i)

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-22051 and PDB model 6X5I. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay ⓘ
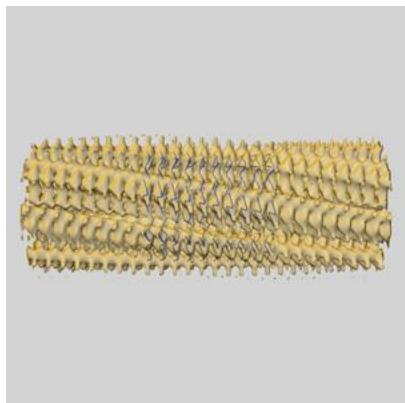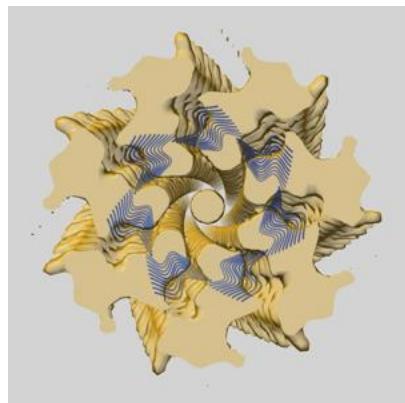
X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.000696 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   ⓘ
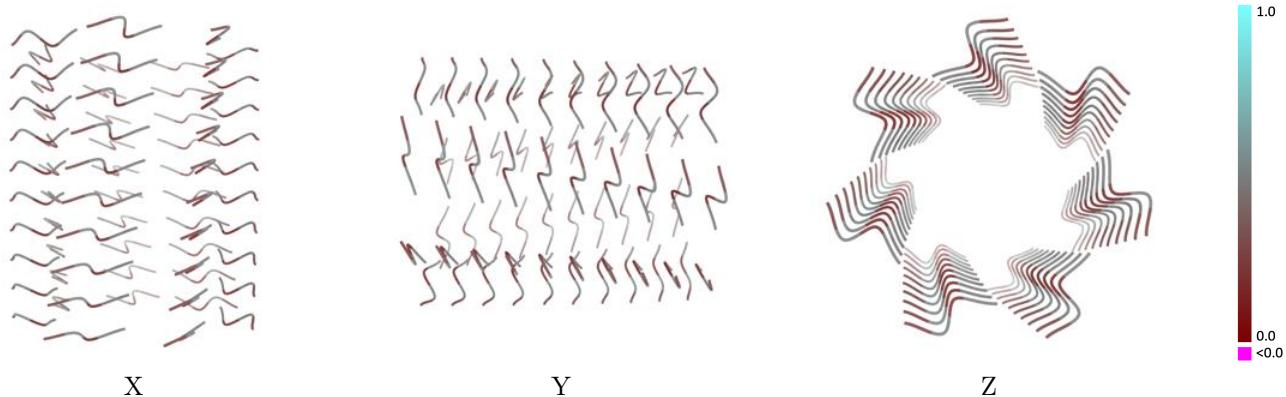
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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   ⓘ
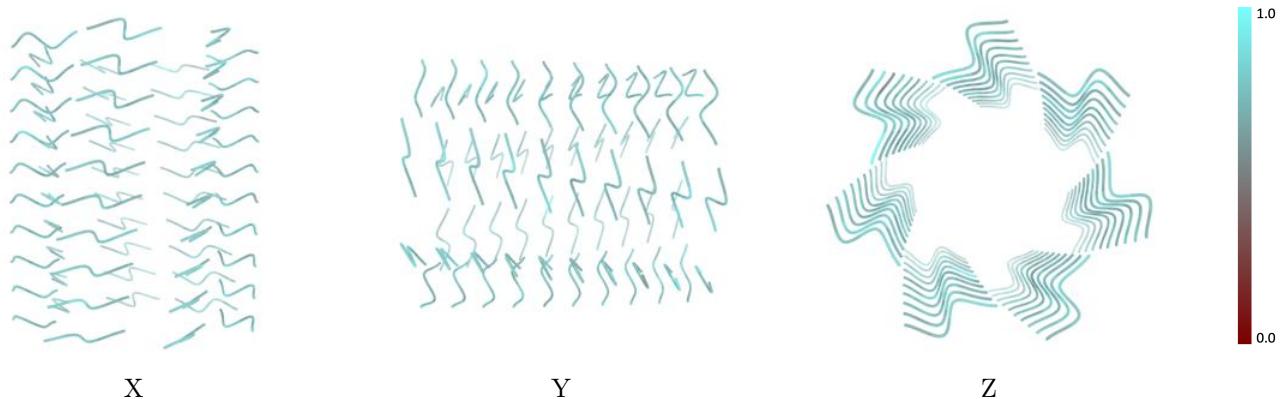
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.000696).

9.4 Atom inclusion ⓘ
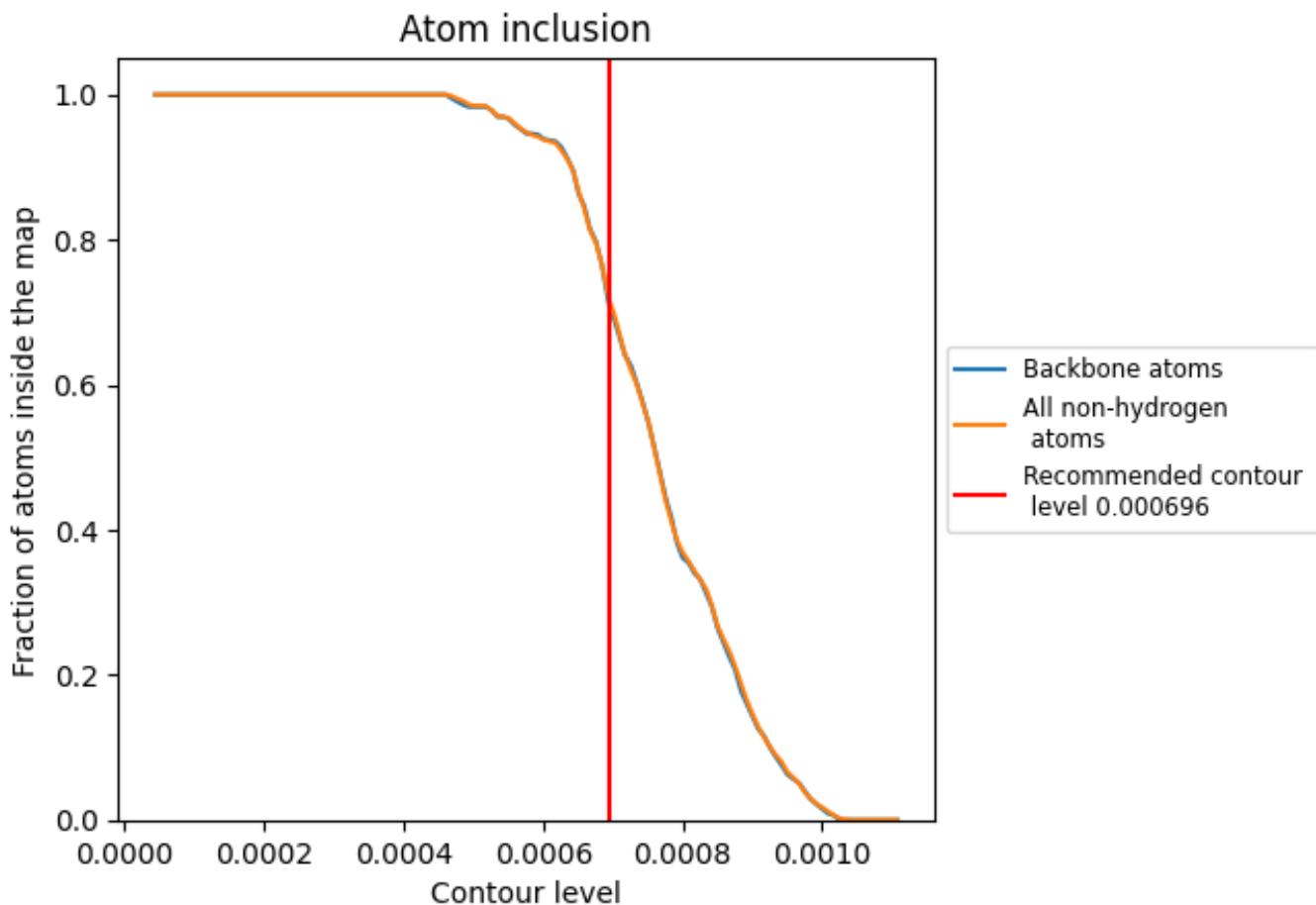
At the recommended contour level, 70% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.000696) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7125	0.3400
0	0.7302	0.3380
AA	0.7302	0.3400
B	0.7302	0.3420
BA	0.7143	0.3420
CA	0.7302	0.3270
D	0.7143	0.3410
DA	0.7619	0.3300
E	0.7302	0.3380
EA	0.7460	0.3380
F	0.7143	0.3340
FA	0.7302	0.3400
G	0.7302	0.3410
GA	0.7143	0.3410
H	0.7460	0.3220
HA	0.7302	0.3410
I	0.7143	0.3370
IA	0.6984	0.3320
J	0.7302	0.3460
JA	0.7143	0.3370
K	0.7302	0.3450
KA	0.7460	0.3370
L	0.7460	0.3430
LA	0.7143	0.3370
M	0.7143	0.3360
MA	0.7302	0.3500
N	0.7460	0.3470
NA	0.6984	0.3440
O	0.7460	0.3410
OA	0.7143	0.3500
P	0.7302	0.3370
PA	0.7143	0.3430
Q	0.7302	0.3410
QA	0.7143	0.3400
R	0.7143	0.3460

1.0

0.0
<0.0

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Chain	Atom inclusion	Q-score
RA	0.7143	0.3420
S	0.7143	0.3440
SA	0.7460	0.3500
T	0.7302	0.3370
U	0.7302	0.3420
V	0.7302	0.3440
W	0.7302	0.3330
X	0.7302	0.3420
Y	0.7302	0.3380
Z	0.7460	0.3400
a	0.7143	0.3340
b	0.7460	0.3330
c	0.7143	0.3350
d	0.7143	0.3320
e	0.7460	0.3430
f	0.6984	0.3440
g	0.7143	0.3500
h	0.7143	0.3400
i	0.7143	0.3370
j	0.7143	0.3420
k	0.7143	0.3440
l	0.7302	0.3450
m	0.7143	0.3440
n	0.7302	0.3540
o	0.7302	0.3380
p	0.7143	0.3410
q	0.7143	0.3350
r	0.7143	0.3390
s	0.7302	0.3430
t	0.7143	0.3370
u	0.7302	0.3490
v	0.6984	0.3360
w	0.7143	0.3340
x	0.6825	0.3320
y	0.7460	0.3420
z	0.7143	0.3420