



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 08:32 PM EST

PDB ID : 7KOR
EMDB ID : EMD-22981
Title : Structure of cardiac native thin filament at pCa=5.8 having upper troponin in Ca²⁺ bound state and lower troponin in Ca²⁺ free state
Authors : Galkin, V.E.; Risi, C.M.
Deposited on : 2020-11-09
Resolution : 7.80 Å (reported)
Based on initial models : 6KN8, 6KN7

This is a Full wwPDB EM Validation 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:

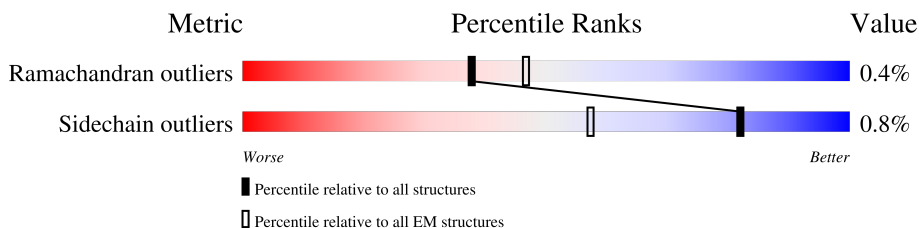
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 7.80 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.



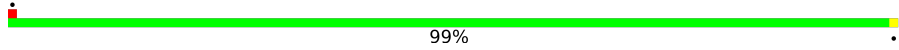
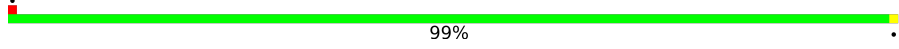
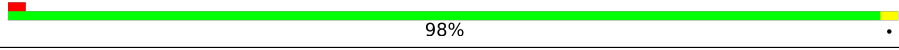
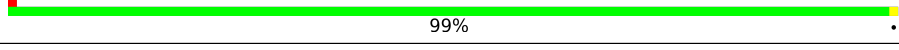
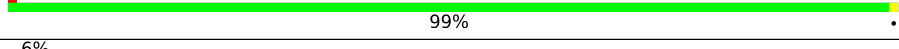
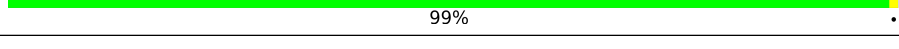
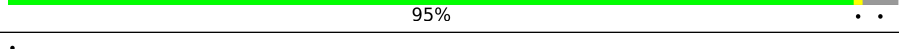
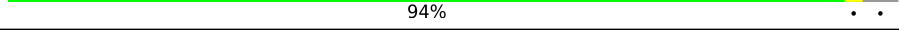
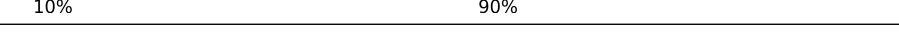
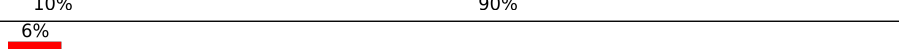
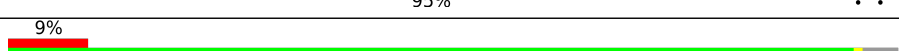
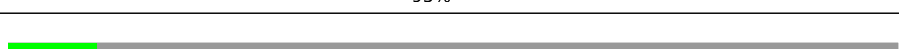


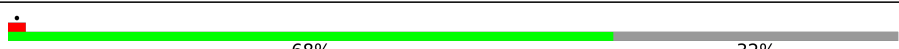

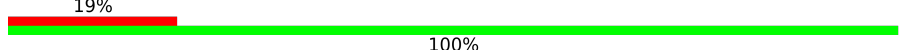
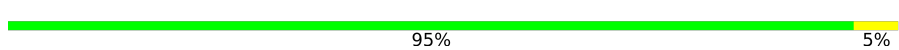
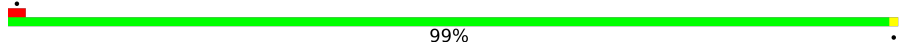

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	375	98% .
1	B	375	99% .
1	C	375	99% .
1	D	375	98% .
1	E	375	99% .
1	F	375	99% .
1	G	375	99% .
1	H	375	99% .
1	I	375	100% .

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Mol	Chain	Length	Quality of chain
1	J	375	 99%
1	K	375	 99%
1	L	375	 98%
1	M	375	 99%
1	N	375	 99%
1	O	375	 99%
2	P	286	 95%
2	Q	286	 94%
2	R	286	 10% 90%
2	S	286	 10% 90%
2	W	286	 95%
2	X	286	 95%
2	Y	286	 10% 90%
2	Z	286	 10% 90%
3	T	186	 72% 26%
3	a	186	 68% 32%
4	U	170	 71% 26%
4	b	170	 19% 100%
5	V	160	 95% 5%
5	c	160	 99%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60981 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	B	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	C	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	G	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	H	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	J	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	K	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	L	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	M	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	N	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		
1	O	375	Total	C	N	O	S	0	0
			2933	1854	493	565	21		

- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Q	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	R	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	S	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	W	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	X	274	Total	C	N	O	S	0	0
			2207	1347	376	480	4		
2	Y	29	Total	C	N	O	S	0	0
			231	141	41	46	3		
2	Z	29	Total	C	N	O	S	0	0
			231	141	41	46	3		

- Molecule 3 is a protein called Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	138	Total	C	N	O	S	0	0
			1205	737	238	229	1		
3	a	126	Total	C	N	O		0	0
			1101	673	219	209			

- Molecule 4 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	126	Total	C	N	O	S	0	0
			1008	624	193	187	4		
4	b	170	Total	C	N	O	S	0	0
			1374	848	263	258	5		

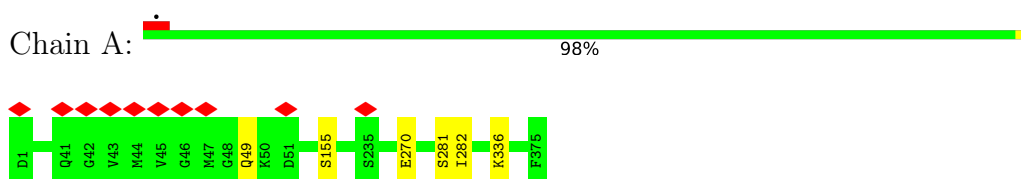
- Molecule 5 is a protein called Troponin C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		
5	c	160	Total	C	N	O	S	0	0
			1273	788	195	278	12		

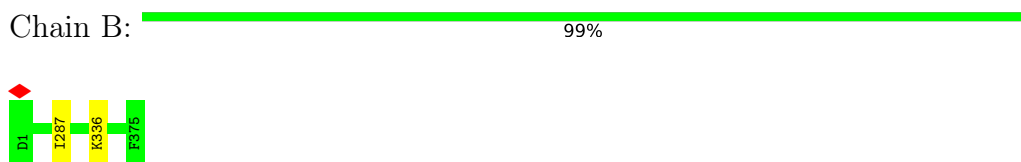
3 Residue-property plots [i](#)

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.

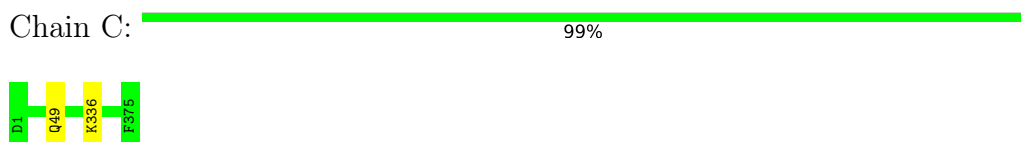
- Molecule 1: Actin, alpha skeletal muscle



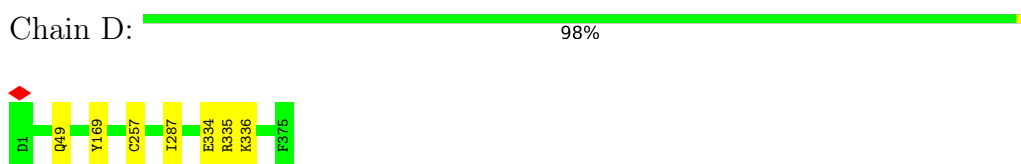
- Molecule 1: Actin, alpha skeletal muscle



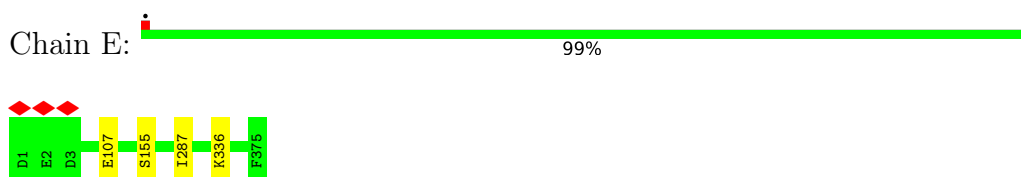
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

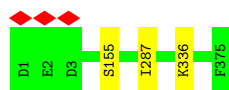


- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle

Chain F:  99%



- Molecule 1: Actin, alpha skeletal muscle

Chain G:  99%



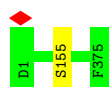
- Molecule 1: Actin, alpha skeletal muscle

Chain H:  99%



- Molecule 1: Actin, alpha skeletal muscle

Chain I:  100%



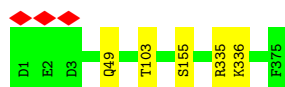
- Molecule 1: Actin, alpha skeletal muscle

Chain J:  99%



- Molecule 1: Actin, alpha skeletal muscle

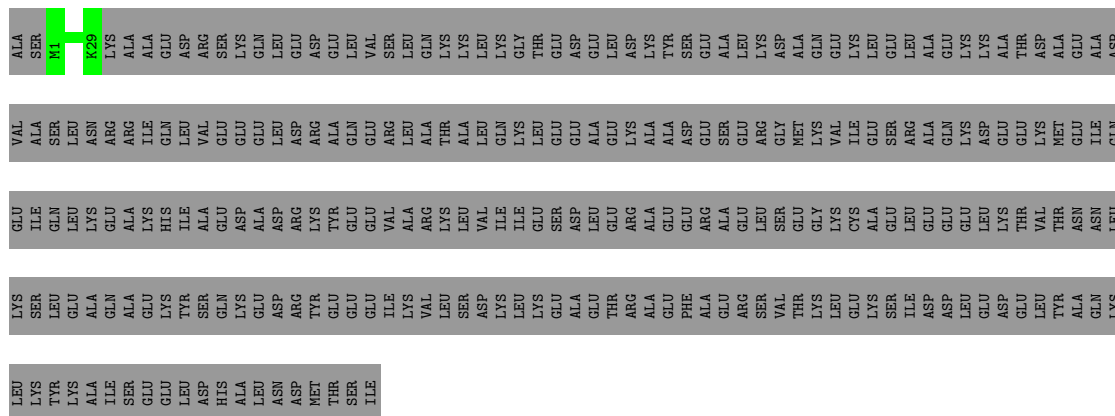
Chain K:  99%



- Molecule 1: Actin, alpha skeletal muscle

Chain L:  98%

- Molecule 2: Tropomyosin alpha-1 chain



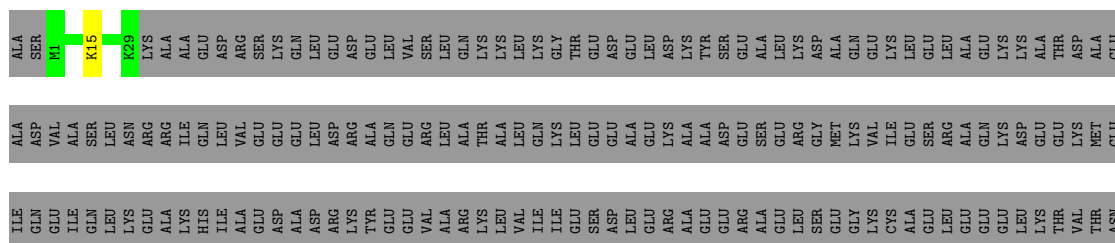
- Molecule 2: Tropomyosin alpha-1 chain



- Molecule 2: Tropomyosin alpha-1 chain

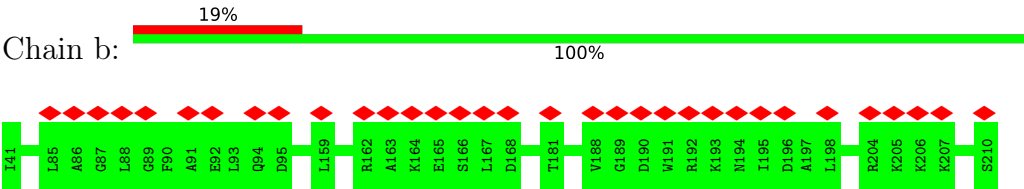


- Molecule 2: Tropomyosin alpha-1 chain

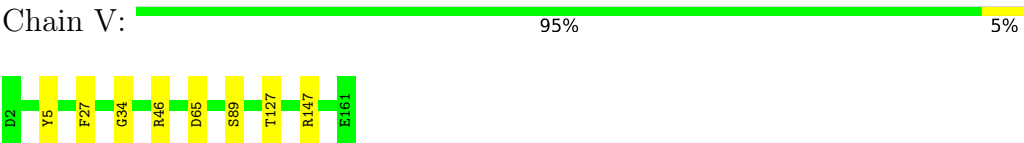


LYS
LYS
PHE
GLU
SER

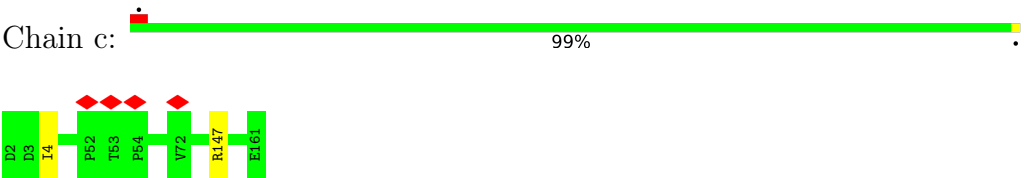
- Molecule 4: Troponin I, cardiac muscle



- Molecule 5: Troponin C



- Molecule 5: Troponin C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	439.344, 439.344, 439.344	wwPDB
Map dimensions	162, 162, 162	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.712, 2.712, 2.712	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	1/2996 (0.0%)	0.88	0/4058
1	B	0.93	0/2996	0.91	0/4058
1	C	0.92	0/2996	0.89	0/4058
1	D	0.93	1/2996 (0.0%)	0.90	1/4058 (0.0%)
1	E	0.91	0/2996	0.91	0/4058
1	F	0.91	0/2996	0.88	0/4058
1	G	0.93	0/2996	0.91	0/4058
1	H	0.91	0/2996	0.90	0/4058
1	I	0.92	0/2996	0.90	0/4058
1	J	0.89	0/2996	0.87	0/4058
1	K	0.91	0/2996	0.87	0/4058
1	L	0.90	0/2996	0.88	0/4058
1	M	0.91	0/2996	0.88	0/4058
1	N	0.92	0/2996	0.90	1/4058 (0.0%)
1	O	0.91	0/2996	0.88	0/4058
2	P	1.27	0/2215	0.82	0/2954
2	Q	1.25	1/2215 (0.0%)	0.89	2/2954 (0.1%)
2	R	1.04	0/230	0.77	0/301
2	S	1.06	0/230	0.82	0/301
2	W	1.30	2/2215 (0.1%)	0.83	0/2954
2	X	1.31	0/2215	0.90	1/2954 (0.0%)
2	Y	1.17	0/230	0.86	0/301
2	Z	1.13	0/230	0.90	0/301
3	T	0.93	0/1214	0.79	1/1606 (0.1%)
3	a	0.31	0/1108	0.49	0/1466
4	U	0.55	0/1014	0.76	1/1352 (0.1%)
4	b	0.29	0/1384	0.50	0/1840
5	V	0.51	0/1286	0.68	0/1719
5	c	0.29	0/1286	0.48	0/1719
All	All	0.94	5/62012 (0.0%)	0.86	7/83592 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	U	0	1
5	V	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	165	VAL	CB-CG1	-5.10	1.42	1.52
1	A	270	GLU	CD-OE1	-5.08	1.20	1.25
2	W	40	GLU	CD-OE1	-5.06	1.20	1.25
1	D	257	CYS	CB-SG	-5.02	1.73	1.81
2	Q	222	GLU	CD-OE1	-5.00	1.20	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	272	GLU	CB-CA-C	10.76	131.91	110.40
2	Q	272	GLU	N-CA-C	-10.75	81.97	111.00
3	T	229	LEU	CA-CB-CG	5.57	128.12	115.30
4	U	76	LEU	CB-CG-CD2	-5.24	102.10	111.00
2	X	238	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	169	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	N	53	TYR	CB-CG-CD2	-5.04	117.97	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	U	79	ARG	Peptide
5	V	27	PHE	Peptide
5	V	89	SER	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/375 (100%)	362 (97%)	9 (2%)	2 (0%)	29	69
1	B	373/375 (100%)	360 (96%)	13 (4%)	0	100	100
1	C	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	41	77
1	D	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	29	69
1	E	373/375 (100%)	359 (96%)	13 (4%)	1 (0%)	41	77
1	F	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	77
1	G	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	29	69
1	H	373/375 (100%)	360 (96%)	11 (3%)	2 (0%)	29	69
1	I	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	41	77
1	J	373/375 (100%)	360 (96%)	10 (3%)	3 (1%)	19	60
1	K	373/375 (100%)	358 (96%)	12 (3%)	3 (1%)	19	60
1	L	373/375 (100%)	359 (96%)	11 (3%)	3 (1%)	19	60
1	M	373/375 (100%)	358 (96%)	13 (4%)	2 (0%)	29	69
1	N	373/375 (100%)	362 (97%)	10 (3%)	1 (0%)	41	77
1	O	373/375 (100%)	358 (96%)	14 (4%)	1 (0%)	41	77
2	P	272/286 (95%)	272 (100%)	0	0	100	100
2	Q	272/286 (95%)	268 (98%)	2 (1%)	2 (1%)	22	63
2	R	27/286 (9%)	27 (100%)	0	0	100	100
2	S	27/286 (9%)	27 (100%)	0	0	100	100
2	W	272/286 (95%)	272 (100%)	0	0	100	100
2	X	272/286 (95%)	272 (100%)	0	0	100	100
2	Y	27/286 (9%)	27 (100%)	0	0	100	100
2	Z	27/286 (9%)	27 (100%)	0	0	100	100
3	T	134/186 (72%)	126 (94%)	6 (4%)	2 (2%)	10	46
3	a	122/186 (66%)	116 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	124/170 (73%)	109 (88%)	13 (10%)	2 (2%)	9	44
4	b	168/170 (99%)	156 (93%)	12 (7%)	0	100	100
5	V	158/160 (99%)	129 (82%)	27 (17%)	2 (1%)	12	48
5	c	158/160 (99%)	139 (88%)	19 (12%)	0	100	100
All	All	7655/8945 (86%)	7366 (96%)	256 (3%)	33 (0%)	38	72

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	155	SER
1	H	155	SER
1	I	155	SER
1	K	155	SER
1	L	155	SER
1	M	155	SER
1	O	155	SER
2	Q	272	GLU
1	A	155	SER
2	Q	273	GLU
5	V	65	ASP
1	G	336	LYS
1	J	336	LYS
3	T	241	TYR
1	F	155	SER
1	J	220	ALA
1	N	155	SER
4	U	42	SER
4	U	143	THR
1	A	49	GLN
1	C	49	GLN
1	D	334	GLU
1	G	49	GLN
1	K	103	THR
1	L	336	LYS
1	M	49	GLN
1	D	49	GLN
1	H	49	GLN
1	J	49	GLN
1	K	49	GLN
1	L	49	GLN
5	V	34	GLY

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Mol	Chain	Res	Type
3	T	240	ILE

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	318/318 (100%)	315 (99%)	3 (1%)	78	87
1	B	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	C	318/318 (100%)	317 (100%)	1 (0%)	92	95
1	D	318/318 (100%)	315 (99%)	3 (1%)	78	87
1	E	318/318 (100%)	315 (99%)	3 (1%)	78	87
1	F	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	G	318/318 (100%)	315 (99%)	3 (1%)	78	87
1	H	318/318 (100%)	315 (99%)	3 (1%)	78	87
1	I	318/318 (100%)	318 (100%)	0	100	100
1	J	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	K	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	L	318/318 (100%)	315 (99%)	3 (1%)	78	87
1	M	318/318 (100%)	315 (99%)	3 (1%)	78	87
1	N	318/318 (100%)	316 (99%)	2 (1%)	86	92
1	O	318/318 (100%)	314 (99%)	4 (1%)	69	81
2	P	236/246 (96%)	234 (99%)	2 (1%)	81	89
2	Q	236/246 (96%)	233 (99%)	3 (1%)	69	81
2	R	24/246 (10%)	23 (96%)	1 (4%)	30	54
2	S	24/246 (10%)	24 (100%)	0	100	100
2	W	236/246 (96%)	235 (100%)	1 (0%)	91	94
2	X	236/246 (96%)	235 (100%)	1 (0%)	91	94
2	Y	24/246 (10%)	23 (96%)	1 (4%)	30	54
2	Z	24/246 (10%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	128/169 (76%)	127 (99%)	1 (1%)	81	89
3	a	117/169 (69%)	117 (100%)	0	100	100
4	U	106/145 (73%)	104 (98%)	2 (2%)	57	75
4	b	145/145 (100%)	145 (100%)	0	100	100
5	V	141/141 (100%)	137 (97%)	4 (3%)	43	65
5	c	141/141 (100%)	139 (99%)	2 (1%)	67	80
All	All	6588/7648 (86%)	6534 (99%)	54 (1%)	82	89

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	SER
1	A	282	ILE
1	A	336	LYS
1	B	287	ILE
1	B	336	LYS
1	C	336	LYS
1	D	287	ILE
1	D	335	ARG
1	D	336	LYS
1	E	107	GLU
1	E	287	ILE
1	E	336	LYS
1	F	287	ILE
1	F	336	LYS
1	G	287	ILE
1	G	335	ARG
1	G	336	LYS
1	H	163	VAL
1	H	254	ARG
1	H	336	LYS
1	J	305	MET
1	J	336	LYS
1	K	335	ARG
1	K	336	LYS
1	L	177	ARG
1	L	287	ILE
1	L	335	ARG
1	M	47	MET
1	M	335	ARG

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Mol	Chain	Res	Type
1	M	336	LYS
1	N	335	ARG
1	N	336	LYS
1	O	37	ARG
1	O	39	ARG
1	O	335	ARG
1	O	336	LYS
2	P	29	LYS
2	P	178	ARG
2	Q	15	LYS
2	Q	261	TYR
2	Q	264	LYS
2	R	15	LYS
3	T	215	ARG
4	U	69	ARG
4	U	112	TYR
5	V	5	TYR
5	V	46	ARG
5	V	127	THR
5	V	147	ARG
2	W	15	LYS
2	X	29	LYS
2	Y	15	LYS
5	c	4	ILE
5	c	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	162	ASN
1	J	162	ASN
1	M	162	ASN
1	O	162	ASN
2	P	153	HIS
2	Q	276	HIS
2	Q	279	ASN
3	T	109	HIS
3	T	149	GLN
3	T	202	GLN
3	T	225	ASN
3	T	238	GLN
3	T	269	ASN

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Mol	Chain	Res	Type
4	U	48	GLN
4	U	55	GLN
4	U	130	GLN
5	V	51	ASN
5	V	143	ASN
2	W	153	HIS
3	a	142	ASN
3	a	225	ASN
3	a	228	GLN
3	a	266	ASN
3	a	269	ASN
3	a	271	ASN
4	b	48	GLN
4	b	94	GLN
4	b	101	HIS
5	c	50	GLN
5	c	122	GLN

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](#)

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 ⓘ

There are no chain breaks in this entry.

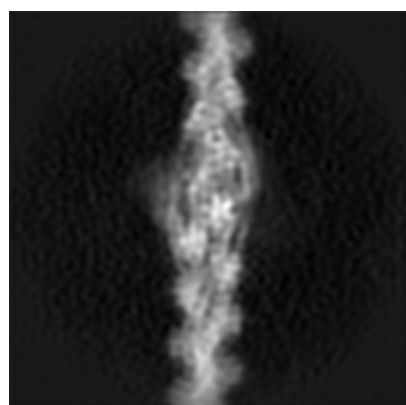
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22981. These allow visual inspection of the internal detail of the map and identification of artifacts.

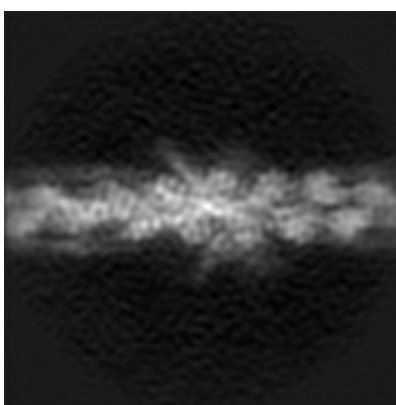
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

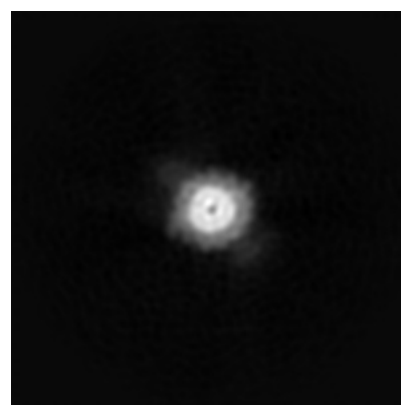
6.1.1 Primary map



X



Y

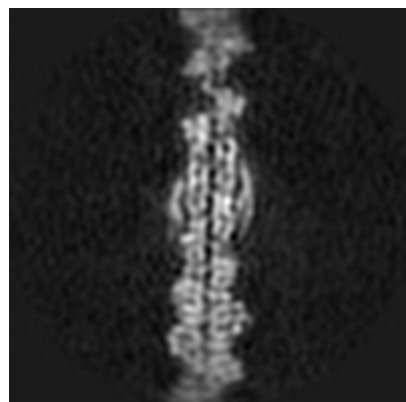


Z

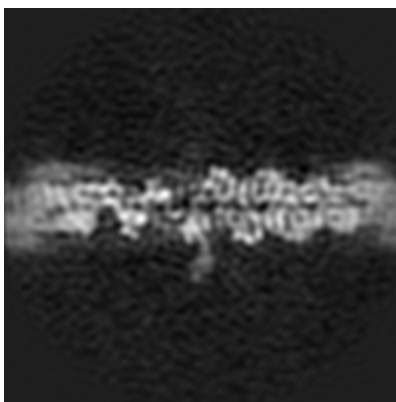
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

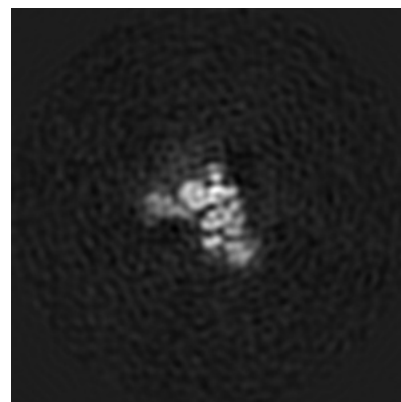
6.2.1 Primary map



X Index: 81



Y Index: 81

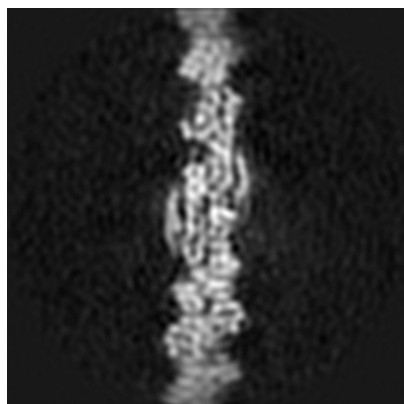


Z Index: 81

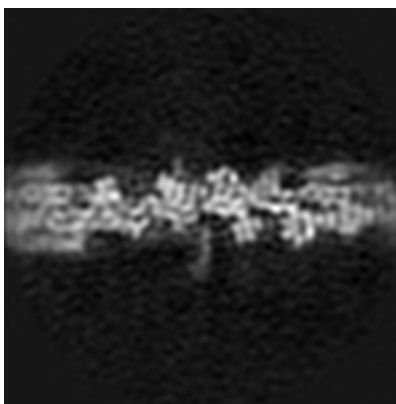
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

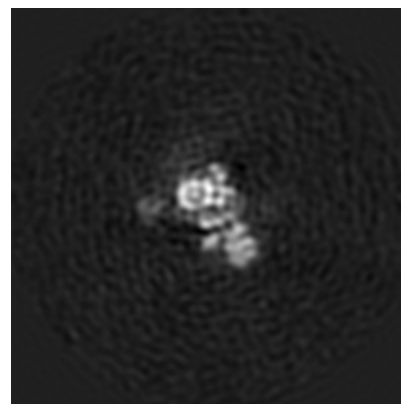
6.3.1 Primary map



X Index: 79



Y Index: 78



Z Index: 78

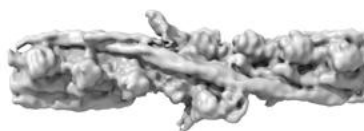
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

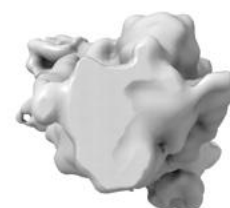
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

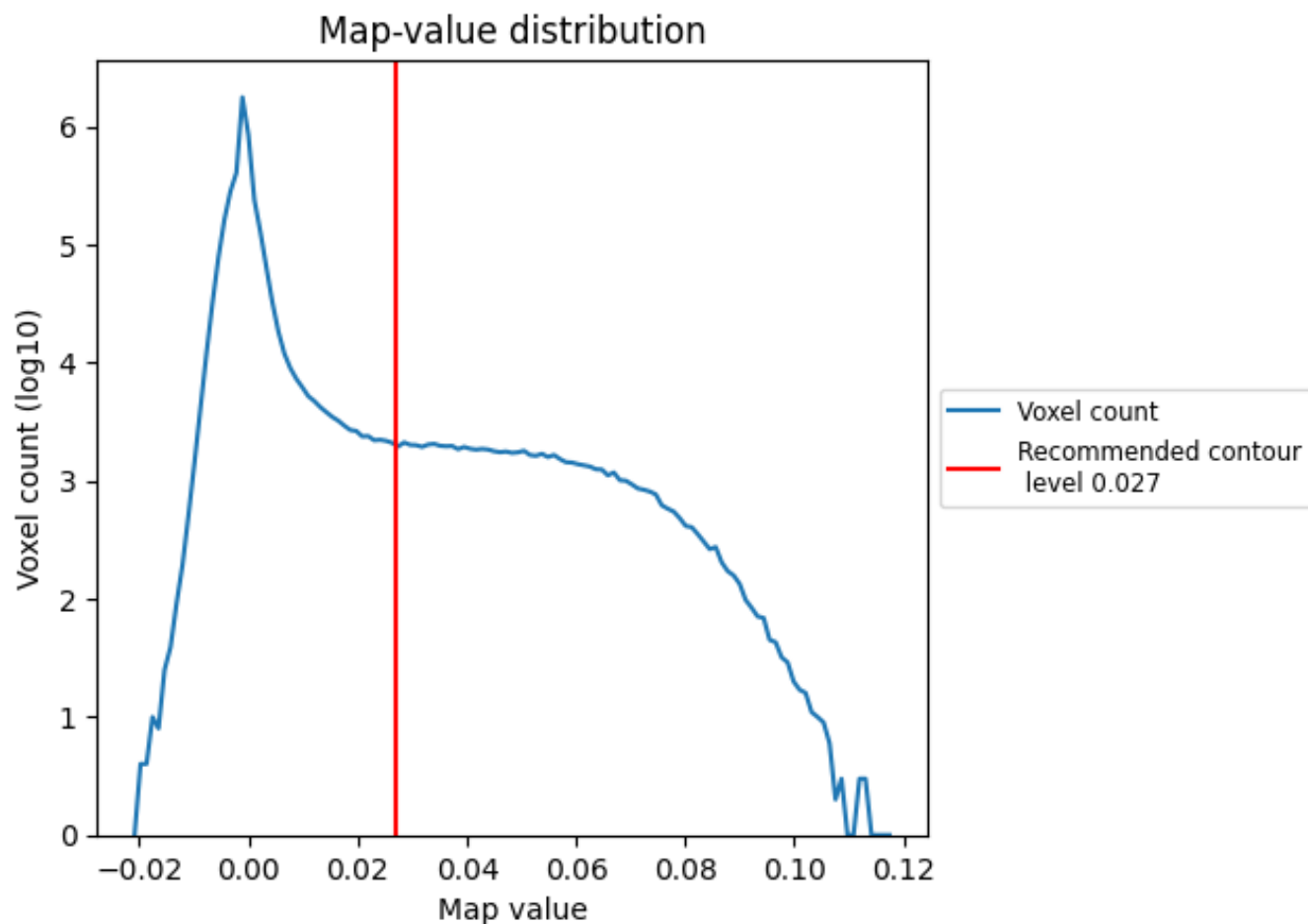
6.5 Mask visualisation

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

7 Map analysis [i](#)

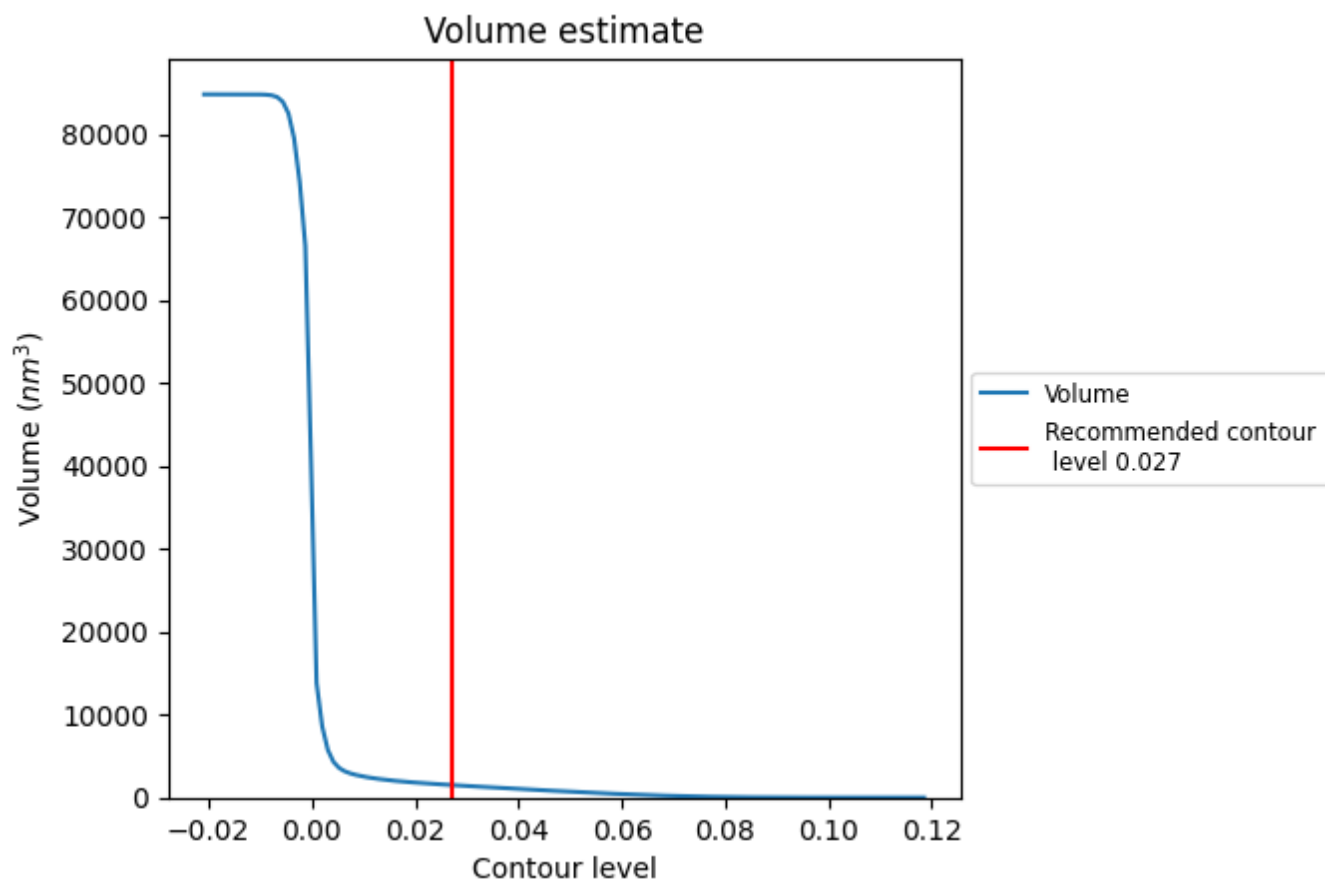
This section contains the results of statistical analysis of the map.

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.

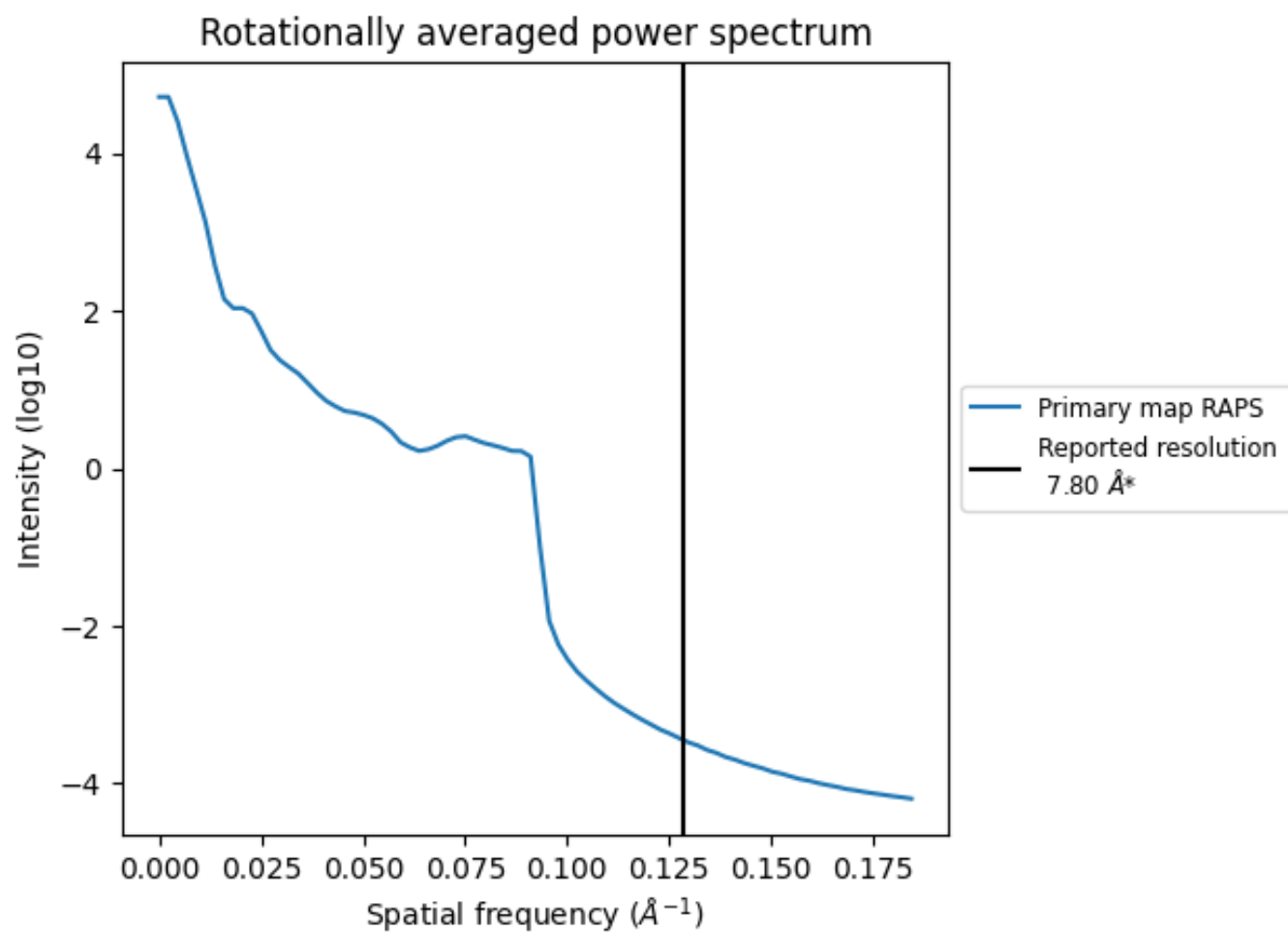
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1513 nm³; this corresponds to an approximate mass of 1367 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 ⓘ

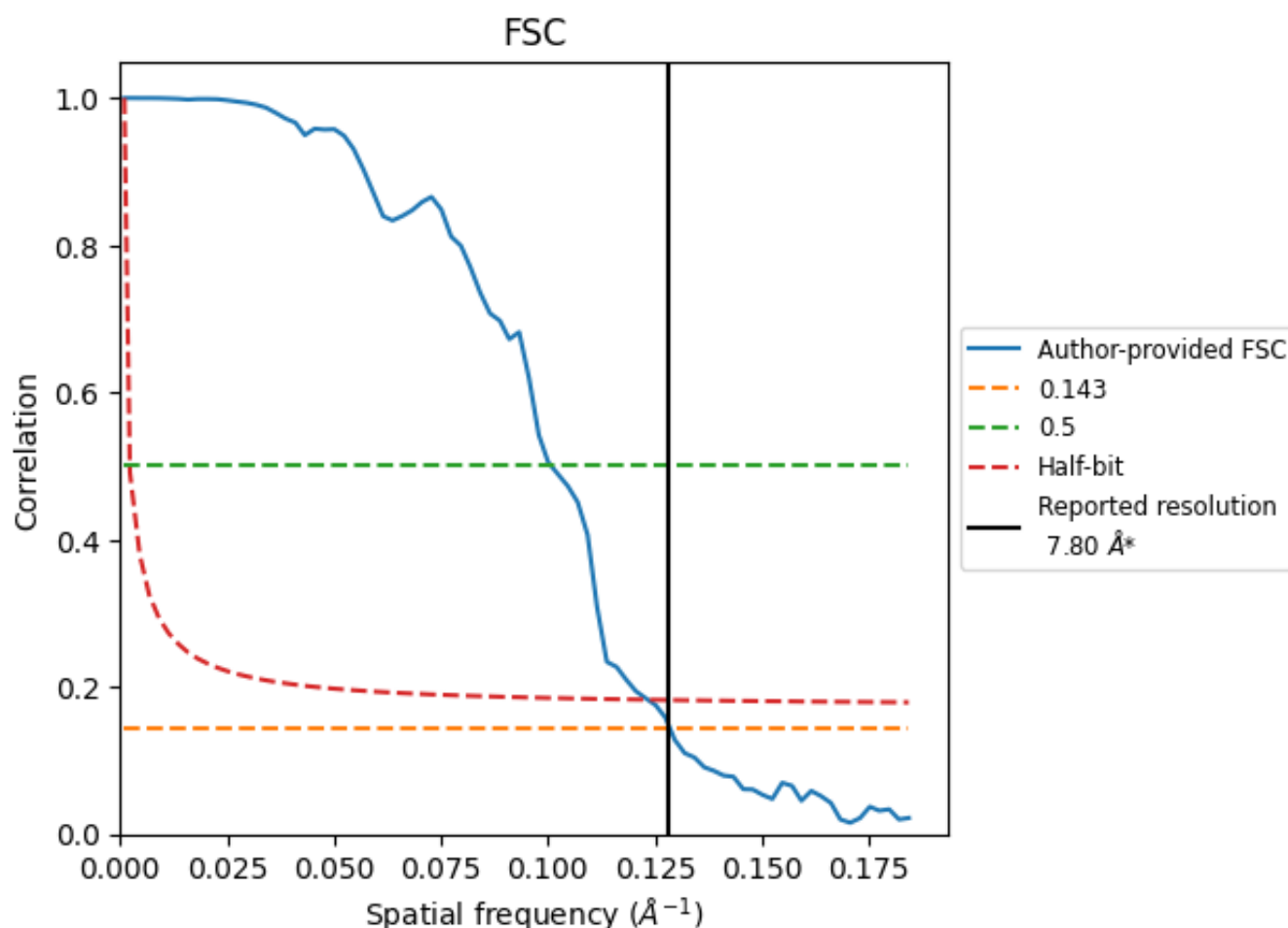


*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

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 0.128 \AA^{-1}

8.2 Resolution estimates [i](#)

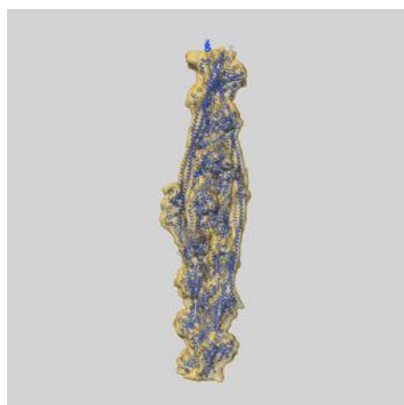
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.78	9.92	8.10
Unmasked-calculated*	-	-	-

*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-22981 and PDB model 7KOR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

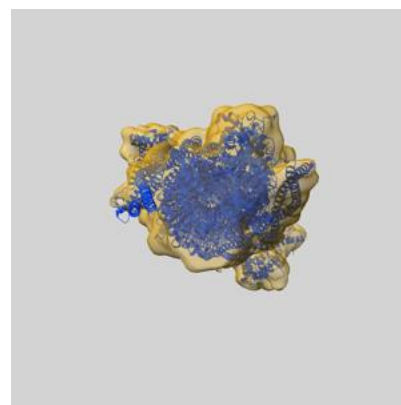
9.1 Map-model overlay [i](#)



X



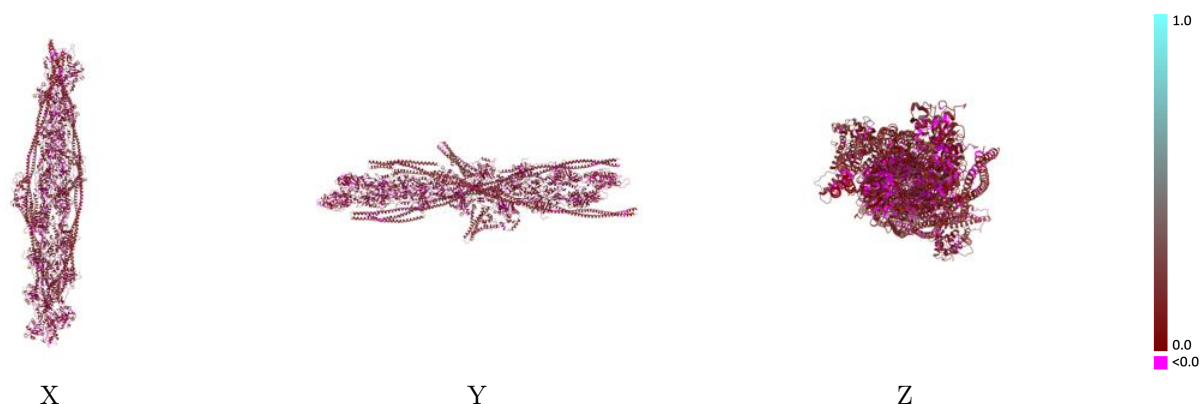
Y



Z

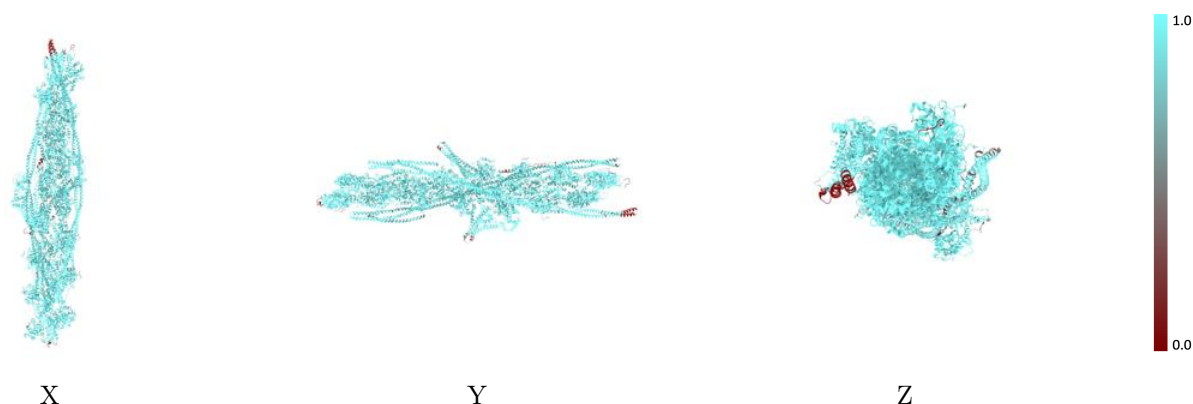
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



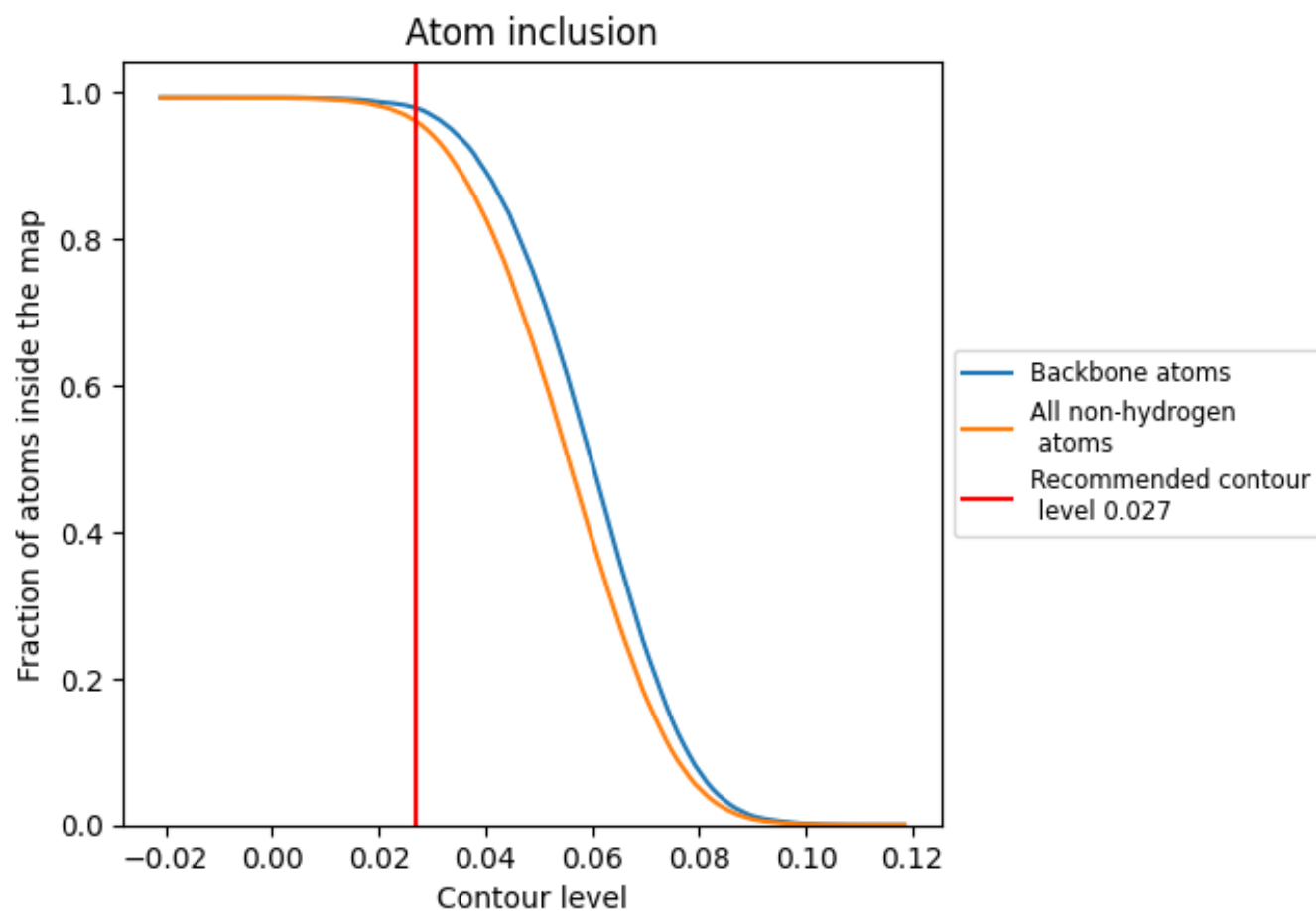
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).





























































9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9607	 0.1130
A	 0.9663	 0.0920
B	 0.9948	 0.0980
C	 0.9944	 0.1050
D	 0.9892	 0.1090
E	 0.9778	 0.1020
F	 0.9771	 0.1080
G	 0.9871	 0.1060
H	 0.9892	 0.1000
I	 0.9864	 0.1030
J	 0.9830	 0.1070
K	 0.9875	 0.1070
L	 0.9778	 0.1020
M	 0.9823	 0.1010
N	 0.9878	 0.0920
O	 0.9291	 0.0740
P	 0.9212	 0.1350
Q	 0.9392	 0.1450
R	 0.9694	 0.0620
S	 0.9825	 0.1720
T	 0.8293	 0.1590
U	 0.9355	 0.1790
V	 0.9952	 0.1720
W	 0.8908	 0.1600
X	 0.8673	 0.1270
Y	 0.9694	 0.1860
Z	 0.9913	 0.1800
a	 0.9314	 0.1690
b	 0.7991	 0.1140
c	 0.9548	 0.1310

