



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 09:38 AM UTC

PDB ID : 8YWT / pdb_00008ywt
EMDB ID : EMD-39644
Title : The isolated Vo domain of V/A-ATPase from *Thermus thermophilus*.
Authors : Kishikawa, J.; Nishida, Y.; Nakano, A.; Yokoyama, K.
Deposited on : 2024-04-01
Resolution : 2.80 Å (reported)
Based on initial model : 6LY9

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

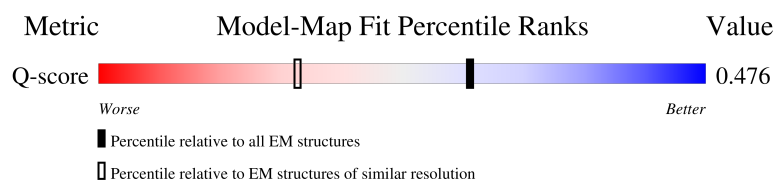
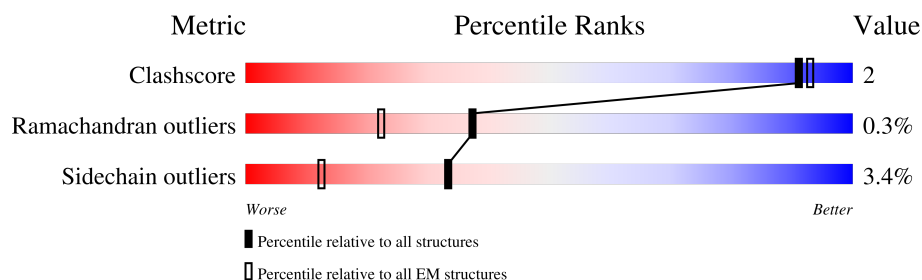
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

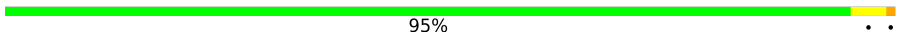
The reported resolution of this entry is 2.80 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	N	652	 95%
2	O	102	 70% 28%
2	P	102	 72% 25%
2	Q	102	 66% 5% 27%

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Mol	Chain	Length	Quality of chain
2	R	102	 63%7% ..27%
2	S	102	 63%7% ..27%
2	T	102	 67%5%28%
2	U	102	 54%14% ..28%
2	V	102	 69%.29%
2	W	102	 71%.27%
2	X	102	 68%.28%
2	Y	102	 70%..28%
2	Z	102	 53%14%5%28%
3	M	323	 95%..
4	K	120	 18%82%
5	L	188	 11%89%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13986 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 V-type ATP synthase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	649	Total	C	N	O	S	0	0
			5089	3344	866	871	8		

- Molecule 2 is a protein called V-type ATP synthase, subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
2	P	76	Total	C	N	O	S	0	0
			524	340	91	92	1		
2	Q	74	Total	C	N	O	S	0	0
			514	334	89	90	1		
2	R	74	Total	C	N	O	S	0	0
			514	334	89	90	1		
2	S	74	Total	C	N	O	S	0	0
			514	334	89	90	1		
2	T	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
2	U	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
2	V	72	Total	C	N	O	S	0	0
			504	329	87	87	1		
2	W	74	Total	C	N	O	S	0	0
			514	334	89	90	1		
2	X	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
2	Y	73	Total	C	N	O	S	0	0
			508	331	88	88	1		
2	Z	73	Total	C	N	O	S	0	0
			508	331	88	88	1		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	81	HIS	-	expression tag	UNP Q5SIT7
O	82	HIS	-	expression tag	UNP Q5SIT7
O	83	HIS	-	expression tag	UNP Q5SIT7
P	81	HIS	-	expression tag	UNP Q5SIT7
P	82	HIS	-	expression tag	UNP Q5SIT7
P	83	HIS	-	expression tag	UNP Q5SIT7
Q	81	HIS	-	expression tag	UNP Q5SIT7
Q	82	HIS	-	expression tag	UNP Q5SIT7
Q	83	HIS	-	expression tag	UNP Q5SIT7
R	81	HIS	-	expression tag	UNP Q5SIT7
R	82	HIS	-	expression tag	UNP Q5SIT7
R	83	HIS	-	expression tag	UNP Q5SIT7
S	81	HIS	-	expression tag	UNP Q5SIT7
S	82	HIS	-	expression tag	UNP Q5SIT7
S	83	HIS	-	expression tag	UNP Q5SIT7
T	81	HIS	-	expression tag	UNP Q5SIT7
T	82	HIS	-	expression tag	UNP Q5SIT7
T	83	HIS	-	expression tag	UNP Q5SIT7
U	81	HIS	-	expression tag	UNP Q5SIT7
U	82	HIS	-	expression tag	UNP Q5SIT7
U	83	HIS	-	expression tag	UNP Q5SIT7
V	81	HIS	-	expression tag	UNP Q5SIT7
V	82	HIS	-	expression tag	UNP Q5SIT7
V	83	HIS	-	expression tag	UNP Q5SIT7
W	81	HIS	-	expression tag	UNP Q5SIT7
W	82	HIS	-	expression tag	UNP Q5SIT7
W	83	HIS	-	expression tag	UNP Q5SIT7
X	81	HIS	-	expression tag	UNP Q5SIT7
X	82	HIS	-	expression tag	UNP Q5SIT7
X	83	HIS	-	expression tag	UNP Q5SIT7
Y	81	HIS	-	expression tag	UNP Q5SIT7
Y	82	HIS	-	expression tag	UNP Q5SIT7
Y	83	HIS	-	expression tag	UNP Q5SIT7
Z	81	HIS	-	expression tag	UNP Q5SIT7
Z	82	HIS	-	expression tag	UNP Q5SIT7
Z	83	HIS	-	expression tag	UNP Q5SIT7

- Molecule 3 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	322	Total	C	N	O	S	0	0
			2527	1607	462	454	4		

- Molecule 4 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	22	Total	C	N	O	0	0
			88	44	22	22		

- Molecule 5 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	20	Total	C	N	O	0	0
			80	40	20	20		

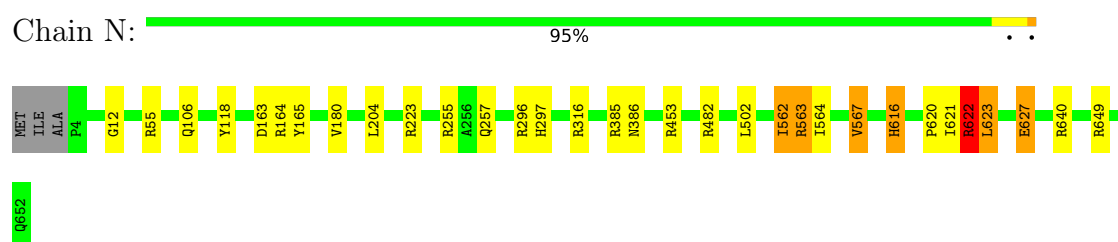
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	N	27	Total	O	0
			27	27	
6	O	2	Total	O	0
			2	2	
6	P	1	Total	O	0
			1	1	
6	Q	1	Total	O	0
			1	1	
6	X	2	Total	O	0
			2	2	
6	Y	2	Total	O	0
			2	2	
6	Z	5	Total	O	0
			5	5	
6	M	30	Total	O	0
			30	30	

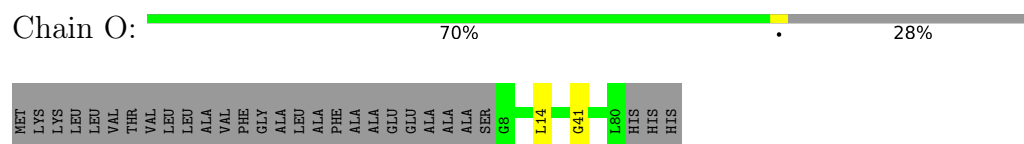
3 Residue-property plots

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.

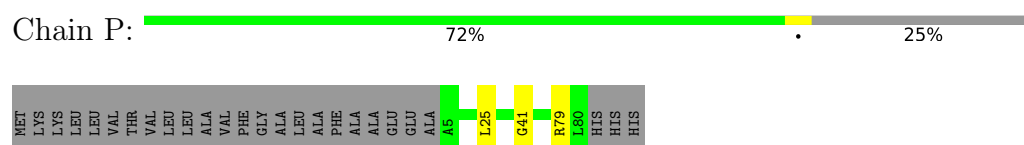
- Molecule 1: V-type ATP synthase subunit I



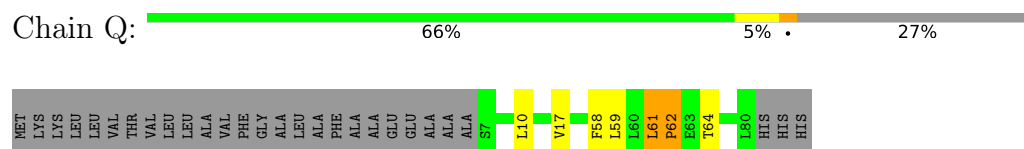
- Molecule 2: V-type ATP synthase, subunit K



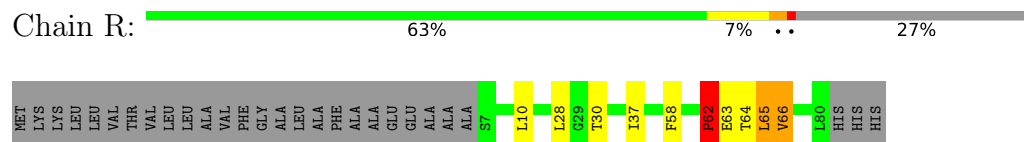
- Molecule 2: V-type ATP synthase, subunit K



- Molecule 2: V-type ATP synthase, subunit K

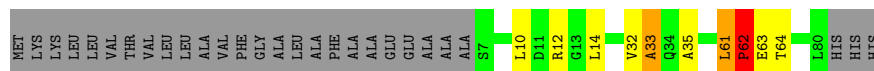


- Molecule 2: V-type ATP synthase, subunit K



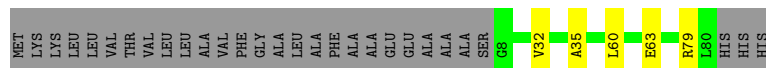
- Molecule 2: V-type ATP synthase, subunit K

Chain S:  63% 7% 27%



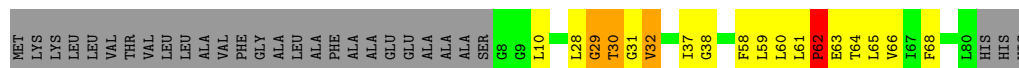
- Molecule 2: V-type ATP synthase, subunit K

Chain T:  67% 5% 28%



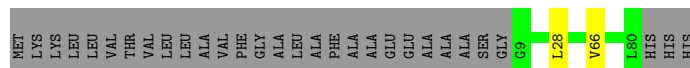
- Molecule 2: V-type ATP synthase, subunit K

Chain U:  54% 14% 28%



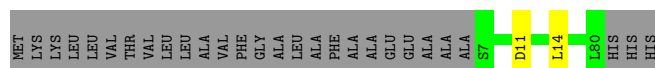
- Molecule 2: V-type ATP synthase, subunit K

Chain V:  69% 0% 29%



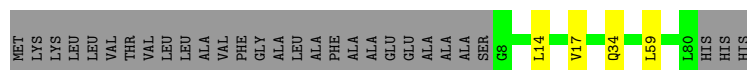
- Molecule 2: V-type ATP synthase, subunit K

Chain W:  71% 0% 27%



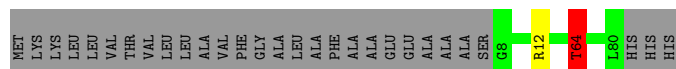
- Molecule 2: V-type ATP synthase, subunit K

Chain X:  68% 0% 28%



- Molecule 2: V-type ATP synthase, subunit K

Chain Y:  70% 0% 28%

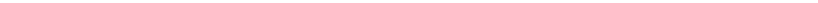


- Molecule 2: V-type ATP synthase, subunit K

HIS	MET
HIS	LYS
	LEU
	LEU
	VAL
	THR
	VAL
	LEU
	LEU
	ALA
	VAL
	PHE
	GLY
	ALA
	LEU
	ALA
	PHE
	ALA
	ALA
	GLU
	GLU
	ALA
	ALA
	ALA
	SER
	G8
	D11
	R12
	V17
	L25
	A26
	A27
	L28
	G29
	T30
	G31
	V32
	A33
	Q34
	R49
	F58
	L59
	L60
	L61
	P62
	E63
	T64
	L65
	V66
	L67
	F68
	L80
	H85

- Chain M: 95% .



- Chain K:  18% 82%

GLU	THR	GLU	GLU	ALA	LEU	LEU	ALA	ARG	TYR	ARG	GLU	GLU	ALA	ALA	GLU	GLU	ALA	ALA	LYS	VAL	VAL	VAL	VAL	LEU	LEU	LEU	LEU	PRO																															
MET	THR	GLY	GLY	LEU	VAL	LEU	ASN	ALA	ILE	SER	ARG	ARG	GLY	GLY	ALA	ALA	MET	GLY	GLY	LEU	G21	G42	GLU	ALA	GLU	GLU	GLU	ARG	VAL	LYS	ARG	ALA	ALA	GLU	ALA	ALA	LYS	ALA	LYS	ALA	LEU	GLU	ALA	ALA	LYS	ALA	ALA	ALA	LYS	VAL	VAL	LEU	LEU	LEU	LYS	GLU	VAL	LEU	PRO

- Chain L: 11% 89%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	370215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.295	Depositor
Minimum map value	-3.337	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	N	0.79	0/5220	1.37	12/7093 (0.2%)
2	O	0.77	0/512	1.45	0/692
2	P	0.73	0/528	1.41	1/714 (0.1%)
2	Q	0.80	1/518 (0.2%)	1.50	3/700 (0.4%)
2	R	0.95	1/518 (0.2%)	1.68	9/700 (1.3%)
2	S	1.02	3/518 (0.6%)	1.68	7/700 (1.0%)
2	T	0.76	0/512	1.41	0/692
2	U	0.96	1/512 (0.2%)	1.67	10/692 (1.4%)
2	V	0.77	0/508	1.43	0/687
2	W	0.72	0/518	1.44	1/700 (0.1%)
2	X	0.76	0/512	1.43	1/692 (0.1%)
2	Y	0.78	0/512	1.54	2/692 (0.3%)
2	Z	0.92	0/512	1.67	7/692 (1.0%)
3	M	0.81	0/2567	1.41	9/3466 (0.3%)
4	K	0.62	0/87	1.47	0/107
5	L	0.73	0/79	1.49	0/97
All	All	0.81	6/14133 (0.0%)	1.45	62/19116 (0.3%)

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
1	N	0	5
2	T	0	1
2	Z	0	1
3	M	0	4
All	All	0	11

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	62	PRO	C-O	-7.37	1.14	1.24
2	S	62	PRO	C-O	-7.11	1.14	1.24
2	S	33	ALA	C-O	-6.55	1.16	1.24
2	Q	62	PRO	C-O	-5.67	1.16	1.24
2	S	35	ALA	CA-CB	-5.40	1.44	1.53
2	U	62	PRO	C-O	-5.02	1.17	1.24

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	32	VAL	O-C-N	-13.13	109.13	121.87
2	S	35	ALA	N-CA-C	-9.77	100.59	111.14
2	R	65	LEU	N-CA-C	-8.95	102.49	113.41
2	Q	64	THR	N-CA-C	-8.60	103.21	114.31
2	Z	32	VAL	O-C-N	-8.49	113.33	121.90
2	U	28	LEU	O-C-N	-8.06	113.77	122.07
2	R	66	VAL	CA-C-N	7.97	131.74	120.42
2	R	66	VAL	C-N-CA	7.97	131.74	120.42
2	Q	64	THR	CA-C-N	7.63	130.73	120.65
2	Q	64	THR	C-N-CA	7.63	130.73	120.65
2	U	64	THR	N-CA-C	-7.53	103.94	113.72
2	Z	28	LEU	O-C-N	-7.50	114.17	122.12
2	R	62	PRO	N-CA-CB	-7.09	95.81	103.25
2	U	32	VAL	O-C-N	-7.01	114.07	122.06
1	N	623	LEU	N-CA-C	-6.93	102.82	112.45
3	M	11	ARG	NE-CZ-NH2	6.90	125.41	119.20
2	Y	12	ARG	NE-CZ-NH2	6.64	125.18	119.20
2	R	64	THR	CB-CA-C	-6.50	98.77	110.35
2	U	68	PHE	CA-C-N	6.42	127.06	119.94
2	U	68	PHE	C-N-CA	6.42	127.06	119.94
2	S	64	THR	N-CA-C	-6.11	105.78	113.72
2	U	31	GLY	CA-C-N	-6.11	110.66	120.86
2	U	31	GLY	C-N-CA	-6.11	110.66	120.86
2	P	79	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	N	386	ASN	CA-CB-CG	6.07	118.67	112.60
2	W	11	ASP	CA-CB-CG	6.06	118.66	112.60
3	M	232	ARG	NE-CZ-NH2	6.04	124.64	119.20
2	S	61	LEU	O-C-N	6.04	126.29	120.55
3	M	202	ARG	NE-CZ-NH2	5.99	124.59	119.20
3	M	305	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	N	620	PRO	CA-C-N	5.92	128.57	120.46
1	N	620	PRO	C-N-CA	5.92	128.57	120.46
3	M	125	ARG	NE-CZ-NH2	5.91	124.52	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	12	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	N	616	HIS	CB-CG-CD2	-5.83	123.62	131.20
3	M	256	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	N	223	ARG	NE-CZ-NH2	5.75	124.38	119.20
2	Z	64	THR	N-CA-C	-5.75	106.27	113.28
2	Y	64	THR	CB-CA-C	-5.73	100.18	110.37
2	R	64	THR	N-CA-C	-5.71	104.16	113.19
2	Z	67	ILE	N-CA-C	-5.60	104.82	113.16
1	N	255	ARG	NE-CZ-NH2	5.57	124.21	119.20
2	S	35	ALA	CA-C-N	-5.56	111.08	120.58
2	S	35	ALA	C-N-CA	-5.56	111.08	120.58
1	N	55	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	N	164	ARG	NE-CZ-NH2	5.54	124.19	119.20
2	U	68	PHE	CA-C-O	-5.47	114.17	120.24
2	R	65	LEU	CA-C-N	5.42	129.22	120.82
2	R	65	LEU	C-N-CA	5.42	129.22	120.82
2	U	29	GLY	N-CA-C	5.33	119.12	112.73
2	X	34	GLN	OE1-CD-NE2	-5.32	117.28	122.60
3	M	63	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	N	564	ILE	N-CA-C	-5.27	105.26	111.00
2	R	66	VAL	CA-C-O	-5.27	114.39	119.92
2	Z	11	ASP	CA-CB-CG	5.25	117.85	112.60
2	Z	68	PHE	CB-CA-C	5.15	120.02	109.67
2	Z	12	ARG	NE-CZ-NH2	5.10	123.79	119.20
2	U	65	LEU	N-CA-C	-5.06	106.95	113.23
3	M	132	ASP	N-CA-CB	-5.05	105.80	111.10
1	N	106	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	N	385	ARG	NE-CZ-NH2	5.03	123.73	119.20
3	M	156	ARG	NE-CZ-NH2	5.02	123.72	119.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	125	ARG	Sidechain
3	M	229	ARG	Sidechain
3	M	266	ARG	Sidechain
3	M	305	ARG	Sidechain
1	N	118	TYR	Sidechain
1	N	453	ARG	Sidechain
1	N	482	ARG	Sidechain
1	N	563	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	N	622	ARG	Sidechain
2	T	79	ARG	Sidechain
2	Z	49	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	5089	0	5236	10	0
2	O	508	0	547	1	0
2	P	524	0	562	1	0
2	Q	514	0	552	7	0
2	R	514	0	552	8	0
2	S	514	0	552	3	0
2	T	508	0	547	2	0
2	U	508	0	547	6	0
2	V	504	0	544	0	0
2	W	514	0	552	0	0
2	X	508	0	547	0	0
2	Y	508	0	547	1	0
2	Z	508	0	547	9	0
3	M	2527	0	2599	1	0
4	K	88	0	23	0	0
5	L	80	0	19	0	0
6	M	30	0	0	1	0
6	N	27	0	0	1	0
6	O	2	0	0	1	0
6	P	1	0	0	1	0
6	Q	1	0	0	0	0
6	X	2	0	0	0	0
6	Y	2	0	0	0	0
6	Z	5	0	0	0	0
All	All	13986	0	14473	44	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:622:ARG:HG3	1:N:622:ARG:HH11	1.36	0.90
2:U:30:THR:HG21	2:U:66:VAL:HB	1.61	0.81
1:N:563:ARG:NH2	2:Y:64:THR:HG21	2.03	0.72
1:N:622:ARG:NH1	1:N:627:GLU:OE2	2.23	0.71
1:N:563:ARG:O	1:N:567:VAL:HG12	1.93	0.68
2:R:10:LEU:HD12	2:S:10:LEU:HG	1.80	0.62
3:M:202:ARG:NH1	6:M:401:HOH:O	2.34	0.61
2:R:58:PHE:O	2:R:62:PRO:HD2	2.03	0.58
2:O:41:GLY:HA3	6:O:101:HOH:O	2.03	0.57
1:N:616:HIS:HD2	6:N:708:HOH:O	1.88	0.56
2:Z:64:THR:O	2:Z:68:PHE:HD2	1.90	0.55
2:R:37:ILE:CD1	2:R:62:PRO:HG2	2.37	0.55
2:R:37:ILE:HD12	2:R:62:PRO:HG2	1.91	0.53
2:Z:61:LEU:N	2:Z:62:PRO:HD2	2.23	0.52
2:Q:58:PHE:O	2:Q:62:PRO:HD3	2.10	0.51
2:Q:10:LEU:HG	2:R:10:LEU:CD2	2.40	0.51
2:Q:10:LEU:HG	2:R:10:LEU:HD21	1.92	0.51
2:T:60:LEU:O	2:T:63:GLU:HB2	2.12	0.50
2:Z:61:LEU:H	2:Z:62:PRO:HD2	1.77	0.49
2:Z:26:ALA:O	2:Z:30:THR:HG22	2.13	0.49
2:Z:30:THR:HG21	2:Z:66:VAL:HB	1.93	0.49
2:Z:58:PHE:O	2:Z:62:PRO:HD2	2.13	0.49
2:U:29:GLY:HA2	2:U:32:VAL:HG22	1.94	0.49
2:U:38:GLY:CA	2:U:59:LEU:HD13	2.43	0.48
2:S:33:ALA:HA	2:T:35:ALA:HB2	1.97	0.47
2:S:61:LEU:HB2	2:S:62:PRO:HD3	1.97	0.46
2:R:58:PHE:O	2:R:62:PRO:CD	2.63	0.46
1:N:622:ARG:HG3	1:N:622:ARG:NH1	2.13	0.46
2:U:58:PHE:O	2:U:62:PRO:CD	2.66	0.44
1:N:296:ARG:HE	1:N:297:HIS:CE1	2.35	0.44
2:U:37:ILE:HD12	2:U:62:PRO:HG2	1.99	0.44
2:Z:64:THR:HG22	2:Z:68:PHE:CD2	2.52	0.43
1:N:562:ILE:O	1:N:562:ILE:HG12	2.17	0.43
2:U:38:GLY:HA2	2:U:59:LEU:HD13	2.01	0.42
1:N:563:ARG:O	1:N:567:VAL:CG1	2.64	0.42
2:Q:58:PHE:O	2:Q:62:PRO:CD	2.67	0.42
2:R:30:THR:HG21	2:R:66:VAL:HB	2.01	0.42
2:Q:61:LEU:N	2:Q:62:PRO:CD	2.83	0.42
1:N:163:ASP:HA	1:N:165:TYR:CE2	2.56	0.41
2:Z:30:THR:O	2:Z:34:GLN:HG3	2.20	0.41
2:P:41:GLY:HA3	6:P:101:HOH:O	2.20	0.41
2:Q:59:LEU:C	2:Q:62:PRO:HD2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:61:LEU:C	2:Z:63:GLU:H	2.28	0.40
2:Q:61:LEU:HD12	2:Q:61:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	647/652 (99%)	626 (97%)	19 (3%)	2 (0%)	36	66
2	O	71/102 (70%)	71 (100%)	0	0	100	100
2	P	74/102 (72%)	74 (100%)	0	0	100	100
2	Q	72/102 (71%)	71 (99%)	1 (1%)	0	100	100
2	R	72/102 (71%)	69 (96%)	2 (3%)	1 (1%)	9	30
2	S	72/102 (71%)	70 (97%)	2 (3%)	0	100	100
2	T	71/102 (70%)	69 (97%)	2 (3%)	0	100	100
2	U	71/102 (70%)	69 (97%)	1 (1%)	1 (1%)	9	30
2	V	70/102 (69%)	69 (99%)	1 (1%)	0	100	100
2	W	72/102 (71%)	72 (100%)	0	0	100	100
2	X	71/102 (70%)	70 (99%)	1 (1%)	0	100	100
2	Y	71/102 (70%)	71 (100%)	0	0	100	100
2	Z	71/102 (70%)	69 (97%)	1 (1%)	1 (1%)	9	30
3	M	320/323 (99%)	312 (98%)	8 (2%)	0	100	100
4	K	20/120 (17%)	20 (100%)	0	0	100	100
5	L	18/188 (10%)	17 (94%)	1 (6%)	0	100	100
All	All	1863/2507 (74%)	1819 (98%)	39 (2%)	5 (0%)	37	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	62	PRO
2	U	62	PRO
2	Z	62	PRO
1	N	562	ILE
1	N	12	GLY

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	N	517/520 (99%)	505 (98%)	12 (2%)	44	78
2	O	47/67 (70%)	46 (98%)	1 (2%)	47	79
2	P	48/67 (72%)	47 (98%)	1 (2%)	47	79
2	Q	48/67 (72%)	46 (96%)	2 (4%)	26	61
2	R	48/67 (72%)	44 (92%)	4 (8%)	10	32
2	S	48/67 (72%)	45 (94%)	3 (6%)	16	45
2	T	47/67 (70%)	46 (98%)	1 (2%)	47	79
2	U	47/67 (70%)	42 (89%)	5 (11%)	6	22
2	V	47/67 (70%)	45 (96%)	2 (4%)	26	60
2	W	48/67 (72%)	47 (98%)	1 (2%)	47	79
2	X	47/67 (70%)	44 (94%)	3 (6%)	16	44
2	Y	47/67 (70%)	46 (98%)	1 (2%)	47	79
2	Z	47/67 (70%)	42 (89%)	5 (11%)	6	22
3	M	255/256 (100%)	251 (98%)	4 (2%)	55	83
All	All	1341/1580 (85%)	1296 (97%)	45 (3%)	33	68

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	180	VAL

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Mol	Chain	Res	Type
1	N	204	LEU
1	N	257	GLN
1	N	316	ARG
1	N	502	LEU
1	N	567	VAL
1	N	621	ILE
1	N	622	ARG
1	N	623	LEU
1	N	627	GLU
1	N	640	ARG
1	N	649	ARG
2	O	14	LEU
2	P	25	LEU
2	Q	17	VAL
2	Q	61	LEU
2	R	28	LEU
2	R	62	PRO
2	R	63	GLU
2	R	65	LEU
2	S	14	LEU
2	S	62	PRO
2	S	63	GLU
2	T	32	VAL
2	U	10	LEU
2	U	30	THR
2	U	60	LEU
2	U	61	LEU
2	U	63	GLU
2	V	28	LEU
2	V	66	VAL
2	W	14	LEU
2	X	14	LEU
2	X	17	VAL
2	X	59	LEU
2	Y	64	THR
2	Z	17	VAL
2	Z	25	LEU
2	Z	30	THR
2	Z	60	LEU
2	Z	61	LEU
3	M	103	LYS
3	M	142	VAL

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Mol	Chain	Res	Type
3	M	241	LEU
3	M	291	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	31	HIS
1	N	44	GLN
1	N	323	ASN
1	N	452	HIS
1	N	491	HIS
1	N	616	HIS
1	N	638	ASN
2	O	34	GLN
2	Q	34	GLN
2	T	51	ASN
2	T	77	ASN
2	U	51	ASN
2	V	51	ASN
2	W	51	ASN
2	W	77	ASN
2	Y	51	ASN
3	M	97	GLN
3	M	159	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

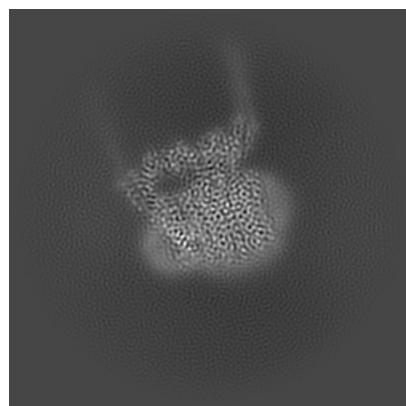
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39644. These allow visual inspection of the internal detail of the map and identification of artifacts.

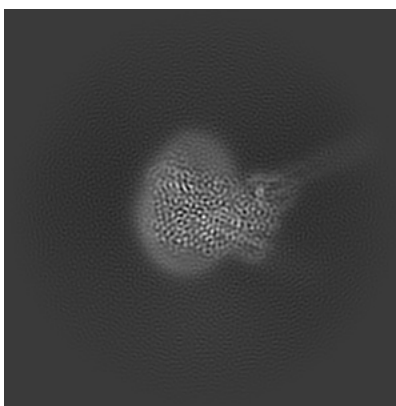
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

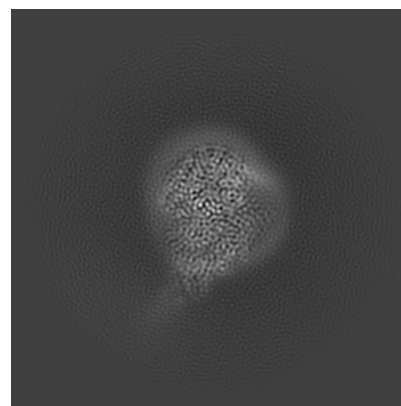
6.1.1 Primary map



X

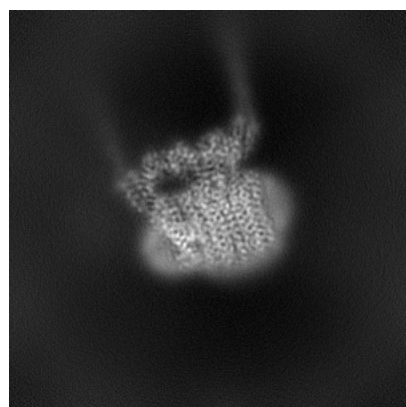


Y

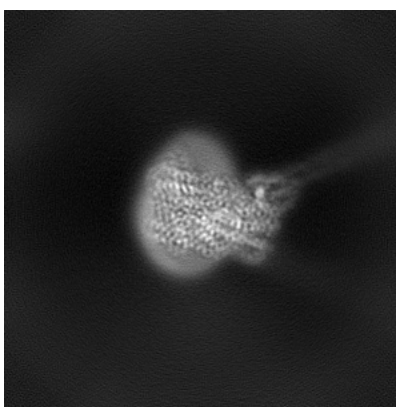


Z

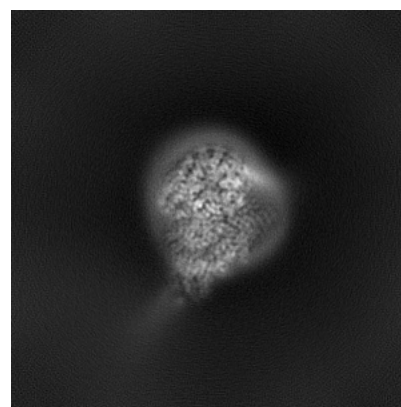
6.1.2 Raw map



X



Y

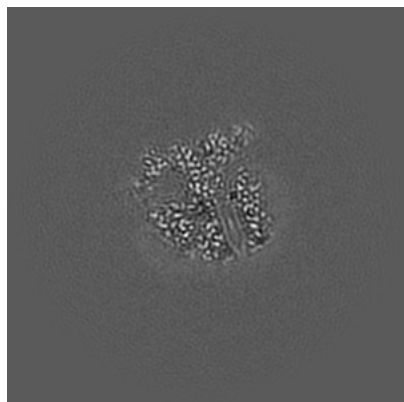


Z

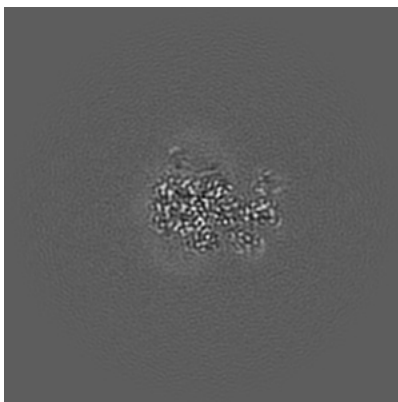
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

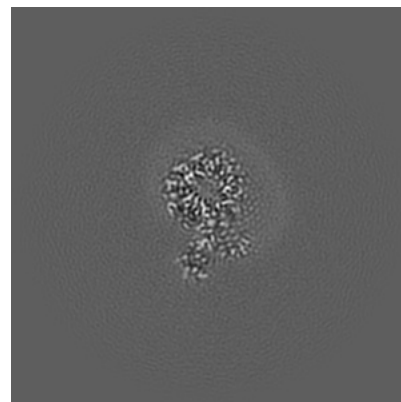
6.2.1 Primary map



X Index: 160

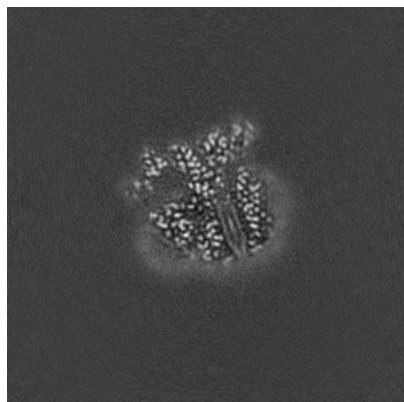


Y Index: 160

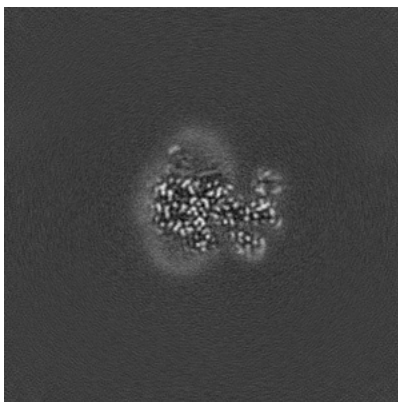


Z Index: 160

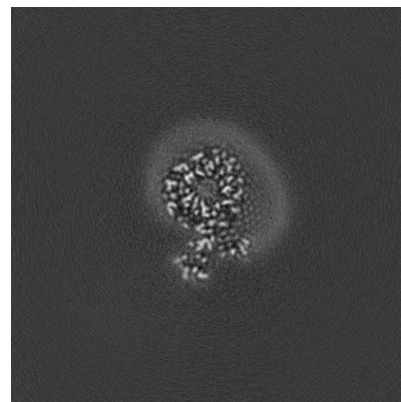
6.2.2 Raw map



X Index: 160



Y Index: 160

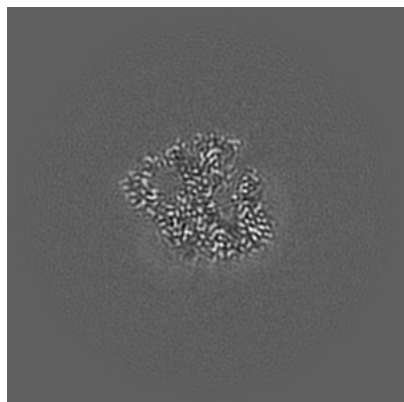


Z Index: 160

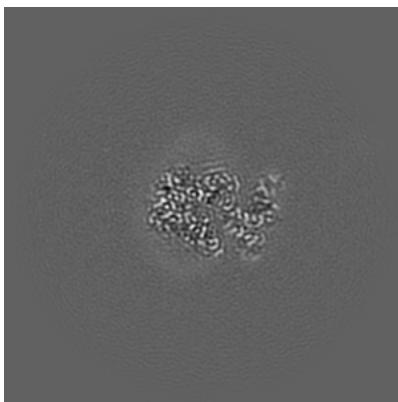
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

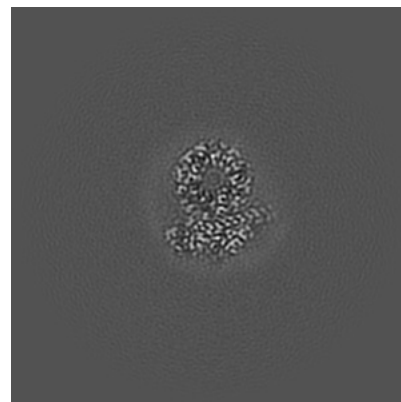
6.3.1 Primary map



X Index: 152

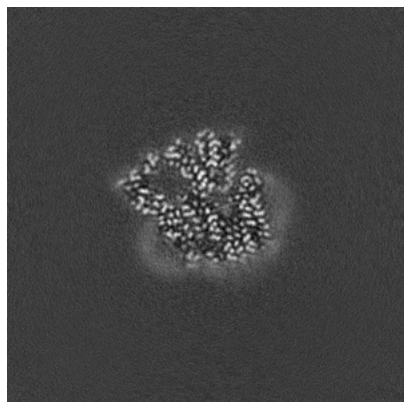


Y Index: 167

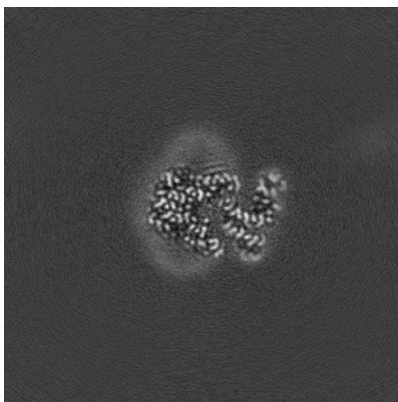


Z Index: 138

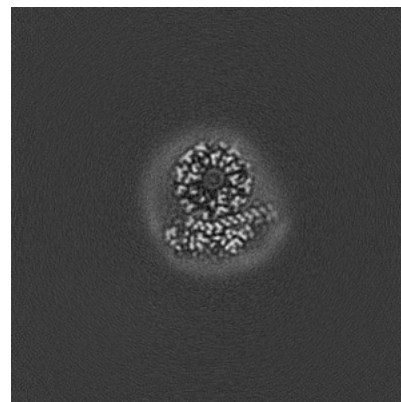
6.3.2 Raw map



X Index: 150



Y Index: 167

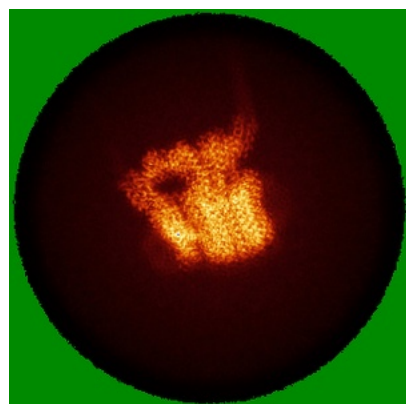


Z Index: 138

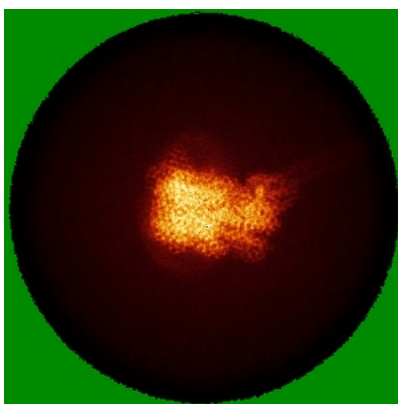
The images above show the largest variance slices of the map in three orthogonal directions.

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

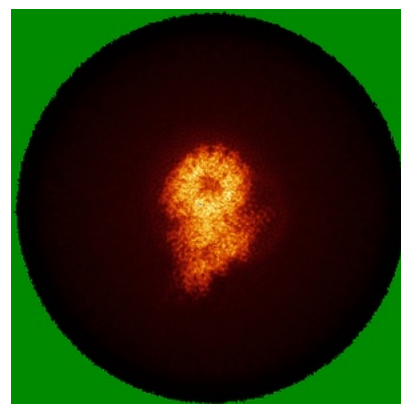
6.4.1 Primary map



X

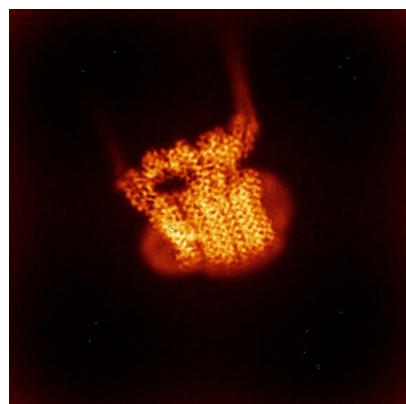


Y

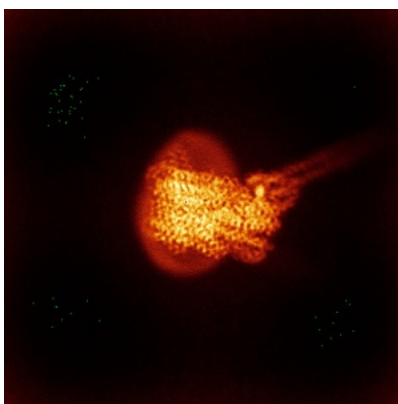


Z

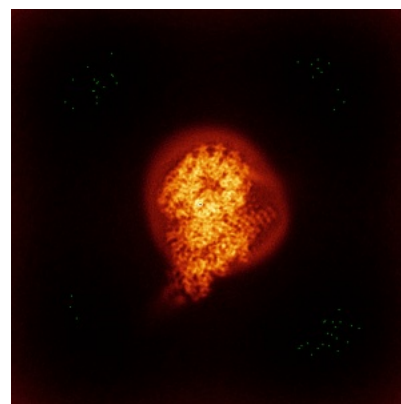
6.4.2 Raw map



X



Y

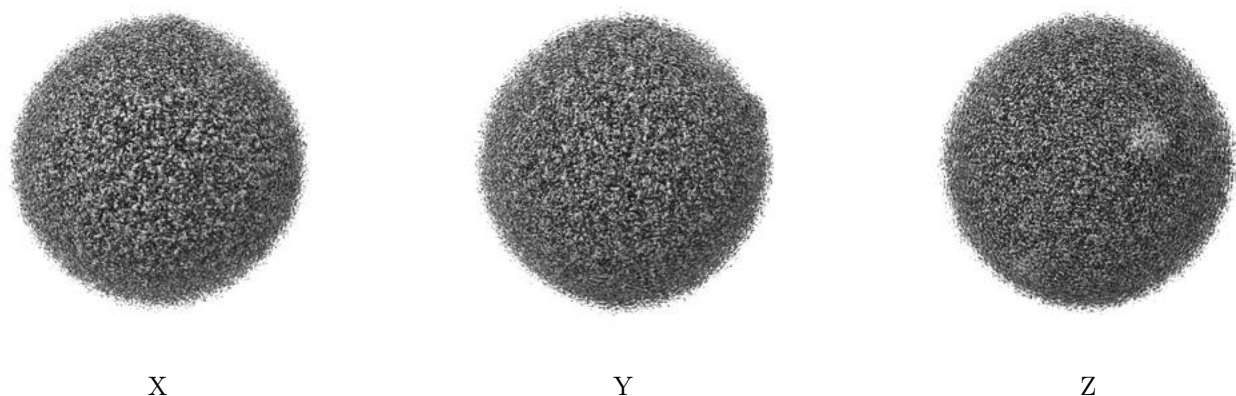


Z

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

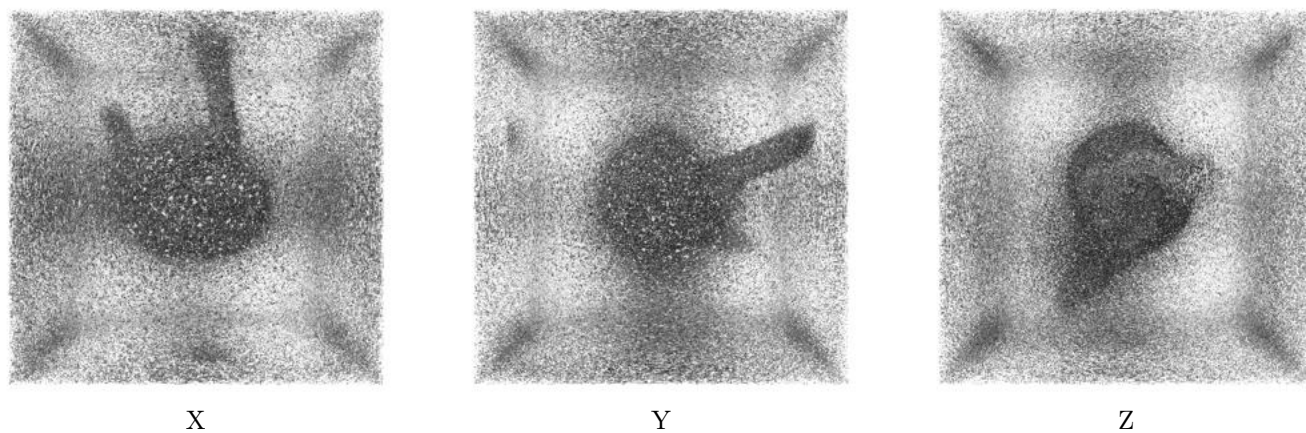
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_39644_msk_1.map [i](#)



X



Y

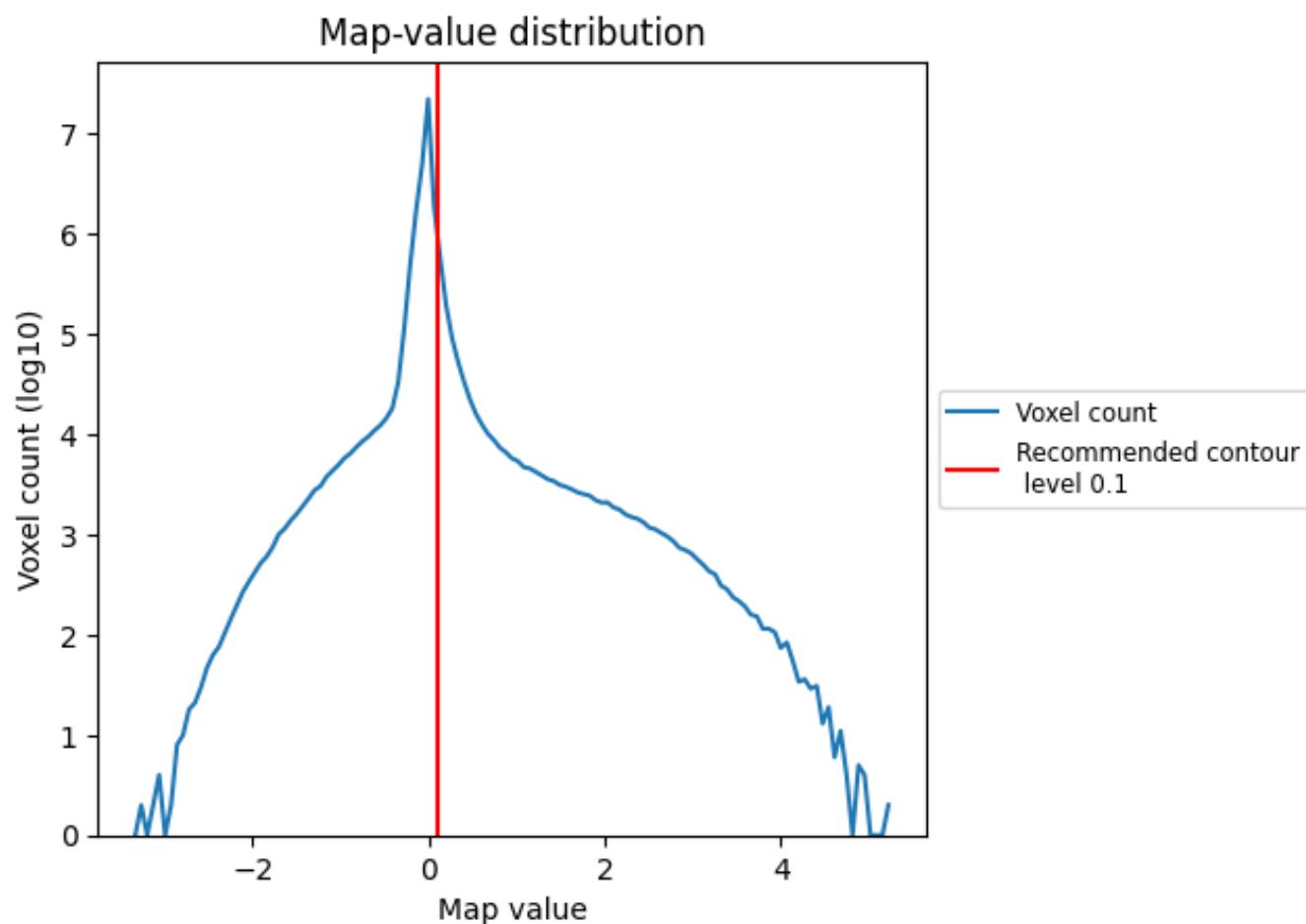


Z

7 Map analysis [i](#)

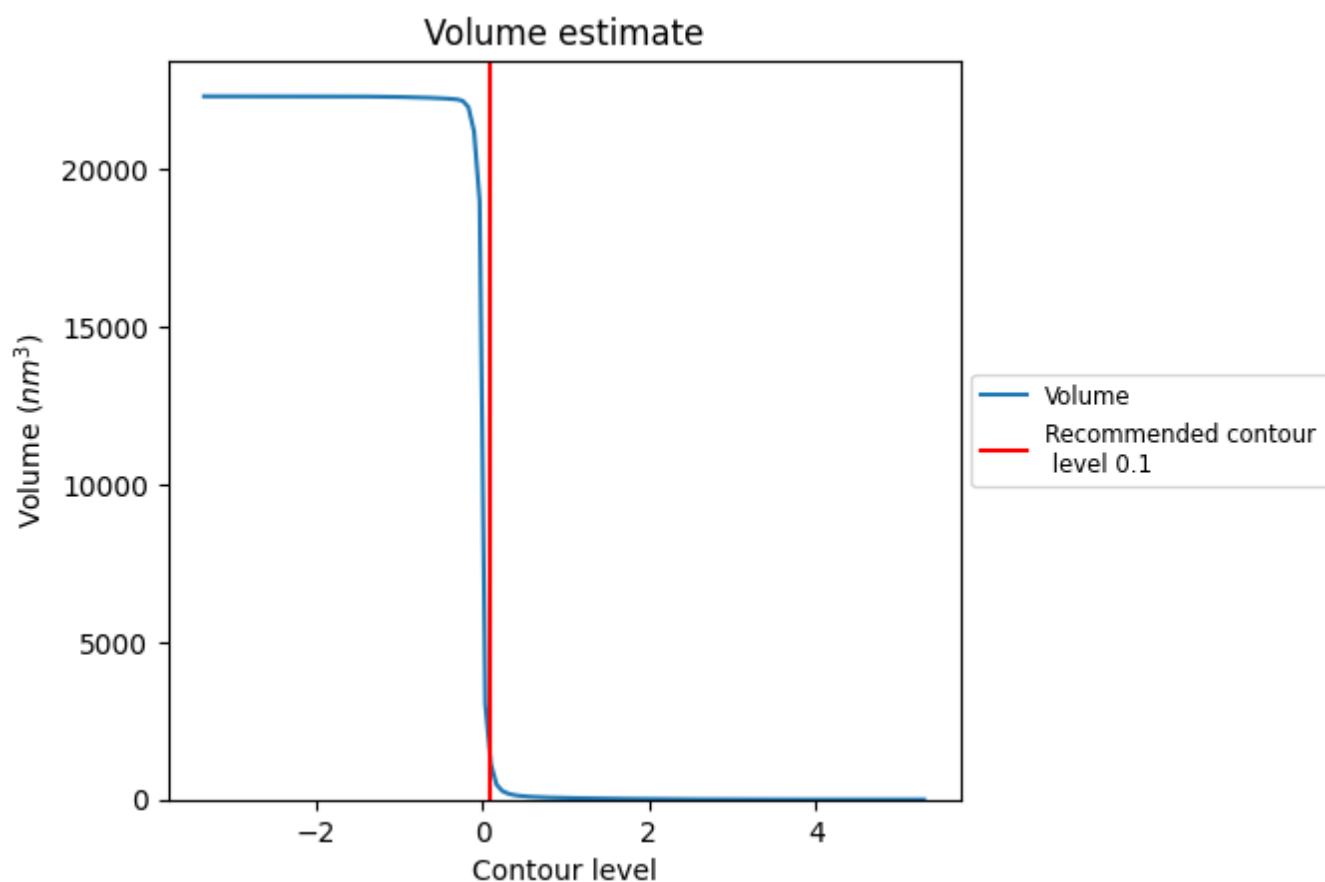
This section contains the results of statistical analysis of the map.

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.

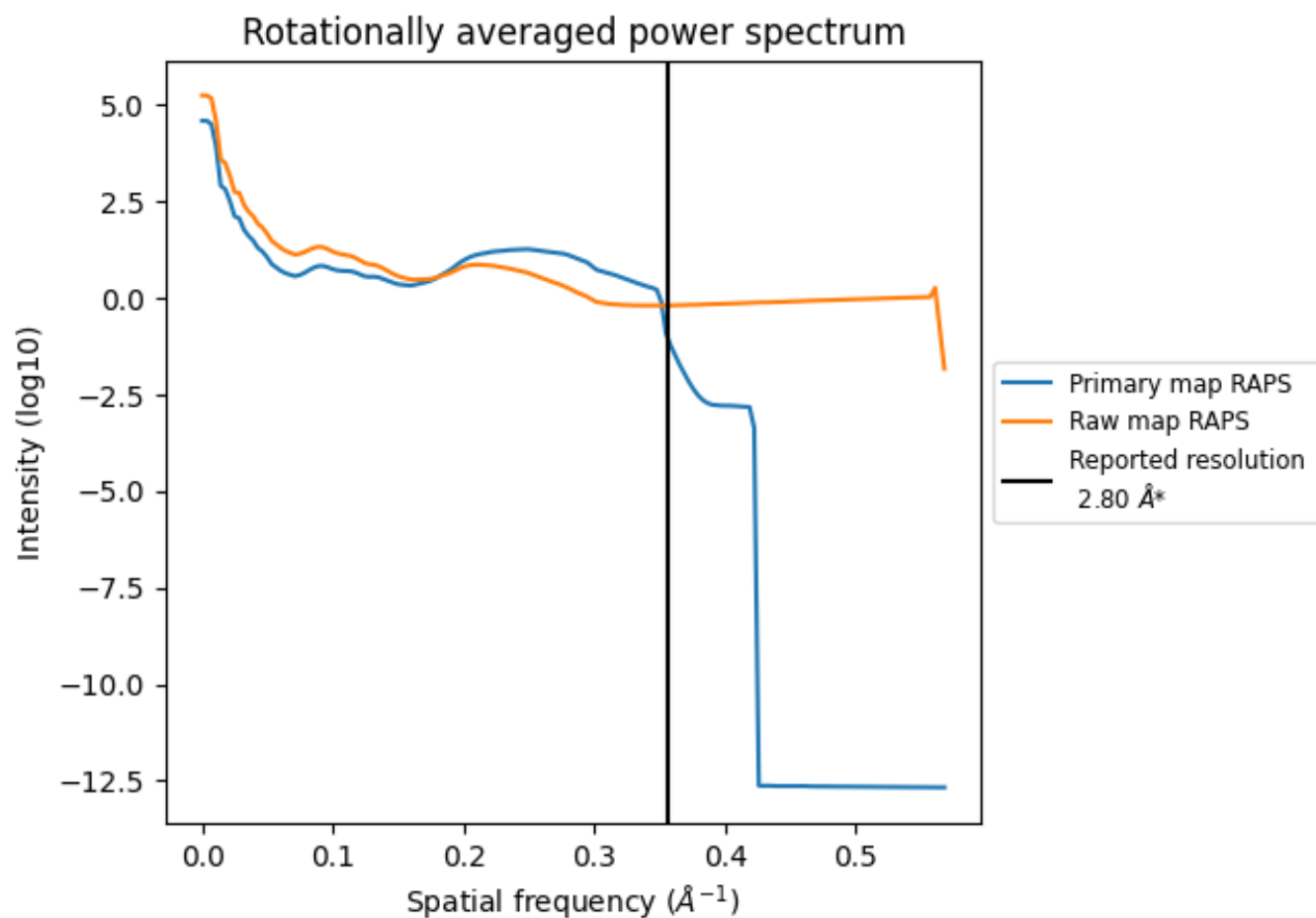
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1186 nm³; this corresponds to an approximate mass of 1071 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 ⓘ

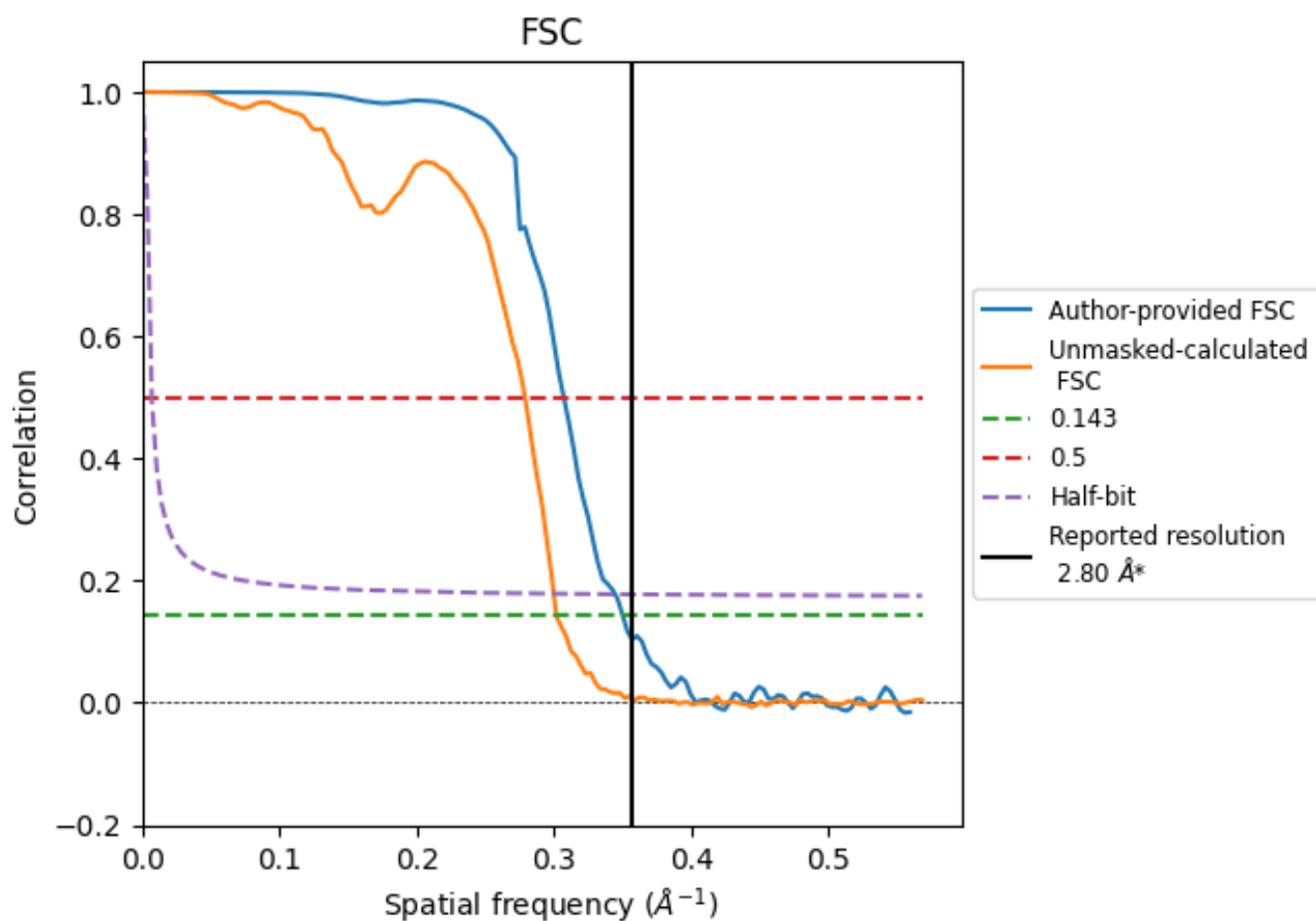


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

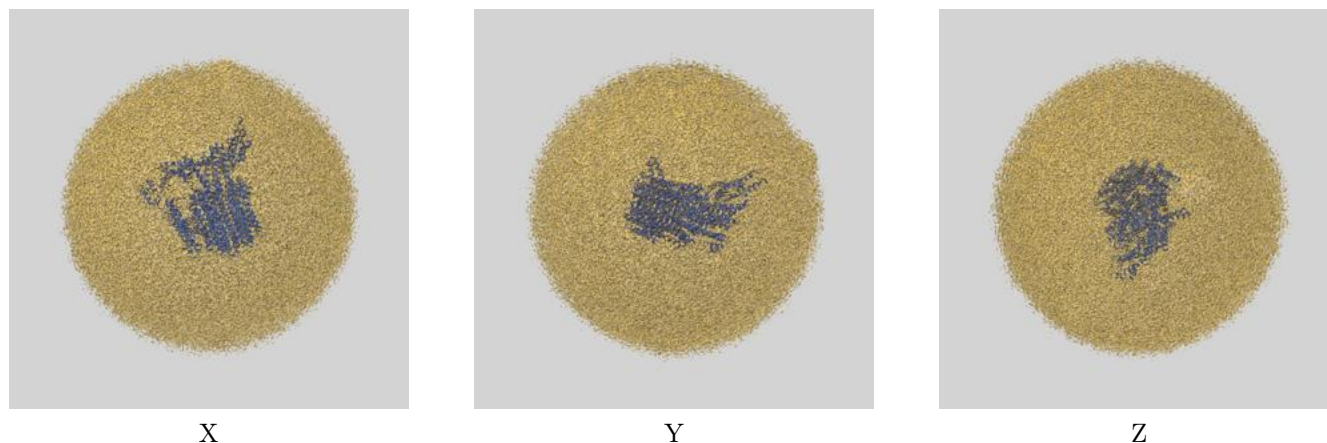
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.86	3.26	2.90
Unmasked-calculated*	3.31	3.59	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

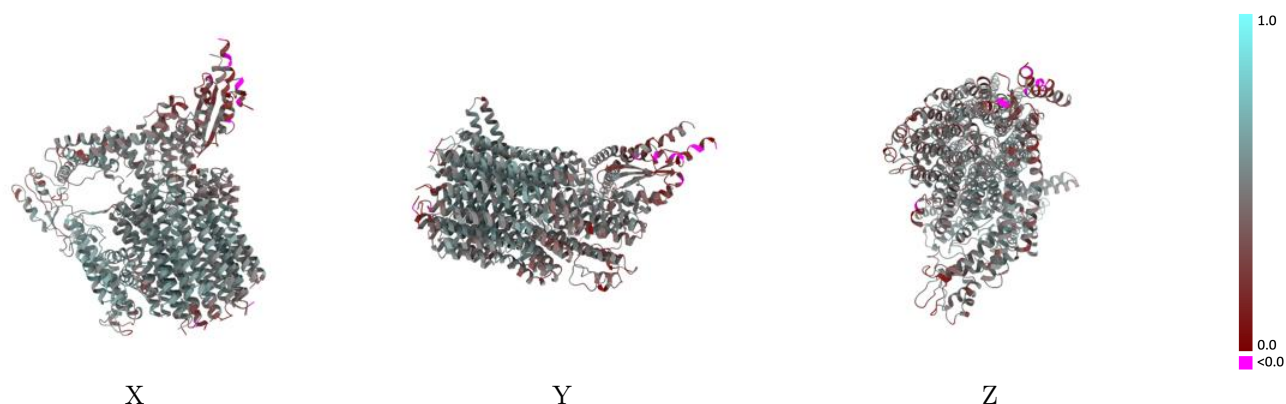
This section contains information regarding the fit between EMDB map EMD-39644 and PDB model 8YWT. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



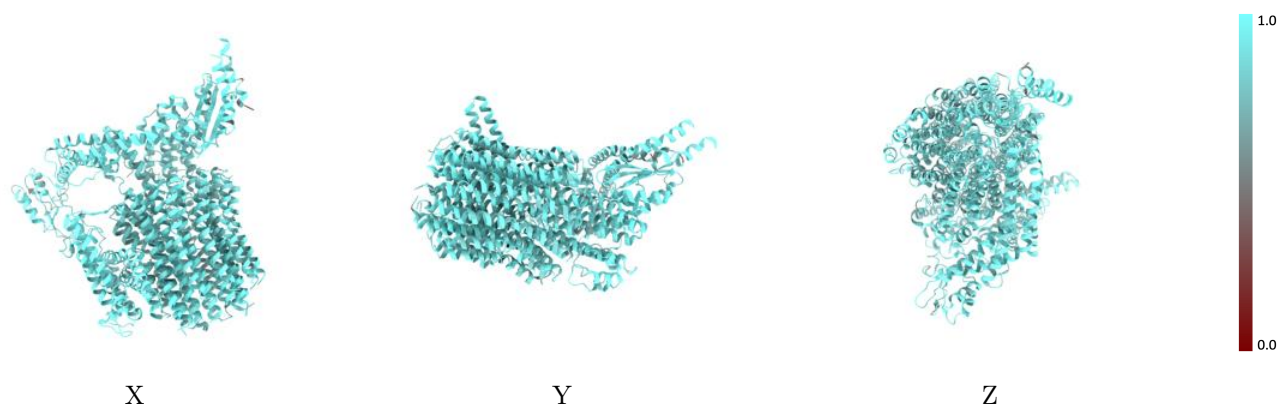
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



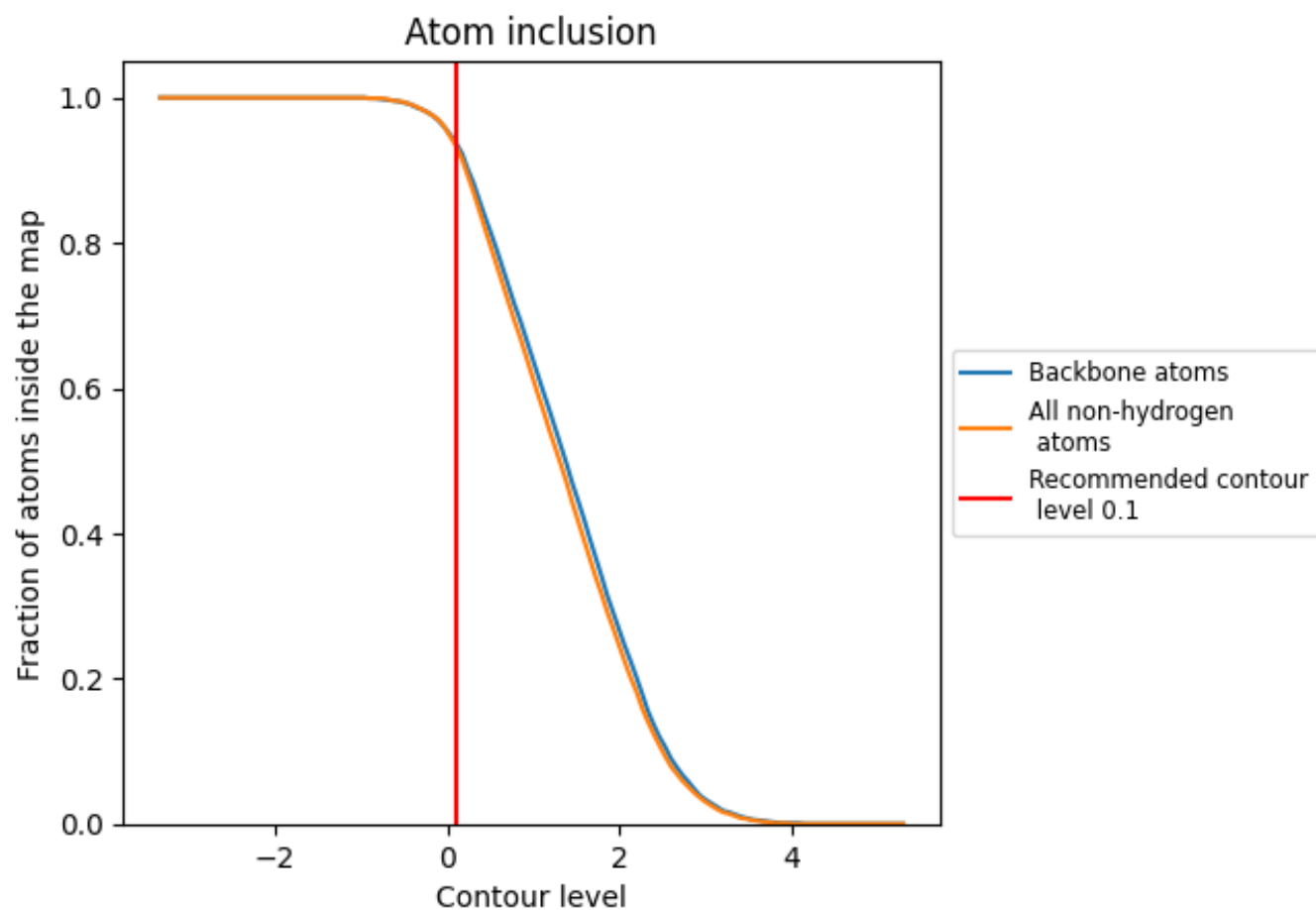
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.4760
K	 0.9660	 0.3040
L	 0.8630	 0.0840
M	 0.9370	 0.4430
N	 0.9430	 0.4710
O	 0.9280	 0.5080
P	 0.9070	 0.4650
Q	 0.9150	 0.4700
R	 0.9050	 0.4710
S	 0.8970	 0.4500
T	 0.9140	 0.4760
U	 0.9360	 0.5150
V	 0.9350	 0.5090
W	 0.9390	 0.5310
X	 0.9500	 0.5320
Y	 0.9640	 0.5540
Z	 0.9420	 0.5380

