



Full wwPDB EM Validation Report ⓘ

Mar 13, 2026 – 01:53 AM UTC

PDB ID : 9R87 / pdb_00009r87
EMDB ID : EMD-53806
Title : Cap of the vault protein from Human Brain
Authors : Lovestam, S.L.; Scheres, S.H.W.
Deposited on : 2025-05-15
Resolution : 3.60 Å(reported)

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

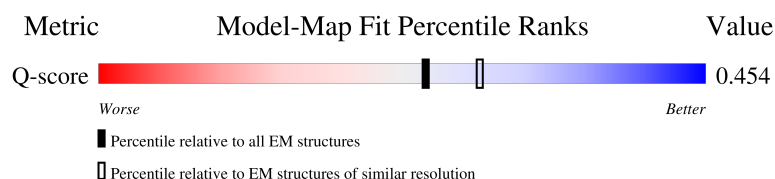
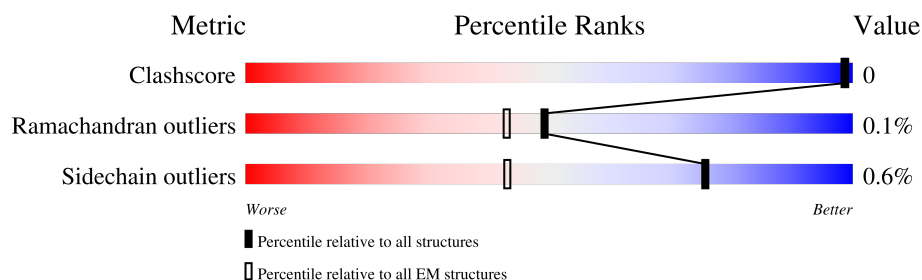
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

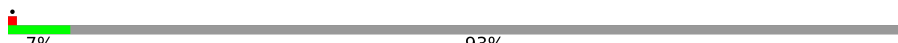
The reported resolution of this entry is 3.60 Å.

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	12797 (3.10 - 4.10)

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	893	
1	A1	893	
1	A2	893	
1	A3	893	

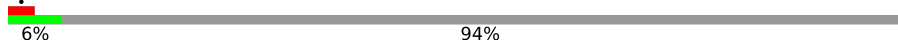
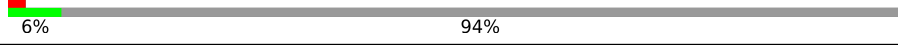
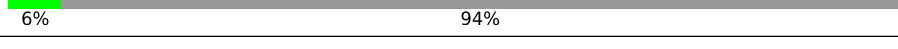
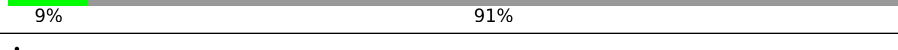
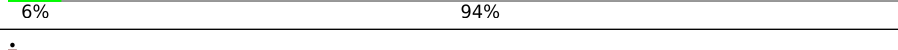
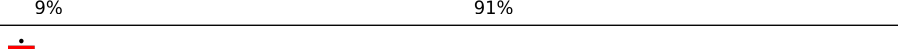
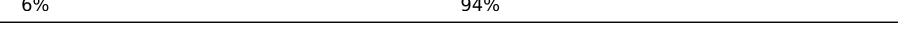
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Mol	Chain	Length	Quality of chain	
1	A4	893		93%
1	Ar	893		93%
1	As	893		93%
1	At	893		93%
1	Au	893		93%
1	Av	893		93%
1	Aw	893		93%
1	Ax	893		93%
1	Ay	893		93%
1	Az	893		93%
1	B	893		94%
1	C	893		91%
1	D	893		94%
1	E	893		91%
1	F	893		94%
1	G	893		91%
1	H	893		94%
1	I	893		91%
1	J	893		94%
1	K	893		91%
1	L	893		94%
1	M	893		91%
1	N	893		94%
1	O	893		91%
1	P	893		94%

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Mol	Chain	Length	Quality of chain
1	Q	893	 9%91%
1	R	893	 6%94%
1	S	893	 9%91%
1	T	893	 6%94%
1	U	893	 9%91%
1	V	893	 6%94%
1	W	893	 9%91%
1	X	893	 6%94%
1	Y	893	 9%91%
1	Z	893	 6%94%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 42419 atoms, of which 21814 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 Major vault protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	A1	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	A2	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	A3	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	A4	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	Ar	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	As	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	At	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	Au	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	Av	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	Aw	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	Ax	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	Ay	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	Az	66	Total	C	H	N	O	S	0	0
			1048	322	541	84	99	2		
1	B	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	C	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	D	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	E	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	F	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	G	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	H	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	I	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	J	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	K	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	L	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	M	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	N	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	O	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	P	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	Q	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	R	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	S	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	T	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	U	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	V	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	W	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		
1	X	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		
1	Y	84	Total	C	H	N	O	S	0	0
			1297	404	665	104	122	2		

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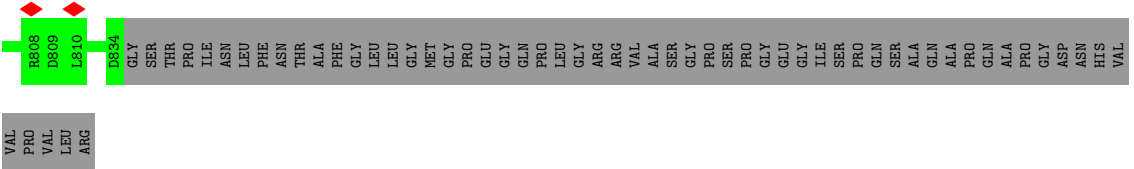
Mol	Chain	Residues	Atoms						AltConf	Trace
1	Z	58	Total	C	H	N	O	S	0	0
			918	283	472	75	86	2		



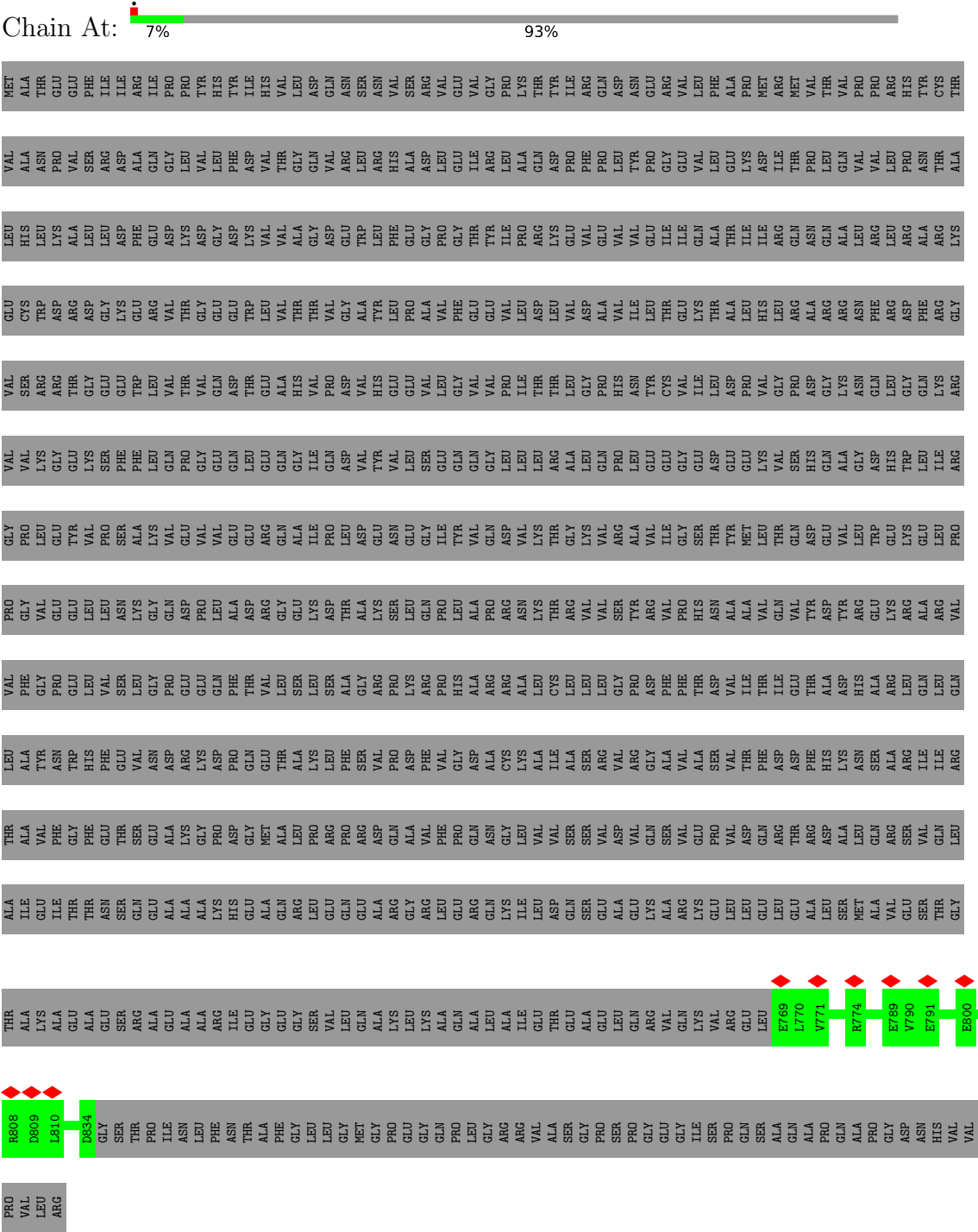


- Molecule 1: Major vault protein

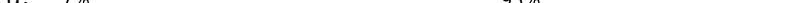




• Molecule 1: Major vault protein

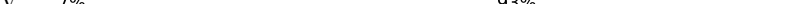


• Molecule 1: Major vault protein

Chain Au:  7% 93%

[illegible]

- Molecule 1: Major vault protein

Chain Av:  7% 93%

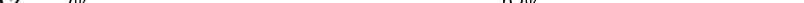
[illegible]



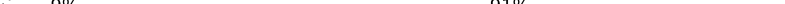


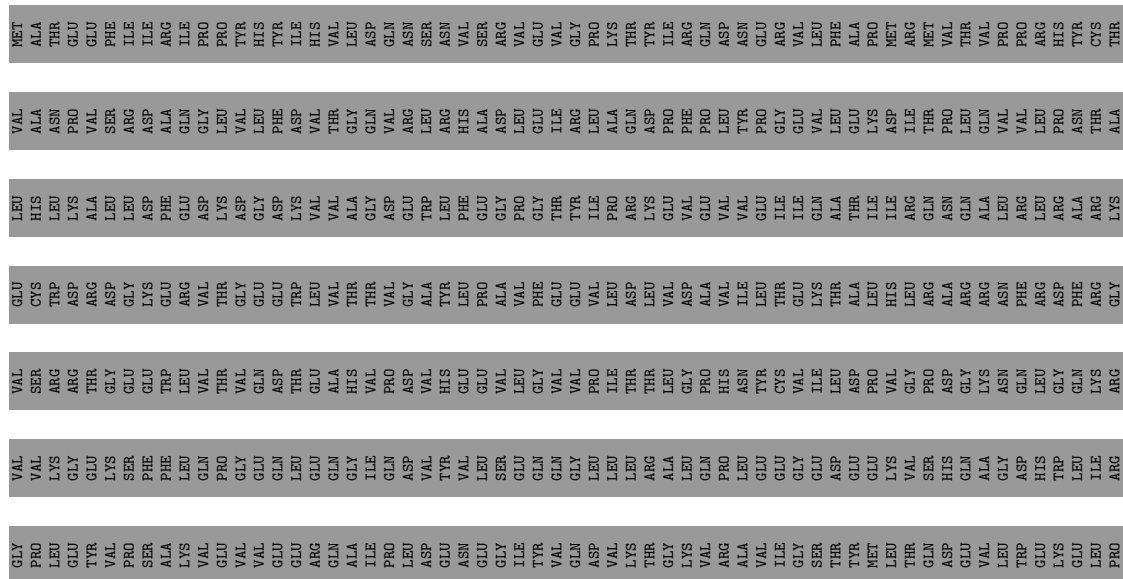
[illegible]

- Molecule 1: Major vault protein

Chain Az:  7% 93%

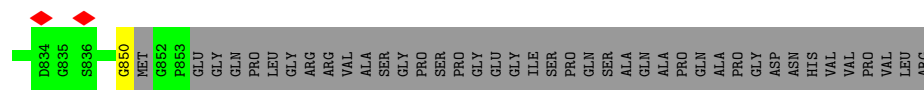


Chain C:  9% 91%



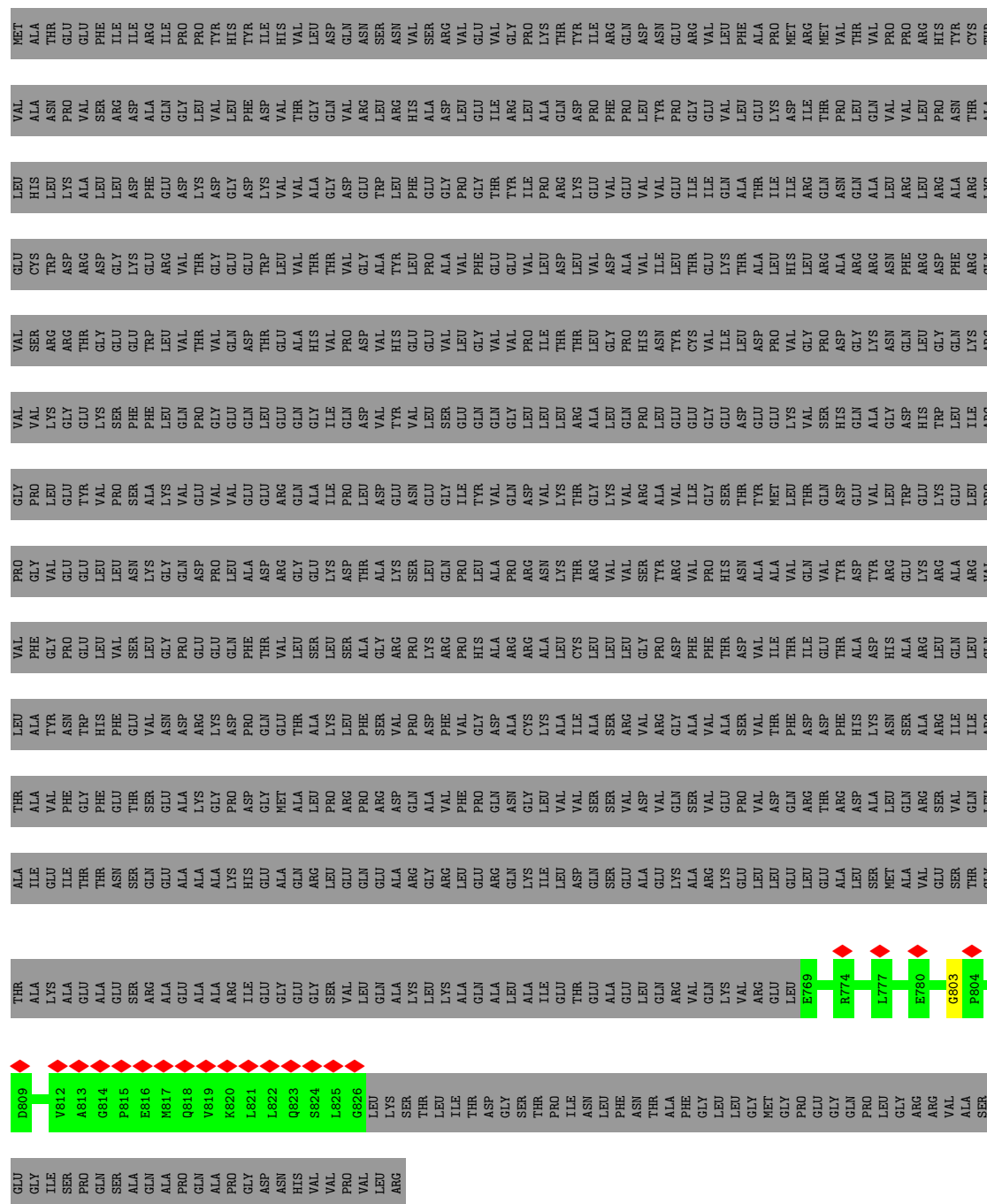






- Molecule 1: Major vault protein

Chain H: 6% 94%



- Molecule 1: Major vault protein

Chain I: 9% 91%



7833	7839	7850	MET	7852	7853	GLU	GLY	GLN	PRO	PRO	GLY	ARG	ARG	VAL	ALA	ALA	GLY	PRO	PRO	PRO	GLY	GLY	ILE	SER	SER	GLN	GLN	ALA	ALA	ALA	GLN	PRO	PRO	GLY	ASP	ASN	HIS	VAL	VAL	PRO	PRO	VAL	VAL	LEU
------	------	------	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

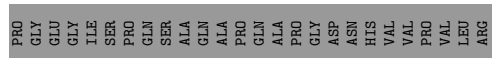
Chain P:

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

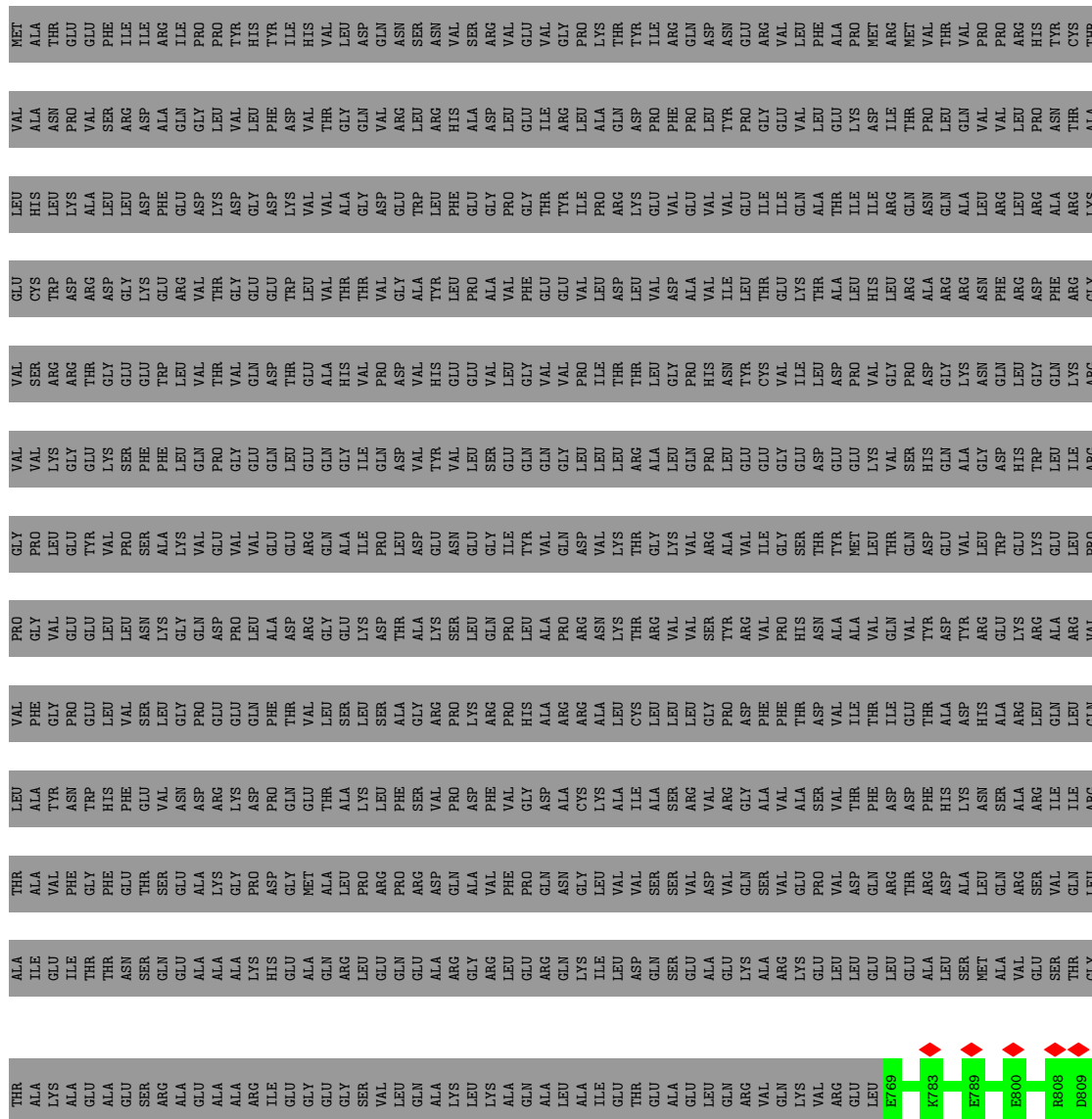
GLY	ILE	SER	PRO	GLN	SER	ALA	GLN	ALA	ALA	PRO	PRO	GLN	GLN	VAL	VAL	VAL	VAL	LEU	ARG																																						
D809	A813	G814	F815	E816	M817	Q818	V819	K820	L821	L822	Q823	S824	L825	Q826	LEU	LYS	SER	THR	LEU	ILE	THR	ASP	GLY	SER	SER	THR	PRO	ILE	ASN	LEU	PHE	ASN	THR	ALA	PHE	GLY	LEU	LEU	GLY	MET	PRO	GLY	GLU	GLN	PRO	LEU	GLY	ARG	VAL	ALA	SER	GLY	PRO	SER	PRO	GLY	GLU

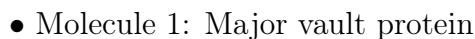
- Chain Q:  9% 91%





Chain S: 9% 91%





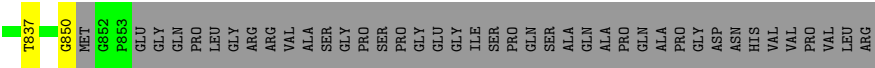
- Molecule 1: Major vault protein

Chain V: 6% 94%

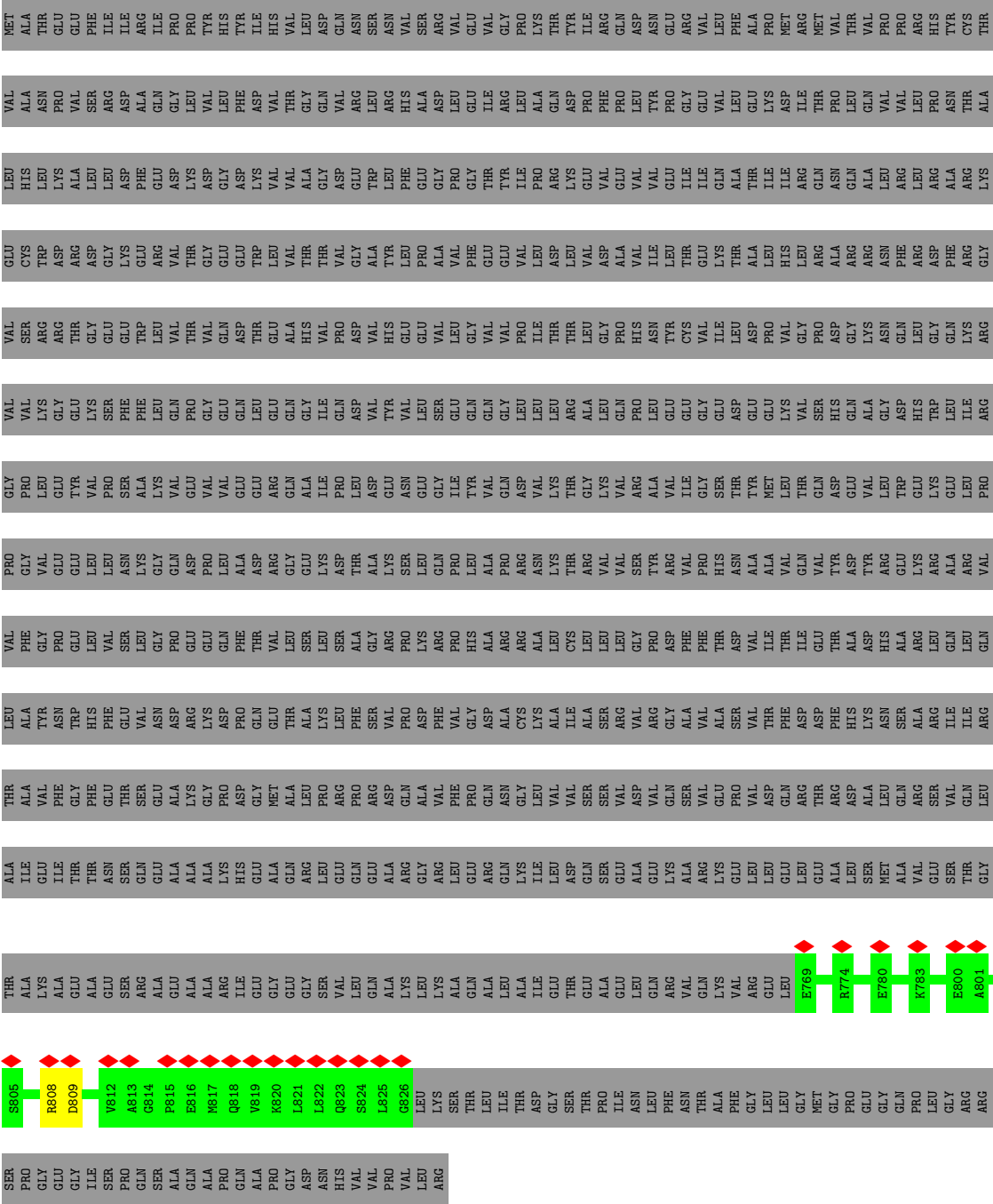
[illegible]







• Molecule 1: Major vault protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65387	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.259	Depositor
Minimum map value	-0.208	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	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	0.65	0/639	1.22	0/863
1	A1	0.63	0/510	1.26	0/686
1	A2	0.64	0/510	1.26	0/686
1	A3	0.63	0/510	1.26	0/686
1	A4	0.62	0/510	1.22	0/686
1	Ar	0.63	0/510	1.23	0/686
1	As	0.63	0/510	1.25	0/686
1	At	0.63	0/510	1.25	0/686
1	Au	0.63	0/510	1.25	0/686
1	Av	0.63	0/510	1.27	0/686
1	Aw	0.64	0/510	1.26	0/686
1	Ax	0.64	0/510	1.25	0/686
1	Ay	0.63	0/510	1.26	0/686
1	Az	0.63	0/510	1.26	0/686
1	B	0.65	0/449	1.31	1/603 (0.2%)
1	C	0.65	0/639	1.23	0/863
1	D	0.68	0/449	1.36	1/603 (0.2%)
1	E	0.64	0/639	1.21	0/863
1	F	0.65	0/449	1.34	1/603 (0.2%)
1	G	0.65	0/639	1.22	0/863
1	H	0.65	0/449	1.33	2/603 (0.3%)
1	I	0.65	0/639	1.19	0/863
1	J	0.64	0/449	1.28	1/603 (0.2%)
1	K	0.66	0/639	1.20	0/863
1	L	0.65	0/449	1.34	1/603 (0.2%)
1	M	0.64	0/639	1.21	0/863
1	N	0.65	0/449	1.32	1/603 (0.2%)
1	O	0.64	0/639	1.24	0/863
1	P	0.65	0/449	1.34	0/603
1	Q	0.64	0/639	1.22	0/863
1	R	0.65	0/449	1.34	0/603
1	S	0.65	0/639	1.26	0/863
1	T	0.65	0/449	1.35	1/603 (0.2%)
1	U	0.65	0/639	1.22	0/863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	V	0.65	0/449	1.33	0/603
1	W	0.64	0/639	1.22	0/863
1	X	0.65	0/449	1.34	0/603
1	Y	0.65	0/639	1.22	0/863
1	Z	0.65	0/449	1.35	1/603 (0.2%)
All	All	0.64	0/20774	1.26	10/27976 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	809	ASP	CA-CB-CG	5.50	118.10	112.60
1	F	809	ASP	CA-CB-CG	5.25	117.85	112.60
1	J	808	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	808	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	B	809	ASP	CA-CB-CG	5.12	117.72	112.60
1	T	774	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	H	803	GLY	CA-C-N	5.03	126.13	119.84
1	H	803	GLY	C-N-CA	5.03	126.13	119.84
1	L	809	ASP	CA-CB-CG	5.03	117.63	112.60
1	N	809	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

There are no planarity outliers.

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	A	632	665	664	1	0
1	A1	507	541	540	0	0
1	A2	507	541	540	1	0
1	A3	507	541	540	0	0
1	A4	507	541	540	0	0
1	Ar	507	541	540	0	0
1	As	507	541	540	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	At	507	541	540	0	0
1	Au	507	541	540	0	0
1	Av	507	541	540	0	0
1	Aw	507	541	540	0	0
1	Ax	507	541	540	0	0
1	Ay	507	541	540	0	0
1	Az	507	541	540	0	0
1	B	446	472	471	0	0
1	C	632	665	664	0	0
1	D	446	472	471	0	0
1	E	632	665	664	0	0
1	F	446	472	471	0	0
1	G	632	665	664	0	0
1	H	446	472	471	0	0
1	I	632	665	664	0	0
1	J	446	472	471	0	0
1	K	632	665	664	0	0
1	L	446	472	471	0	0
1	M	632	665	664	0	0
1	N	446	472	471	0	0
1	O	632	665	664	1	0
1	P	446	472	471	0	0
1	Q	632	665	664	0	0
1	R	446	472	471	0	0
1	S	632	665	664	1	0
1	T	446	472	471	0	0
1	U	632	665	664	0	0
1	V	446	472	471	0	0
1	W	632	665	664	0	0
1	X	446	472	471	0	0
1	Y	632	665	664	0	0
1	Z	446	472	471	0	0
All	All	20605	21814	21775	3	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 0.

All (3) 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:O:833:THR:HG22	1:O:839:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:817:MET:HE1	1:S:812:VAL:HG13	1.99	0.45
1:A:770:LEU:HD21	1:As:775:ALA:HB1	2.01	0.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	A1	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	A2	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	A3	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	A4	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	Ar	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	As	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	At	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	Au	64/893 (7%)	60 (94%)	4 (6%)	0	100	100
1	Av	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	Aw	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	Ax	64/893 (7%)	63 (98%)	1 (2%)	0	100	100
1	Ay	64/893 (7%)	61 (95%)	3 (5%)	0	100	100
1	Az	64/893 (7%)	62 (97%)	2 (3%)	0	100	100
1	B	56/893 (6%)	56 (100%)	0	0	100	100
1	C	82/893 (9%)	79 (96%)	3 (4%)	0	100	100
1	D	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	E	82/893 (9%)	78 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	G	82/893 (9%)	78 (95%)	3 (4%)	1 (1%)	10	41
1	H	56/893 (6%)	52 (93%)	4 (7%)	0	100	100
1	I	82/893 (9%)	79 (96%)	3 (4%)	0	100	100
1	J	35/893 (4%)	35 (100%)	0	0	100	100
1	K	82/893 (9%)	80 (98%)	1 (1%)	1 (1%)	10	41
1	L	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	M	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	N	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	O	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	P	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	Q	82/893 (9%)	79 (96%)	3 (4%)	0	100	100
1	R	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	S	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	T	56/893 (6%)	53 (95%)	3 (5%)	0	100	100
1	U	82/893 (9%)	78 (95%)	4 (5%)	0	100	100
1	V	56/893 (6%)	52 (93%)	4 (7%)	0	100	100
1	W	82/893 (9%)	76 (93%)	6 (7%)	0	100	100
1	X	56/893 (6%)	52 (93%)	4 (7%)	0	100	100
1	Y	82/893 (9%)	78 (95%)	3 (4%)	1 (1%)	10	41
1	Z	56/893 (6%)	54 (96%)	2 (4%)	0	100	100
All	All	2605/34827 (8%)	2490 (96%)	112 (4%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	850	GLY
1	G	850	GLY
1	K	850	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	A	69/755 (9%)	69 (100%)	0	100	100
1	A1	56/755 (7%)	56 (100%)	0	100	100
1	A2	56/755 (7%)	55 (98%)	1 (2%)	51	68
1	A3	56/755 (7%)	56 (100%)	0	100	100
1	A4	56/755 (7%)	56 (100%)	0	100	100
1	Ar	56/755 (7%)	56 (100%)	0	100	100
1	As	56/755 (7%)	56 (100%)	0	100	100
1	At	56/755 (7%)	56 (100%)	0	100	100
1	Au	56/755 (7%)	56 (100%)	0	100	100
1	Av	56/755 (7%)	56 (100%)	0	100	100
1	Aw	56/755 (7%)	56 (100%)	0	100	100
1	Ax	56/755 (7%)	56 (100%)	0	100	100
1	Ay	56/755 (7%)	56 (100%)	0	100	100
1	Az	56/755 (7%)	56 (100%)	0	100	100
1	B	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	C	69/755 (9%)	69 (100%)	0	100	100
1	D	48/755 (6%)	48 (100%)	0	100	100
1	E	69/755 (9%)	69 (100%)	0	100	100
1	F	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	G	69/755 (9%)	69 (100%)	0	100	100
1	H	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	I	69/755 (9%)	69 (100%)	0	100	100
1	J	48/755 (6%)	48 (100%)	0	100	100
1	K	69/755 (9%)	69 (100%)	0	100	100
1	L	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	M	69/755 (9%)	68 (99%)	1 (1%)	59	71
1	N	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	O	69/755 (9%)	69 (100%)	0	100	100
1	P	48/755 (6%)	47 (98%)	1 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	69/755 (9%)	69 (100%)	0	100	100
1	R	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	S	69/755 (9%)	69 (100%)	0	100	100
1	T	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	U	69/755 (9%)	69 (100%)	0	100	100
1	V	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	W	69/755 (9%)	69 (100%)	0	100	100
1	X	48/755 (6%)	47 (98%)	1 (2%)	47	65
1	Y	69/755 (9%)	68 (99%)	1 (1%)	59	71
1	Z	48/755 (6%)	47 (98%)	1 (2%)	47	65
All	All	2249/29445 (8%)	2235 (99%)	14 (1%)	76	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A2	817	MET
1	B	808	ARG
1	F	808	ARG
1	H	808	ARG
1	L	808	ARG
1	M	806	THR
1	N	808	ARG
1	P	808	ARG
1	R	808	ARG
1	T	808	ARG
1	V	808	ARG
1	X	808	ARG
1	Y	837	THR
1	Z	808	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	786	GLN
1	A	818	GLN
1	A	823	GLN
1	A2	786	GLN

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Mol	Chain	Res	Type
1	A2	818	GLN
1	A3	797	GLN
1	Ar	786	GLN
1	As	786	GLN
1	At	786	GLN
1	Au	786	GLN
1	Aw	786	GLN
1	Ax	786	GLN
1	Ay	776	GLN
1	Ay	786	GLN
1	Az	786	GLN
1	B	776	GLN
1	B	797	GLN
1	B	823	GLN
1	C	786	GLN
1	D	797	GLN
1	D	823	GLN
1	E	818	GLN
1	E	823	GLN
1	F	797	GLN
1	G	823	GLN
1	H	797	GLN
1	I	776	GLN
1	I	818	GLN
1	I	823	GLN
1	J	776	GLN
1	J	797	GLN
1	J	823	GLN
1	K	818	GLN
1	K	823	GLN
1	L	776	GLN
1	L	797	GLN
1	L	823	GLN
1	N	797	GLN
1	O	818	GLN
1	P	776	GLN
1	P	797	GLN
1	Q	786	GLN
1	Q	818	GLN
1	R	776	GLN
1	R	797	GLN
1	R	823	GLN

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Mol	Chain	Res	Type
1	S	786	GLN
1	T	776	GLN
1	T	797	GLN
1	T	823	GLN
1	U	786	GLN
1	U	818	GLN
1	V	797	GLN
1	W	823	GLN
1	X	797	GLN
1	Y	786	GLN
1	Y	823	GLN
1	Z	797	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 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.

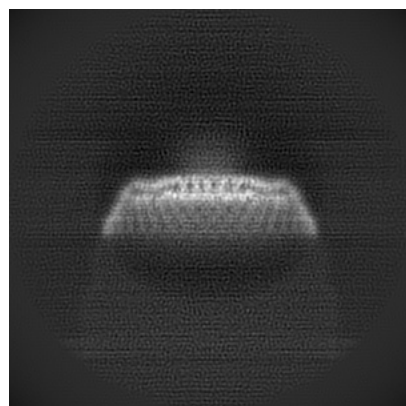
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53806. These allow visual inspection of the internal detail of the map and identification of artifacts.

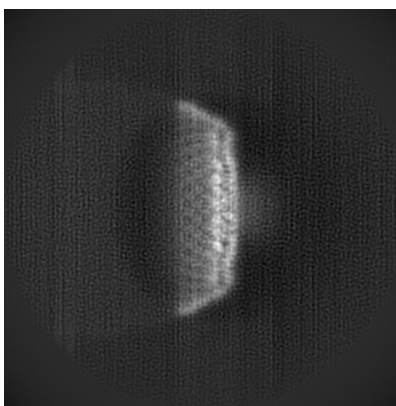
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

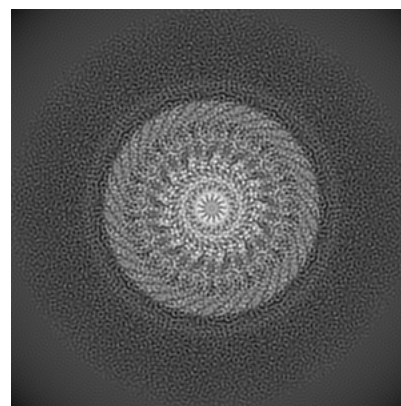
6.1.1 Primary map



X

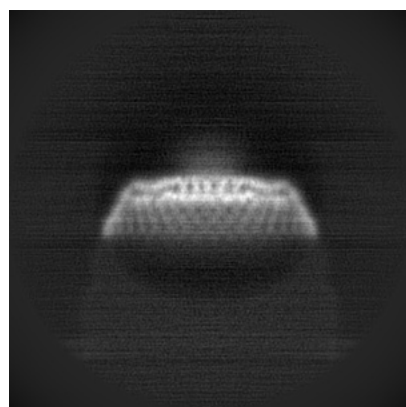


Y

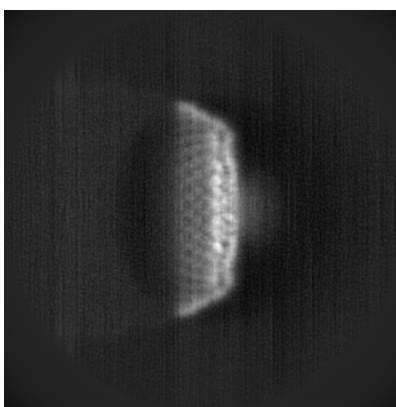


Z

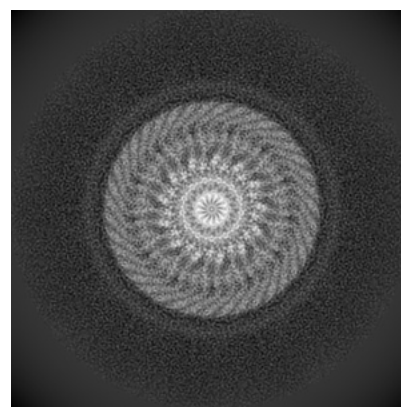
6.1.2 Raw map



X



Y

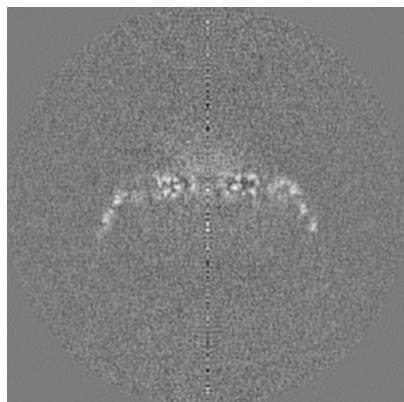


Z

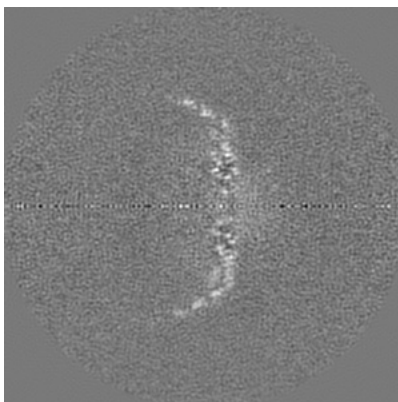
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

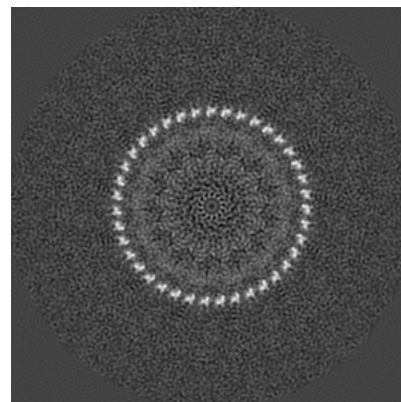
6.2.1 Primary map



X Index: 128



Y Index: 128

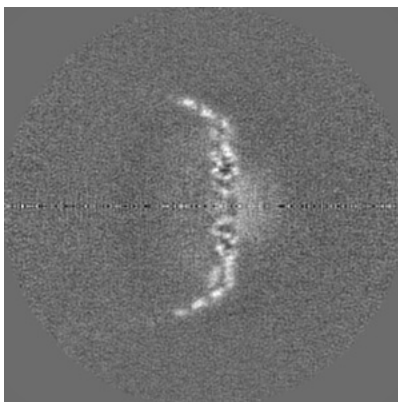


Z Index: 128

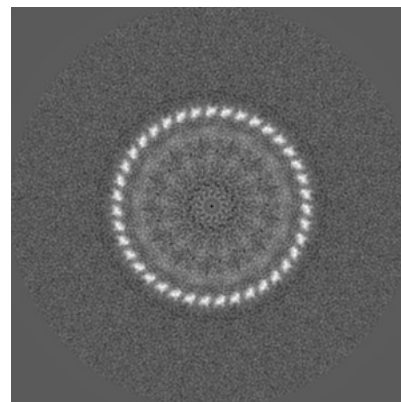
6.2.2 Raw map



X Index: 128



Y Index: 128

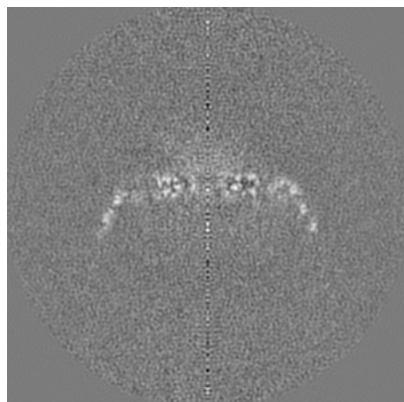


Z Index: 128

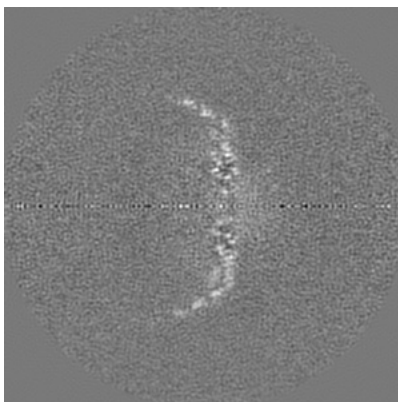
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

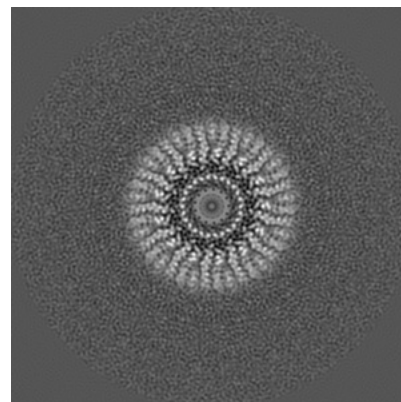
6.3.1 Primary map



X Index: 128

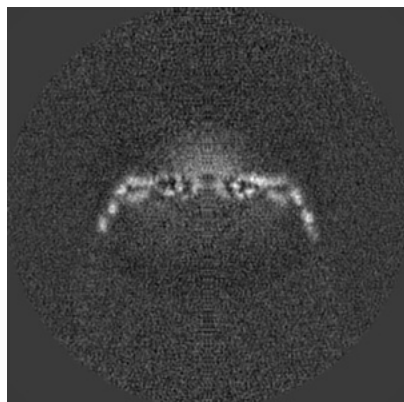


Y Index: 128

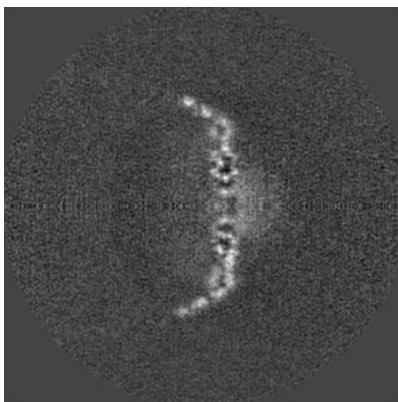


Z Index: 143

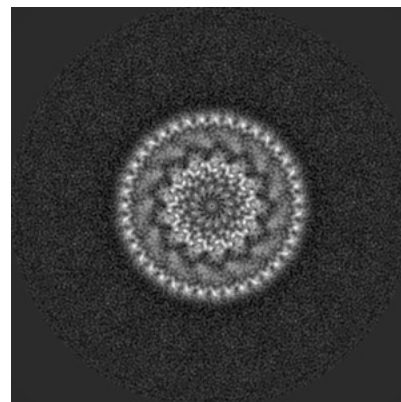
6.3.2 Raw map



X Index: 123



Y Index: 127

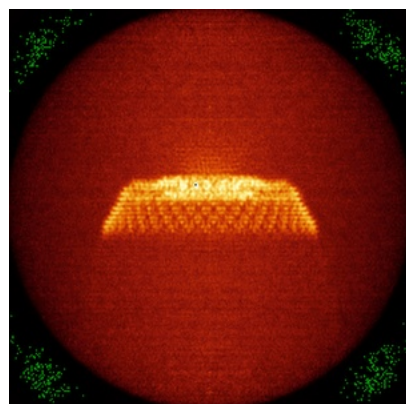


Z Index: 136

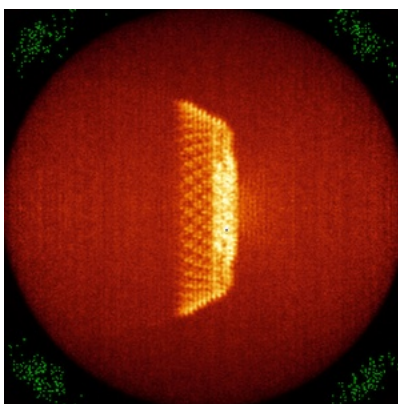
The images above show the largest variance slices of the map in three orthogonal directions.

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

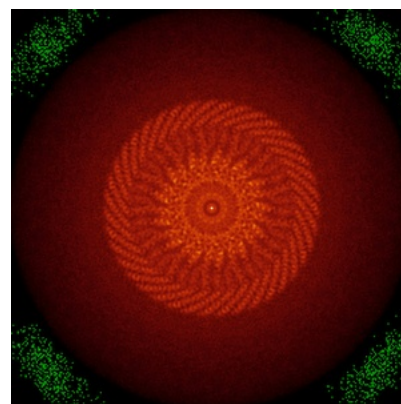
6.4.1 Primary map



X

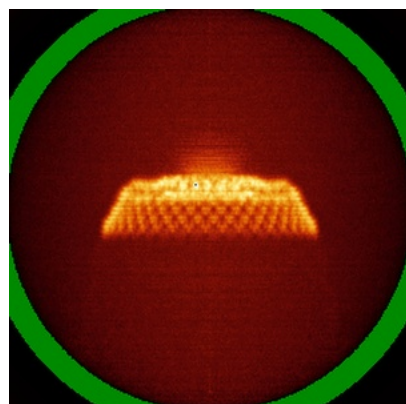


Y

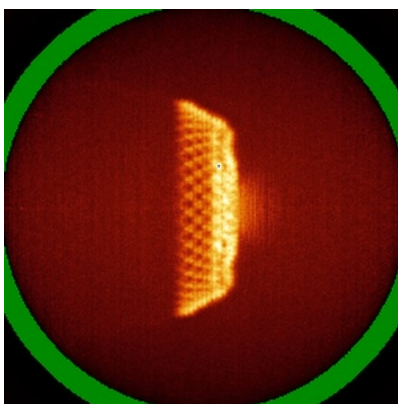


Z

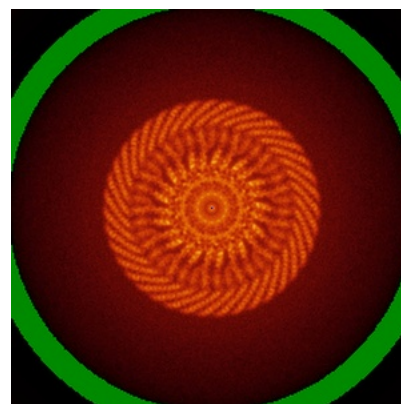
6.4.2 Raw map



X



Y

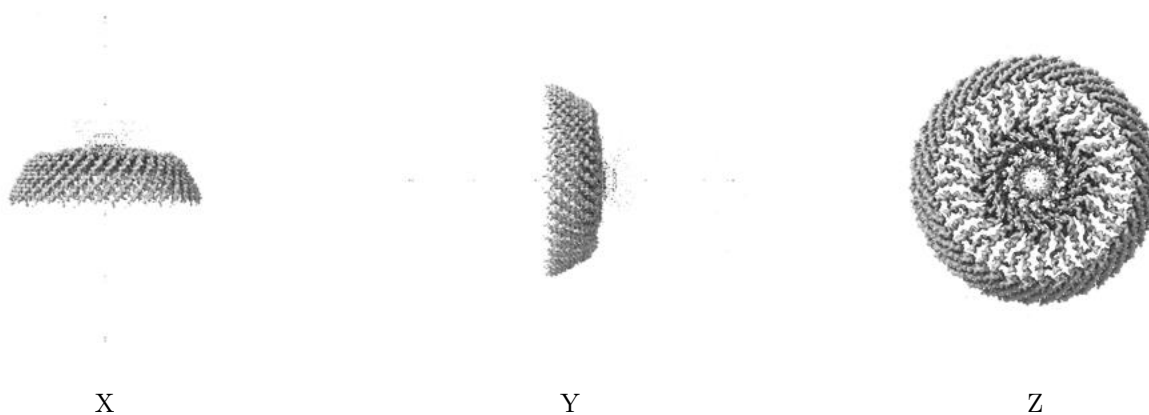


Z

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.

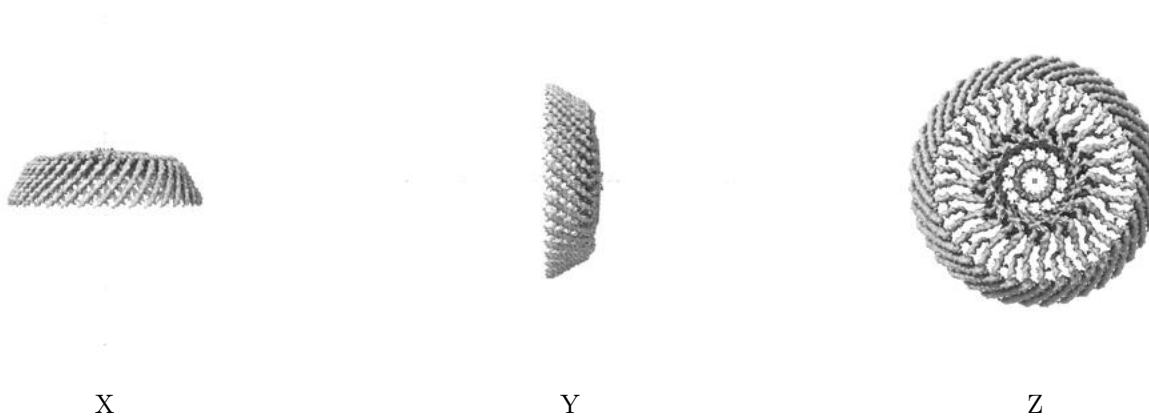
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

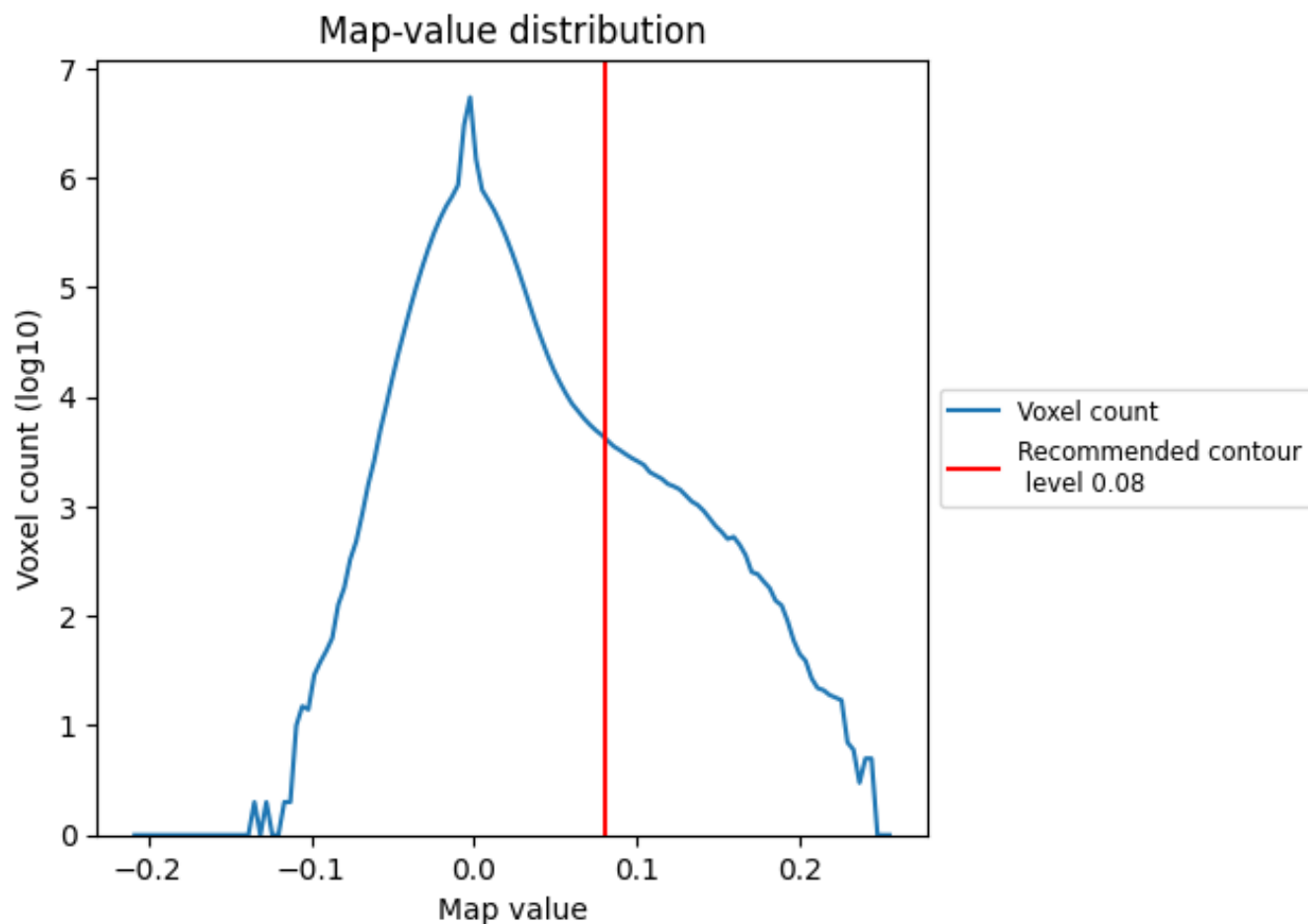
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

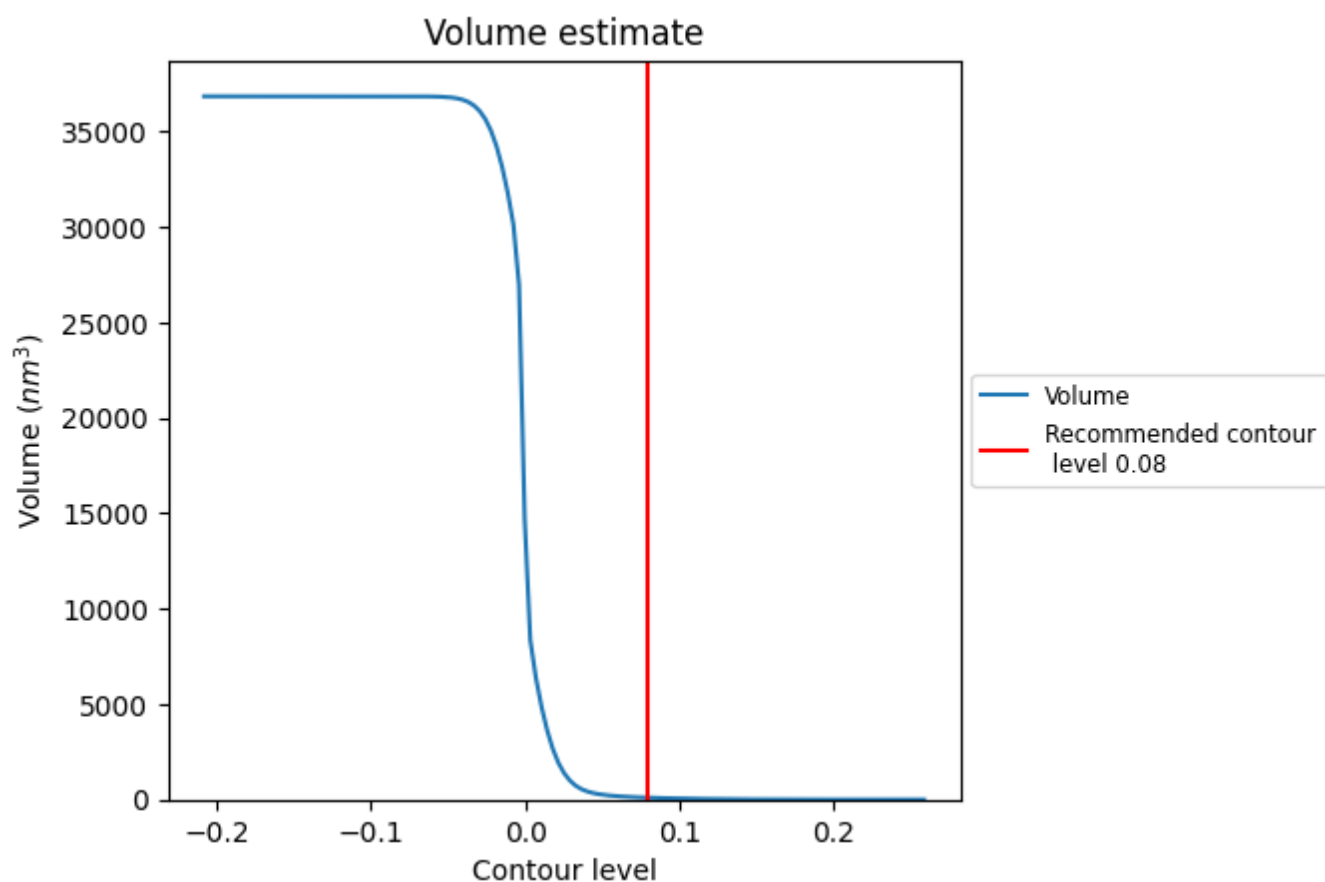
This section contains the results of statistical analysis of the map.

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.

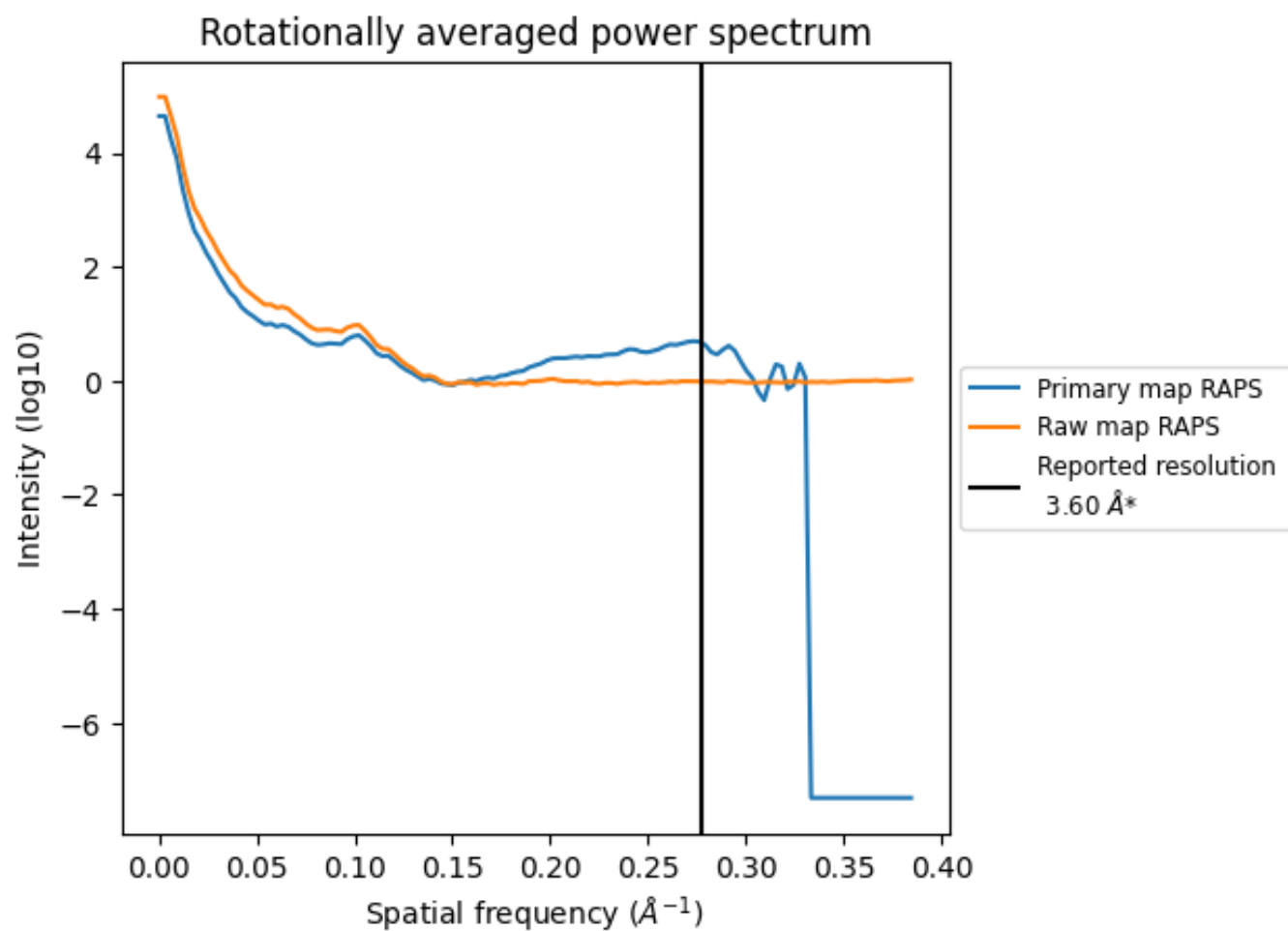
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm^3 ; this corresponds to an approximate mass of 88 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 ⓘ

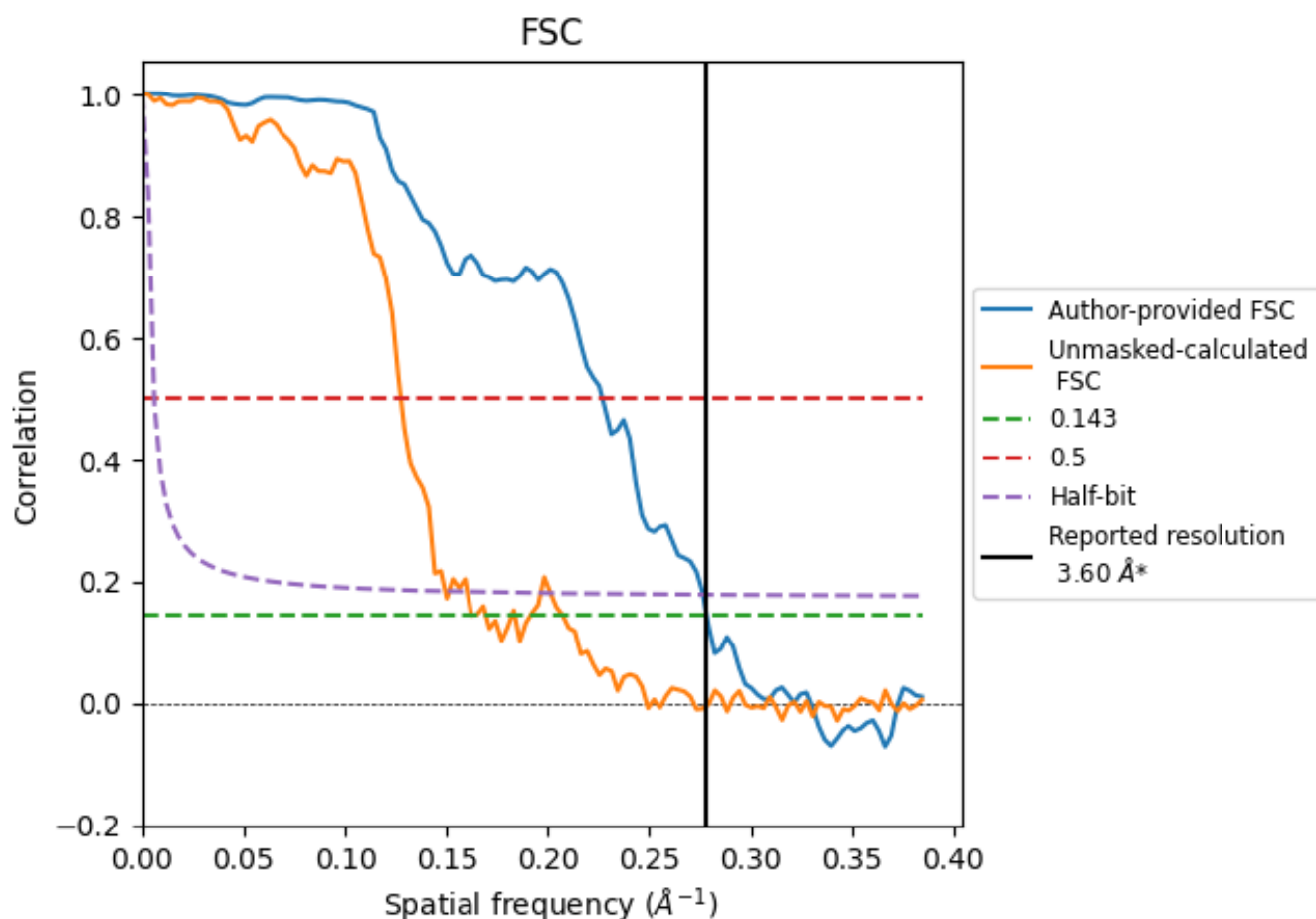


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

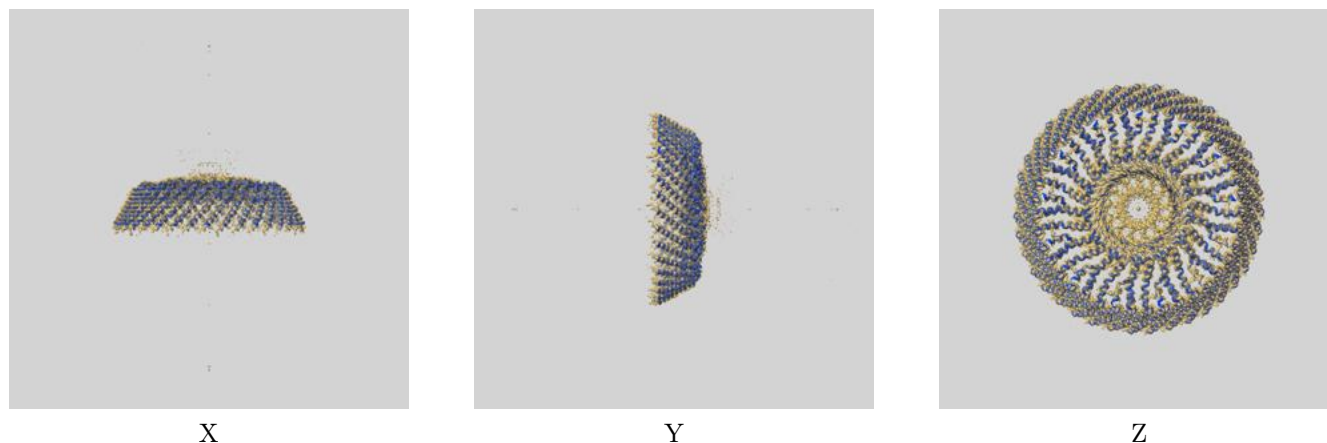
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.41	3.62
Unmasked-calculated*	5.90	7.84	6.69

*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 5.90 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

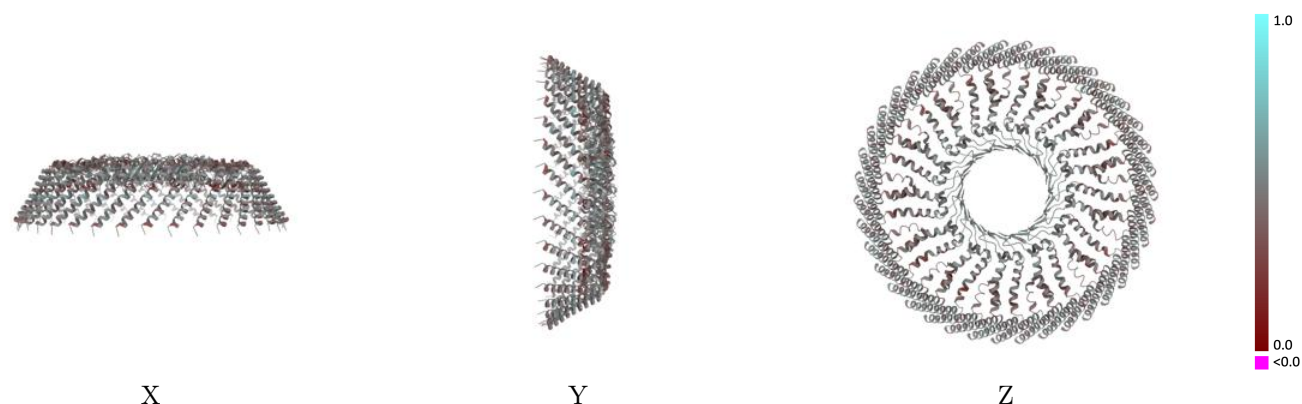
This section contains information regarding the fit between EMDB map EMD-53806 and PDB model 9R87. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



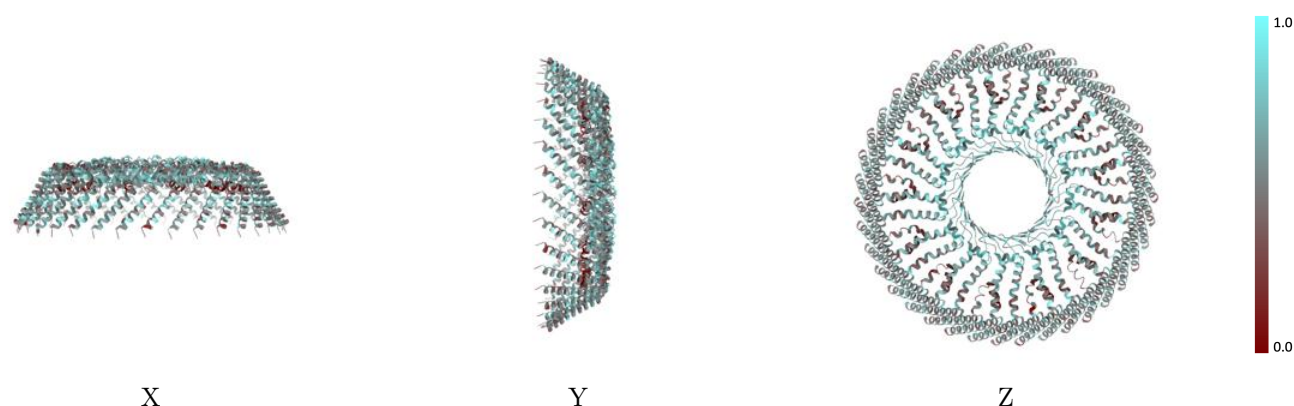
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



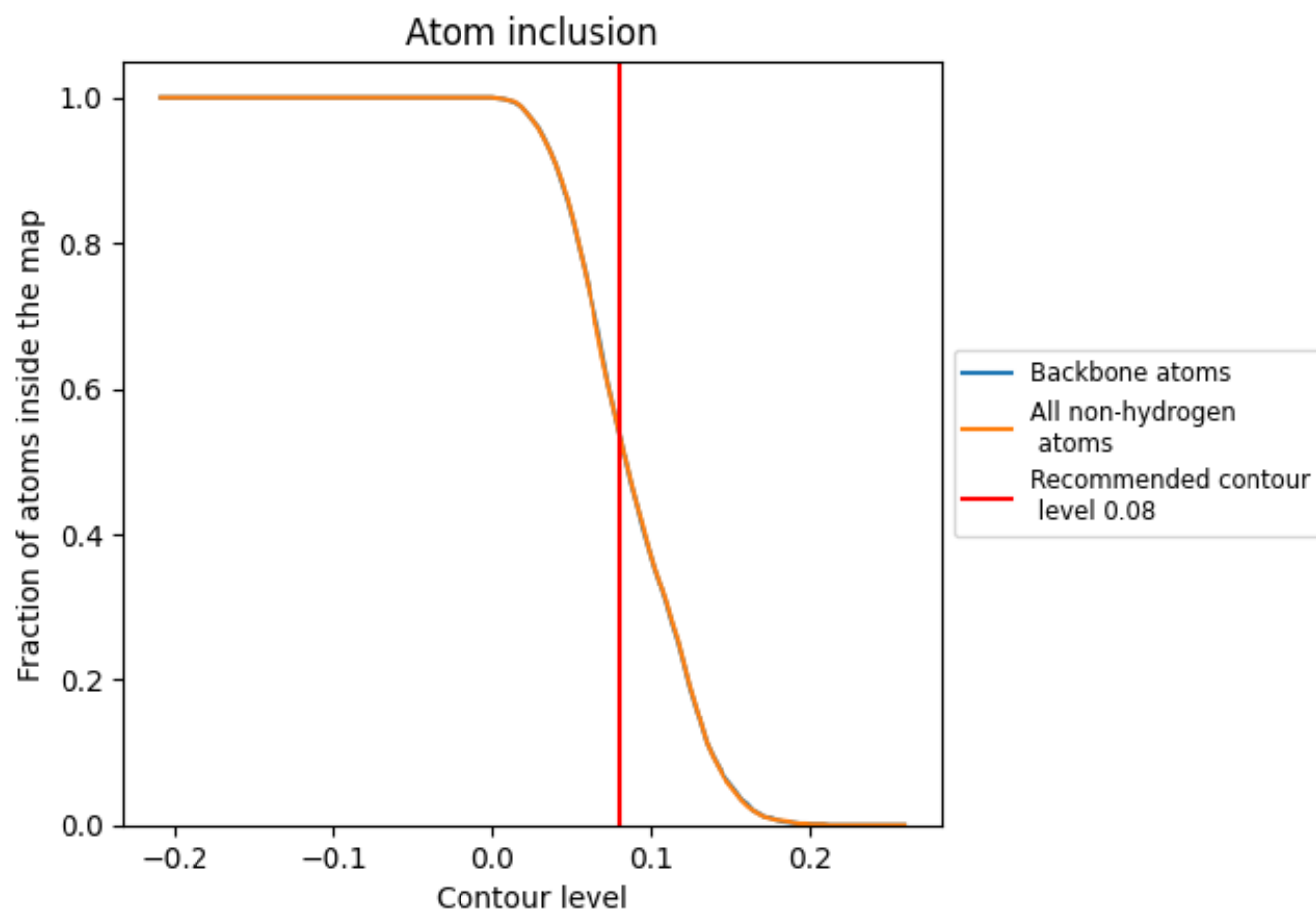
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5380	 0.4540
A	 0.6030	 0.4740
A1	 0.5620	 0.4550
A2	 0.5900	 0.4590
A3	 0.5800	 0.4530
A4	 0.5700	 0.4550
Ar	 0.5720	 0.4620
As	 0.5680	 0.4560
At	 0.5680	 0.4620
Au	 0.5620	 0.4590
Av	 0.5740	 0.4630
Aw	 0.5740	 0.4590
Ax	 0.5720	 0.4590
Ay	 0.5820	 0.4570
Az	 0.5840	 0.4540
B	 0.4420	 0.4300
C	 0.6000	 0.4670
D	 0.4240	 0.4250
E	 0.6010	 0.4720
F	 0.4220	 0.4280
G	 0.5920	 0.4710
H	 0.4420	 0.4380
I	 0.5930	 0.4690
J	 0.4330	 0.4340
K	 0.5980	 0.4720
L	 0.4150	 0.4220
M	 0.6080	 0.4760
N	 0.4310	 0.4240
O	 0.6050	 0.4720
P	 0.4380	 0.4240
Q	 0.5970	 0.4730
R	 0.4240	 0.4230
S	 0.6140	 0.4720
T	 0.4420	 0.4240
U	 0.5970	 0.4680



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Chain	Atom inclusion	Q-score
V	 0.4400	 0.4220
W	 0.6010	 0.4680
X	 0.4290	 0.4150
Y	 0.6010	 0.4690
Z	 0.4330	 0.4260