



wwPDB EM Validation Summary Report ⓘ

Jan 28, 2025 – 07:14 pm GMT

PDB ID : 9GOT
EMDB ID : EMD-51500
Title : Partial (48mer) encapsulin shell assembly from Mycobacterium tuberculosis
Authors : Lewis, C.J.; Berger, C.; Ravelli, R.B.G.
Deposited on : 2024-09-06
Resolution : 5.42 Å(reported)
Based on initial model : 7P1T

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

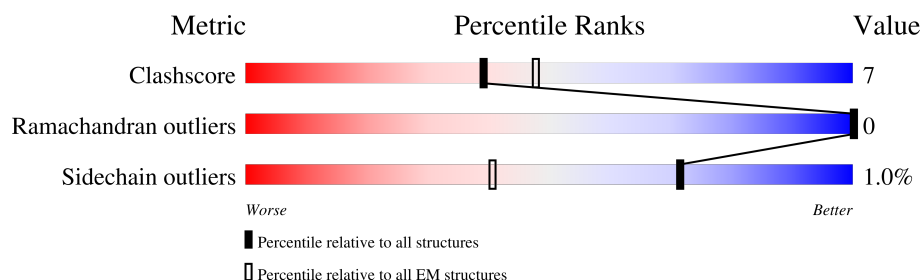
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.42 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.













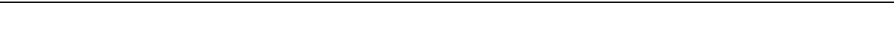

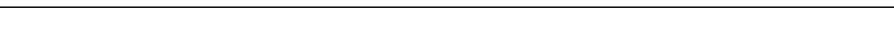
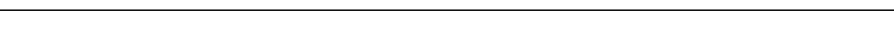







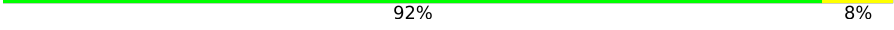



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	265	89% 11%
1	AB	265	91% 8% .
1	BA	265	90% 10%
1	CA	265	92% 8%
1	D	265	89% 11%
1	DA	265	91% 9%
1	DB	265	91% 8%
1	E	265	90% 10%

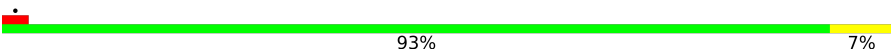



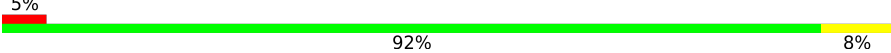
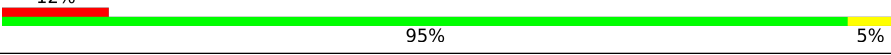

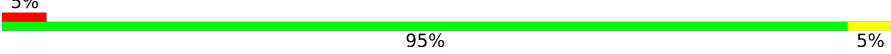

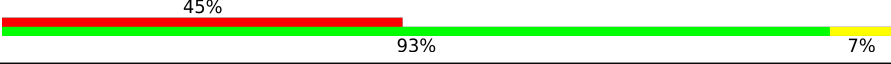

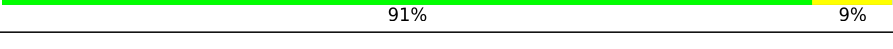


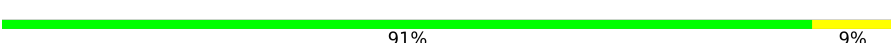
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Mol	Chain	Length	Quality of chain
1	EA	265	 91% 9%
1	FA	265	 92% 8%
1	FB	265	 90% 10%
1	G	265	 91% 8%
1	GA	265	 92% 8%
1	GB	265	 89% 11%
1	H	265	 89% 11%
1	HA	265	 93% 7%
1	HB	265	 88% 12%
1	I	265	 94% 6%
1	IA	265	 89% 10%
1	JA	265	 88% 12%
1	K	265	 90% 9%
1	KA	265	 90% 10%
1	L	265	 88% 12%
1	LA	265	 89% 11%
1	M	265	 91% 9%
1	MA	265	 90% 10%
1	N	265	 88% 11%
1	NA	265	 91% 9%
1	O	265	 92% 8%
1	OA	265	 91% 9%
1	P	265	 88% 12%
1	PA	265	 89% 11%
1	Q	265	 88% 11%

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Mol	Chain	Length	Quality of chain
1	R	265	 93%7%
1	S	265	 89%11%
1	SA	265	 90%10%
1	T	265	 90%10%
1	TA	265	 5%92%8%
1	U	265	 12%95%5%
1	UA	265	 88%11%
1	V	265	 5%95%5%
1	VA	265	 88%12%
1	W	265	 45%93%7%
1	WA	265	 90%10%
1	X	265	 31%93%6%
1	XA	265	 89%11%
1	YA	265	 91%9%
1	ZA	265	 91%9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 97632 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 Type 1 encapsulin shell protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	D	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	E	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	G	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	H	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	I	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	K	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	L	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	M	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	N	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	O	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	P	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Q	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	R	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	S	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	T	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	U	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	W	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	X	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	BA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	CA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	DA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	EA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	FA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	GA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	HA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	IA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	JA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	KA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	LA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	MA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	NA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	OA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	PA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	SA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	TA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	UA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	VA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	WA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	XA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	YA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	ZA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	DB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	FB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	GB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	HB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

3 Residue-property plots [i](#)


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

- Molecule 1: Type 1 encapsulin shell protein

Chain A: 




- Molecule 1: Type 1 encapsulin shell protein

Chain D: 



- Molecule 1: Type 1 encapsulin shell protein

Chain E: 




- Molecule 1: Type 1 encapsulin shell protein

Chain G: 




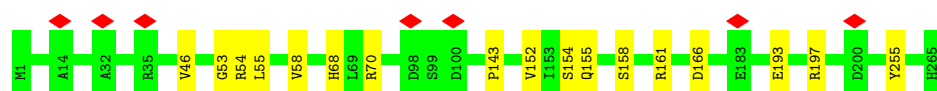
- Molecule 1: Type 1 encapsulin shell protein

Chain H: 



- Molecule 1: Type 1 encapsulin shell protein

Chain I:  94% 6%




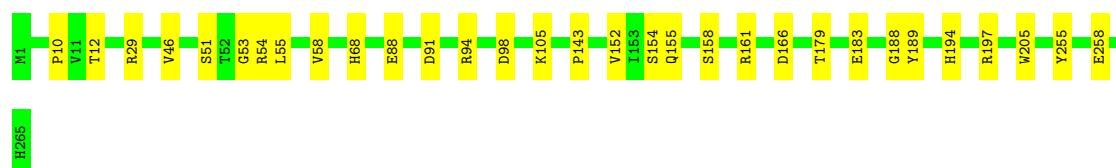
- Molecule 1: Type 1 encapsulin shell protein

Chain K:  90% 9%



- Molecule 1: Type 1 encapsulin shell protein

Chain L:  88% 12%




- Molecule 1: Type 1 encapsulin shell protein

Chain M:  91% 9%



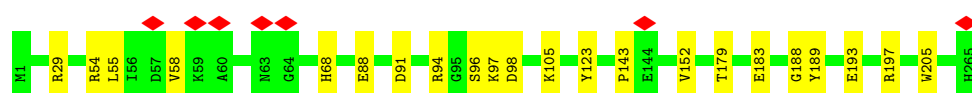
- Molecule 1: Type 1 encapsulin shell protein

Chain N:  88% 11%




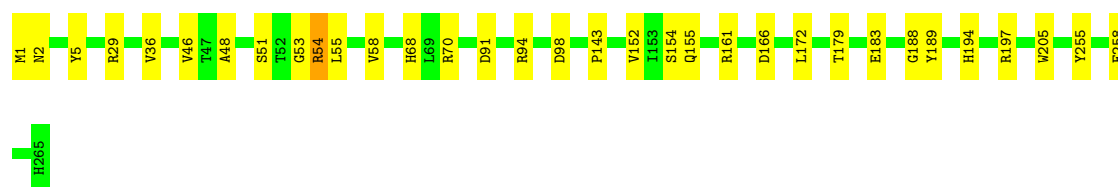
- Molecule 1: Type 1 encapsulin shell protein

Chain O:  92% 8%

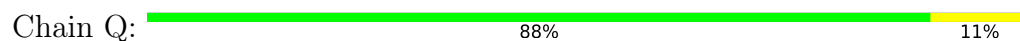


- Molecule 1: Type 1 encapsulin shell protein

Chain P:  88% 12%



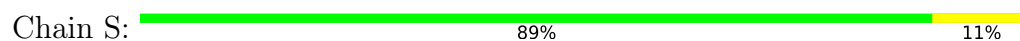
- Molecule 1: Type 1 encapsulin shell protein



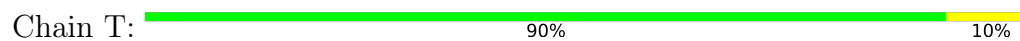
- Molecule 1: Type 1 encapsulin shell protein



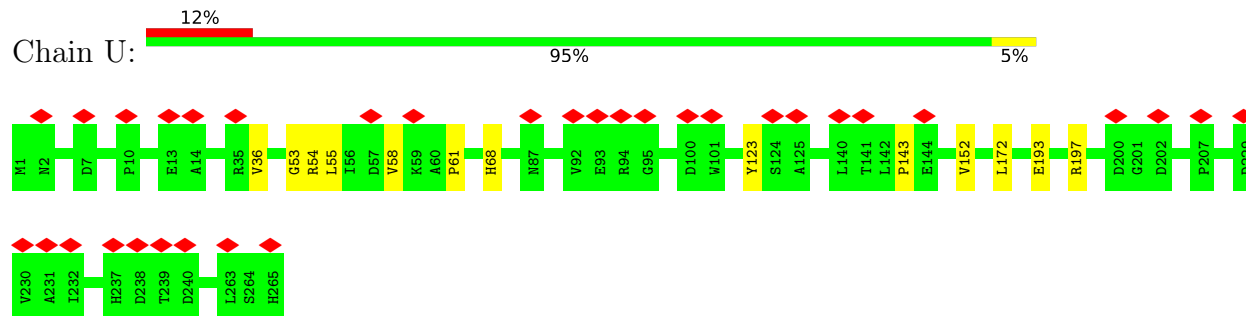
- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein

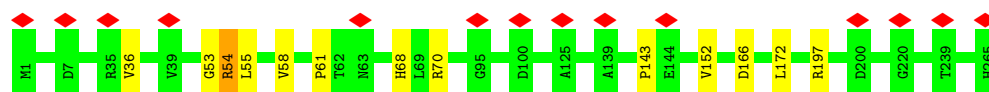


- Molecule 1: Type 1 encapsulin shell protein

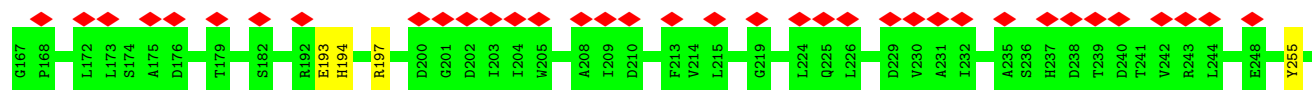
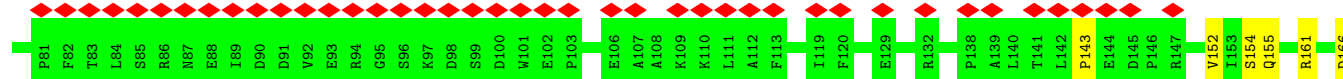
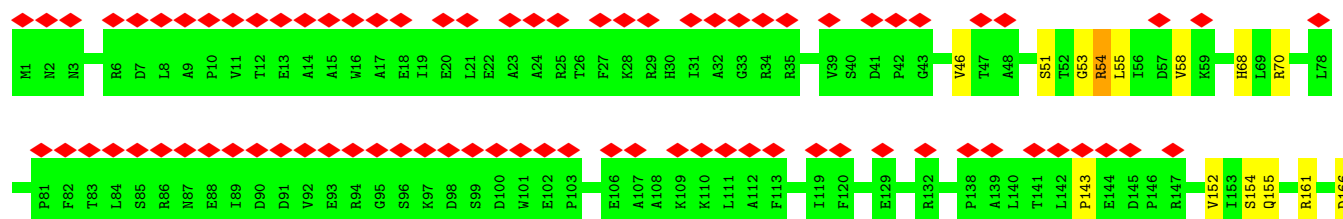


- Molecule 1: Type 1 encapsulin shell protein

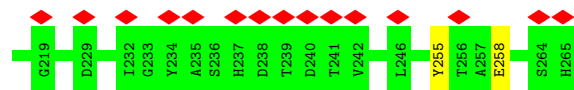
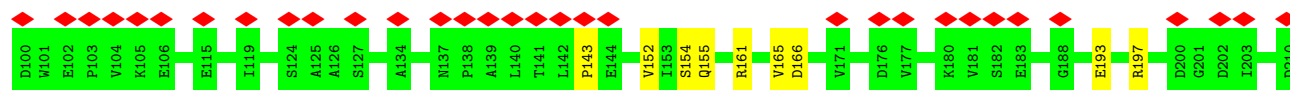
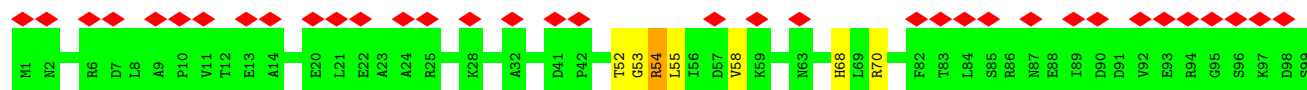




- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein

Chain DA:  91% 9%



- Molecule 1: Type 1 encapsulin shell protein

Chain EA:  91% 9%



- Molecule 1: Type 1 encapsulin shell protein

Chain FA:  92% 8%



- Molecule 1: Type 1 encapsulin shell protein

Chain GA:  92% 8%




- Molecule 1: Type 1 encapsulin shell protein

Chain HA:  93% 7%



- Molecule 1: Type 1 encapsulin shell protein

Chain IA:  89% 10%



- Molecule 1: Type 1 encapsulin shell protein

Chain JA:  88% 12%



H265

- Molecule 1: Type 1 encapsulin shell protein

Chain KA:  90% 10%


- Molecule 1: Type 1 encapsulin shell protein

Chain LA:  89% 11%


- Molecule 1: Type 1 encapsulin shell protein

Chain MA:  90% 10%



- Molecule 1: Type 1 encapsulin shell protein

Chain NA:  91% 9%


- Molecule 1: Type 1 encapsulin shell protein

Chain OA:  91% 9%


- Molecule 1: Type 1 encapsulin shell protein

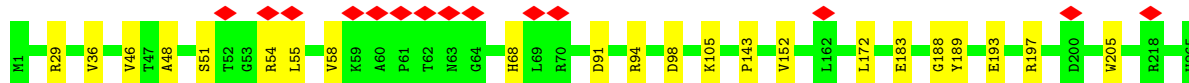
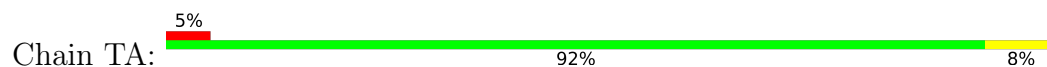
Chain PA:  89% 11%


- Molecule 1: Type 1 encapsulin shell protein

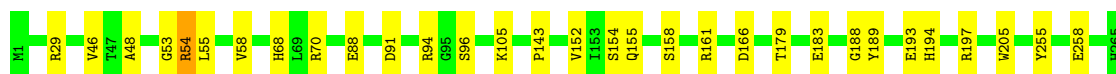
Chain SA:  90% 10%



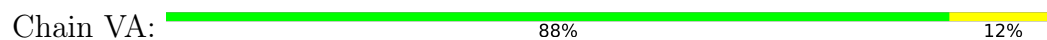
- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein

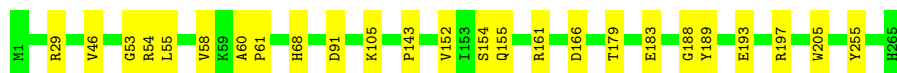


- Molecule 1: Type 1 encapsulin shell protein



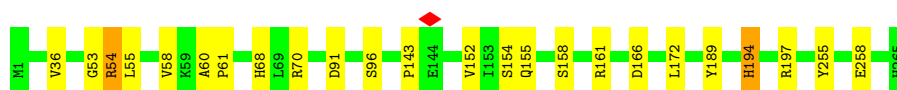
- Molecule 1: Type 1 encapsulin shell protein

Chain ZA:  91% 9%



- Molecule 1: Type 1 encapsulin shell protein

Chain AB:  91% 8%



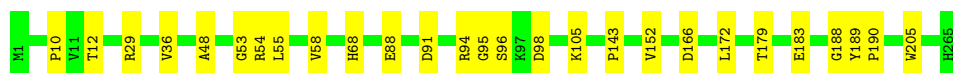
- Molecule 1: Type 1 encapsulin shell protein

Chain DB:  91% 8%



- Molecule 1: Type 1 encapsulin shell protein

Chain FB:  90% 10%



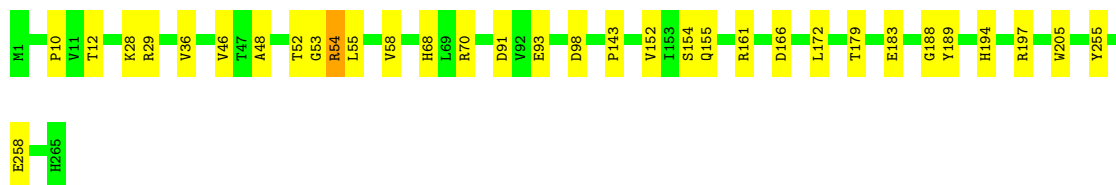
- Molecule 1: Type 1 encapsulin shell protein

Chain GB:  89% 11%



- Molecule 1: Type 1 encapsulin shell protein

Chain HB:  88% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3427	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	163000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	320.25598, 320.25598, 320.25598	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83399993, 0.83399993, 0.83399993	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	0.37	0/2074	0.57	0/2828
1	AB	0.37	0/2074	0.57	0/2828
1	BA	0.37	0/2074	0.57	0/2828
1	CA	0.37	0/2074	0.57	0/2828
1	D	0.37	0/2074	0.57	0/2828
1	DA	0.37	0/2074	0.57	0/2828
1	DB	0.37	0/2074	0.57	0/2828
1	E	0.37	0/2074	0.57	0/2828
1	EA	0.37	0/2074	0.57	0/2828
1	FA	0.37	0/2074	0.57	0/2828
1	FB	0.37	0/2074	0.57	0/2828
1	G	0.37	0/2074	0.57	0/2828
1	GA	0.37	0/2074	0.57	0/2828
1	GB	0.37	0/2074	0.57	0/2828
1	H	0.37	0/2074	0.57	0/2828
1	HA	0.37	0/2074	0.57	0/2828
1	HB	0.37	0/2074	0.57	0/2828
1	I	0.37	0/2074	0.57	0/2828
1	IA	0.37	0/2074	0.57	0/2828
1	JA	0.37	0/2074	0.57	0/2828
1	K	0.37	0/2074	0.57	0/2828
1	KA	0.37	0/2074	0.57	0/2828
1	L	0.37	0/2074	0.57	0/2828
1	LA	0.37	0/2074	0.57	0/2828
1	M	0.37	0/2074	0.57	0/2828
1	MA	0.37	0/2074	0.57	0/2828
1	N	0.37	0/2074	0.57	0/2828
1	NA	0.37	0/2074	0.57	0/2828
1	O	0.37	0/2074	0.57	0/2828
1	OA	0.37	0/2074	0.57	0/2828
1	P	0.37	0/2074	0.57	0/2828
1	PA	0.37	0/2074	0.57	0/2828
1	Q	0.37	0/2074	0.57	0/2828
1	R	0.37	0/2074	0.57	0/2828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	S	0.37	0/2074	0.57	0/2828
1	SA	0.37	0/2074	0.57	0/2828
1	T	0.37	0/2074	0.57	0/2828
1	TA	0.37	0/2074	0.57	0/2828
1	U	0.37	0/2074	0.57	0/2828
1	UA	0.37	0/2074	0.56	0/2828
1	V	0.37	0/2074	0.57	0/2828
1	VA	0.37	0/2074	0.57	0/2828
1	W	0.37	0/2074	0.57	0/2828
1	WA	0.37	0/2074	0.57	0/2828
1	X	0.37	0/2074	0.57	0/2828
1	XA	0.37	0/2074	0.57	0/2828
1	YA	0.37	0/2074	0.57	0/2828
1	ZA	0.37	0/2074	0.57	0/2828
All	All	0.37	0/99552	0.57	0/135744

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2034	0	2013	59	0
1	AB	2034	0	2013	41	0
1	BA	2034	0	2013	58	0
1	CA	2034	0	2013	41	0
1	D	2034	0	2013	70	0
1	DA	2034	0	2013	39	0
1	DB	2034	0	2010	52	0
1	E	2034	0	2013	53	0
1	EA	2034	0	2013	58	0
1	FA	2034	0	2013	30	0
1	FB	2034	0	2013	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2034	0	2013	41	0
1	GA	2034	0	2013	28	0
1	GB	2034	0	2013	58	0
1	H	2034	0	2013	61	0
1	HA	2034	0	2013	50	0
1	HB	2034	0	2013	62	0
1	I	2034	0	2013	25	0
1	IA	2034	0	2013	53	0
1	JA	2034	0	2013	87	0
1	K	2034	0	2013	48	0
1	KA	2034	0	2013	47	0
1	L	2034	0	2013	78	0
1	LA	2034	0	2013	65	0
1	M	2034	0	2013	38	0
1	MA	2034	0	2013	44	0
1	N	2034	0	2012	73	0
1	NA	2034	0	2012	53	0
1	O	2034	0	2013	42	0
1	OA	2034	0	2013	54	0
1	P	2034	0	2013	78	0
1	PA	2034	0	2012	66	0
1	Q	2034	0	2013	75	0
1	R	2034	0	2012	35	0
1	S	2034	0	2012	60	0
1	SA	2034	0	2013	63	0
1	T	2034	0	2013	79	0
1	TA	2034	0	2012	49	0
1	U	2034	0	2013	9	0
1	UA	2034	0	2013	74	0
1	V	2034	0	2013	11	0
1	VA	2034	0	2013	83	0
1	W	2034	0	2013	30	0
1	WA	2034	0	2013	49	0
1	X	2034	0	2013	32	0
1	XA	2034	0	2012	88	0
1	YA	2034	0	2013	49	0
1	ZA	2034	0	2013	54	0
All	All	97632	0	96614	1353	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 7.

The worst 5 of 1353 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:S:29:ARG:CD	1:NA:166:ASP:HB3	1.24	1.54
1:R:29:ARG:CD	1:DB:166:ASP:HB3	1.41	1.47
1:R:188:GLY:O	1:DB:197:ARG:CD	1.66	1.43
1:R:29:ARG:HD3	1:DB:166:ASP:CB	1.50	1.40
1:N:166:ASP:HB3	1:TA:29:ARG:CD	1.53	1.36

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	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	BA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	CA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	D	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	DA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	DB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	E	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	EA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	FA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	FB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	G	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	GA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	GB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	H	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	HA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	I	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	IA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	JA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	K	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	KA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	L	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	LA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	M	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	MA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	N	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	NA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	O	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	OA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	P	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	PA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Q	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	R	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	S	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	SA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	T	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	TA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	U	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	UA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	V	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	VA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	W	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	WA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	X	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	XA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	YA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ZA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
All	All	12624/12720 (99%)	12432 (98%)	192 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	AB	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	BA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	CA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	D	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	DA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	DB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	E	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	EA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	FA	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	FB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	G	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	GA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	GB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	H	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	HA	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	HB	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	I	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	IA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	JA	218/218 (100%)	216 (99%)	2 (1%)	75	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	KA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	L	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	LA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	M	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	MA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	N	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	NA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	O	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	OA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	P	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	PA	218/218 (100%)	215 (99%)	3 (1%)	62	75
1	Q	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	R	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	S	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	SA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	T	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	TA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	U	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	UA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	V	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	VA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	W	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	WA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	X	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	XA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	YA	218/218 (100%)	216 (99%)	2 (1%)	75	83
1	ZA	218/218 (100%)	216 (99%)	2 (1%)	75	83
All	All	10464/10464 (100%)	10361 (99%)	103 (1%)	71	82

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HA	58	VAL
1	OA	54	ARG
1	GB	54	ARG
1	IA	54	ARG
1	LA	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	WA	194	HIS
1	XA	194	HIS
1	GB	194	HIS
1	T	194	HIS
1	P	194	HIS

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.

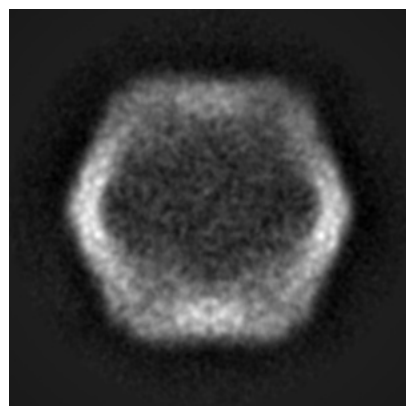
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51500. These allow visual inspection of the internal detail of the map and identification of artifacts.

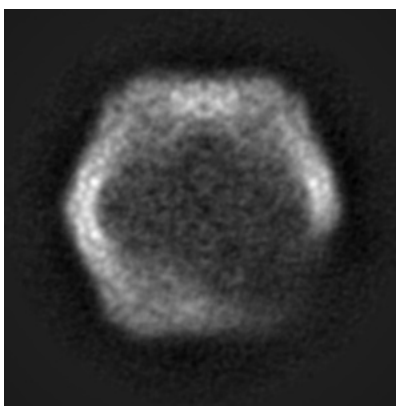
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

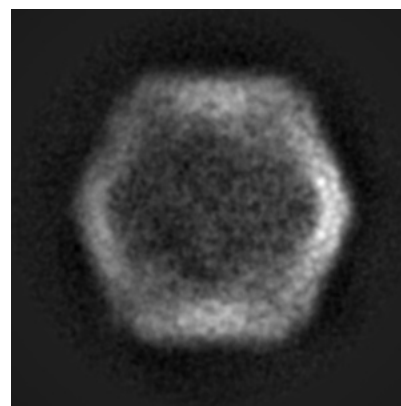
6.1.1 Primary map



X

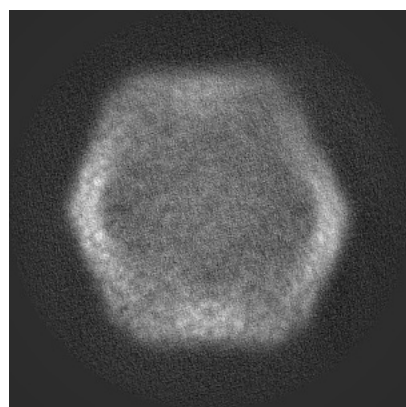


Y

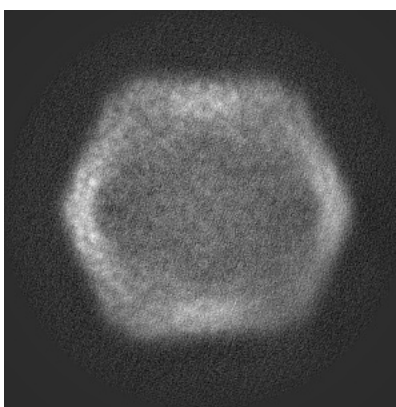


Z

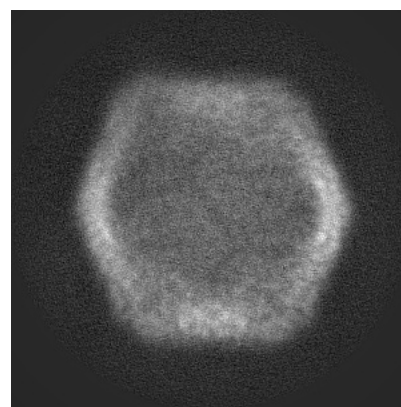
6.1.2 Raw map



X



Y

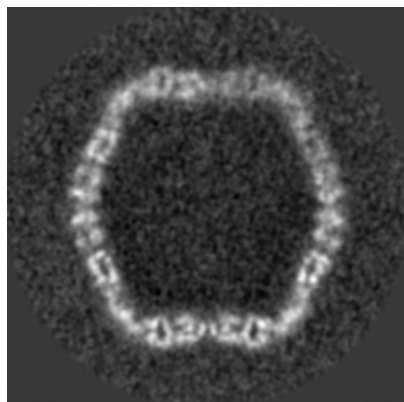


Z

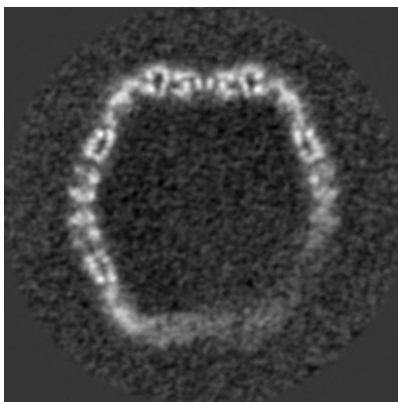
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

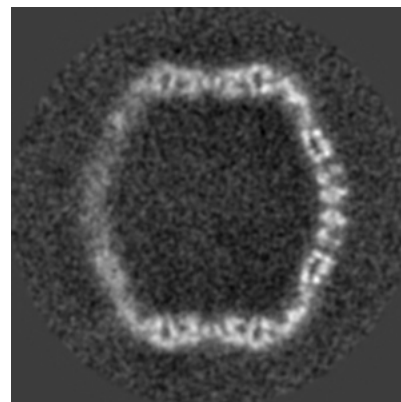
6.2.1 Primary map



X Index: 192

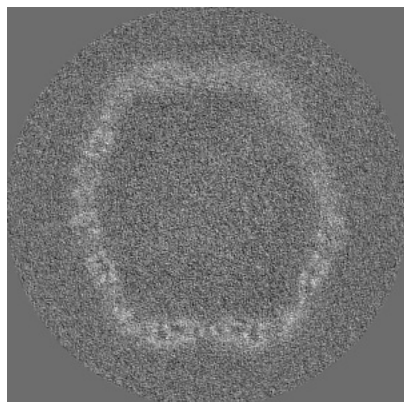


Y Index: 192

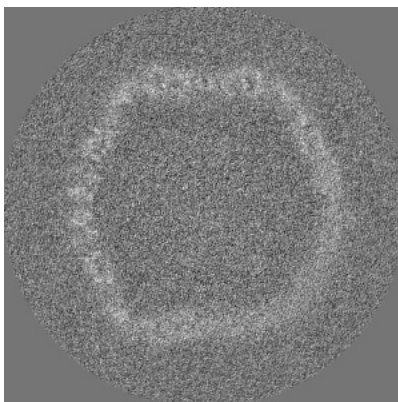


Z Index: 192

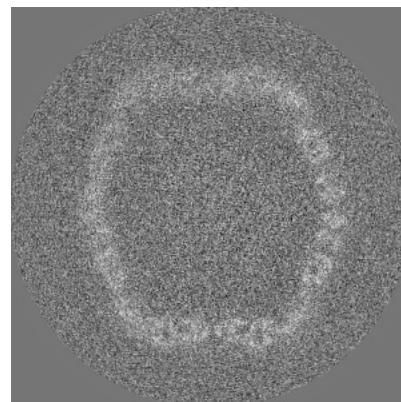
6.2.2 Raw map



X Index: 192



Y Index: 192

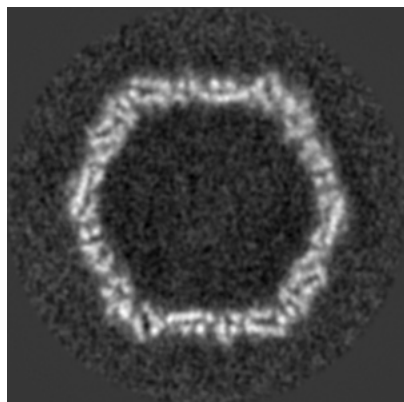


Z Index: 192

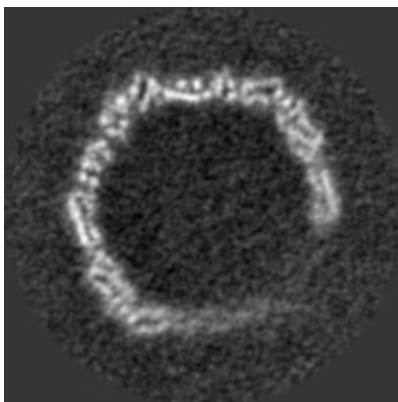
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

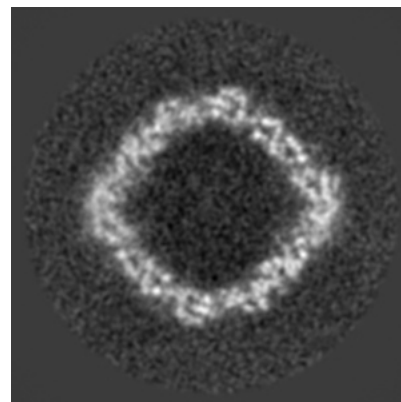
6.3.1 Primary map



X Index: 216

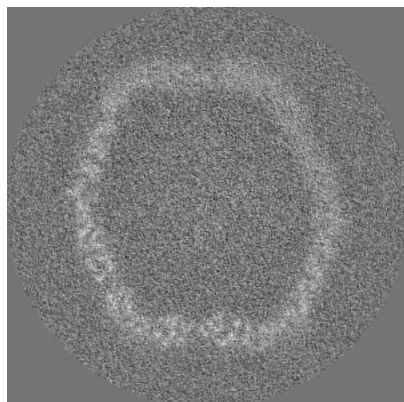


Y Index: 167

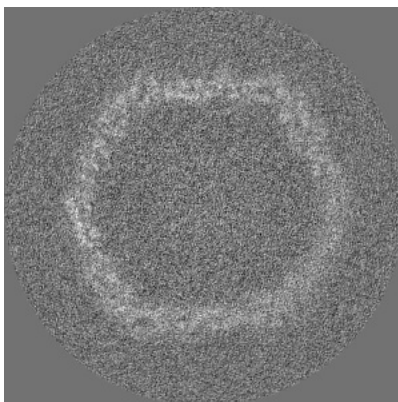


Z Index: 119

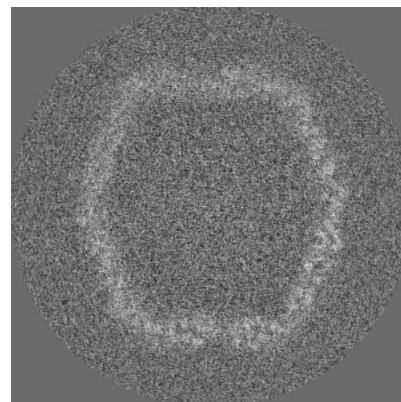
6.3.2 Raw map



X Index: 199



Y Index: 167

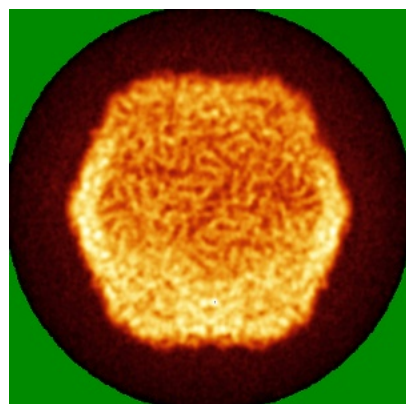


Z Index: 186

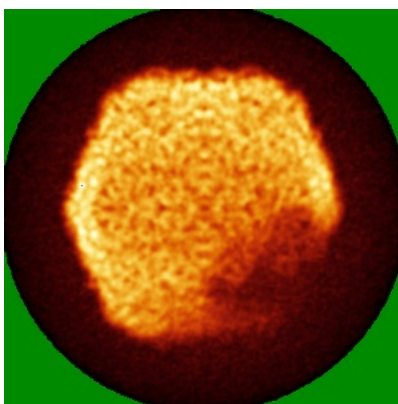
The images above show the largest variance slices of the map in three orthogonal directions.

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

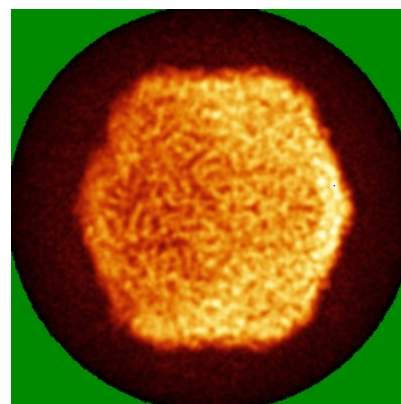
6.4.1 Primary map



X

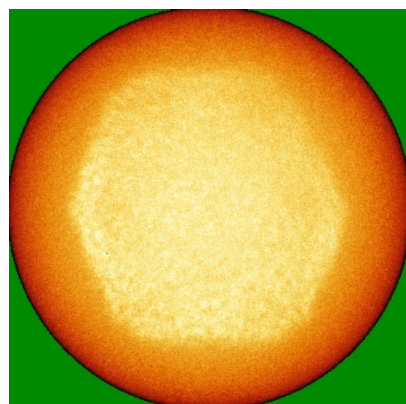


Y

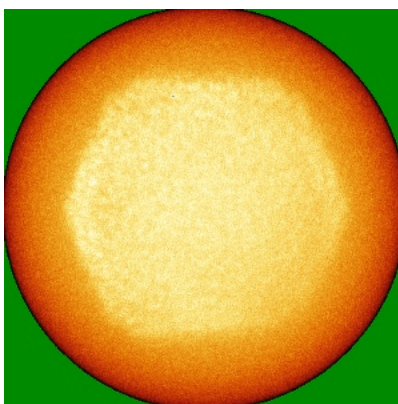


Z

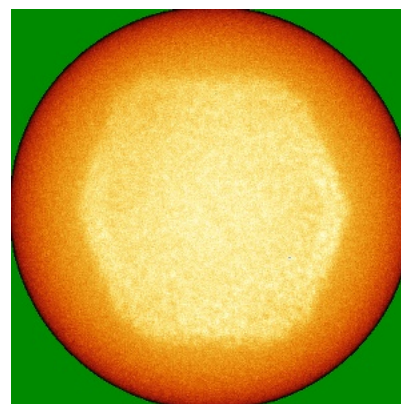
6.4.2 Raw map



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.

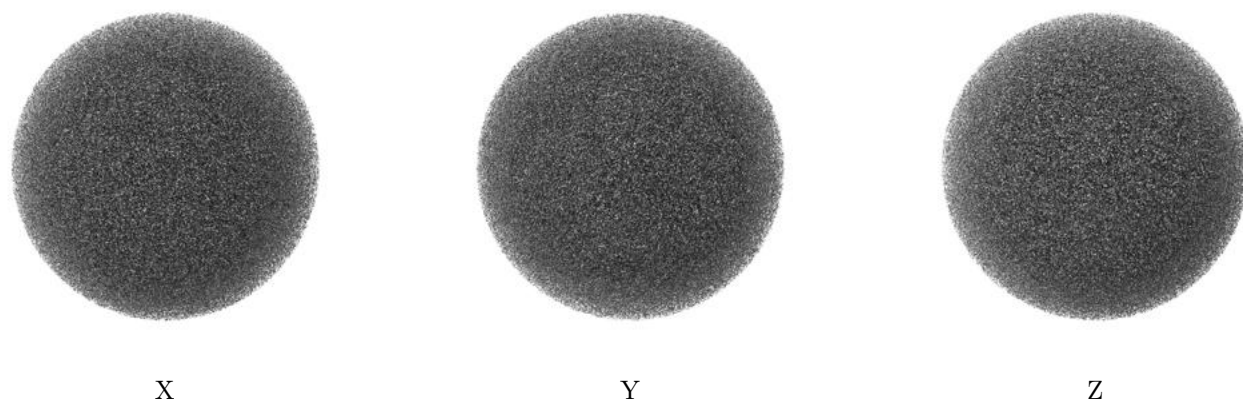
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

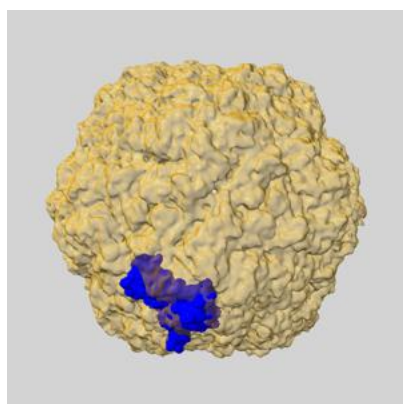
6.6 Mask visualisation [i](#)

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

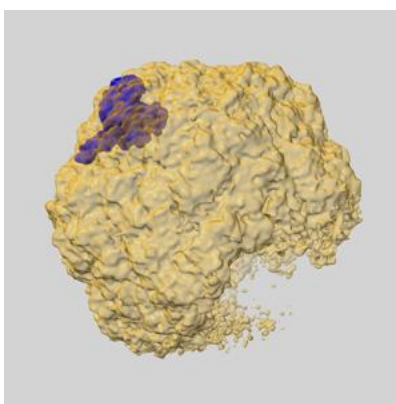
A mask typically either:

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

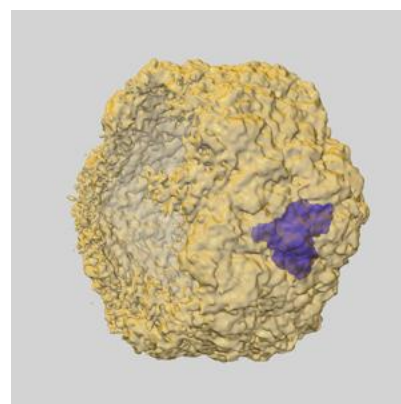
6.6.1 emd_51500_msk_1.map [i](#)



X

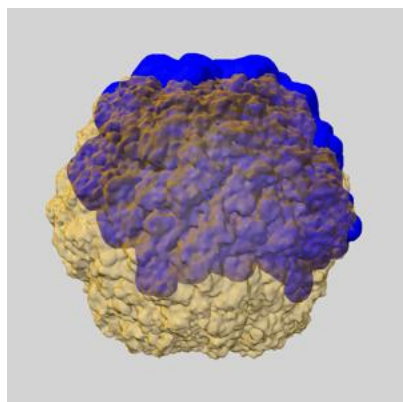


Y

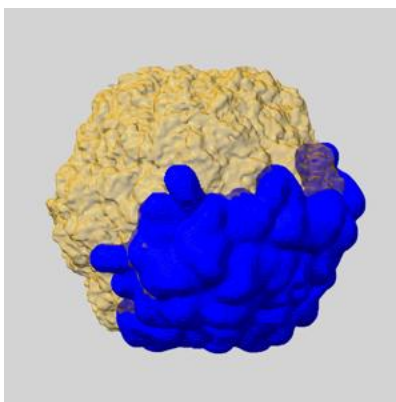


Z

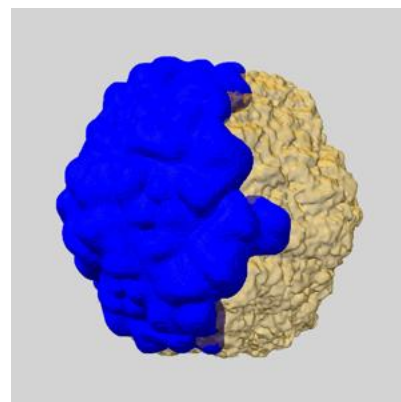
6.6.2 emd_51500_msk_2.map [i](#)



X

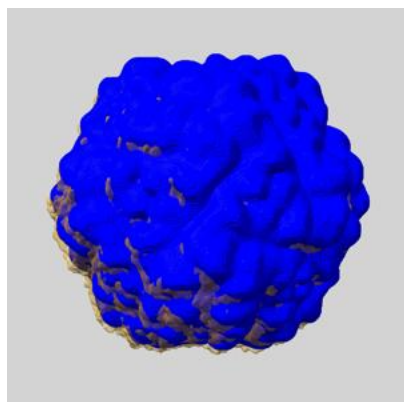


Y

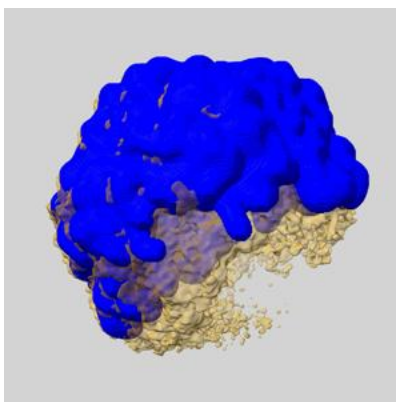


Z

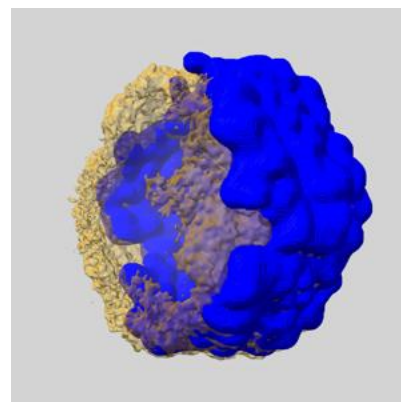
6.6.3 emd_51500_msk_3.map [i](#)



X



Y

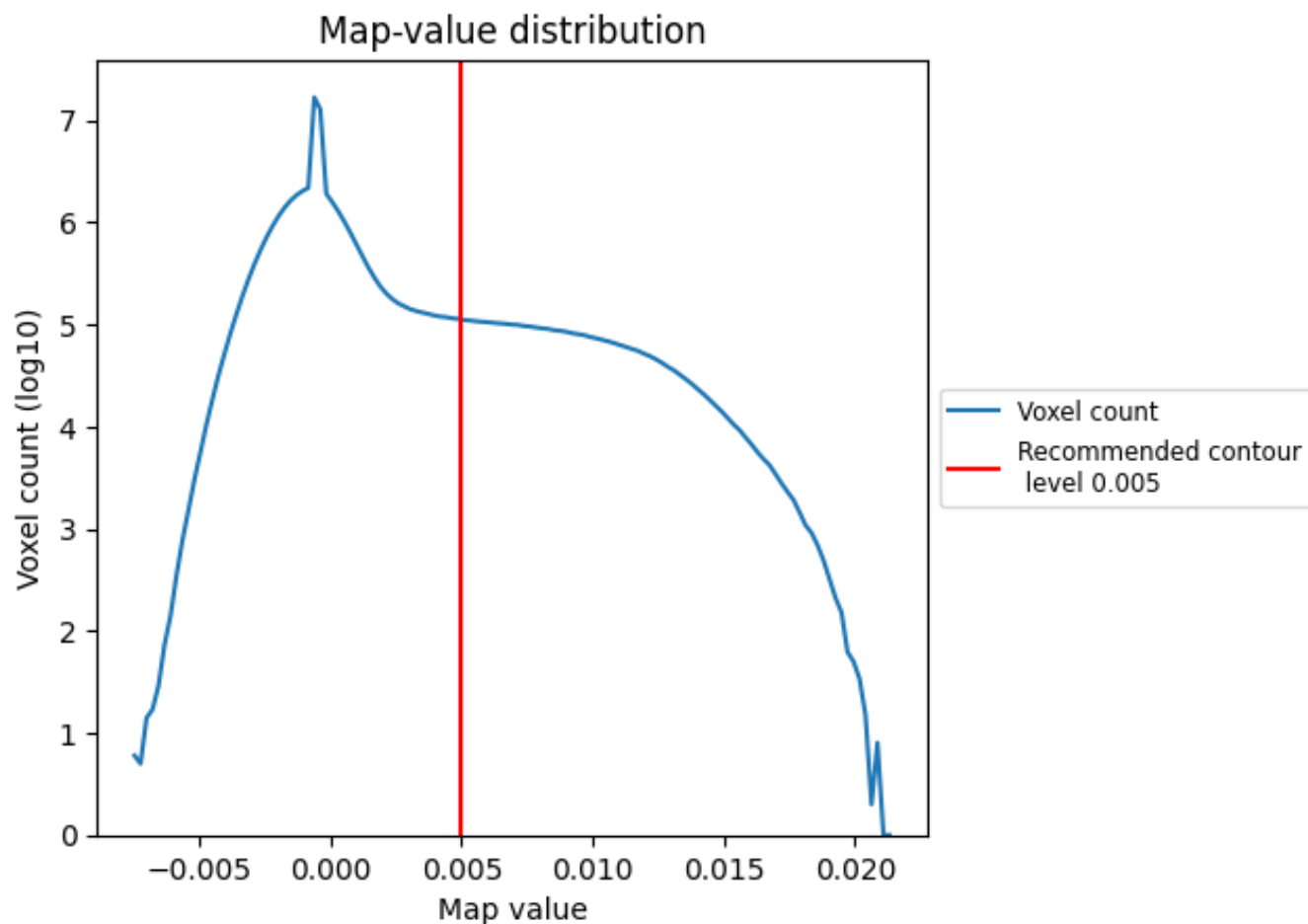


Z

7 Map analysis [i](#)

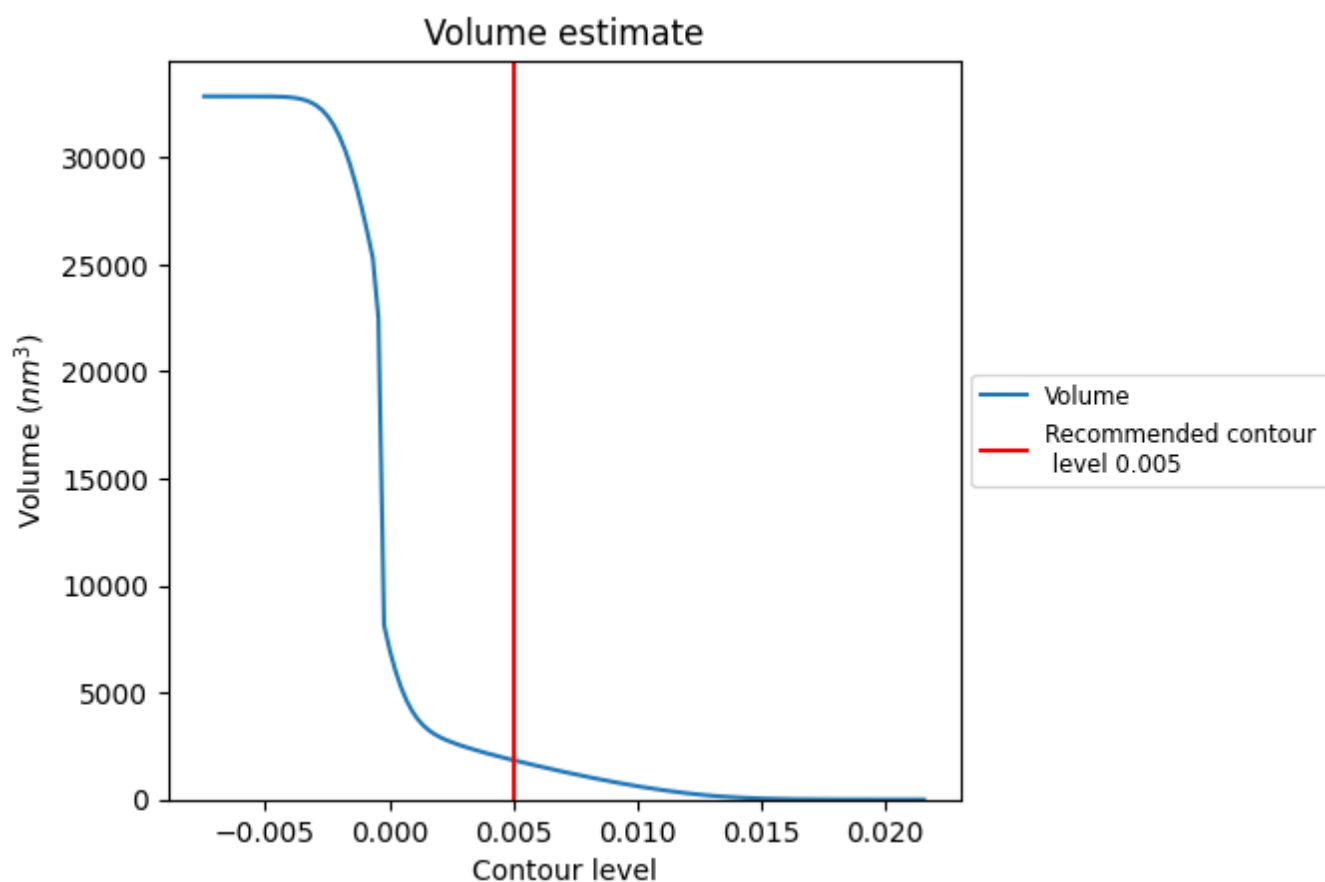
This section contains the results of statistical analysis of the map.

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.

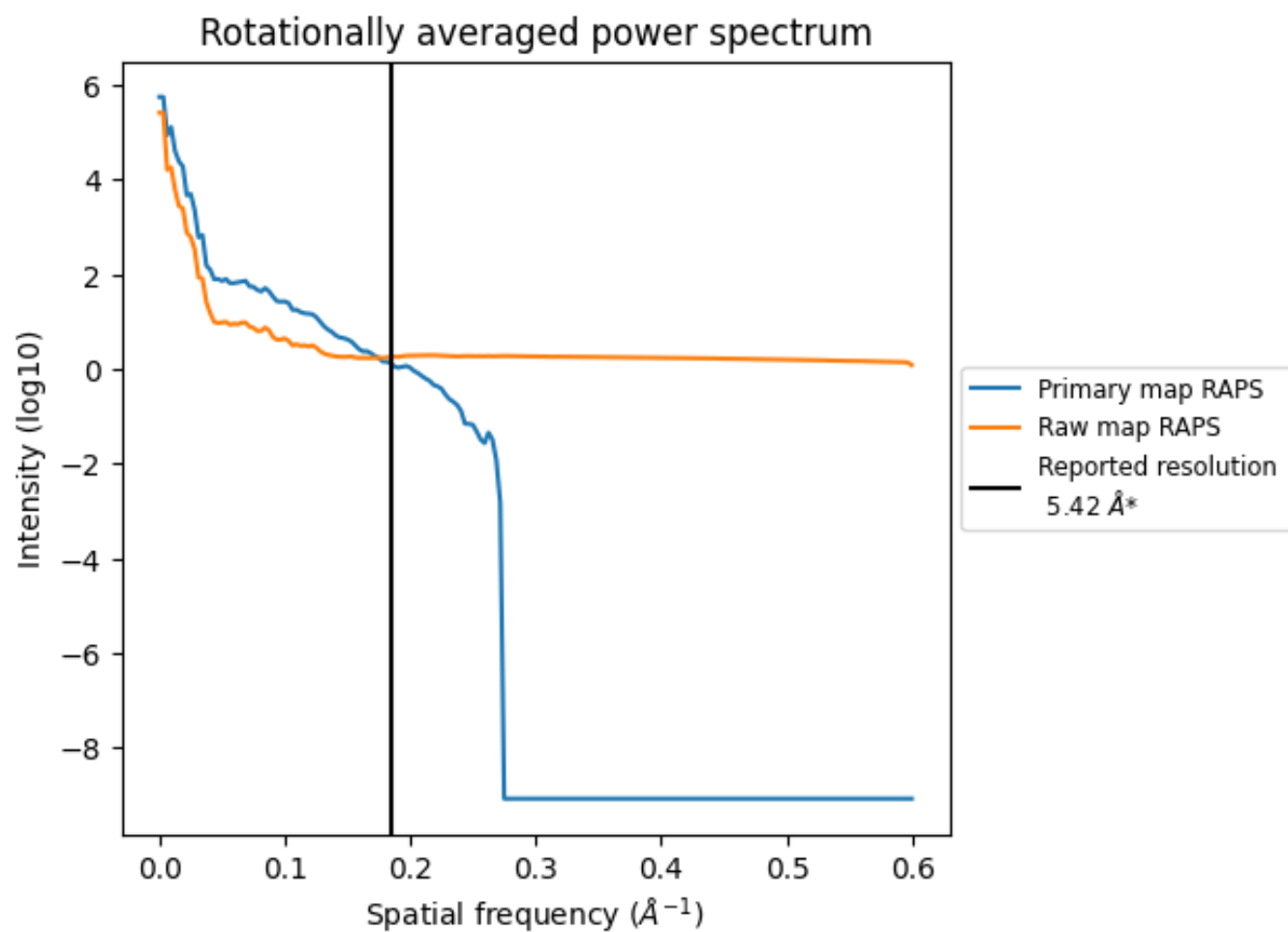
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1841 nm³; this corresponds to an approximate mass of 1663 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 ⓘ

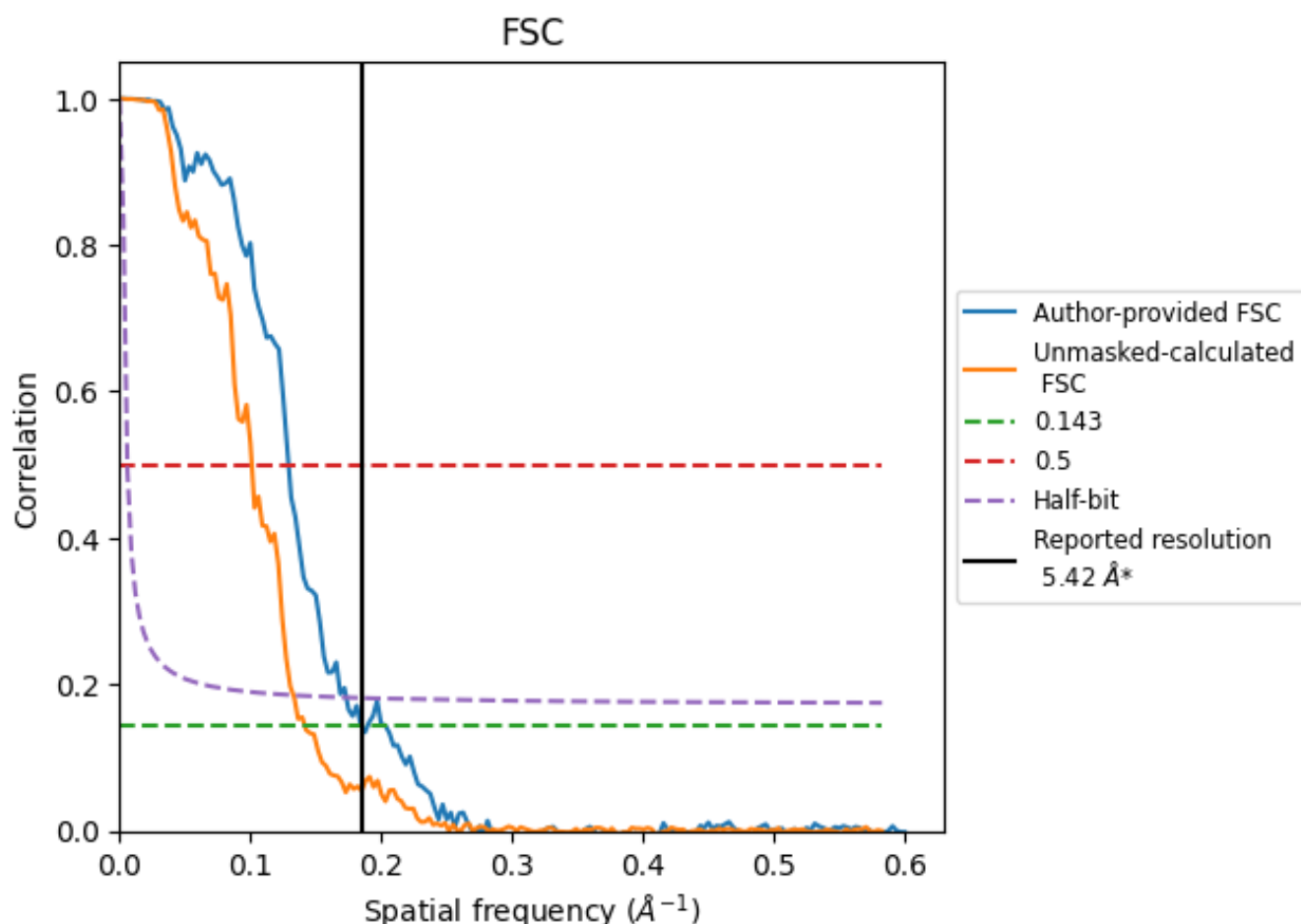


*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

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 0.185 Å⁻¹

8.2 Resolution estimates [i](#)

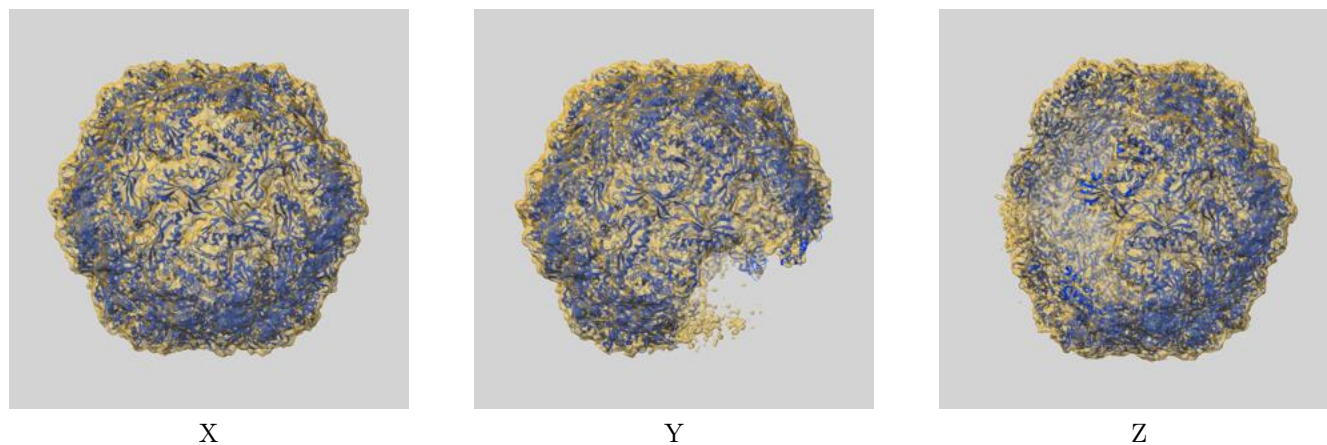
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.42	-	-
Author-provided FSC curve	5.41	7.75	5.78
Unmasked-calculated*	7.07	9.90	7.53

*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 7.07 differs from the reported value 5.42 by more than 10 %

9 Map-model fit [i](#)

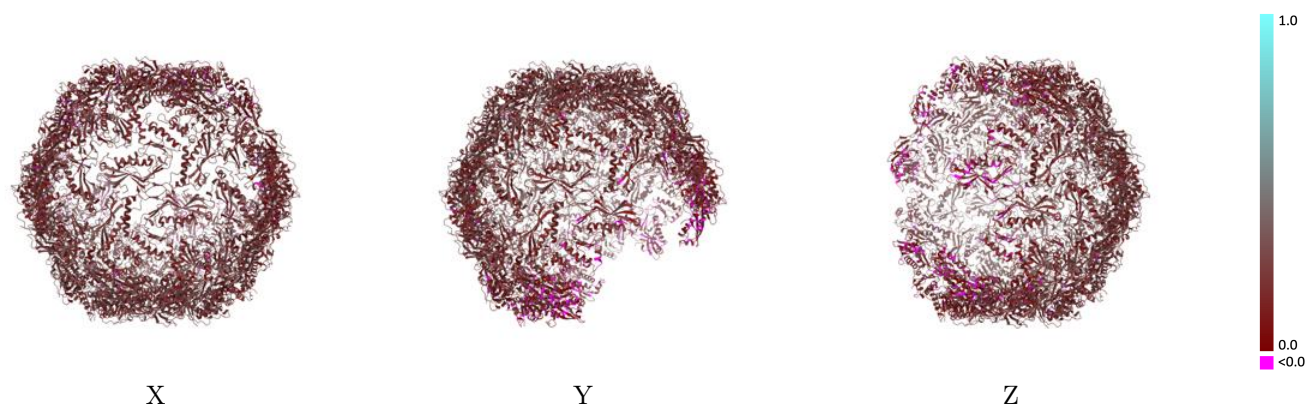
This section contains information regarding the fit between EMDB map EMD-51500 and PDB model 9GOT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



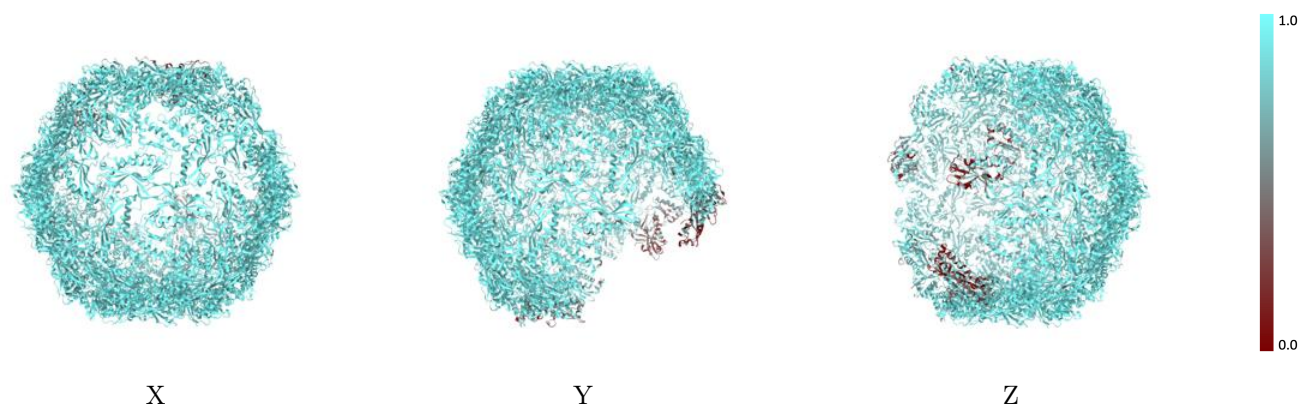
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



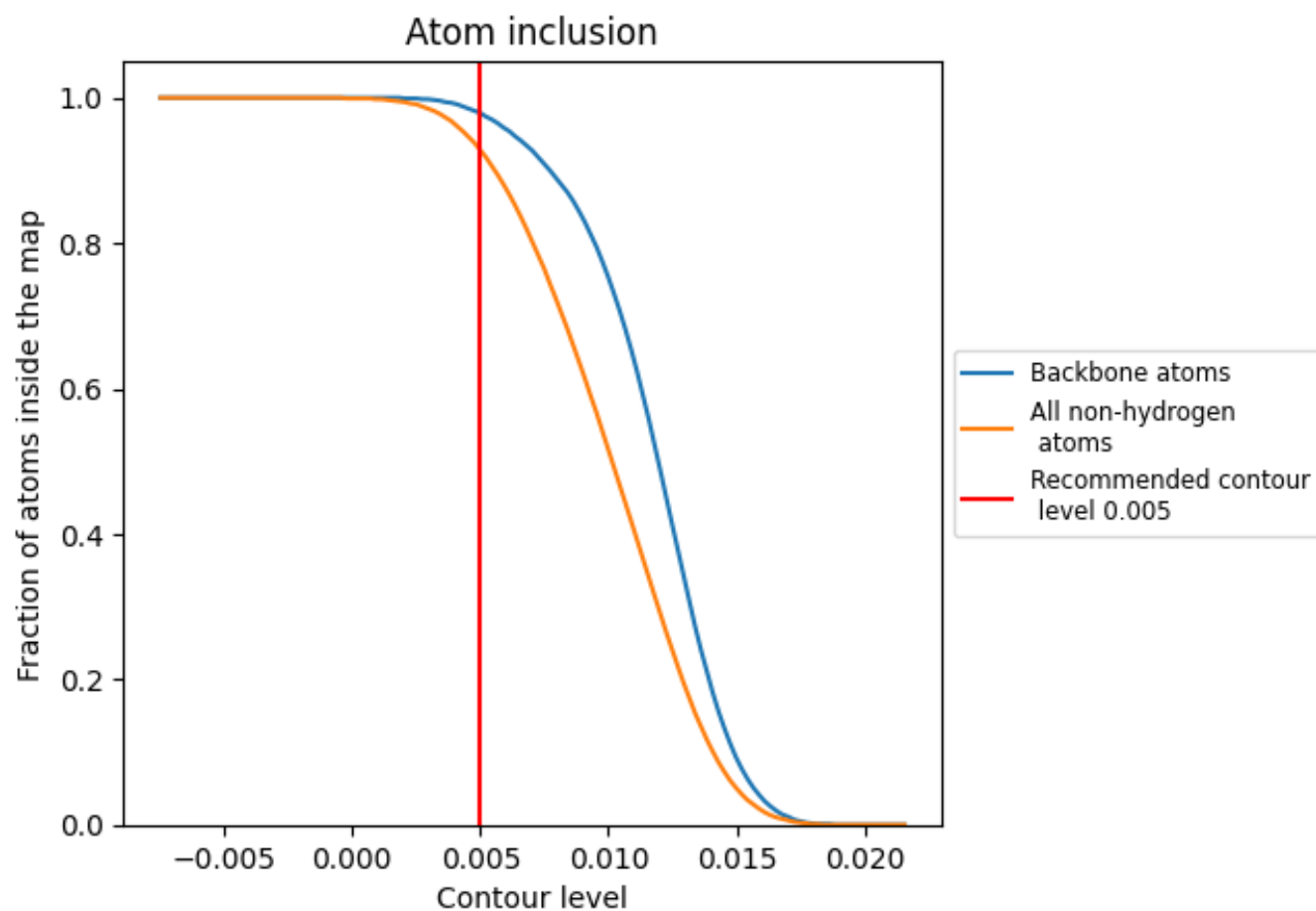
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.2200
A	 0.9560	 0.2020
AB	 0.9570	 0.2070
BA	 0.9640	 0.2190
CA	 0.9620	 0.2480
D	 0.9630	 0.2280
DA	 0.9600	 0.2200
DB	 0.9590	 0.1900
E	 0.9610	 0.2490
EA	 0.9550	 0.2440
FA	 0.9590	 0.2530
FB	 0.9630	 0.2400
G	 0.9590	 0.2350
GA	 0.9480	 0.1850
GB	 0.9650	 0.2580
H	 0.9560	 0.2360
HA	 0.9070	 0.1710
HB	 0.9550	 0.2550
I	 0.8960	 0.1820
IA	 0.9610	 0.2280
JA	 0.9620	 0.2500
K	 0.9600	 0.2340
KA	 0.9540	 0.2480
L	 0.9670	 0.2580
LA	 0.9550	 0.2530
M	 0.9570	 0.2560
MA	 0.9610	 0.2500
N	 0.9620	 0.2210
NA	 0.9510	 0.2210
O	 0.9260	 0.1900
OA	 0.9640	 0.2510
P	 0.9590	 0.2590
PA	 0.9620	 0.2110
Q	 0.9610	 0.2120
R	 0.8870	 0.1620



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Chain	Atom inclusion	Q-score
S	 0.9600	 0.2250
SA	 0.9620	 0.2340
T	 0.9570	 0.2520
TA	 0.8520	 0.1730
U	 0.7320	 0.1160
UA	 0.9590	 0.2310
V	 0.8480	 0.1520
VA	 0.9660	 0.2570
W	 0.4850	 0.1340
WA	 0.9600	 0.2500
X	 0.6030	 0.1320
XA	 0.9610	 0.2160
YA	 0.9600	 0.2140
ZA	 0.9570	 0.2360