



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 05:45 AM UTC

PDB ID : 8TVR / pdb_00008tvr
EMDB ID : EMD-41649
Title : In situ cryo-EM structure of bacteriophage P22 tail hub protein: tailspike protein complex at 2.8Å resolution
Authors : Iglesias, S.; Cingolani, G.; Feng-Hou, C.
Deposited on : 2023-08-18
Resolution : 2.80 Å(reported)

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.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

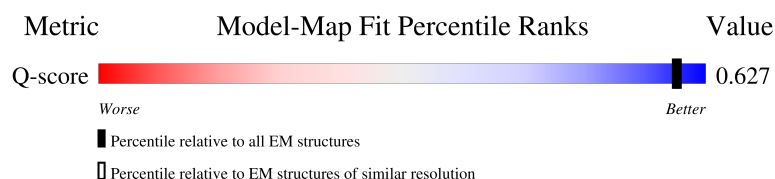
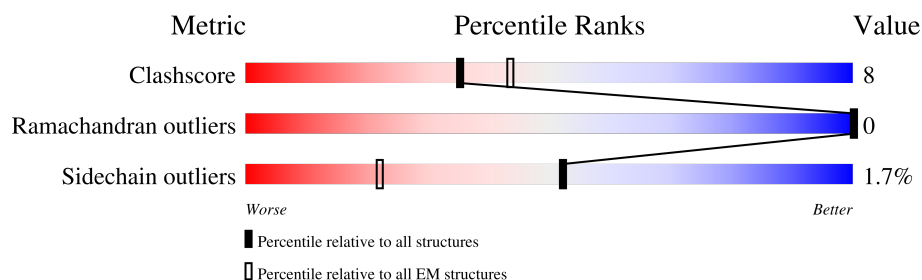
1 Overall quality at a glance

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.



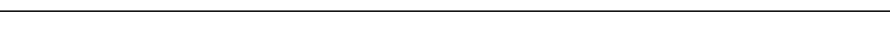
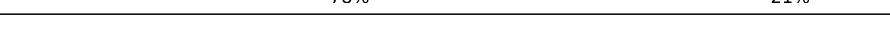
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A	667	
1	B	667	
1	C	667	
1	D	667	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	667	 14% . 82%
1	F	667	 15% . 82%
1	H	667	 15% . 82%
1	I	667	 13% 5% . 82%
1	J	667	 15% . 82%
1	L	667	 14% . 82%
1	M	667	 13% . 82%
1	N	667	 15% . 82%
1	P	667	 15% . 82%
1	Q	667	 14% . 82%
1	R	667	 15% . 82%
1	V	667	 15% . 82%
1	W	667	 14% . 82%
1	X	667	 15% . 82%
2	G	472	 78% 21% .
2	K	472	 74% 25% .
2	O	472	 74% 25% .
2	S	472	 76% 23% .
2	T	472	 79% 20% .
2	Y	472	 77% 22% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38532 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 Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	B	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	C	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	D	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	E	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	F	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	H	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	I	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	J	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	L	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	M	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	N	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	P	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	Q	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	R	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	V	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	W	118	Total 913	C 580	N 153	O 179	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	118	Total	C	N	O	S	0	0
			913	580	153	179	1		

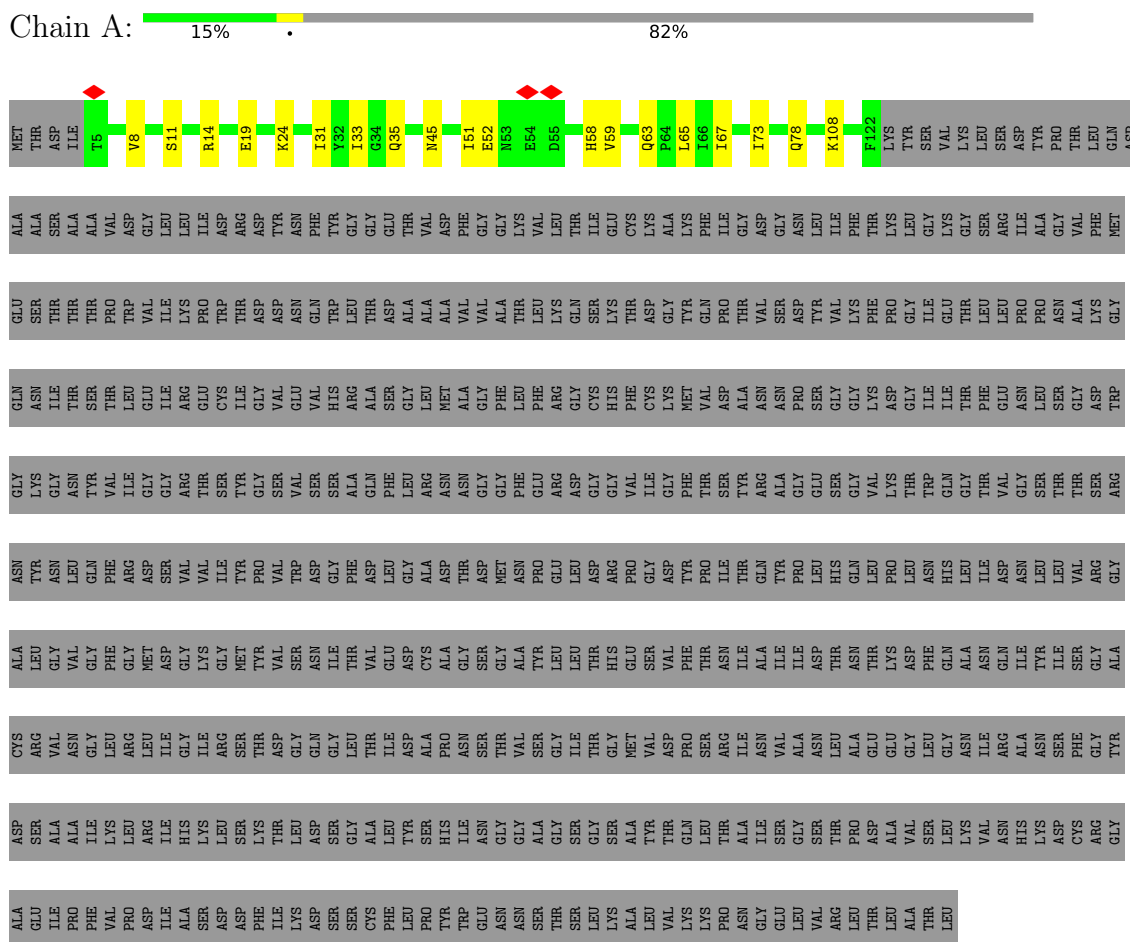
- Molecule 2 is a protein called Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	G	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	K	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	O	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	T	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	Y	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		

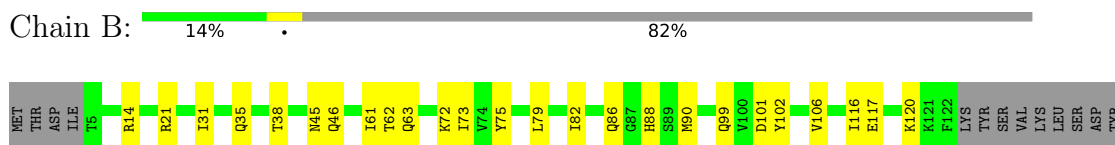
3 Residue-property plots

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: Tail spike protein

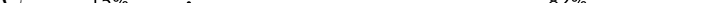


• Molecule 1: Tail spike protein



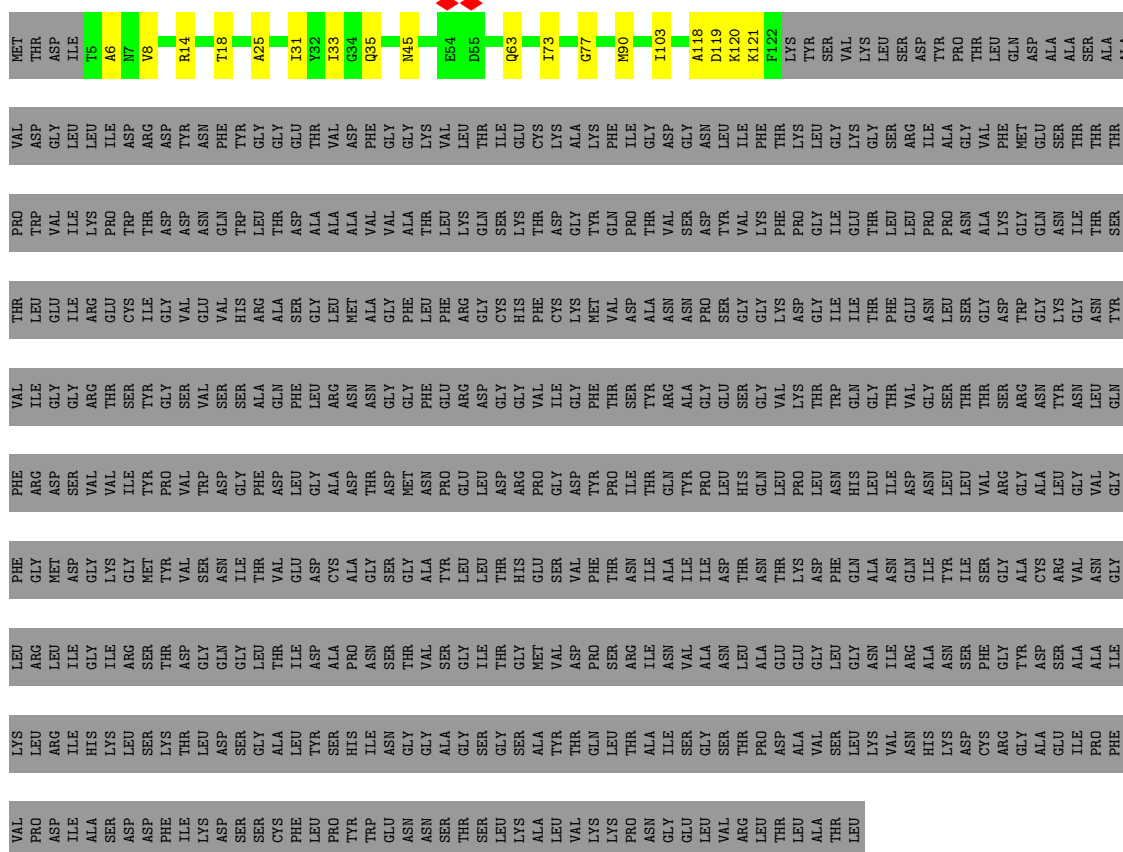
[illegible]

- Molecule 1: Tail spike protein

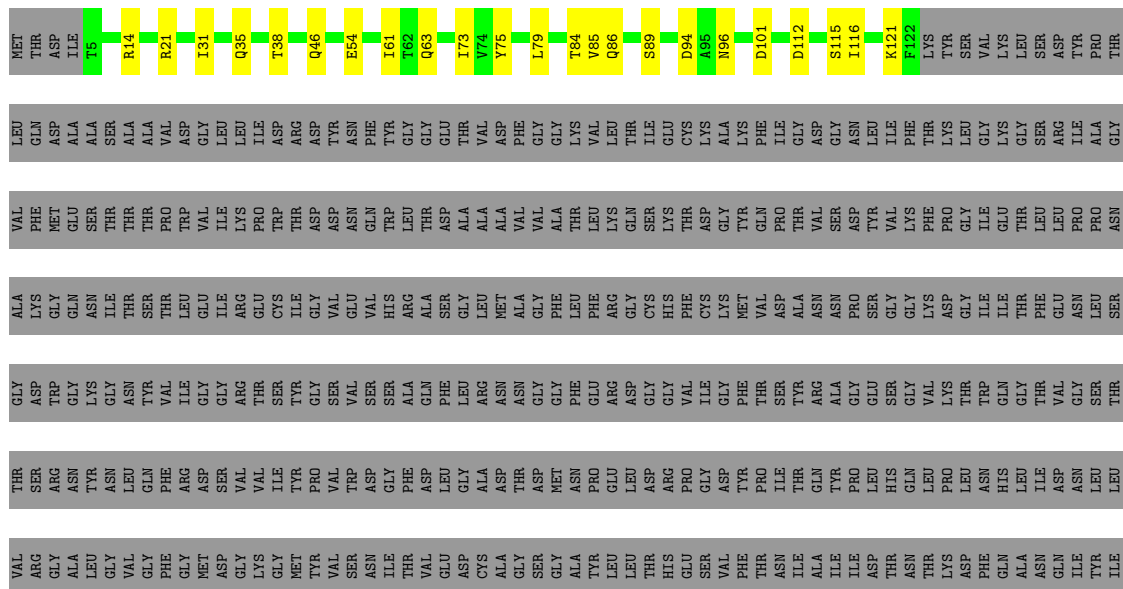
Chain C:  15% 2% 82%

[illegible]

Chain D: 15% . 82%

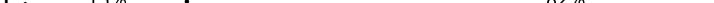


Chain E: 14% 82%



[illegible]

- Molecule 1: Tail spike protein

Chain F:  15% 2% 82%

[illegible]

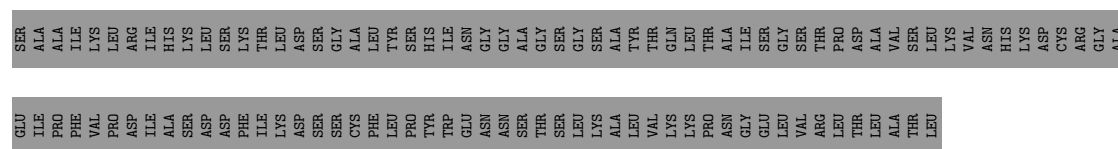
- Molecule 1: Tail spike protein

Chain H: 15% 2% 82%

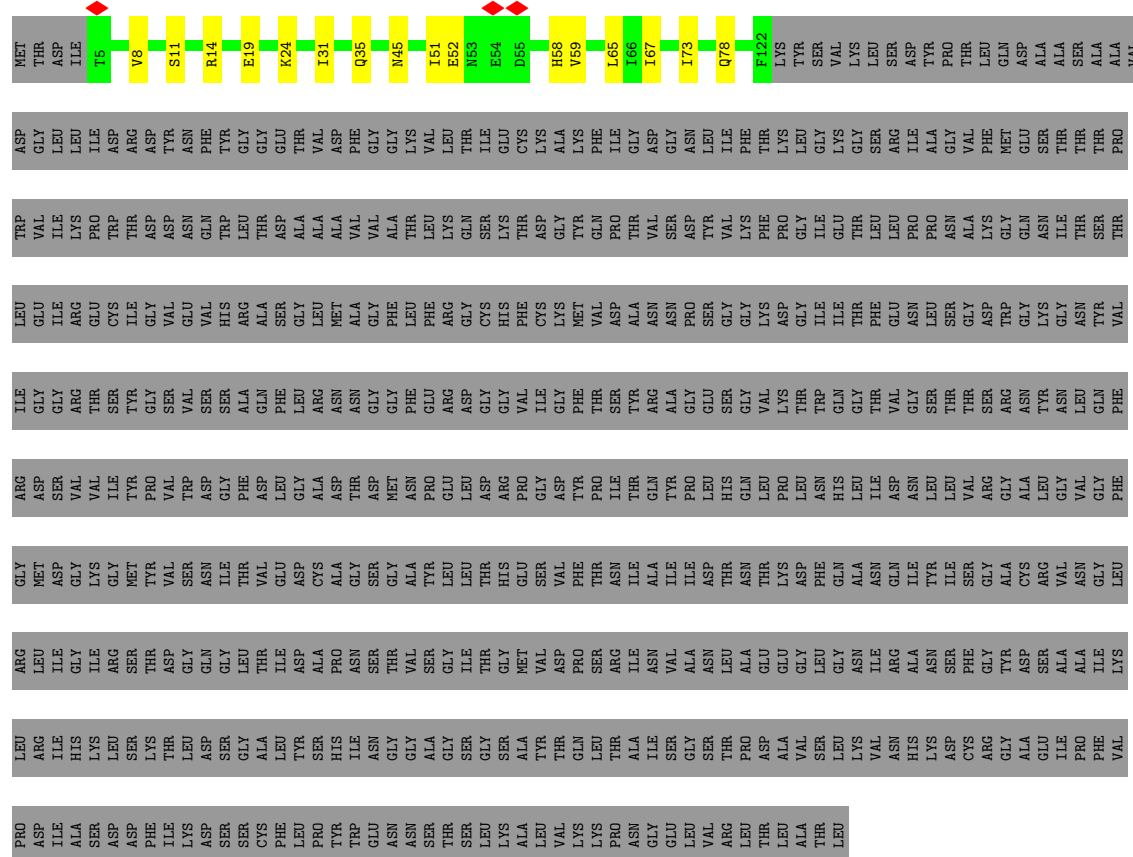
ALA	LYS	PHE	VAL	GLN	LEU	MET
GLY	GLY	GLY	GLY	ASP	ASP	THR
GLN	GLN	GLU	GLU	ALA	ILE	ASP
ILE	ASN	THR	THR	SER	ALA	T5
THR	THR	THR	THR	ALA	ALA	A6
THR	THR	THR	THR	VAL	VAL	I7
THR	THR	THR	THR	ASP	ASP	V8
LEU	LEU	VAL	VAL	GLY	GLY	S11
GLU	ILE	ILE	ILE	LEU	LEU	R14
ARG	LYS	LYS	LYS	LEU	LEU	R14
GLU	GLU	PRO	PRO	ILE	ILE	T18
CYS	CYS	TRP	TRP	ASP	ASP	E19
ILE	ILE	THR	THR	ARG	ARG	T18
GLY	GLY	ASP	ASP	ASP	ASP	K24
VAL	VAL	ASP	ASP	TYR	TYR	A25
GLU	GLU	ASN	ASN	ASN	ASN	N28
VAL	VAL	GLN	GLN	PHE	PHE	N28
HIS	HIS	TRP	TRP	TYR	TYR	I31
ARG	ARG	LEU	LEU	GLY	GLY	Y32
ALA	ALA	THR	THR	GLY	GLY	I33
SER	SER	ALA	ALA	GLU	GLU	I33
GLY	GLY	ALA	ALA	THR	THR	Q46
LEU	LEU	ALA	ALA	VAL	VAL	Q46
MET	MET	ALA	ALA	ASP	ASP	E54
ALA	ALA	VAL	VAL	PHE	PHE	D55
GLY	GLY	VAL	VAL	GLY	GLY	D55
PHE	PHE	ALA	ALA	GLY	GLY	D55
LEU	LEU	THR	THR	LYS	LYS	Q63
PHE	PHE	LEU	LEU	VAL	VAL	P64
ARG	ARG	LYS	LYS	LEU	LEU	P64
GLY	GLY	GLN	GLN	THR	THR	L65
CYS	CYS	SER	SER	ILE	ILE	L65
HIS	HIS	LYS	LYS	GLU	GLU	I67
PHE	PHE	THR	THR	GLU	GLU	I67
CYS	CYS	ASP	ASP	CYS	CYS	I73
LYS	LYS	GLY	GLY	ALA	ALA	I73
MET	MET	TYR	TYR	LYS	LYS	G77
VAL	VAL	GLN	GLN	PHE	PHE	G77
ASP	ASP	PRO	PRO	ILE	ILE	L79
ALA	ALA	THR	THR	GLY	GLY	L79
ASN	ASN	VAL	VAL	ASP	ASP	I82
ASN	ASN	SER	SER	GLY	GLY	I82
PRO	PRO	ASP	ASP	ASN	ASN	M90
SER	SER	TYR	TYR	LEU	LEU	A91
GLY	GLY	THR	THR	ILE	ILE	I92
LYS	LYS	PHE	PHE	PHE	PHE	F122
ASP	ASP	PRO	PRO	LYS	LYS	L93
GLY	GLY	GLY	GLY	LEU	LEU	TYR
ILE	ILE	ILE	ILE	GLY	GLY	SER
ILE	ILE	GLU	GLU	LYS	LYS	VAL
THR	THR	THR	THR	GLY	GLY	LYS
PHE	PHE	LEU	LEU	SER	SER	LEU
GLU	GLU	LEU	LEU	ARG	ARG	SER
ASN	ASN	PRO	PRO	ILE	ILE	ASP
LEU	LEU	PRO	PRO	ALA	ALA	TYR
SER	SER	ASN	ASN	GLY	GLY	PRO



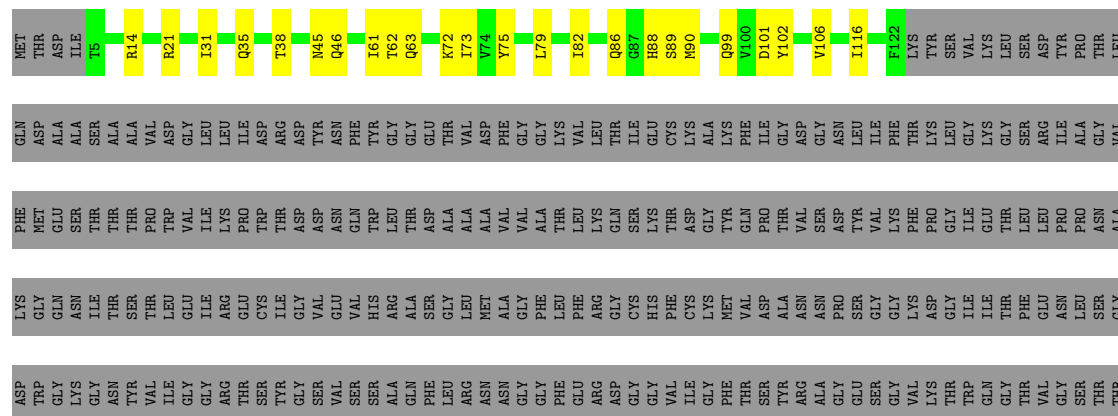




- Molecule 1: Tail spike protein



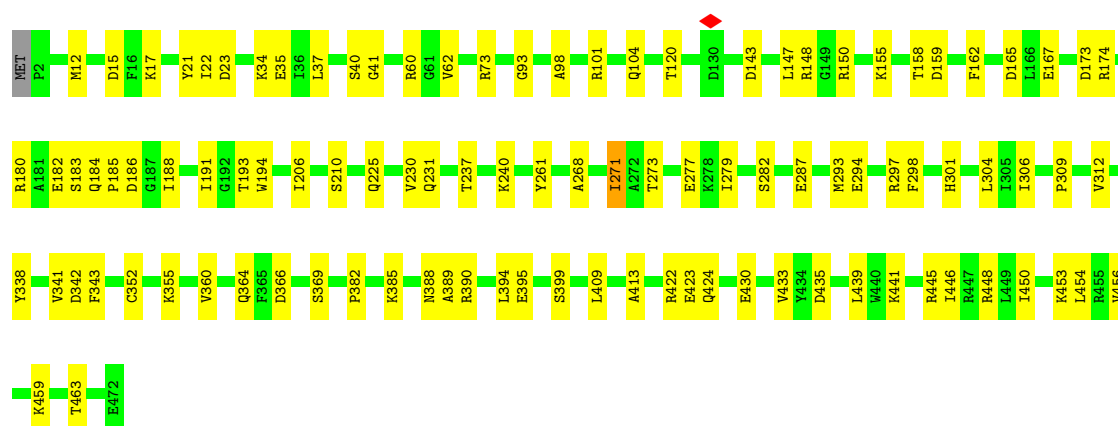
- Molecule 1: Tail spike protein





- Molecule 2: Packaged DNA stabilization protein gp10

Chain G: 78% 21%



- Molecule 2: Packaged DNA stabilization protein gp10

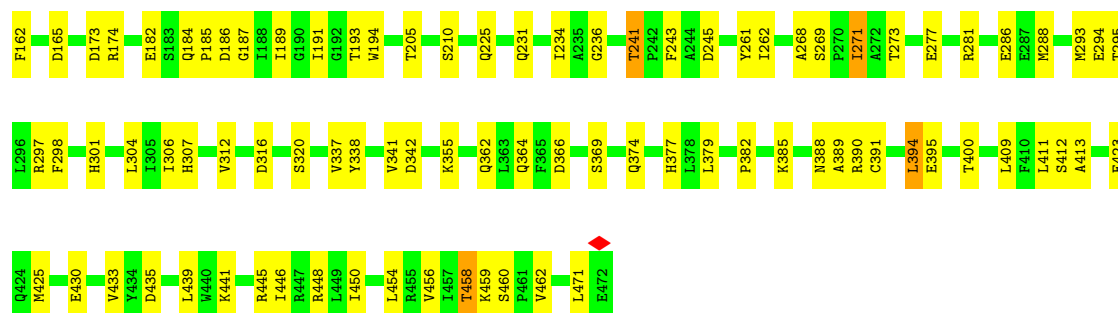
Chain K: 74% 25%



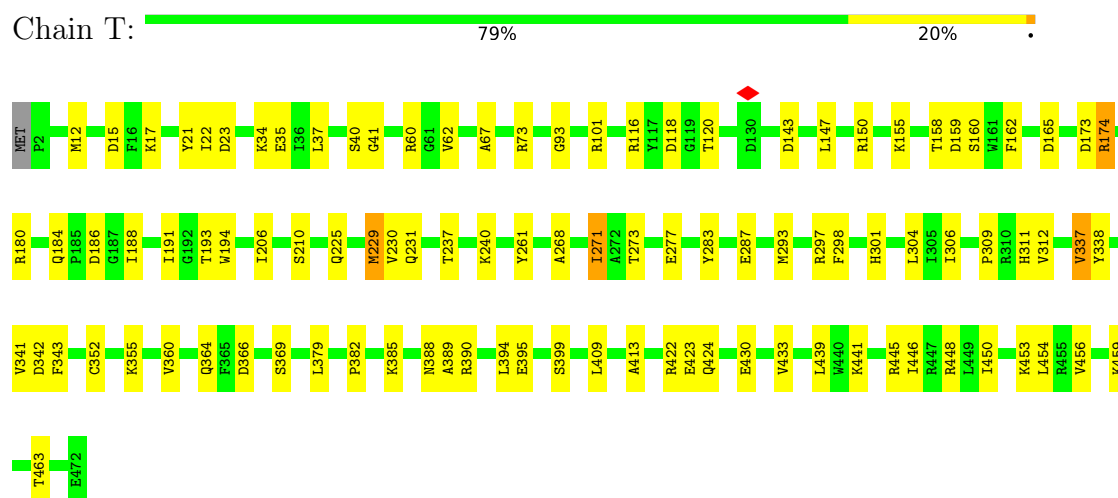
- Molecule 2: Packaged DNA stabilization protein gp10

Chain O: 74% 25%

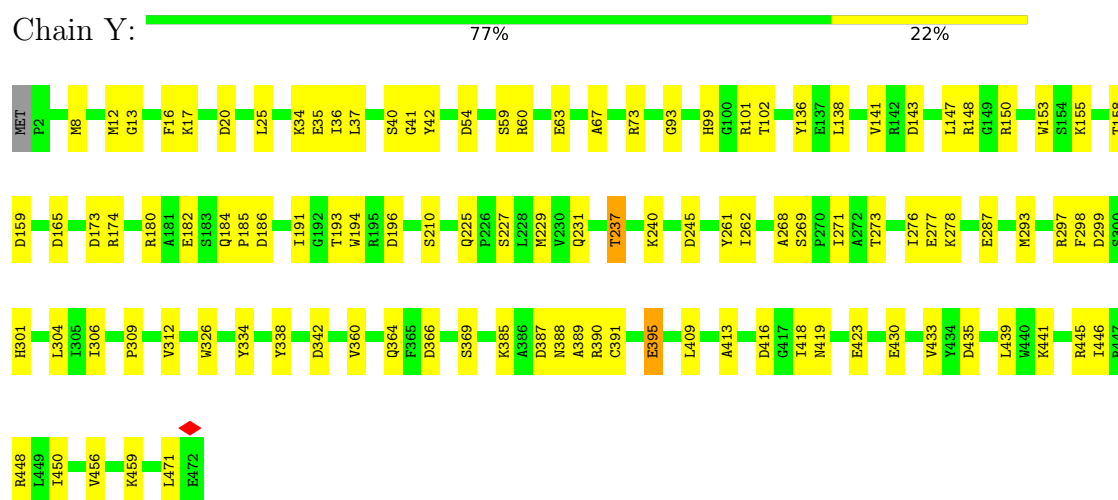




• Molecule 2: Packaged DNA stabilization protein gp10



• Molecule 2: Packaged DNA stabilization protein gp10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	38155	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 ($e^-/\text{\AA}^2$)	1.08	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	35.452	Depositor
Minimum map value	-27.985	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	512.9599, 512.9599, 512.9599	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.165818, 1.165818, 1.165818	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	0.11	0/931	0.29	0/1270
1	B	0.15	0/931	0.33	0/1270
1	C	0.15	0/931	0.31	0/1270
1	D	0.11	0/931	0.29	0/1270
1	E	0.13	0/931	0.29	0/1270
1	F	0.12	0/931	0.30	0/1270
1	H	0.10	0/931	0.28	0/1270
1	I	0.12	0/931	0.29	0/1270
1	J	0.14	0/931	0.30	0/1270
1	L	0.10	0/931	0.29	0/1270
1	M	0.13	0/931	0.28	0/1270
1	N	0.14	0/931	0.30	0/1270
1	P	0.11	0/931	0.29	0/1270
1	Q	0.15	0/931	0.30	0/1270
1	R	0.12	0/931	0.29	0/1270
1	V	0.10	0/931	0.29	0/1270
1	W	0.13	0/931	0.29	0/1270
1	X	0.15	0/931	0.33	0/1270
2	G	0.13	0/3764	0.34	0/5097
2	K	0.12	0/3764	0.33	0/5097
2	O	0.12	0/3764	0.32	0/5097
2	S	0.12	0/3764	0.34	0/5097
2	T	0.12	0/3764	0.32	0/5097
2	Y	0.12	0/3764	0.34	0/5097
All	All	0.12	0/39342	0.32	0/53442

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 ⓘ

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	913	0	903	13	0
1	B	913	0	903	18	0
1	C	913	0	903	10	0
1	D	913	0	903	12	0
1	E	913	0	903	16	0
1	F	913	0	903	10	0
1	H	913	0	903	21	0
1	I	913	0	903	24	0
1	J	913	0	903	12	0
1	L	913	0	903	21	0
1	M	913	0	903	21	0
1	N	913	0	903	12	0
1	P	913	0	903	12	0
1	Q	913	0	903	16	0
1	R	913	0	903	11	0
1	V	913	0	903	11	0
1	W	913	0	903	18	0
1	X	913	0	903	10	0
2	G	3683	0	3590	68	0
2	K	3683	0	3590	82	0
2	O	3683	0	3590	80	0
2	S	3683	0	3590	71	0
2	T	3683	0	3590	66	0
2	Y	3683	0	3590	69	0
All	All	38532	0	37794	603	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 8.

The worst 5 of 603 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)
2:G:395:GLU:HG2	2:G:439:LEU:HD13	1.67	0.76
2:T:395:GLU:HG2	2:T:439:LEU:HD13	1.67	0.76
2:S:409:LEU:HD12	2:S:456:VAL:HG22	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:262:ILE:HD12	2:S:271:ILE:HG13	1.68	0.76
2:K:395:GLU:HG2	2:K:439:LEU:HD13	1.68	0.75

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	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	B	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	C	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	D	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	E	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	F	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	H	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	I	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	J	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	L	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	M	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	N	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	P	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	Q	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	R	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	V	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	W	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	X	116/667 (17%)	113 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
2	K	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
2	O	469/472 (99%)	439 (94%)	30 (6%)	0	100	100
2	S	469/472 (99%)	437 (93%)	32 (7%)	0	100	100
2	T	469/472 (99%)	439 (94%)	30 (6%)	0	100	100
2	Y	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
All	All	4902/14838 (33%)	4662 (95%)	240 (5%)	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	101/548 (18%)	101 (100%)	0	100	100
1	B	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	C	101/548 (18%)	97 (96%)	4 (4%)	28	63
1	D	101/548 (18%)	101 (100%)	0	100	100
1	E	101/548 (18%)	100 (99%)	1 (1%)	68	88
1	F	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	H	101/548 (18%)	101 (100%)	0	100	100
1	I	101/548 (18%)	101 (100%)	0	100	100
1	J	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	L	101/548 (18%)	101 (100%)	0	100	100
1	M	101/548 (18%)	101 (100%)	0	100	100
1	N	101/548 (18%)	100 (99%)	1 (1%)	68	88
1	P	101/548 (18%)	101 (100%)	0	100	100
1	Q	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	R	101/548 (18%)	99 (98%)	2 (2%)	48	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V	101/548 (18%)	101 (100%)	0	100	100
1	W	101/548 (18%)	100 (99%)	1 (1%)	68	88
1	X	101/548 (18%)	96 (95%)	5 (5%)	22	54
2	G	394/395 (100%)	389 (99%)	5 (1%)	61	86
2	K	394/395 (100%)	383 (97%)	11 (3%)	38	73
2	O	394/395 (100%)	384 (98%)	10 (2%)	42	76
2	S	394/395 (100%)	386 (98%)	8 (2%)	48	80
2	T	394/395 (100%)	387 (98%)	7 (2%)	51	82
2	Y	394/395 (100%)	386 (98%)	8 (2%)	48	80
All	All	4182/12234 (34%)	4111 (98%)	71 (2%)	52	83

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	62	THR
1	X	57	SER
2	Y	196	ASP
2	K	50	THR
1	J	84	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	86	GLN
1	X	68	ASN
2	T	377	HIS
1	V	46	GLN
2	G	419	ASN

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 [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.

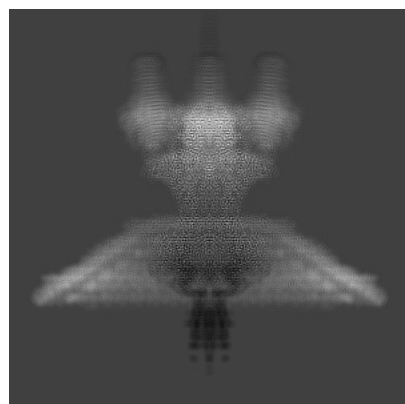
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41649. These allow visual inspection of the internal detail of the map and identification of artifacts.

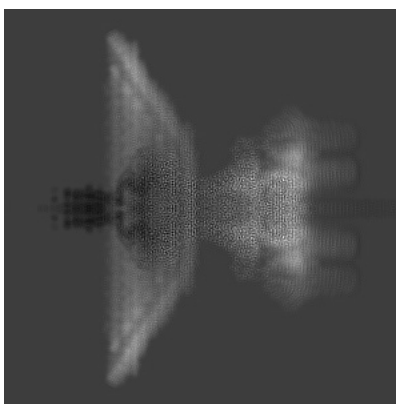
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

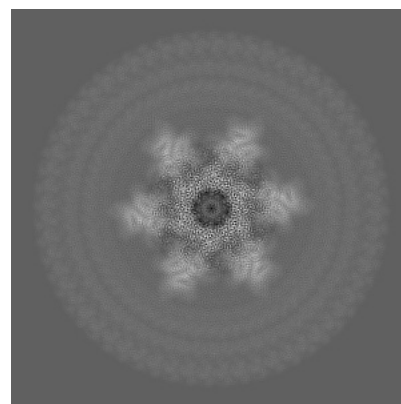
6.1.1 Primary map



X

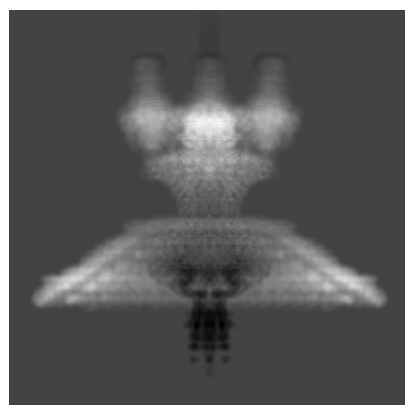


Y

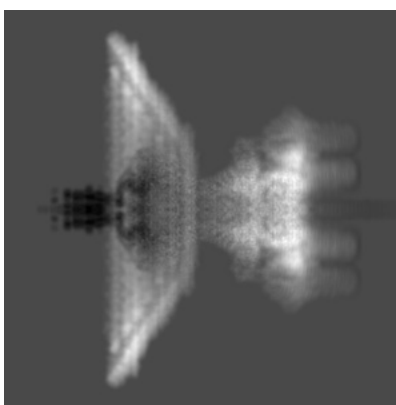


Z

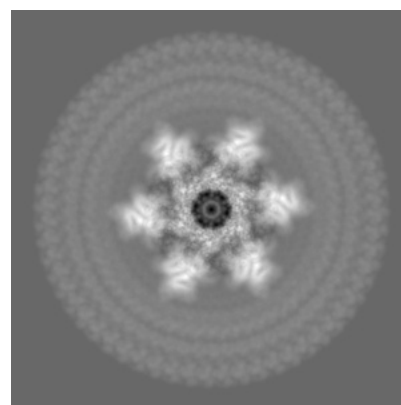
6.1.2 Raw map



X



Y



Z

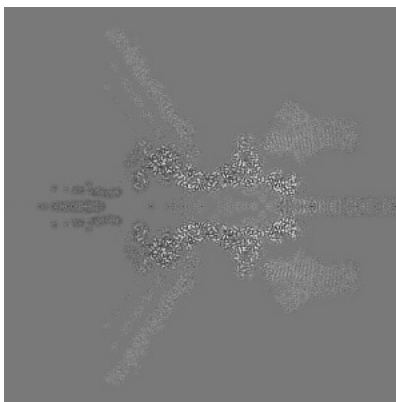
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

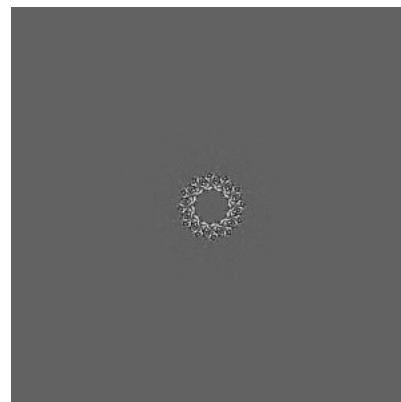
6.2.1 Primary map



X Index: 220

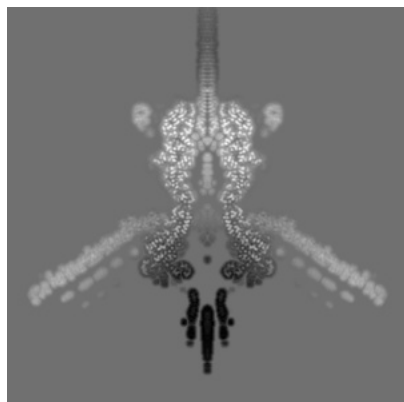


Y Index: 220

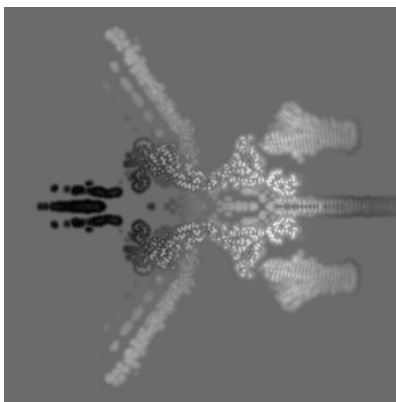


Z Index: 220

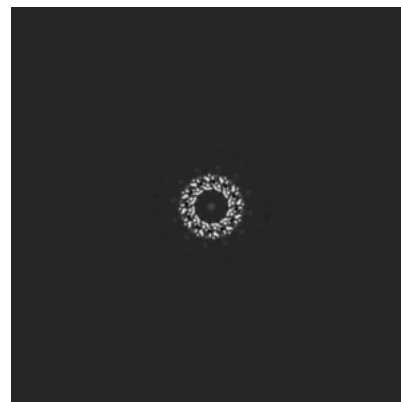
6.2.2 Raw map



X Index: 220



Y Index: 220

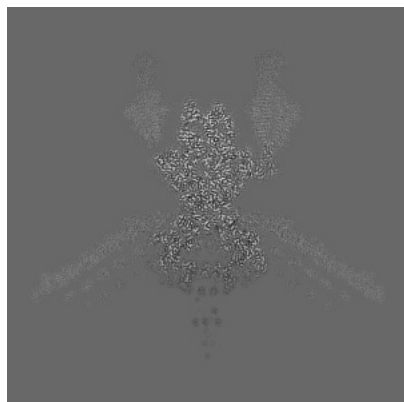


Z Index: 220

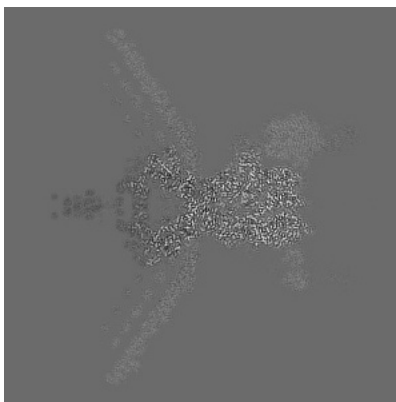
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

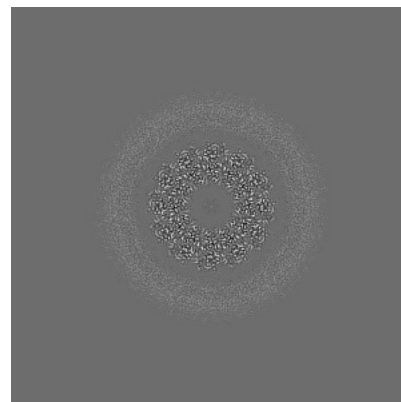
6.3.1 Primary map



X Index: 244



Y Index: 241

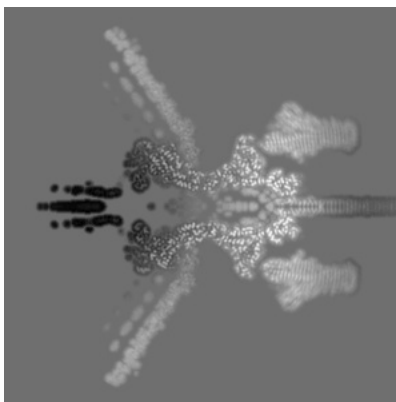


Z Index: 182

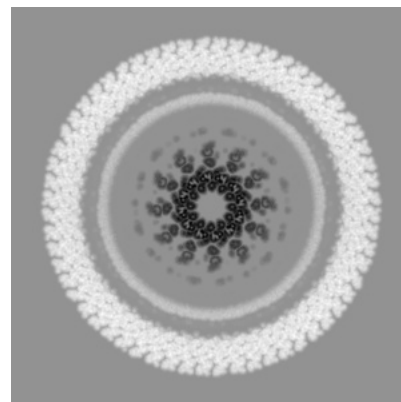
6.3.2 Raw map



X Index: 236



Y Index: 221

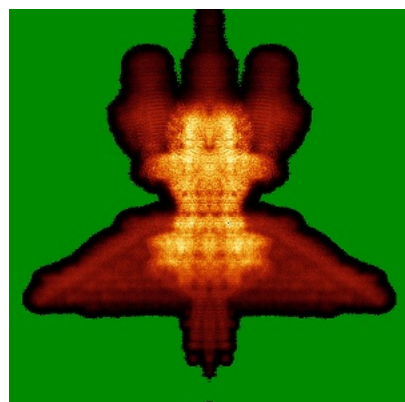


Z Index: 143

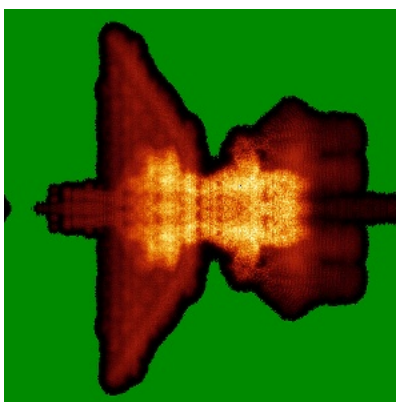
The images above show the largest variance slices of the map in three orthogonal directions.

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

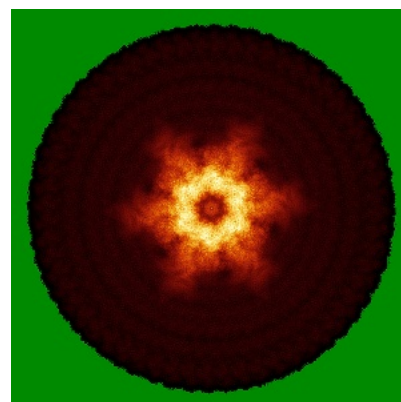
6.4.1 Primary map



X

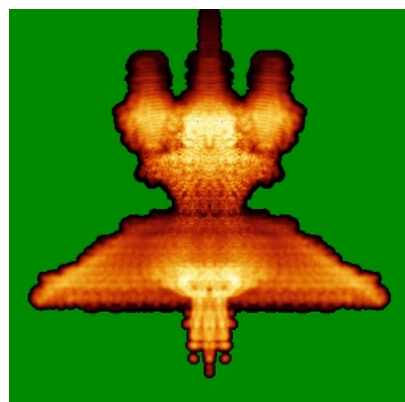


Y

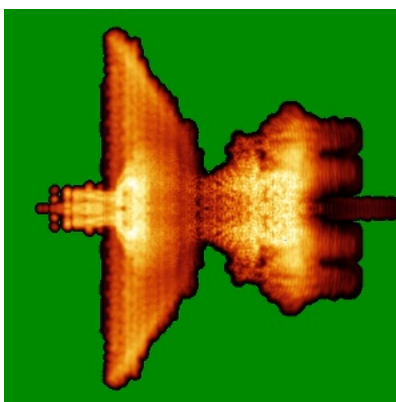


Z

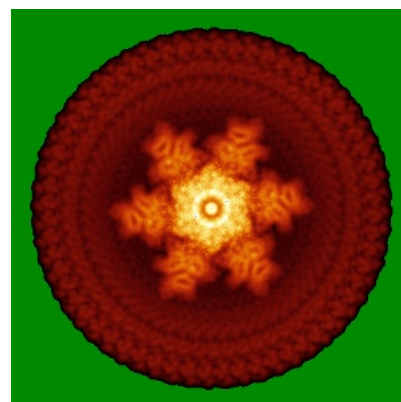
6.4.2 Raw map



X



Y

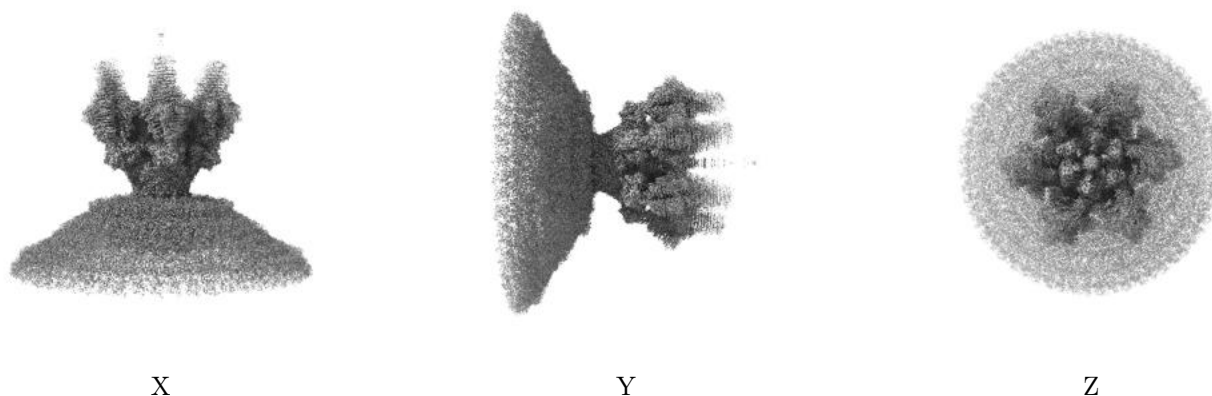


Z

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.

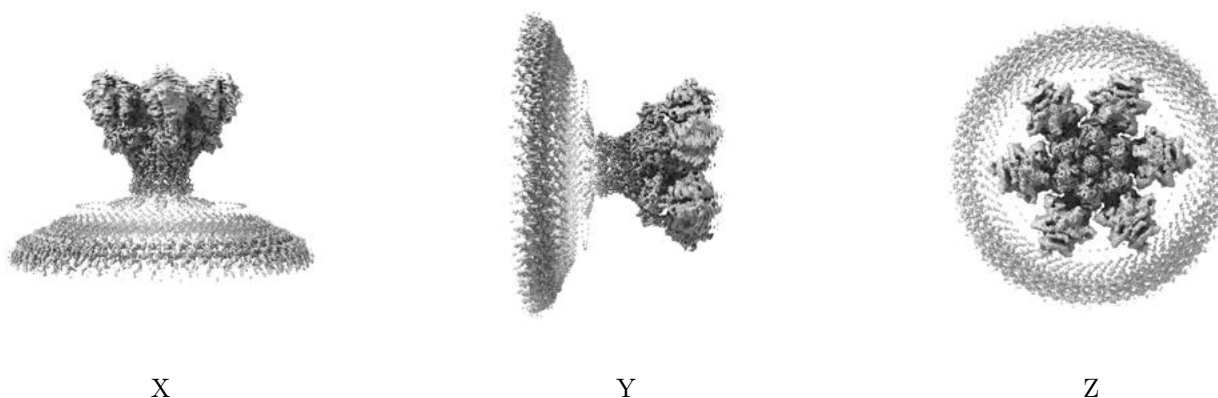
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. 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.

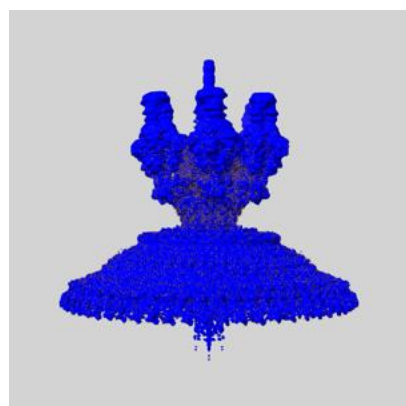
6.6 Mask visualisation [i](#)

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

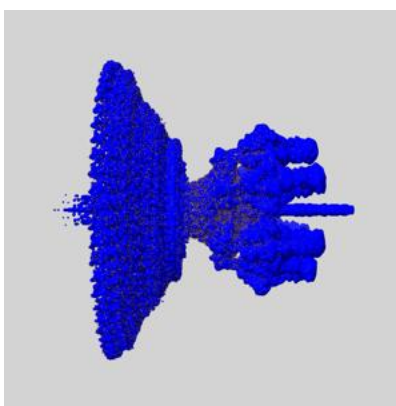
A mask typically either:

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

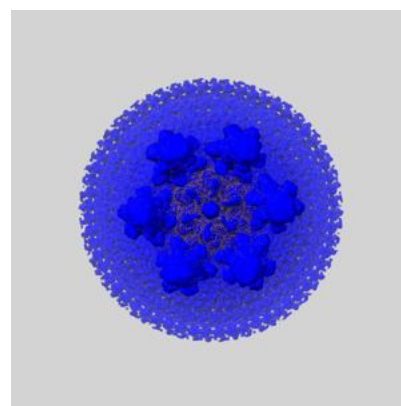
6.6.1 emd_41649_msk_1.map [i](#)



X



Y

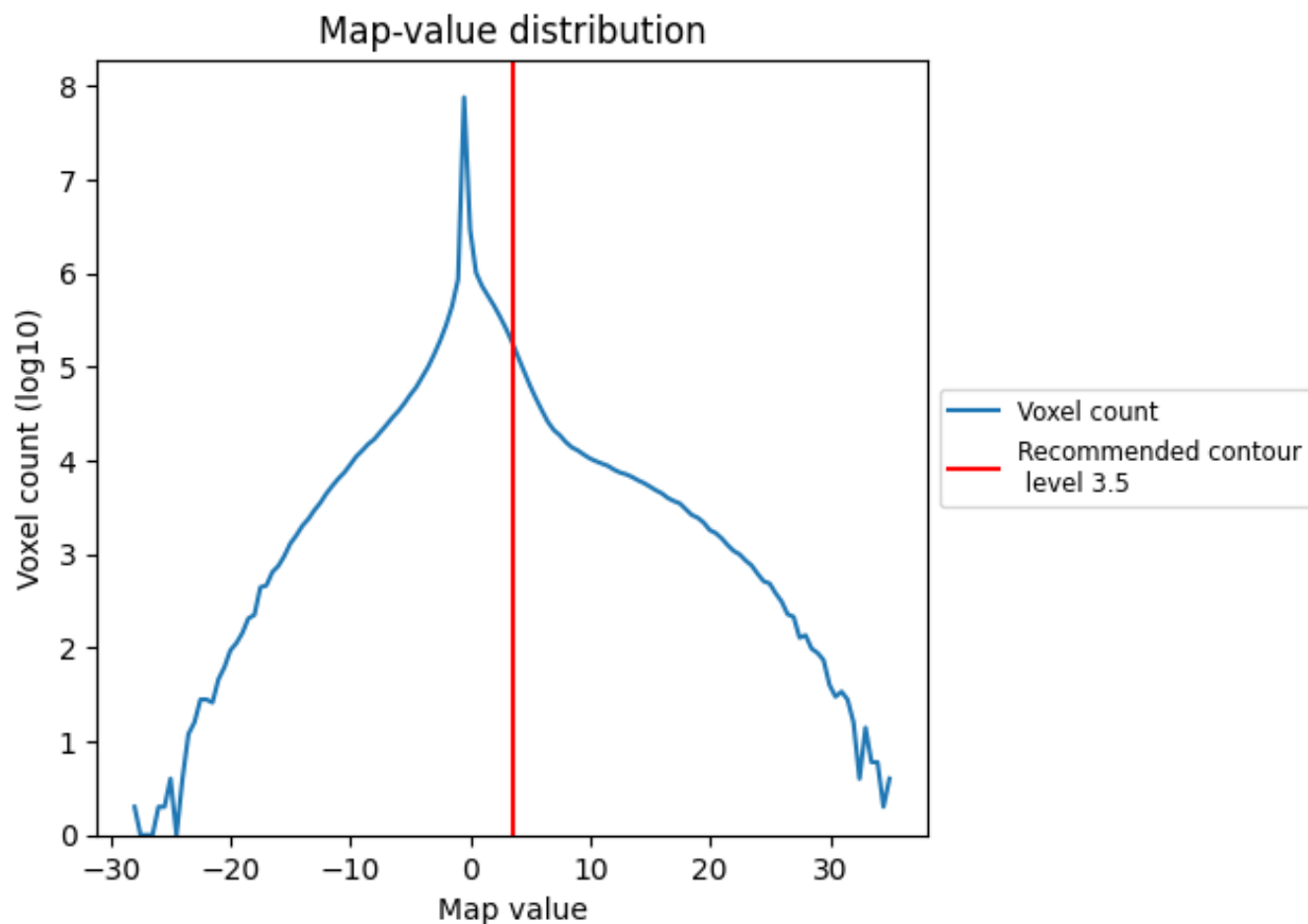


Z

7 Map analysis [i](#)

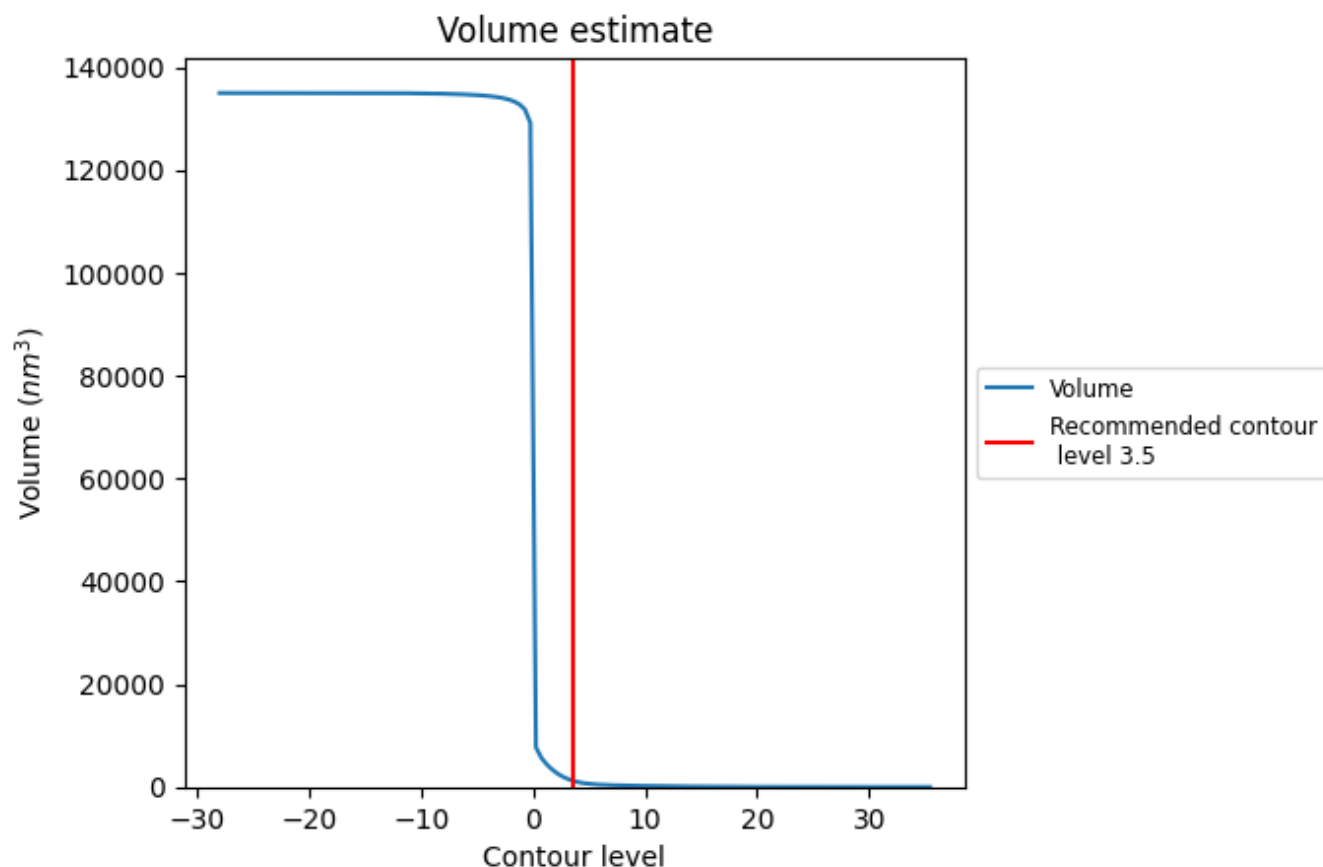
This section contains the results of statistical analysis of the map.

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.

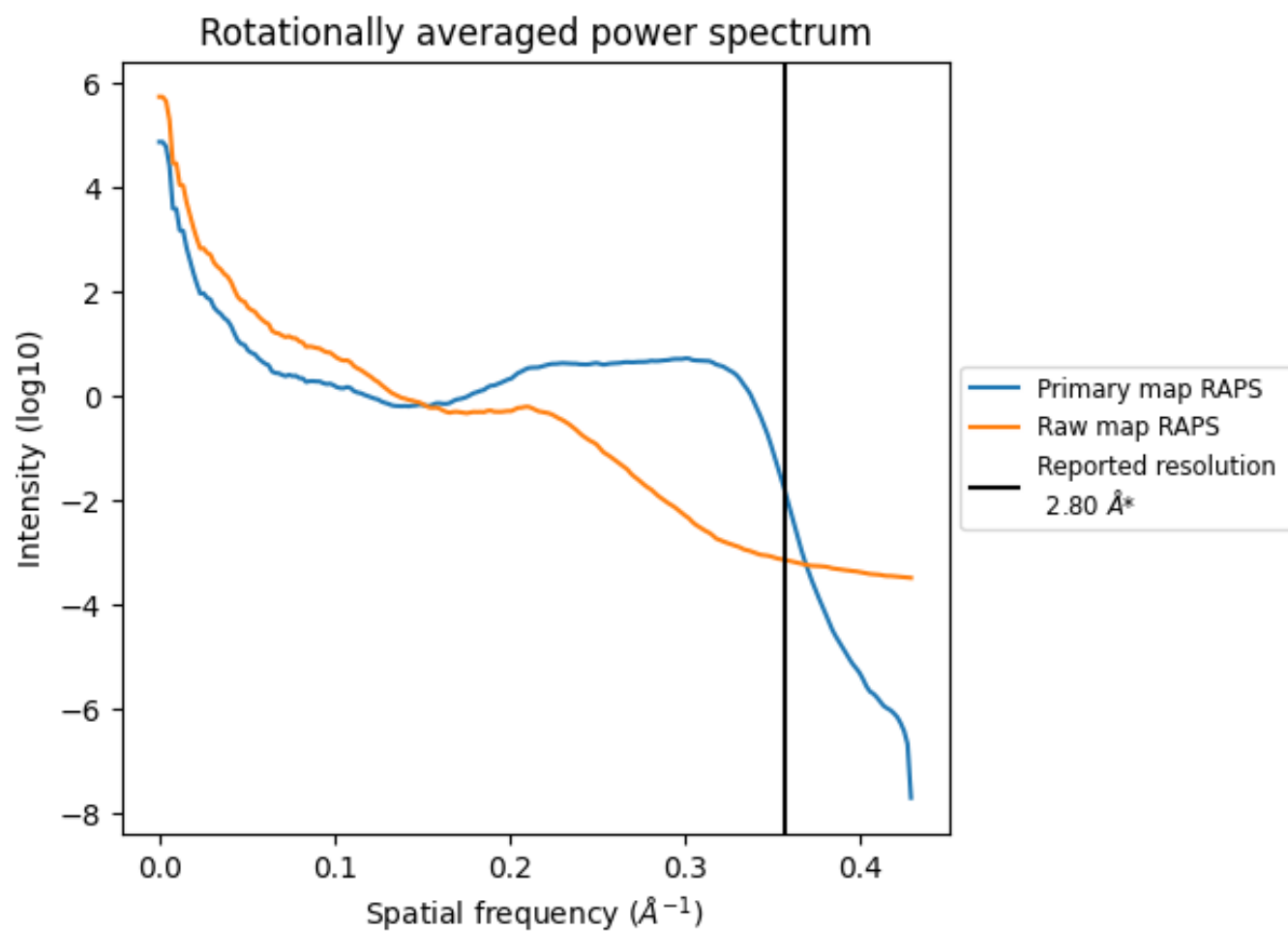
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1261 nm^3 ; this corresponds to an approximate mass of 1139 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 ⓘ

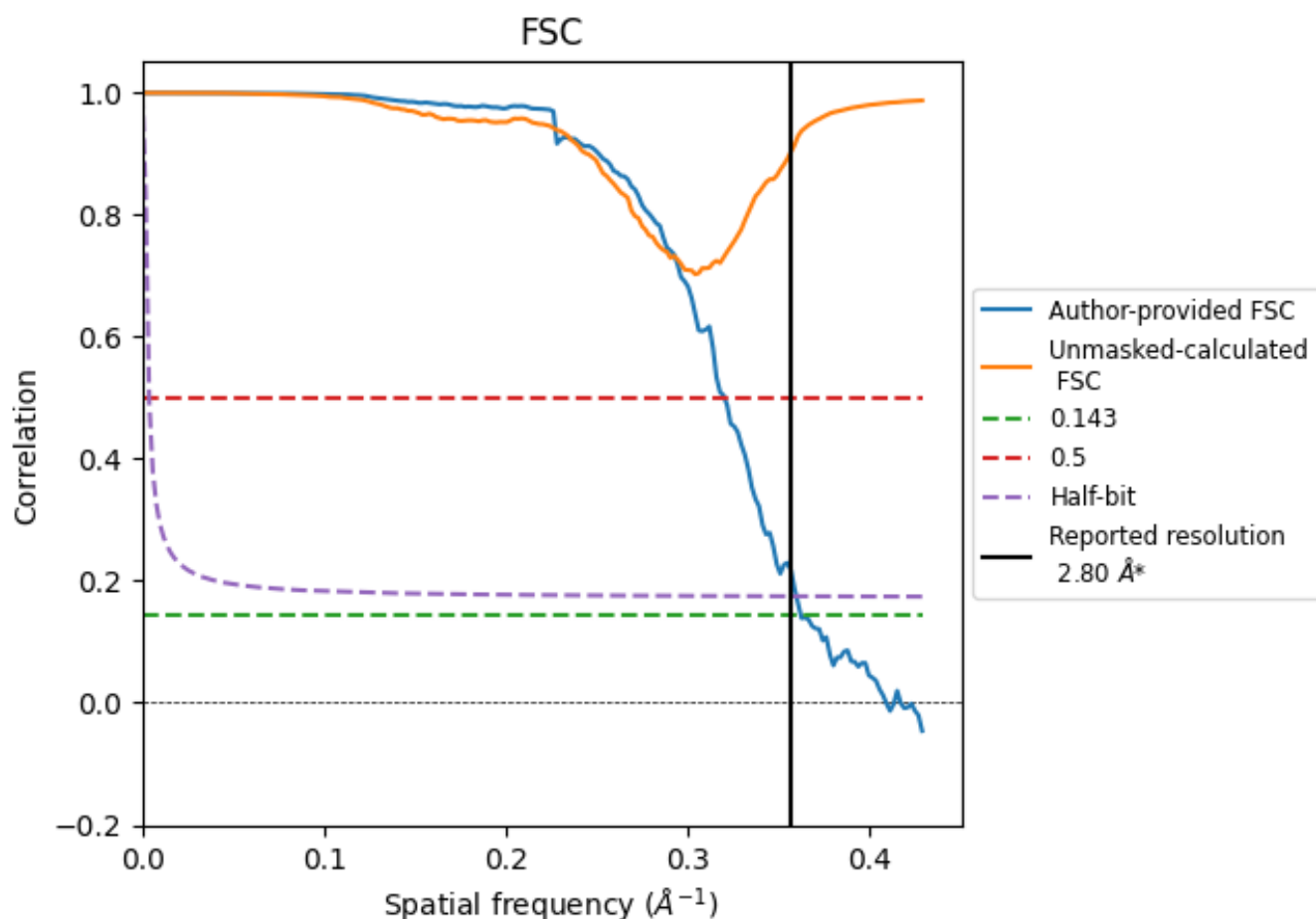


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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](#)

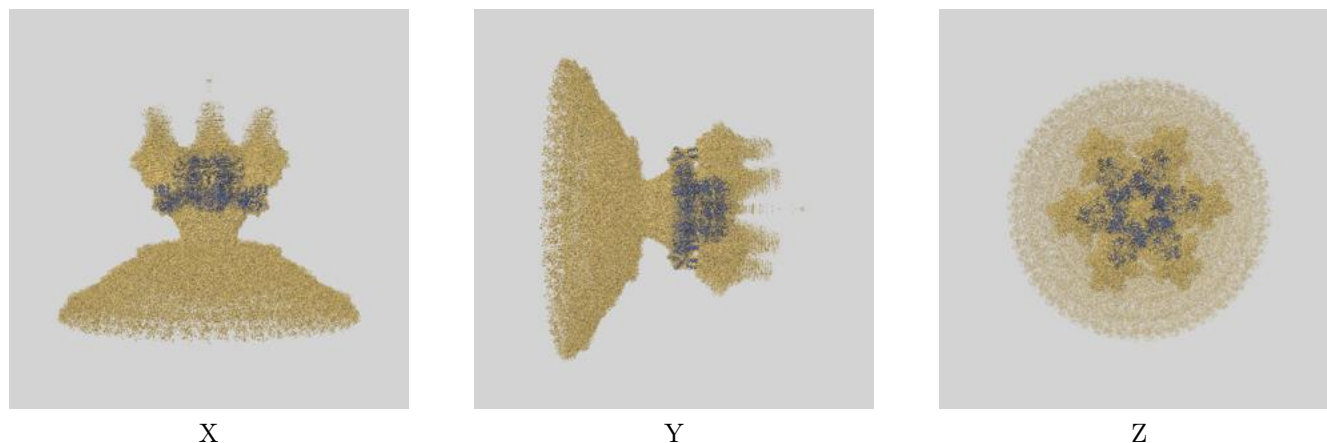
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.12	2.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

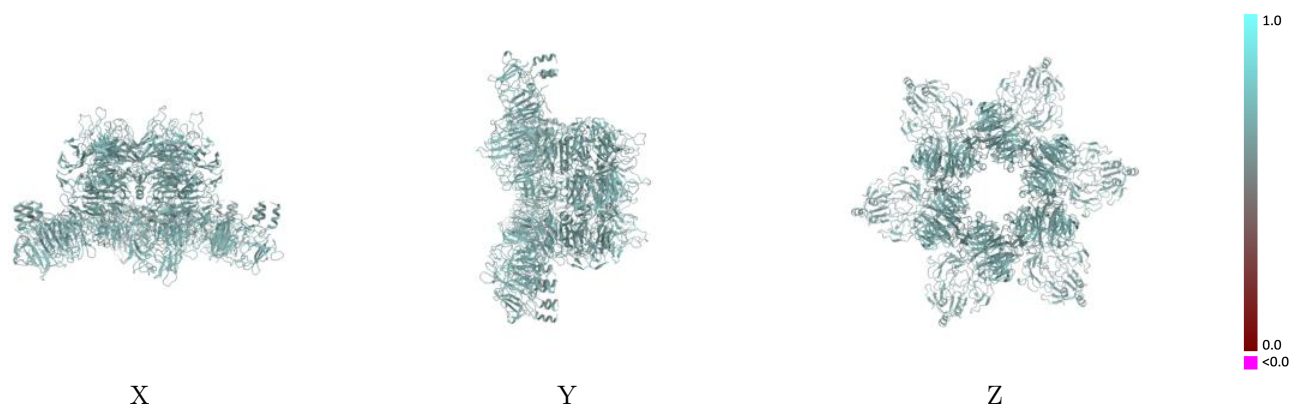
This section contains information regarding the fit between EMDB map EMD-41649 and PDB model 8TVR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



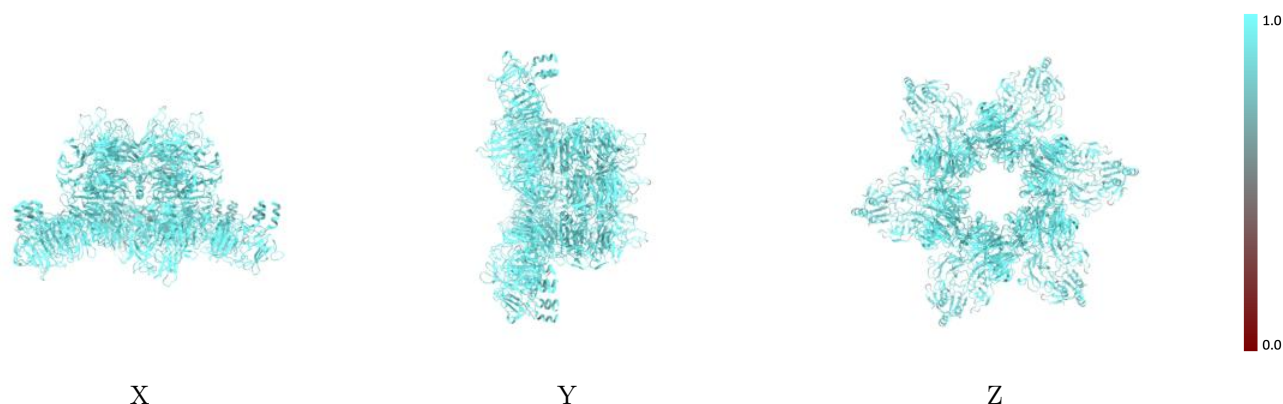
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



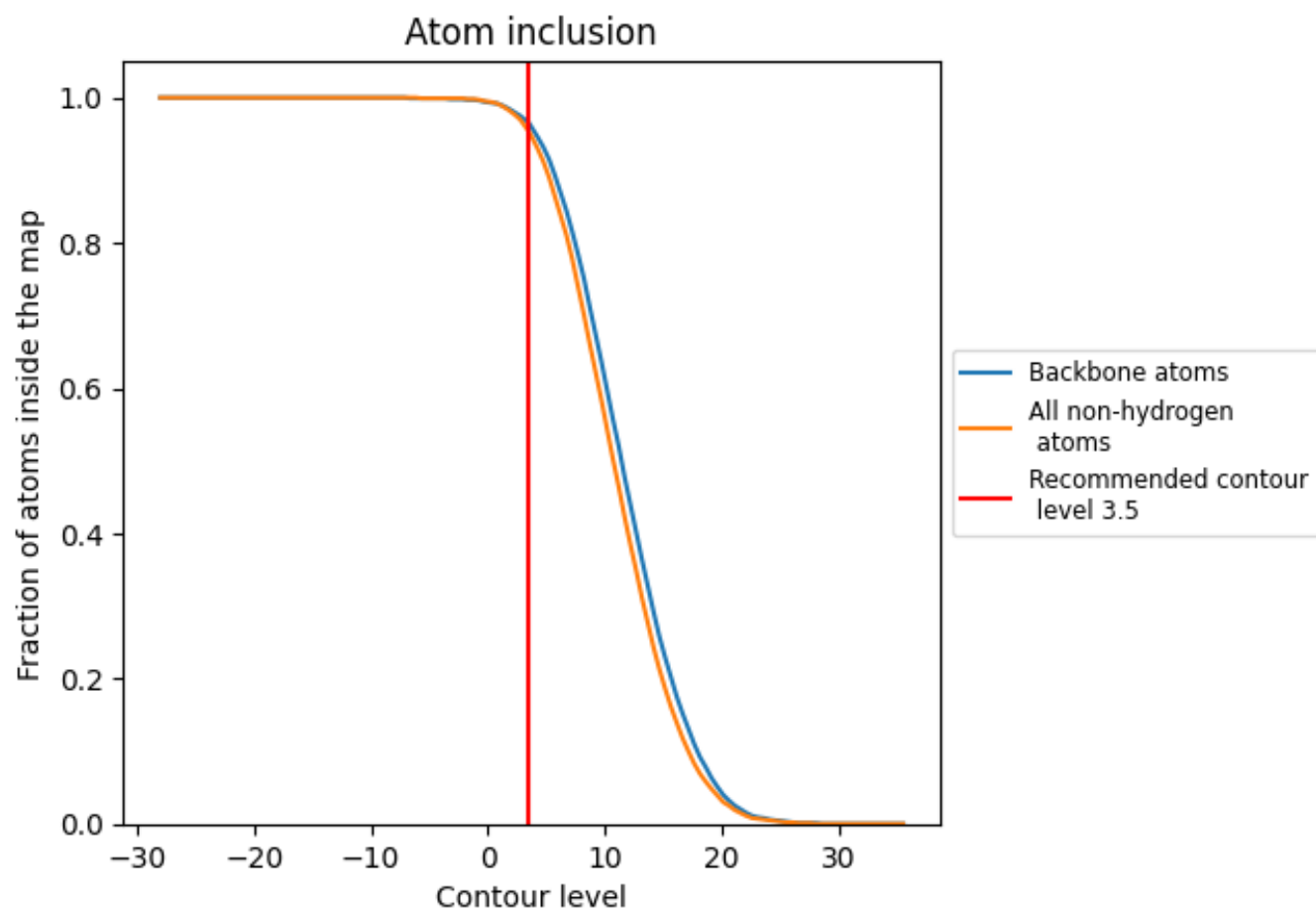
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.6270
A	 0.8980	 0.6060
B	 0.9520	 0.6230
C	 0.9510	 0.6290
D	 0.8940	 0.6060
E	 0.9520	 0.6250
F	 0.9530	 0.6280
G	 0.9680	 0.6320
H	 0.8990	 0.6080
I	 0.9470	 0.6270
J	 0.9530	 0.6280
K	 0.9690	 0.6340
L	 0.8990	 0.6070
M	 0.9490	 0.6260
N	 0.9520	 0.6300
O	 0.9670	 0.6340
P	 0.8910	 0.6080
Q	 0.9510	 0.6230
R	 0.9510	 0.6310
S	 0.9670	 0.6330
T	 0.9680	 0.6310
V	 0.8980	 0.6070
W	 0.9500	 0.6230
X	 0.9480	 0.6280
Y	 0.9680	 0.6330

