



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:21 AM UTC

PDB ID : 9OP4 / pdb_00009op4
EMDB ID : EMD-70678
Title : Herpes simplex virus type 1 (HSV-1) A-capsid pUL6 portal protein, dodecameric complex
Authors : Crofut, E.H.; Kashyap, S.; Stevens, A.; Jih, J.; Liu, Y.-T.; Zhou, Z.H.
Deposited on : 2025-05-16
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

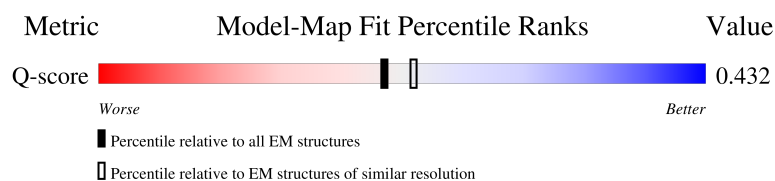
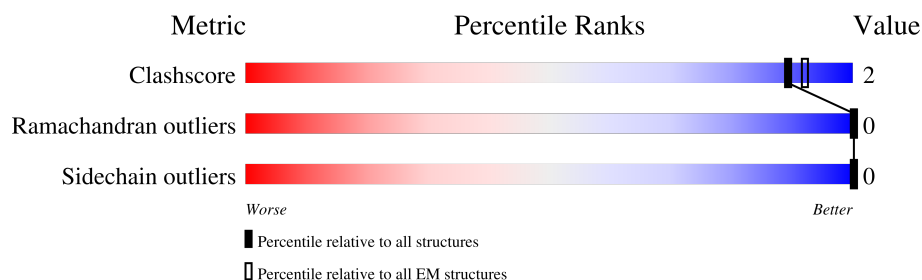
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

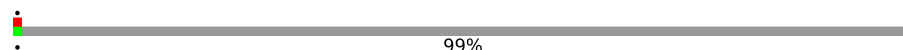
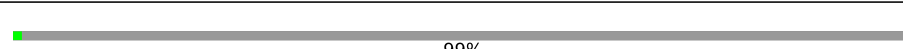
The reported resolution of this entry is 3.60 Å.

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.



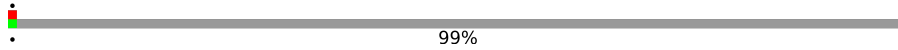
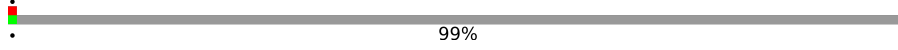
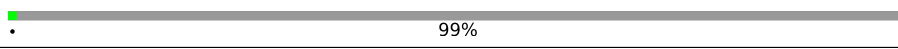
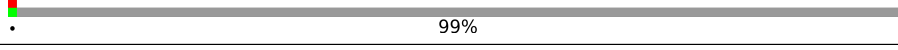
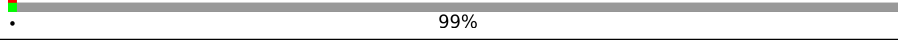
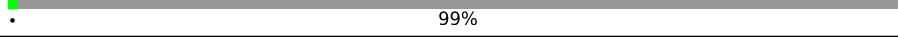
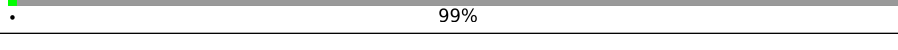
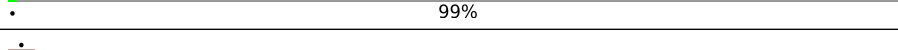
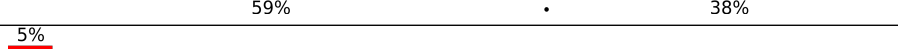
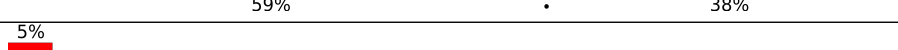
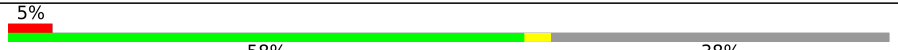
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	635	 99%
1	B	635	 99%
1	C	635	 99%
1	D	635	 99%

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Mol	Chain	Length	Quality of chain
1	E	635	 99%
1	F	635	 99%
1	G	635	 99%
1	H	635	 99%
1	I	635	 99%
1	J	635	 99%
1	K	635	 99%
1	L	635	 99%
2	a	676	 59% 38%
2	b	676	 59% 38%
2	c	676	 58% 38%
2	d	676	 59% 38%
2	e	676	 60% 38%
2	f	676	 59% 38%
2	g	676	 59% 38%
2	h	676	 58% 38%
2	i	676	 58% 38%
2	j	676	 58% 38%
2	k	676	 57% 5% 38%
2	l	676	 60% 38%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 40476 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 Capsid scaffolding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	7	Total	C	N	O	0	0
			56	38	7	11		
1	B	7	Total	C	N	O	0	0
			56	38	7	11		
1	C	7	Total	C	N	O	0	0
			56	38	7	11		
1	D	7	Total	C	N	O	0	0
			56	38	7	11		
1	E	7	Total	C	N	O	0	0
			56	38	7	11		
1	F	7	Total	C	N	O	0	0
			56	38	7	11		
1	G	7	Total	C	N	O	0	0
			56	38	7	11		
1	H	7	Total	C	N	O	0	0
			56	38	7	11		
1	I	7	Total	C	N	O	0	0
			56	38	7	11		
1	J	7	Total	C	N	O	0	0
			56	38	7	11		
1	K	7	Total	C	N	O	0	0
			56	38	7	11		
1	L	7	Total	C	N	O	0	0
			56	38	7	11		

- Molecule 2 is a protein called Capsid portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	416	Total	C	N	O	S	0	0
			3317	2110	601	597	9		
2	b	416	Total	C	N	O	S	0	0
			3317	2110	601	597	9		
2	c	416	Total	C	N	O	S	0	0
			3317	2110	601	597	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	e	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	f	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	g	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	h	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	i	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	j	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	k	416	Total 3317	C 2110	N 601	O 597	S 9	0	0
2	l	416	Total 3317	C 2110	N 601	O 597	S 9	0	0

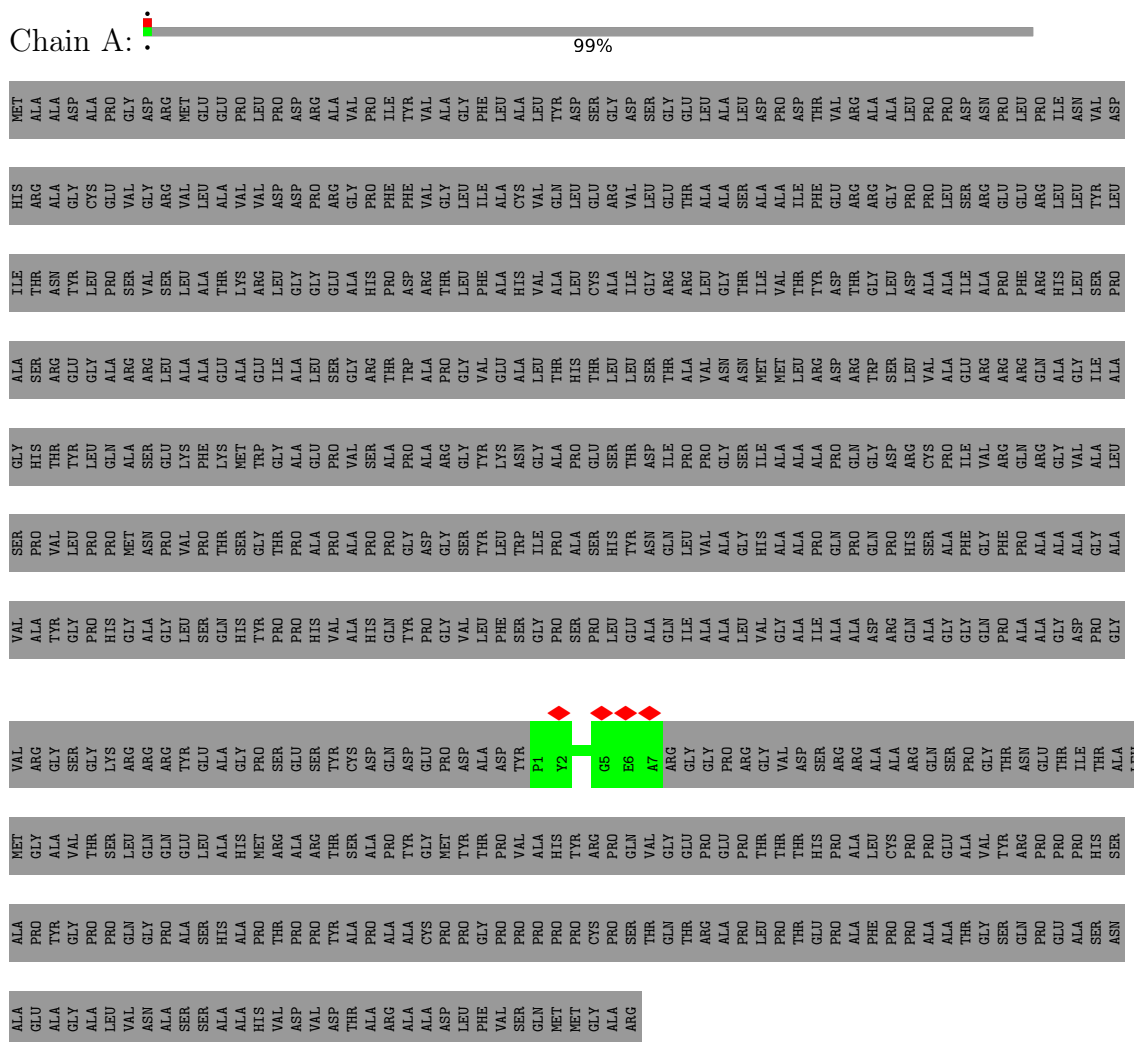
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	363	SER	ALA	conflict	UNP H9E912
b	363	SER	ALA	conflict	UNP H9E912
c	363	SER	ALA	conflict	UNP H9E912
d	363	SER	ALA	conflict	UNP H9E912
e	363	SER	ALA	conflict	UNP H9E912
f	363	SER	ALA	conflict	UNP H9E912
g	363	SER	ALA	conflict	UNP H9E912
h	363	SER	ALA	conflict	UNP H9E912
i	363	SER	ALA	conflict	UNP H9E912
j	363	SER	ALA	conflict	UNP H9E912
k	363	SER	ALA	conflict	UNP H9E912
l	363	SER	ALA	conflict	UNP H9E912

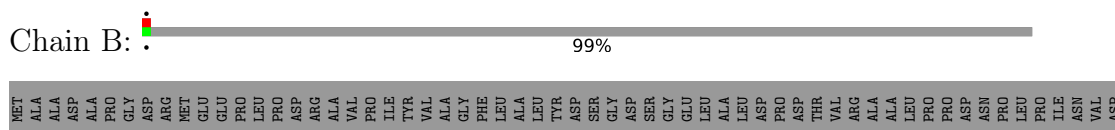
3 Residue-property plots

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: Capsid scaffolding protein



- Molecule 1: Capsid scaffolding protein





- Molecule 1: Capsid scaffolding protein

Chain D: 99%

GLY	ALA	PRO	GLY	VAL	VAL	SER	GLY	ALA	TLE	ALA	TLE	HIS	MET
ALA	GLY	GLY	ARG	VAL	ALA	PRO	THR	SER	THR	SER	THR	ARG	ALA
ALA	VAL	PRO	SER	GLY	TYR	VAL	THR	GLY	GLY	GLY	TYR	GLY	ALA
VAL	LEU	PRO	SER	PRO	PRO	PRO	LEU	LEU	LEU	LEU	LEU	CYS	ALA
ASN	VAL	GLN	ARG	HIS	HIS	PRO	HIS	ALA	ALA	ALA	PRO	GLU	PRO
ALA	ASN	GLY	GLY	GLY	GLY	MET	GLY	GLY	GLY	ARG	SER	VAL	GLY
ALA	ASN	GLY	ARG	ALA	ALA	ALA	GLY	GLY	GLY	ARG	VAL	GLY	ASP
ALA	SER	ALA	ARG	GLY	GLY	PRO	GLY	PRO	GLY	ARG	VAL	GLY	MET
ALA	SER	HIS	TYR	SER	SER	PRO	GLY	GLY	ALA	ALA	ALA	LEU	GLU
ALA	ALA	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	ALA	GLU
HIS	HIS	PRO	MET	ALA	ALA	SER	GLY	GLY	GLY	GLY	LYS	VAL	PRO
VAL	VAL	PRO	ARG	TYR	TYR	GLY	THR	GLY	ARG	GLY	ARG	VAL	LEU
ASP	ASP	PRO	ALA	SER	PRO	THR	THR	THR	TLE	TLE	ASP	ASP	LEU
VAL	VAL	PRO	ARG	GLY	GLY	PRO	PRO	ALA	ALA	GLY	GLY	VAL	VAL
ASP	ASP	TYR	SER	SER	HIS	ALA	ALA	GLY	LEU	LEU	GLY	ALA	LEU
THR	THR	ALA	SER	TYR	VAL	PRO	VAL	SER	GLY	GLY	GLY	ARG	ALA
ALA	ALA	PRO	ALA	CYS	ALA	ALA	ALA	ALA	VAL	GLY	ALA	GLY	VAL
ARG	ARG	ALA	PRO	GLN	GLN	PRO	GLY	GLY	THR	ALA	ALA	GLY	ALA
ALA	ALA	ALA	TYR	GLY	TYR	GLY	TYR	GLY	ARG	ALA	ARG	GLY	ALA
ALA	ALA	CYS	GLY	ASP	ASP	ASP	GLY	GLY	GLY	PRO	THR	GLY	ALA
ASP	ASP	PRO	MET	GLY	GLY	GLY	GLY	GLY	GLY	ALA	ARG	VAL	VAL
PHE	PHE	PRO	TYR	ASP	VAL	SER	THR	SER	GLY	PRO	THR	LEU	ALA
VAL	VAL	PRO	VAL	ALA	PHE	LEU	LEU	TYR	VAL	ALA	PHE	LEU	PHE
SER	SER	PRO	VAL	ASP	SER	LEU	LEU	LEU	GLY	ALA	ALA	LEU	ALA
GLN	GLN	PRO	ALA	ASP	SER	TRP	TRP	ASN	ALA	ALA	HIS	CYS	ALA
MET	MET	PRO	PRO	GLY	GLY	ILE	ILE	GLY	THR	THR	VAL	VAL	LEU
MET	MET	PRO	PRO	P1	P1	PRO	ALA	ALA	ALA	GLN	ALA	GLN	TYR
GLY	GLY	CYS	ARG	P2	P2	ALA	PRO	PRO	THR	THR	HIS	LEU	ASP
ALA	ALA	PRO	PRO	S6	S6	SER	ALA	SER	GLY	GLY	CYS	GLY	GLY
ARG	ARG	SER	GLN	A7	A7	HIS	LEU	LEU	LEU	VAL	ALA	ARG	ALA
		THR	THR	ARG	ARG	ALA	ASN	ASN	THR	THR	ASN	LEU	SER
		GLN	GLY	GLY	GLN	GLN	GLN	ILE	ILE	ARG	GLY	GLY	GLY
		ARG	GLY	PRO	ILE	LEU	VAL	PRO	ARG	ALA	THR	THR	THR
		ALA	GLY	ARG	ALA	VAL	VAL	ALA	VAL	VAL	ALA	ALA	ALA
		PRO	PRO	ARG	ALA	ALA	GLY	GLY	GLY	ASN	THR	SER	ALA
		LEU	THR	ALA	VAL	HIS	GLY	ILE	ILE	MET	VAL	ALA	ASP
		PRO	THR	SER	GLY	ALA	ALA	ALA	VAL	ALA	THR	THR	PRO
		GLY	HIS	ARG	TLE	ALA	ALA	ALA	THR	LEU	TLE	ALA	ASP
		PRO	PRO	ARG	ARG	PRO	PRO	PRO	TYR	ARG	PHE	VAL	THR
		ALA	LEU	ALA	ALA	GLN	GLN	GLN	GLN	GLY	GLY	ARG	ALA
		PRO	CYS	ALA	ALA	PRO	PRO	ASP	THR	SER	THR	GLY	ALA
		PRO	PRO	GLN	ARG	PRO	PRO	ARG	GLY	LEU	ALA	PRO	ALA
		ALA	PRO	GLN	GLN	HIS	HIS	ASN	ASN	THR	ALA	ASN	ASN
		ALA	PRO	GLN	ARG	GLY	GLY	VAL	VAL	GLY	GLY	GLY	GLY
		THR	THR	THR	THR	PHE	PHE	THR	THR	THR	THR	THR	THR
		GLY</											

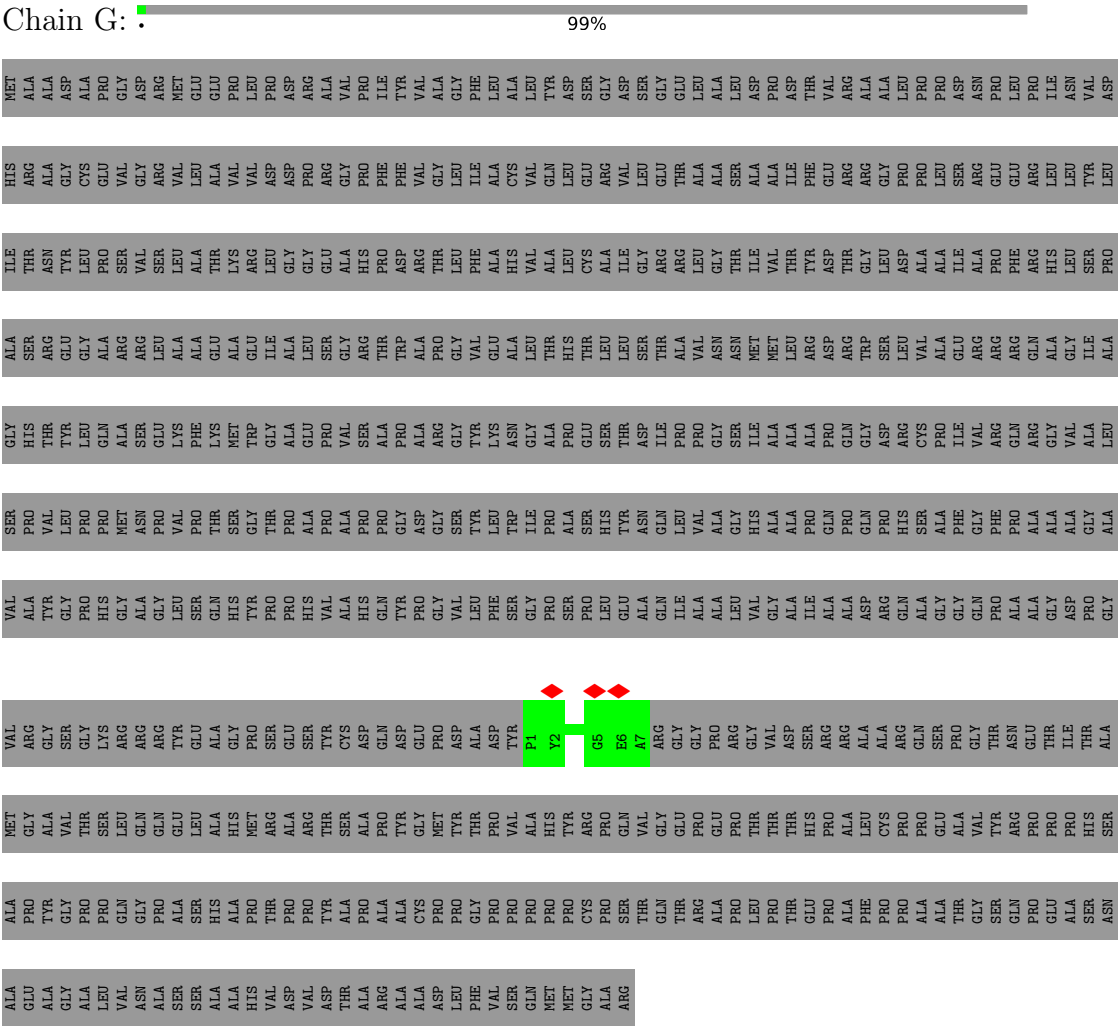
- Molecule 1: Capsid scaffolding protein

Chain E: 99%

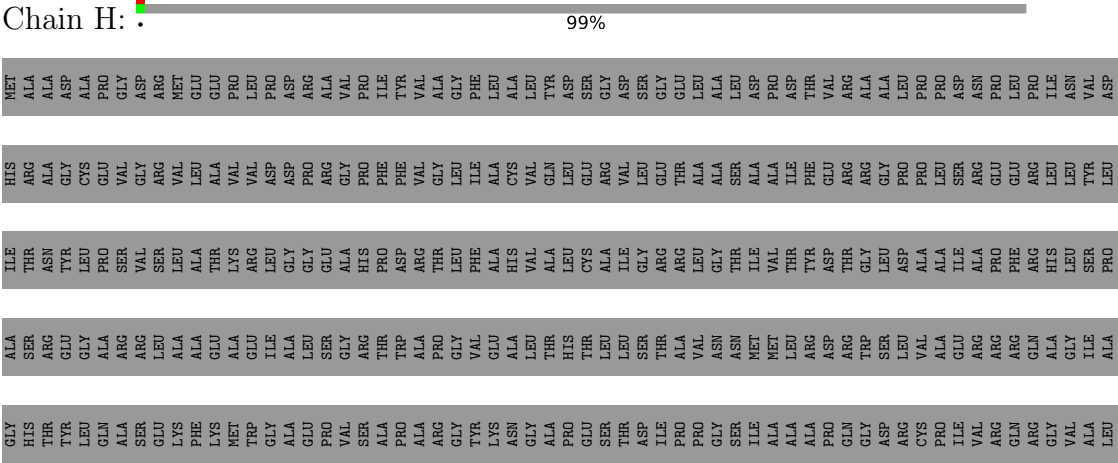
[illegible]

ALA	GLU	ALA	GLY	ALA	ALA	LEU	VAL	GLY	ASP	ASN	SER	SER	ALA	ALA	HIS	VAL	ASP	VAL	THR	ALA	ARG	ALA	ALA	ASP	LEU	PHE	SER	SER	GLN	MET	MET	GLY	ALA	ARG
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● Molecule 1: Capsid scaffolding protein



● Molecule 1: Capsid scaffolding protein



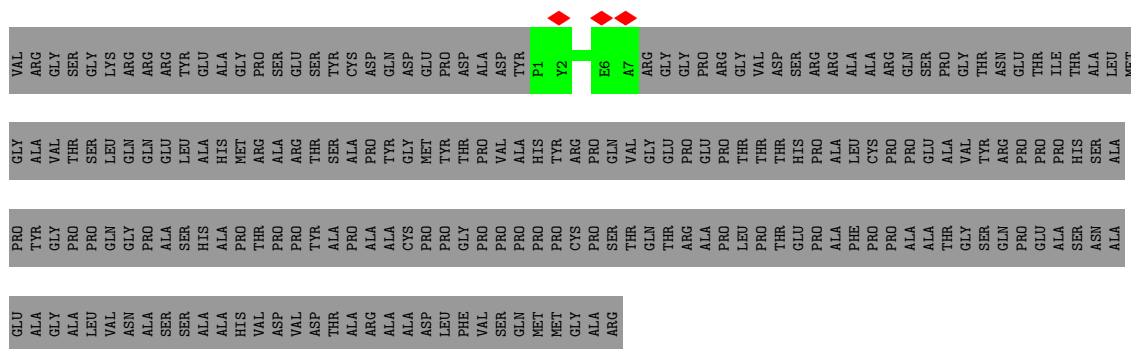
99%

[illegible]

- Molecule 1: Capsid scaffolding protein

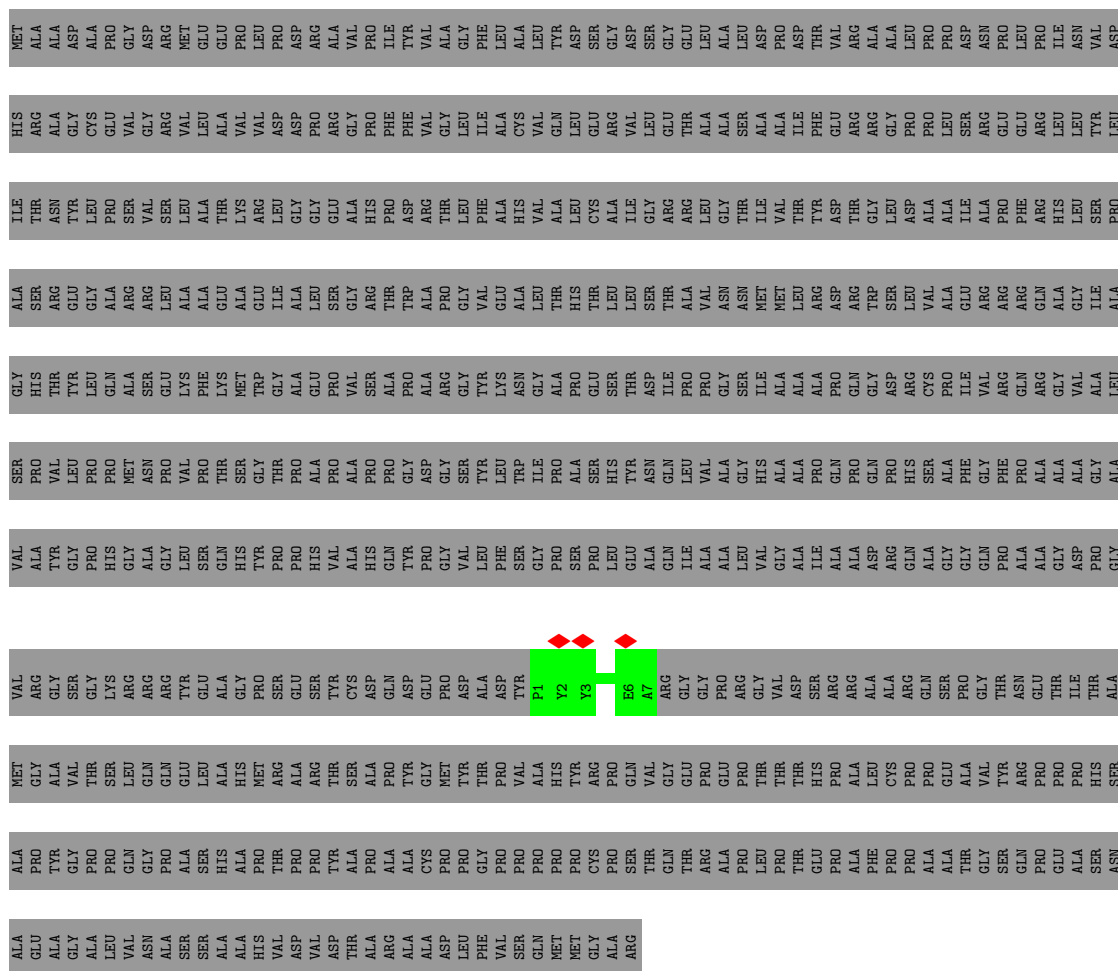
99%

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

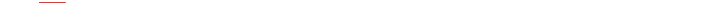


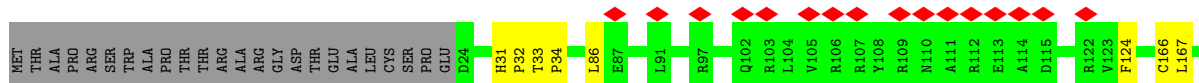
- Molecule 1: Capsid scaffolding protein

Chain L: 99%



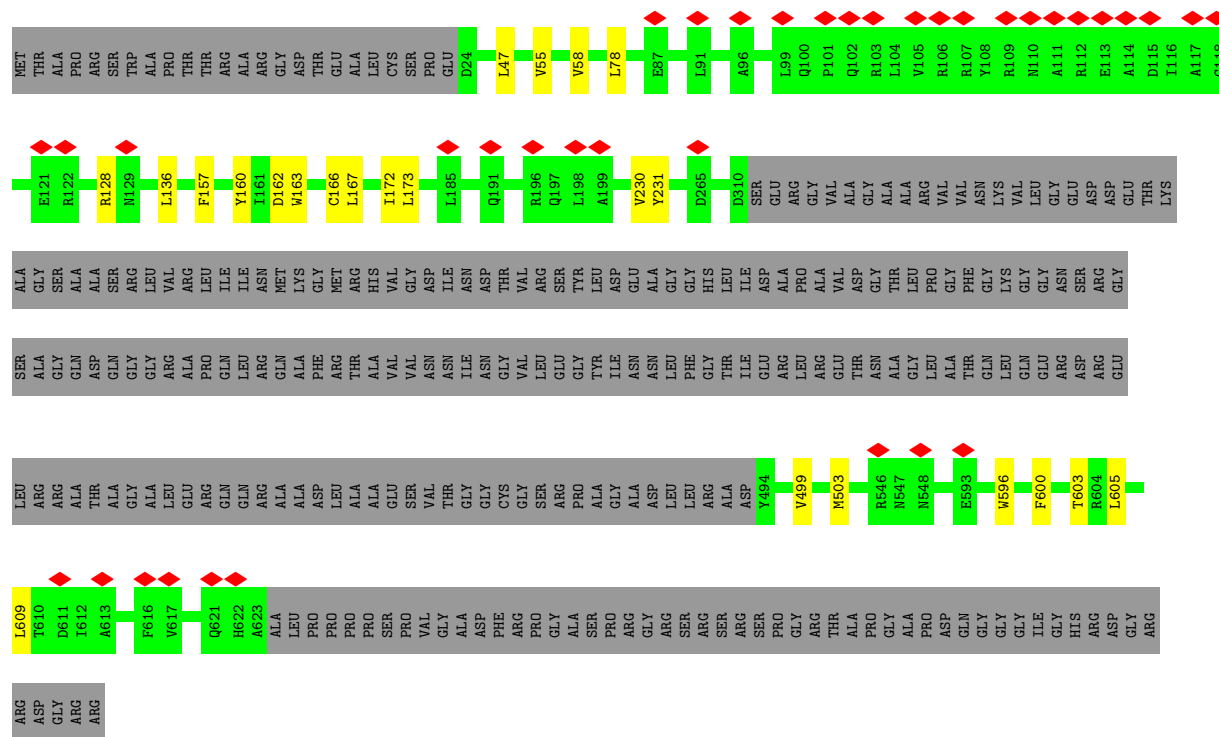
- Molecule 2: Capsid portal protein

Chain a:  59% . 38%

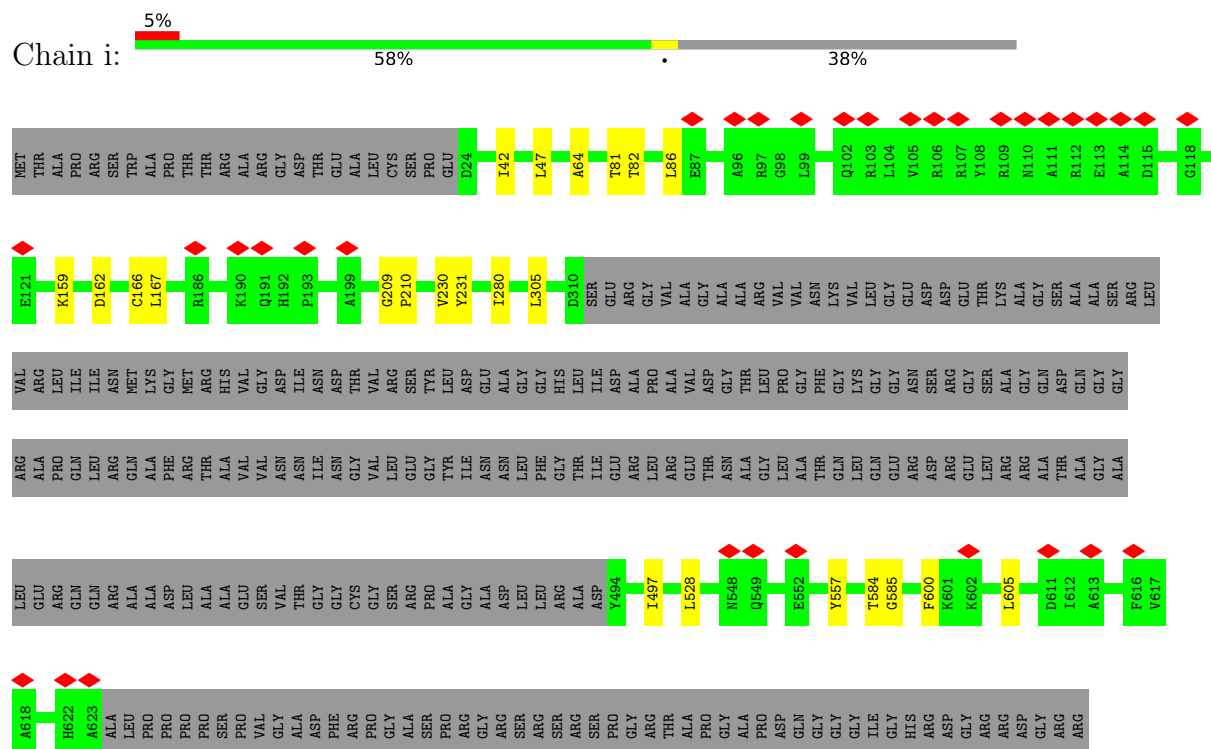


Chain f:





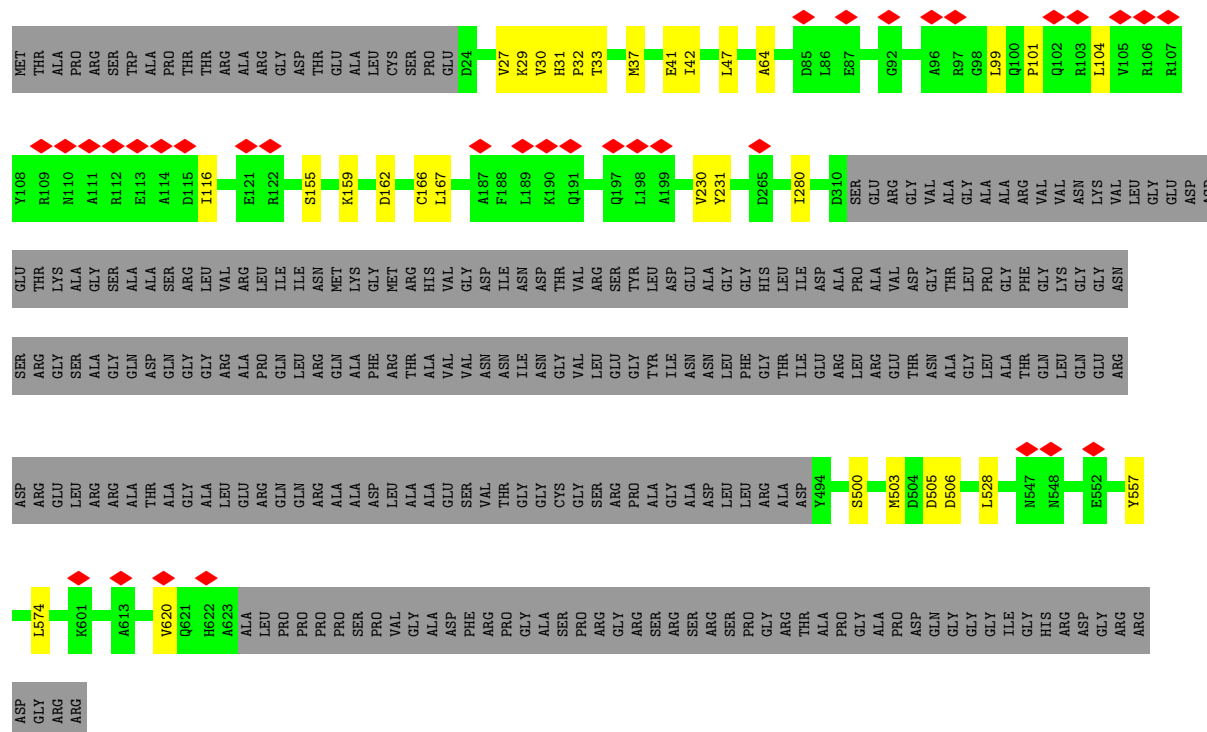
- Molecule 2: Capsid portal protein



- Molecule 2: Capsid portal protein

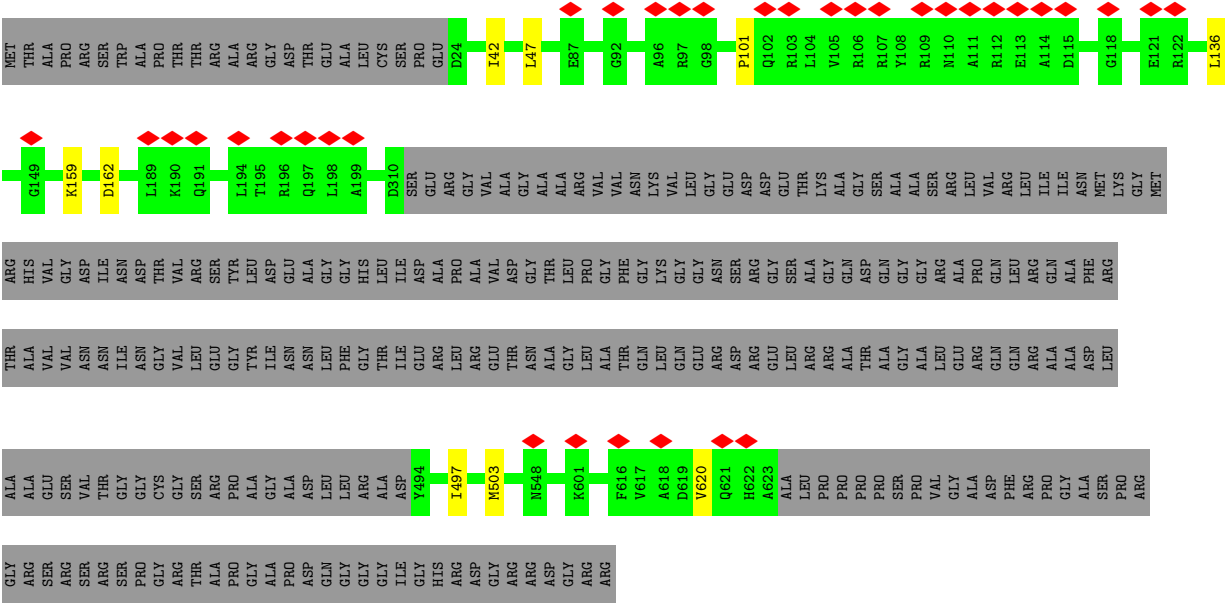


- Molecule 2: Capsid portal protein



- Molecule 2: Capsid portal protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	363576	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.326	Depositor
Minimum map value	-1.598	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.228	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0/59	0.38	0/80
1	B	0.12	0/59	0.35	0/80
1	C	0.10	0/59	0.28	0/80
1	D	0.10	0/59	0.32	0/80
1	E	0.12	0/59	0.31	0/80
1	F	0.12	0/59	0.36	0/80
1	G	0.09	0/59	0.25	0/80
1	H	0.11	0/59	0.30	0/80
1	I	0.09	0/59	0.28	0/80
1	J	0.13	0/59	0.27	0/80
1	K	0.12	0/59	0.35	0/80
1	L	0.11	0/59	0.27	0/80
2	a	0.14	0/3401	0.32	0/4626
2	b	0.15	0/3401	0.32	0/4626
2	c	0.15	0/3401	0.34	0/4626
2	d	0.15	0/3401	0.32	0/4626
2	e	0.15	0/3401	0.33	0/4626
2	f	0.15	0/3401	0.33	0/4626
2	g	0.16	0/3401	0.35	0/4626
2	h	0.15	0/3401	0.33	0/4626
2	i	0.15	0/3401	0.33	0/4626
2	j	0.15	0/3401	0.33	0/4626
2	k	0.16	0/3401	0.34	0/4626
2	l	0.16	0/3401	0.34	0/4626
All	All	0.15	0/41520	0.33	0/56472

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	56	0	48	0	0
1	B	56	0	48	0	0
1	C	56	0	48	0	0
1	D	56	0	48	0	0
1	E	56	0	48	0	0
1	F	56	0	48	0	0
1	G	56	0	48	0	0
1	H	56	0	48	0	0
1	I	56	0	48	0	0
1	J	56	0	48	0	0
1	K	56	0	48	0	0
1	L	56	0	48	0	0
2	a	3317	0	3264	12	0
2	b	3317	0	3264	9	0
2	c	3317	0	3264	19	0
2	d	3317	0	3264	11	0
2	e	3317	0	3264	8	0
2	f	3317	0	3264	7	0
2	g	3317	0	3264	12	0
2	h	3317	0	3264	17	0
2	i	3317	0	3264	16	0
2	j	3317	0	3264	12	0
2	k	3317	0	3264	20	0
2	l	3317	0	3264	8	0
All	All	40476	0	39744	142	0

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

All (142) 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:d:47:LEU:HD12	2:d:47:LEU:O	1.91	0.70
2:e:47:LEU:HD12	2:e:47:LEU:O	1.94	0.67
2:i:64:ALA:HB2	2:i:557:TYR:HD2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:47:LEU:HD12	2:g:47:LEU:O	1.97	0.64
2:j:42:ILE:HG12	2:j:47:LEU:HD21	1.83	0.61
2:h:499:VAL:HG12	2:h:499:VAL:O	2.01	0.60
2:i:42:ILE:HG12	2:i:47:LEU:HD21	1.86	0.57
2:c:42:ILE:HG12	2:c:47:LEU:HD21	1.85	0.57
2:g:36:THR:HG23	2:g:167:LEU:HD11	1.88	0.56
2:k:500:SER:HB2	2:k:503:MET:HE2	1.89	0.55
2:j:101:PRO:HG3	2:j:620:VAL:HG12	1.89	0.54
2:k:280:ILE:HG22	2:k:528:LEU:HD11	1.88	0.54
2:a:124:PHE:CE2	2:a:613:ALA:HB2	2.43	0.54
2:a:500:SER:HB2	2:a:503:MET:HE2	1.90	0.54
2:h:128:ARG:HG3	2:h:609:LEU:HD23	1.90	0.54
2:j:64:ALA:HB2	2:j:557:TYR:HD2	1.74	0.53
2:f:36:THR:HG22	2:f:227:TYR:OH	2.09	0.53
2:g:166:CYS:C	2:g:167:LEU:HD12	2.34	0.53
2:c:124:PHE:CE2	2:c:613:ALA:HB2	2.44	0.52
2:k:503:MET:HE1	2:l:497:ILE:HG12	1.91	0.52
2:g:64:ALA:HB2	2:g:557:TYR:HD2	1.74	0.52
2:h:47:LEU:HD12	2:h:47:LEU:O	2.10	0.52
2:d:78:LEU:O	2:d:81:THR:HG22	2.10	0.52
2:k:503:MET:SD	2:l:497:ILE:HD13	2.50	0.52
2:g:600:PHE:CE2	2:g:605:LEU:HD23	2.45	0.51
2:k:64:ALA:HB2	2:k:557:TYR:HD2	1.75	0.51
2:c:280:ILE:HG22	2:c:528:LEU:HD11	1.93	0.51
2:a:503:MET:HE1	2:c:497:ILE:HD13	1.93	0.51
2:l:136:LEU:O	2:l:136:LEU:HD23	2.11	0.51
2:b:280:ILE:HG22	2:b:528:LEU:HD21	1.93	0.50
2:c:166:CYS:C	2:c:167:LEU:HD12	2.36	0.50
2:c:69:LEU:HD21	2:c:219:PHE:HZ	1.75	0.50
2:c:125:ASP:OD1	2:c:126:THR:N	2.44	0.50
2:h:136:LEU:O	2:h:136:LEU:HD23	2.12	0.50
2:a:600:PHE:CE2	2:a:605:LEU:HD23	2.47	0.50
2:h:172:ILE:C	2:h:173:LEU:HD12	2.37	0.50
2:i:600:PHE:CE2	2:i:605:LEU:HD23	2.47	0.50
2:l:101:PRO:HB3	2:l:620:VAL:HG23	1.94	0.50
2:l:159:LYS:HA	2:l:162:ASP:OD2	2.12	0.49
2:g:280:ILE:HG22	2:g:528:LEU:HD21	1.94	0.49
2:h:503:MET:HE1	2:i:497:ILE:CG2	2.42	0.49
2:d:507:THR:HG21	2:e:501:LYS:HE2	1.94	0.49
2:a:166:CYS:C	2:a:167:LEU:HD12	2.37	0.49
2:k:166:CYS:C	2:k:167:LEU:HD12	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:69:LEU:HD21	2:b:219:PHE:HZ	1.78	0.48
2:i:280:ILE:HG22	2:i:528:LEU:HD11	1.95	0.48
2:c:263:THR:HG23	2:c:263:THR:O	2.14	0.48
2:i:166:CYS:C	2:i:167:LEU:HD12	2.38	0.48
2:j:27:VAL:HG22	2:j:234:TYR:O	2.14	0.47
2:h:136:LEU:HD23	2:h:136:LEU:C	2.39	0.47
2:k:505:ASP:O	2:k:506:ASP:OD1	2.32	0.47
2:h:166:CYS:C	2:h:167:LEU:HD12	2.40	0.47
2:d:78:LEU:HD13	2:d:603:THR:HG21	1.96	0.47
2:b:499:VAL:HG12	2:b:501:LYS:HG3	1.95	0.46
2:i:47:LEU:O	2:i:47:LEU:HG	2.15	0.46
2:d:256:VAL:O	2:d:256:VAL:HG13	2.16	0.46
2:h:605:LEU:O	2:h:609:LEU:HD13	2.16	0.45
2:i:82:THR:O	2:i:86:LEU:HD13	2.16	0.45
2:k:104:LEU:CD2	2:k:116:ILE:HD11	2.45	0.45
2:i:230:VAL:HG22	2:i:231:TYR:N	2.31	0.45
2:j:160:TYR:CD1	2:j:170:VAL:HG11	2.52	0.45
2:l:42:ILE:HG12	2:l:47:LEU:HD21	1.98	0.45
2:g:36:THR:HG22	2:g:227:TYR:OH	2.16	0.45
2:l:47:LEU:O	2:l:47:LEU:HG	2.17	0.45
2:a:503:MET:HE1	2:c:497:ILE:CD1	2.47	0.45
2:d:31:HIS:HB3	2:d:32:PRO:HD3	1.99	0.45
2:i:159:LYS:O	2:i:162:ASP:OD1	2.35	0.45
2:i:86:LEU:HD21	2:i:605:LEU:CD1	2.47	0.44
2:k:42:ILE:HG12	2:k:47:LEU:HD21	1.98	0.44
2:c:30:VAL:O	2:c:33:THR:HG22	2.17	0.44
2:k:506:ASP:OD1	2:k:506:ASP:C	2.60	0.44
2:f:30:VAL:HG13	2:f:31:HIS:N	2.31	0.44
2:i:64:ALA:HB2	2:i:557:TYR:CD2	2.46	0.44
2:c:47:LEU:HG	2:c:47:LEU:O	2.17	0.44
2:d:36:THR:HG22	2:d:227:TYR:OH	2.17	0.44
2:h:78:LEU:HD13	2:h:603:THR:HG21	1.99	0.44
2:k:47:LEU:HG	2:k:47:LEU:O	2.18	0.44
2:f:597:ASP:O	2:f:601:LYS:HG2	2.17	0.44
2:g:162:ASP:OD1	2:g:163:TRP:N	2.51	0.44
2:f:600:PHE:CE2	2:f:605:LEU:HD23	2.53	0.44
2:j:78:LEU:HD23	2:j:603:THR:HG21	2.00	0.44
2:e:256:VAL:HG13	2:e:256:VAL:O	2.18	0.44
2:d:616:PHE:O	2:d:620:VAL:HG23	2.18	0.44
2:k:37:MET:O	2:k:41:GLU:HG2	2.18	0.44
2:d:584:THR:HG22	2:d:585:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:280:ILE:HG22	2:j:528:LEU:HD21	2.01	0.43
2:a:86:LEU:CD2	2:a:612:ILE:HD12	2.48	0.43
2:h:230:VAL:HG22	2:h:231:TYR:N	2.34	0.43
2:b:497:ILE:HD13	2:l:503:MET:SD	2.59	0.43
2:c:280:ILE:HG22	2:c:528:LEU:HD21	2.01	0.43
2:f:230:VAL:HG22	2:f:231:TYR:N	2.33	0.43
2:h:503:MET:HE3	2:i:305:LEU:HD11	2.00	0.43
2:h:162:ASP:OD1	2:h:163:TRP:N	2.52	0.43
2:j:31:HIS:HB3	2:j:32:PRO:HD3	2.00	0.42
2:j:230:VAL:HG22	2:j:231:TYR:N	2.33	0.42
2:j:47:LEU:O	2:j:47:LEU:HG	2.19	0.42
2:d:147:ALA:N	2:d:148:PRO:HD2	2.34	0.42
2:c:160:TYR:CD1	2:c:170:VAL:HG11	2.55	0.42
2:j:600:PHE:CE2	2:j:605:LEU:HD23	2.54	0.42
2:a:503:MET:CE	2:c:497:ILE:HD13	2.50	0.42
2:c:125:ASP:HA	2:c:128:ARG:HG2	2.01	0.42
2:g:64:ALA:HB2	2:g:557:TYR:CD2	2.54	0.42
2:b:171:PRO:HB3	2:b:243:VAL:HG21	2.02	0.42
2:c:219:PHE:HE1	2:c:574:LEU:HD13	1.85	0.42
2:k:99:LEU:HD11	2:k:104:LEU:HD22	2.00	0.42
2:k:31:HIS:HB3	2:k:32:PRO:HD3	2.00	0.42
2:i:584:THR:HG22	2:i:585:GLY:N	2.34	0.42
2:h:136:LEU:HD12	2:h:596:TRP:CD1	2.54	0.42
2:h:55:VAL:O	2:h:58:VAL:HG12	2.19	0.42
2:k:155:SER:HB2	2:k:574:LEU:HD21	2.01	0.42
2:e:280:ILE:HG22	2:e:528:LEU:HD21	2.01	0.41
2:b:208:ALA:HB1	2:b:212:PHE:CZ	2.55	0.41
2:b:64:ALA:HB2	2:b:557:TYR:HD2	1.85	0.41
2:f:147:ALA:N	2:f:148:PRO:HD2	2.35	0.41
2:d:280:ILE:HG22	2:d:528:LEU:HD21	2.02	0.41
2:b:157:PHE:O	2:b:160:TYR:HB3	2.20	0.41
2:i:81:THR:CG2	2:i:86:LEU:HD11	2.50	0.41
2:a:219:PHE:HD1	2:a:574:LEU:HD22	1.86	0.41
2:c:33:THR:OG1	2:c:34:PRO:HD2	2.21	0.41
2:c:617:VAL:O	2:c:620:VAL:HG12	2.21	0.41
2:k:101:PRO:HG3	2:k:620:VAL:HG12	2.03	0.41
2:e:36:THR:HG22	2:e:227:TYR:OH	2.21	0.41
2:e:309:SER:O	2:e:310:ASP:HB3	2.21	0.41
2:i:209:GLY:N	2:i:210:PRO:HD2	2.35	0.41
2:k:27:VAL:HG12	2:k:29:LYS:N	2.36	0.41
2:a:31:HIS:HB3	2:a:32:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:617:VAL:O	2:a:620:VAL:HG12	2.21	0.41
2:g:31:HIS:HB3	2:g:32:PRO:HD3	2.02	0.41
2:j:82:THR:HG22	2:j:83:TYR:N	2.35	0.41
2:k:159:LYS:O	2:k:162:ASP:OD1	2.39	0.41
2:a:33:THR:OG1	2:a:34:PRO:HD2	2.21	0.40
2:e:147:ALA:N	2:e:148:PRO:HD2	2.35	0.40
2:e:301:VAL:O	2:e:301:VAL:HG23	2.21	0.40
2:f:33:THR:OG1	2:f:34:PRO:HD2	2.21	0.40
2:h:157:PHE:O	2:h:160:TYR:HB3	2.22	0.40
2:b:147:ALA:N	2:b:148:PRO:HD2	2.36	0.40
2:k:230:VAL:HG22	2:k:231:TYR:N	2.35	0.40
2:g:30:VAL:O	2:g:33:THR:HG22	2.21	0.40
2:c:129:ASN:O	2:c:132:ARG:HG2	2.21	0.40
2:g:159:LYS:O	2:g:162:ASP:OD1	2.39	0.40
2:h:600:PHE:CE2	2:h:605:LEU:HD23	2.56	0.40
2:k:30:VAL:O	2:k:33:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	5/635 (1%)	5 (100%)	0	0	100	100
1	B	5/635 (1%)	5 (100%)	0	0	100	100
1	C	5/635 (1%)	5 (100%)	0	0	100	100
1	D	5/635 (1%)	5 (100%)	0	0	100	100
1	E	5/635 (1%)	5 (100%)	0	0	100	100
1	F	5/635 (1%)	5 (100%)	0	0	100	100
1	G	5/635 (1%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	5/635 (1%)	5 (100%)	0	0	100	100
1	I	5/635 (1%)	5 (100%)	0	0	100	100
1	J	5/635 (1%)	5 (100%)	0	0	100	100
1	K	5/635 (1%)	5 (100%)	0	0	100	100
1	L	5/635 (1%)	5 (100%)	0	0	100	100
2	a	412/676 (61%)	404 (98%)	8 (2%)	0	100	100
2	b	412/676 (61%)	405 (98%)	7 (2%)	0	100	100
2	c	412/676 (61%)	401 (97%)	11 (3%)	0	100	100
2	d	412/676 (61%)	401 (97%)	11 (3%)	0	100	100
2	e	412/676 (61%)	403 (98%)	9 (2%)	0	100	100
2	f	412/676 (61%)	404 (98%)	8 (2%)	0	100	100
2	g	412/676 (61%)	403 (98%)	9 (2%)	0	100	100
2	h	412/676 (61%)	398 (97%)	14 (3%)	0	100	100
2	i	412/676 (61%)	400 (97%)	12 (3%)	0	100	100
2	j	412/676 (61%)	403 (98%)	9 (2%)	0	100	100
2	k	412/676 (61%)	405 (98%)	7 (2%)	0	100	100
2	l	412/676 (61%)	402 (98%)	10 (2%)	0	100	100
All	All	5004/15732 (32%)	4889 (98%)	115 (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	5/475 (1%)	5 (100%)	0	100	100
1	B	5/475 (1%)	5 (100%)	0	100	100
1	C	5/475 (1%)	5 (100%)	0	100	100
1	D	5/475 (1%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	5/475 (1%)	5 (100%)	0	100	100
1	F	5/475 (1%)	5 (100%)	0	100	100
1	G	5/475 (1%)	5 (100%)	0	100	100
1	H	5/475 (1%)	5 (100%)	0	100	100
1	I	5/475 (1%)	5 (100%)	0	100	100
1	J	5/475 (1%)	5 (100%)	0	100	100
1	K	5/475 (1%)	5 (100%)	0	100	100
1	L	5/475 (1%)	5 (100%)	0	100	100
2	a	347/535 (65%)	347 (100%)	0	100	100
2	b	347/535 (65%)	347 (100%)	0	100	100
2	c	347/535 (65%)	347 (100%)	0	100	100
2	d	347/535 (65%)	347 (100%)	0	100	100
2	e	347/535 (65%)	347 (100%)	0	100	100
2	f	347/535 (65%)	347 (100%)	0	100	100
2	g	347/535 (65%)	347 (100%)	0	100	100
2	h	347/535 (65%)	347 (100%)	0	100	100
2	i	347/535 (65%)	347 (100%)	0	100	100
2	j	347/535 (65%)	347 (100%)	0	100	100
2	k	347/535 (65%)	347 (100%)	0	100	100
2	l	347/535 (65%)	347 (100%)	0	100	100
All	All	4224/12120 (35%)	4224 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	31	HIS
2	a	515	HIS
2	a	548	ASN
2	b	515	HIS
2	d	93	HIS
2	d	284	HIS
2	d	515	HIS
2	e	75	HIS

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Mol	Chain	Res	Type
2	e	545	HIS
2	e	622	HIS
2	f	192	HIS
2	f	548	ASN
2	g	236	HIS
2	h	515	HIS
2	i	236	HIS
2	j	93	HIS
2	j	236	HIS
2	k	140	HIS
2	k	548	ASN
2	k	622	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.

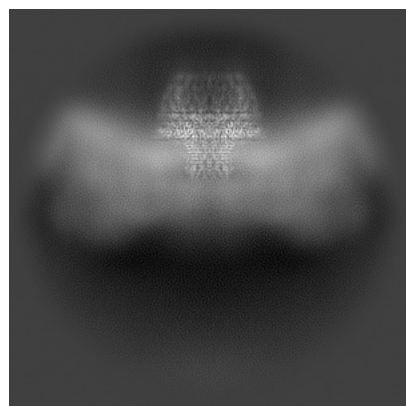
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70678. These allow visual inspection of the internal detail of the map and identification of artifacts.

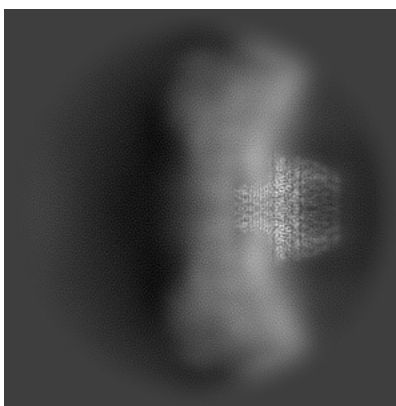
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

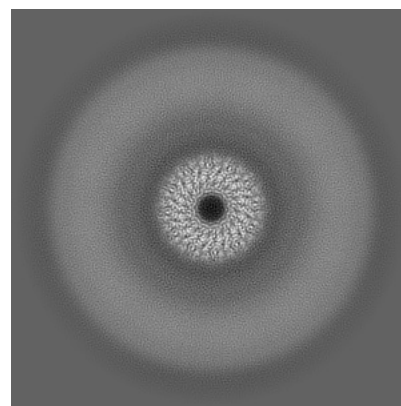
6.1.1 Primary map



X

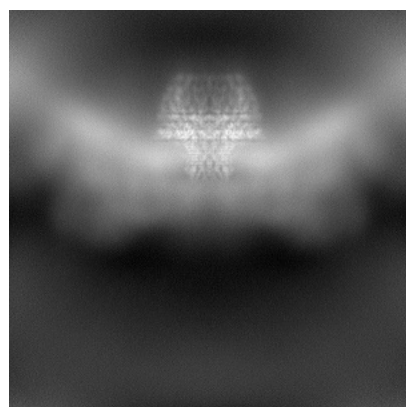


Y

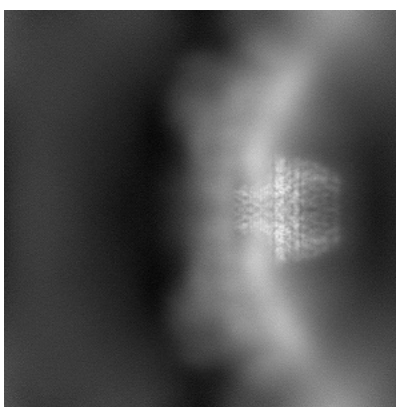


Z

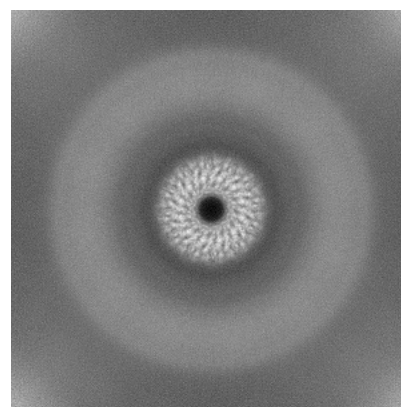
6.1.2 Raw map



X



Y

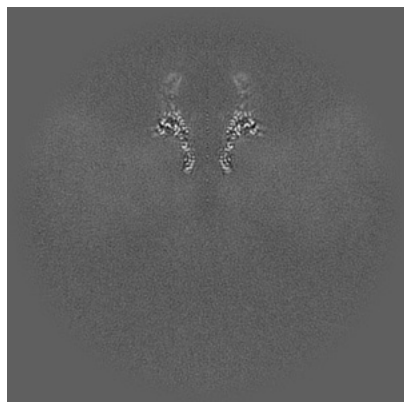


Z

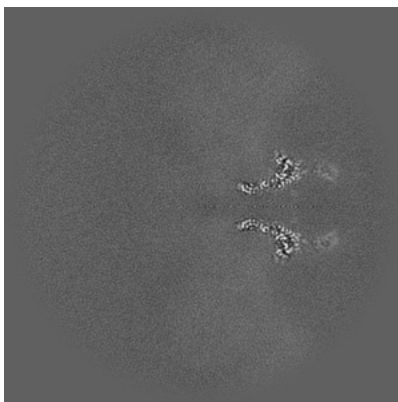
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

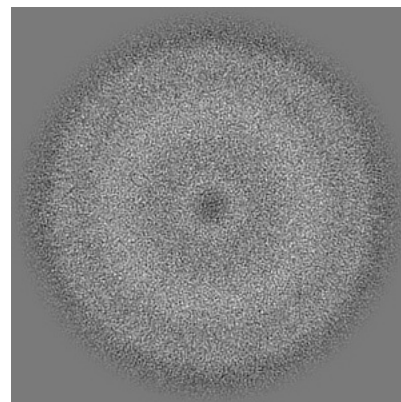
6.2.1 Primary map



X Index: 240

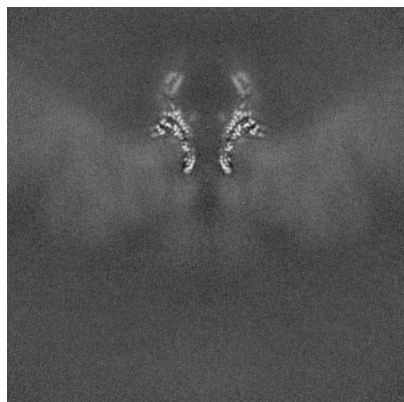


Y Index: 240

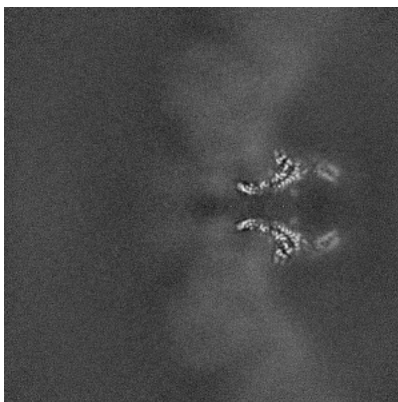


Z Index: 240

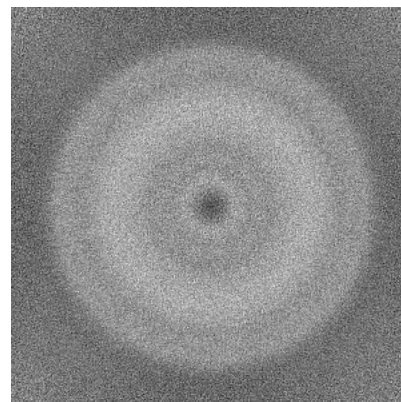
6.2.2 Raw map



X Index: 240



Y Index: 240

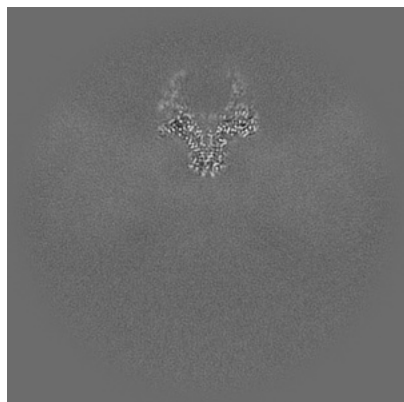


Z Index: 240

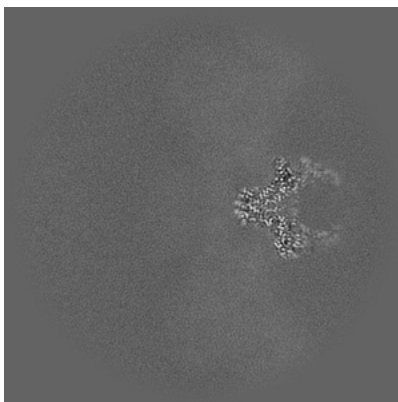
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

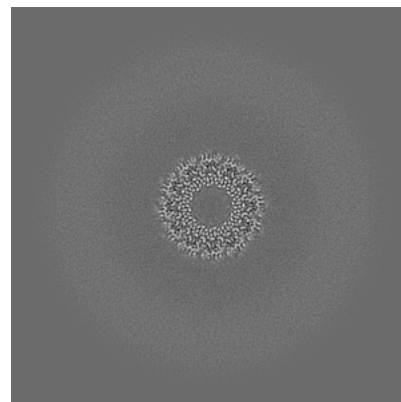
6.3.1 Primary map



X Index: 261

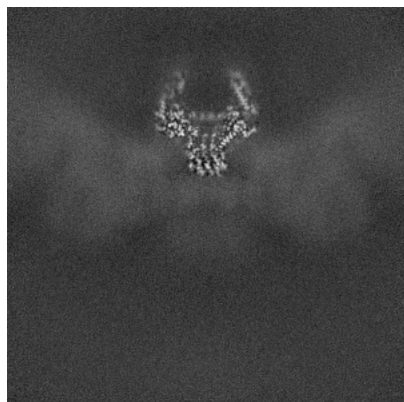


Y Index: 261

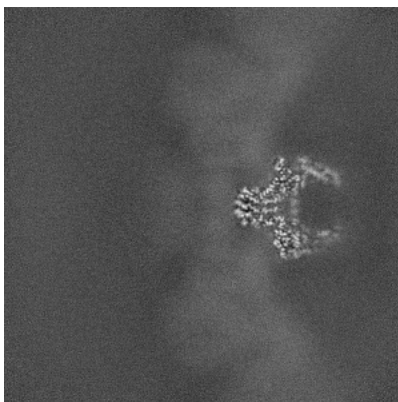


Z Index: 333

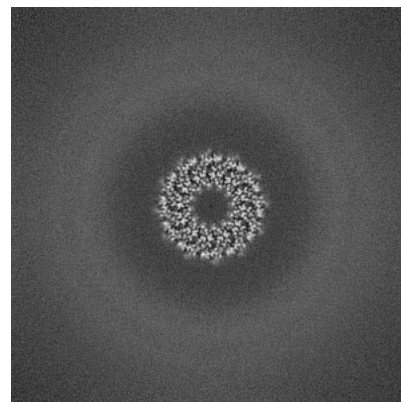
6.3.2 Raw map



X Index: 221



Y Index: 260

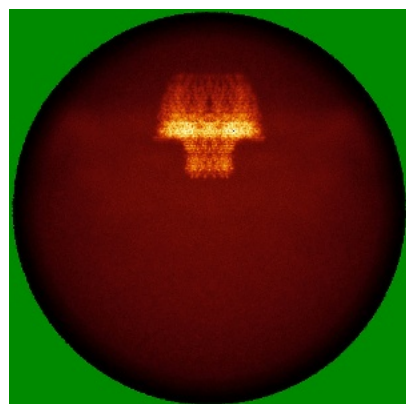


Z Index: 332

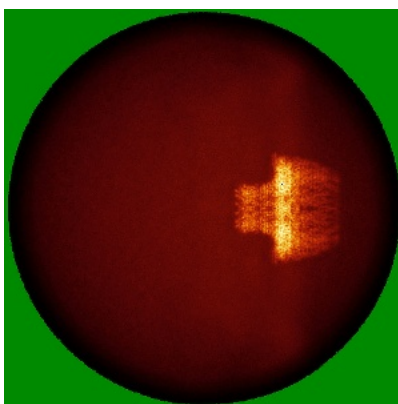
The images above show the largest variance slices of the map in three orthogonal directions.

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

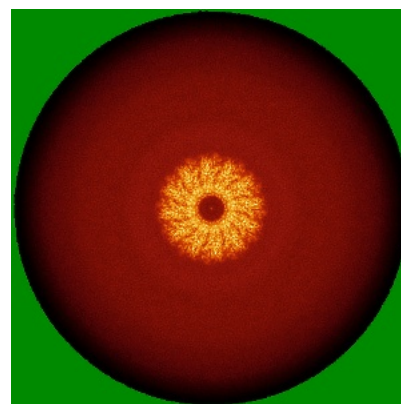
6.4.1 Primary map



X

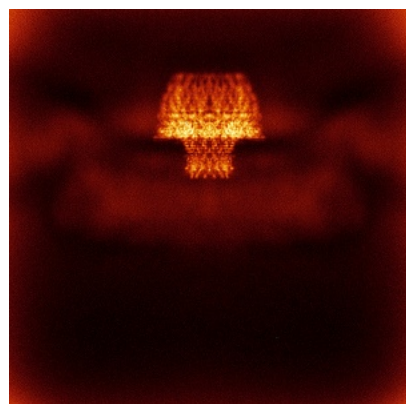


Y

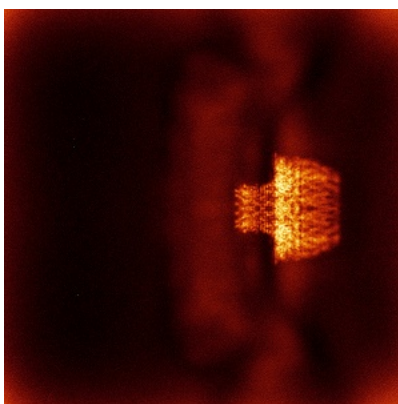


Z

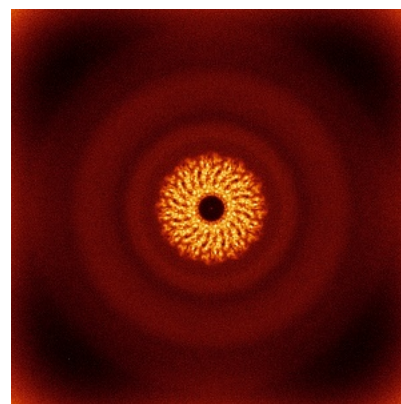
6.4.2 Raw map



X



Y

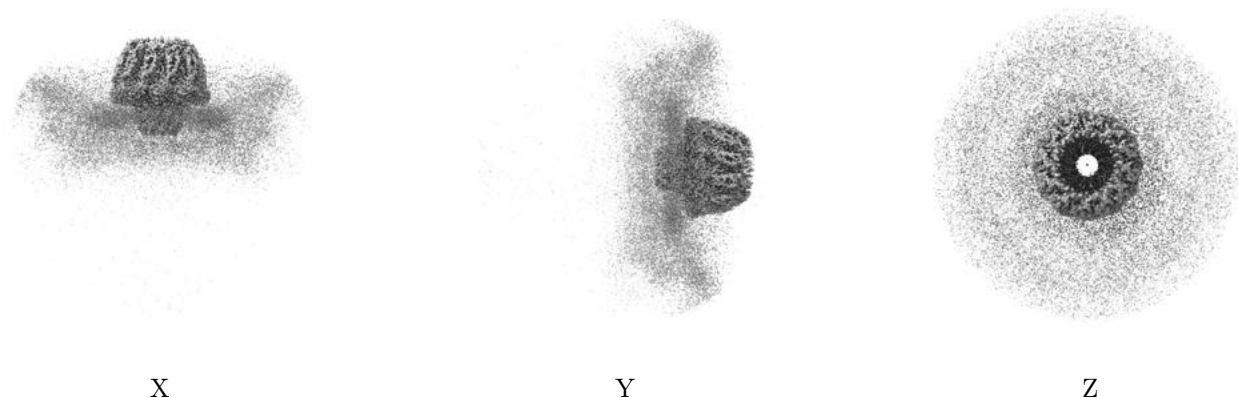


Z

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.

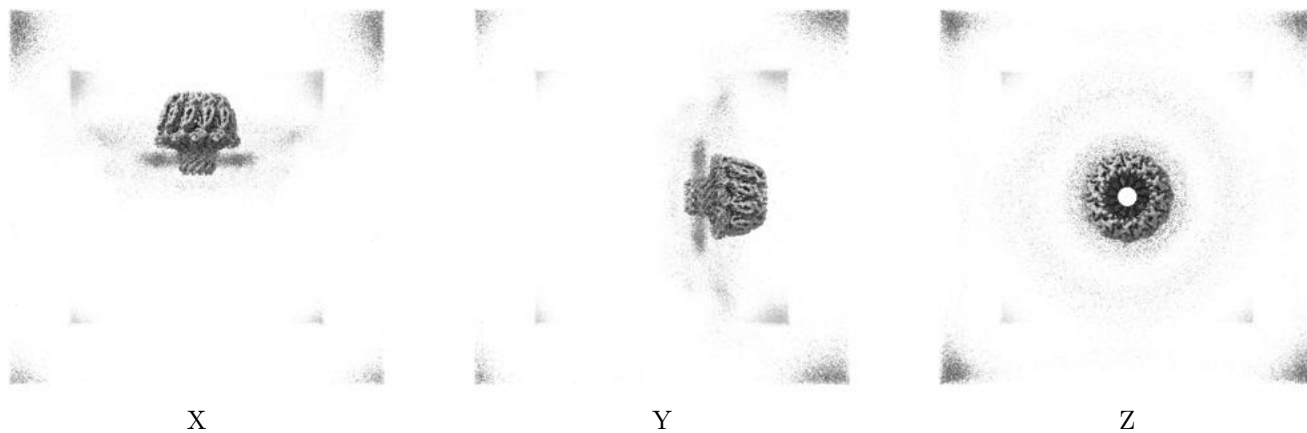
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.228. 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.

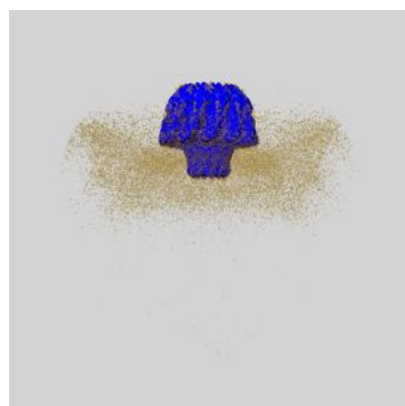
6.6 Mask visualisation [i](#)

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

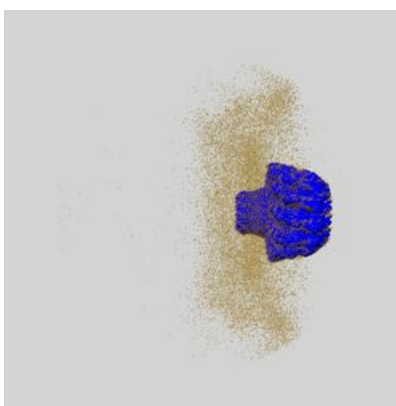
A mask typically either:

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

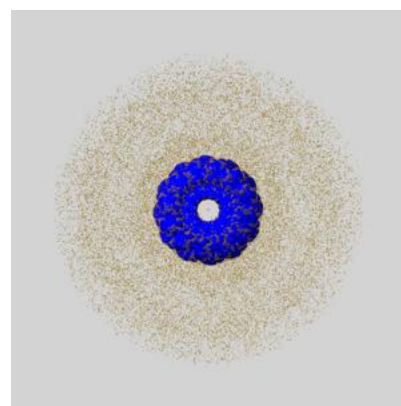
6.6.1 emd_70678_msk_1.map [i](#)



X



Y

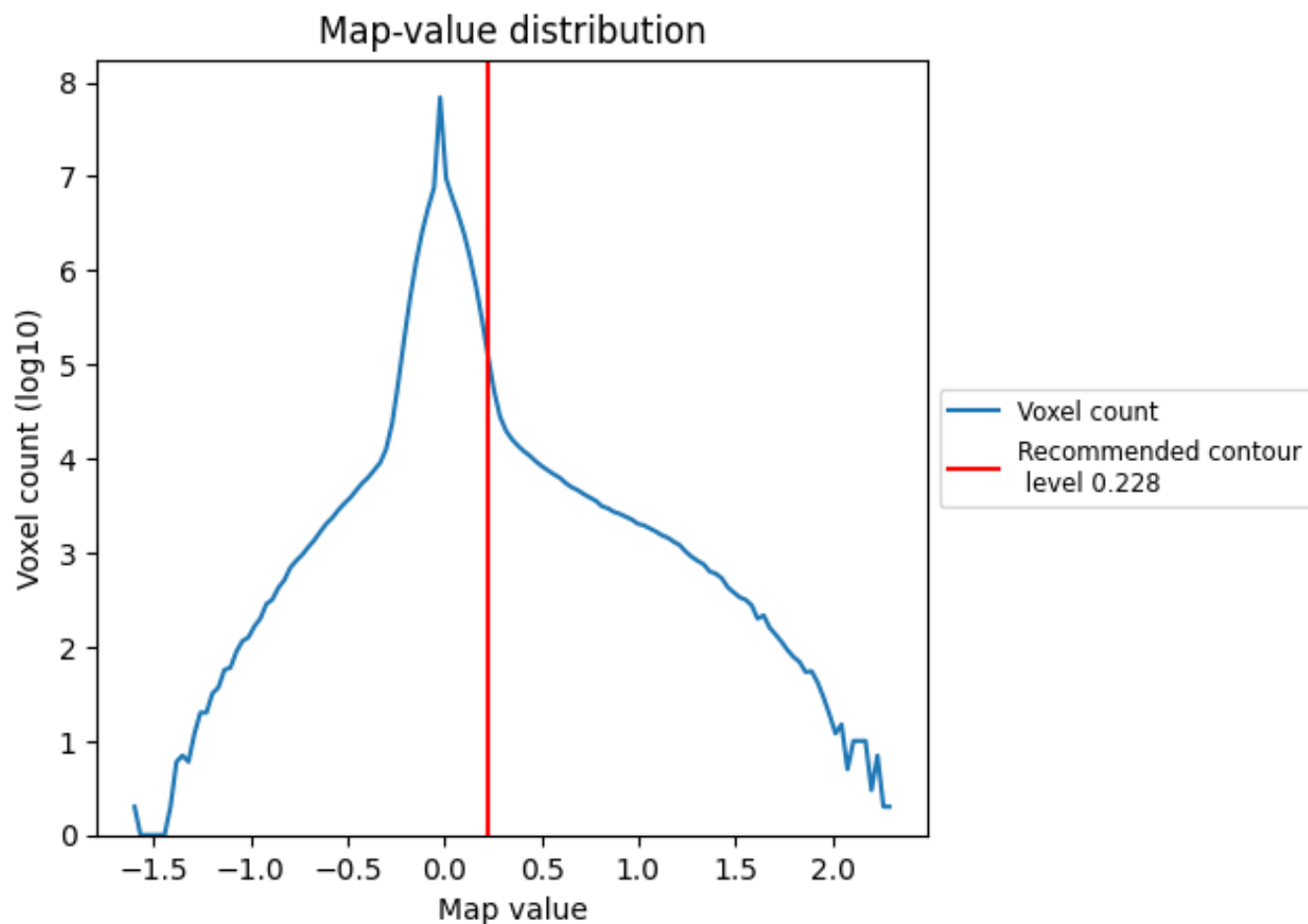


Z

7 Map analysis [i](#)

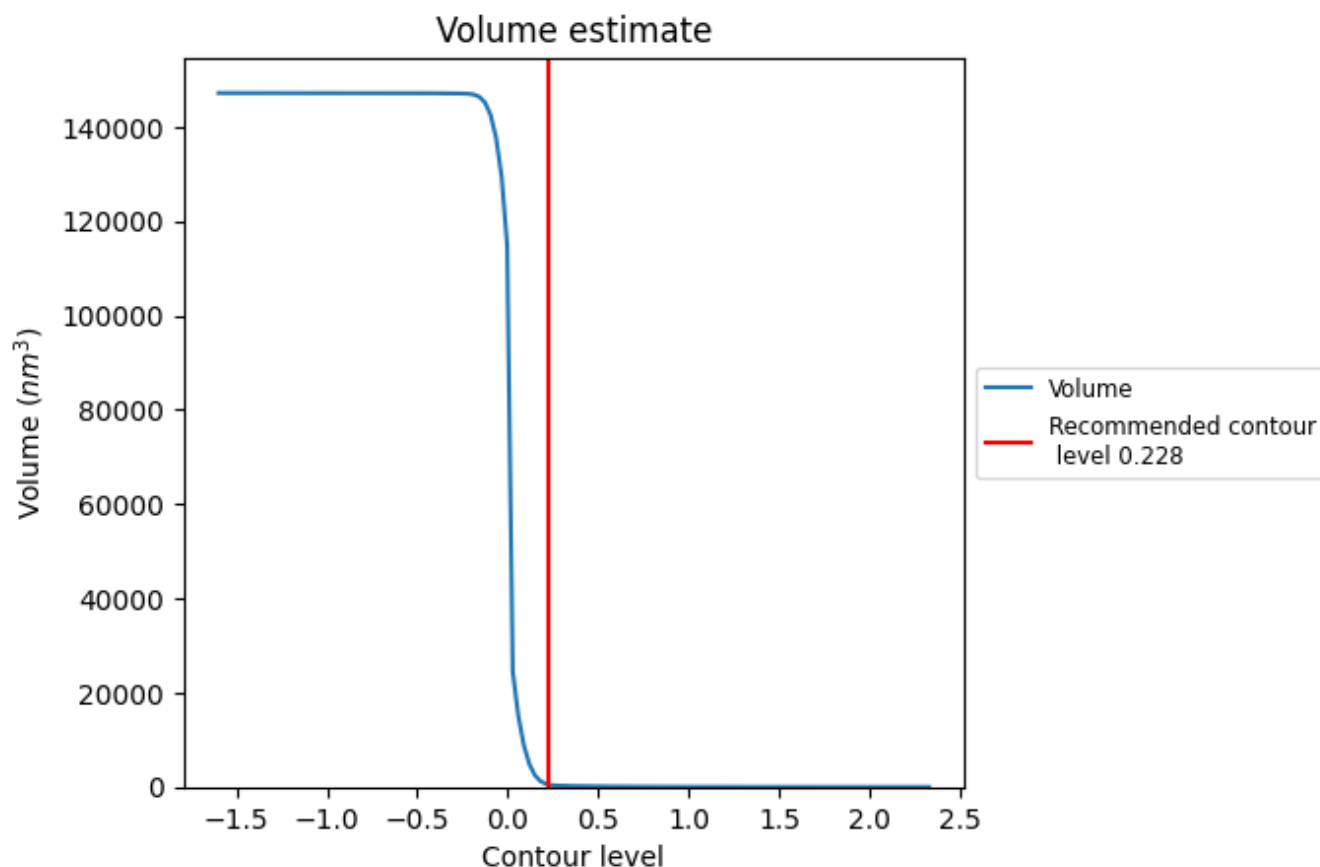
This section contains the results of statistical analysis of the map.

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.

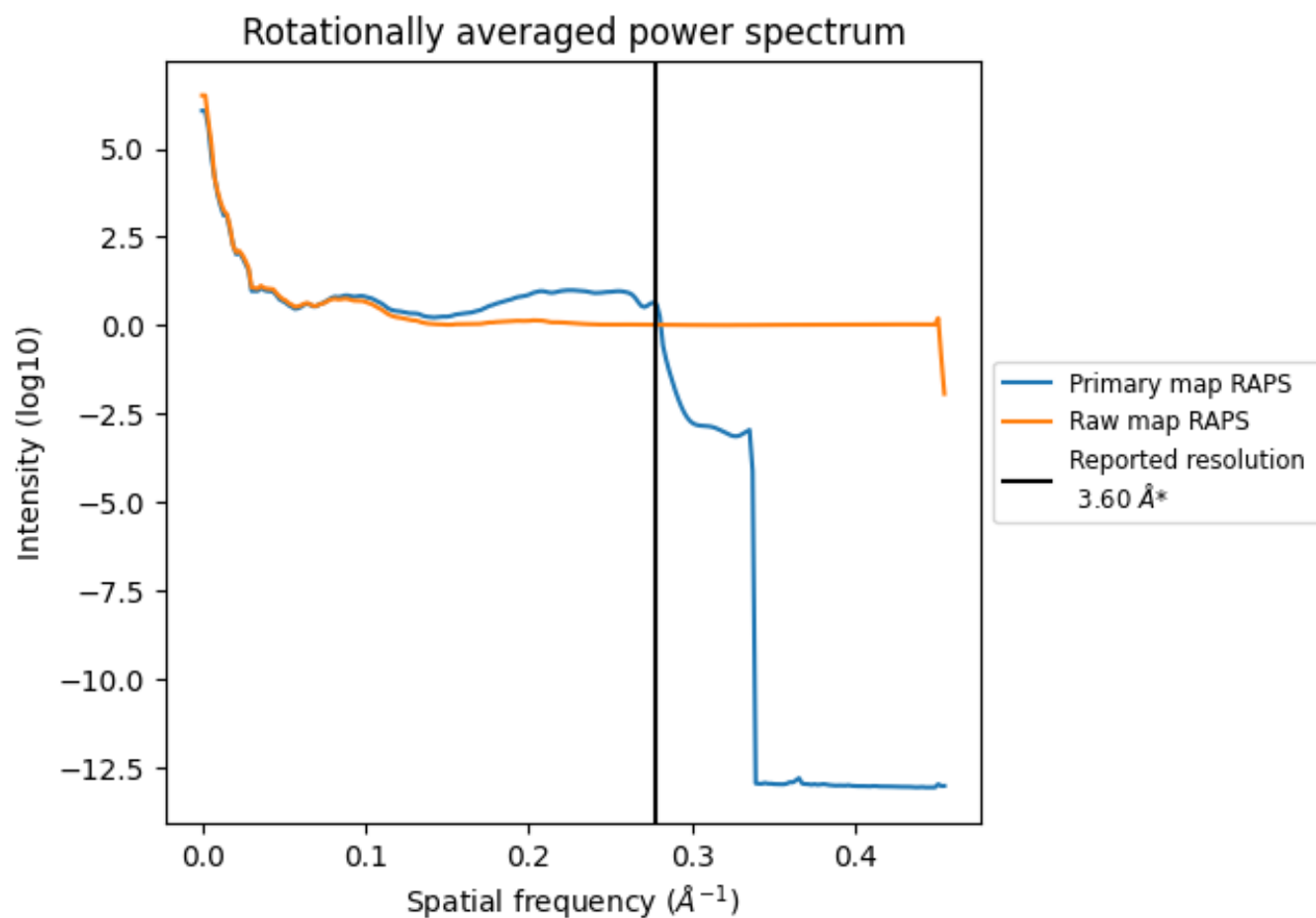
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 505 nm^3 ; this corresponds to an approximate mass of 456 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 ⓘ

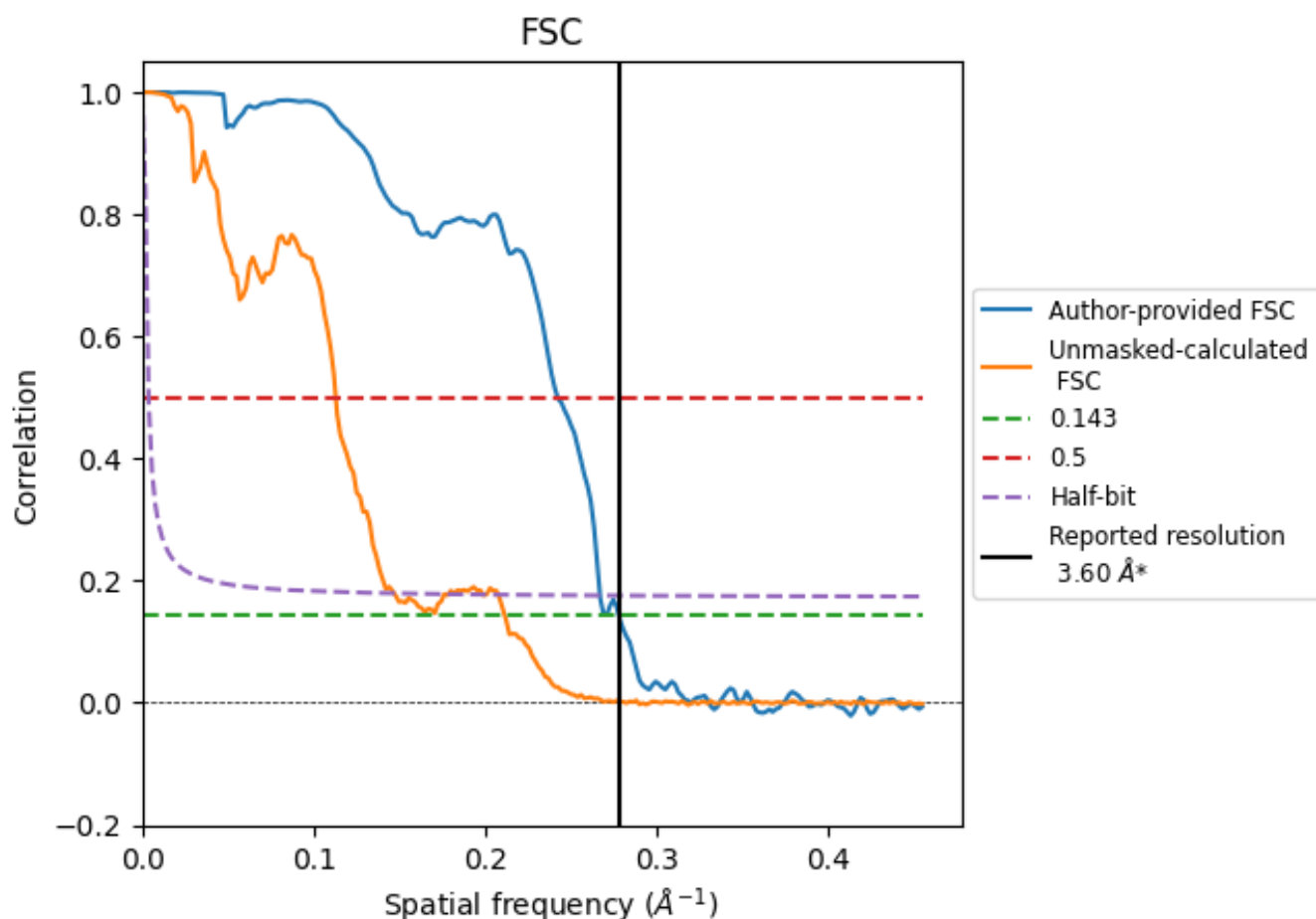


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

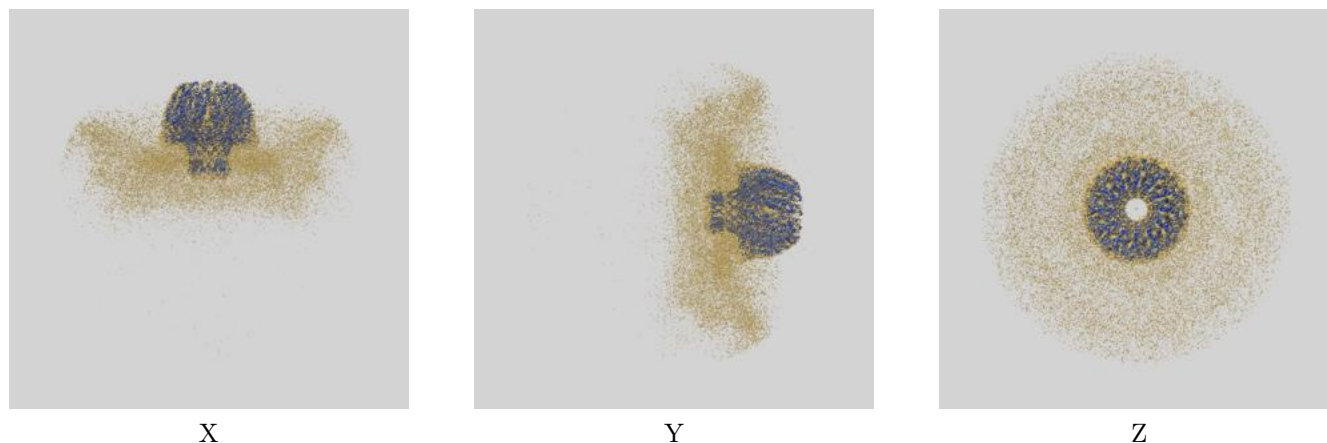
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.13	3.75
Unmasked-calculated*	4.73	8.87	6.81

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

9 Map-model fit [i](#)

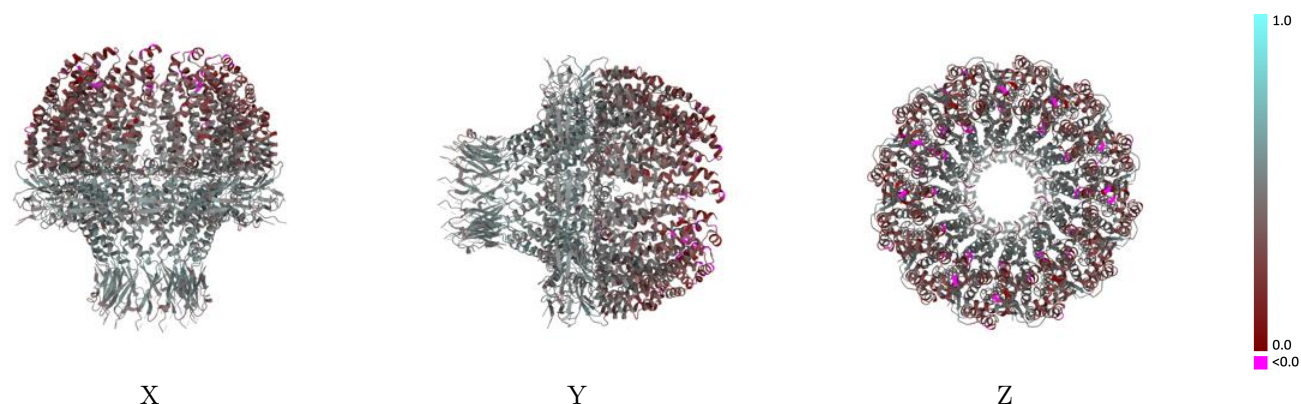
This section contains information regarding the fit between EMDB map EMD-70678 and PDB model 9OP4. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



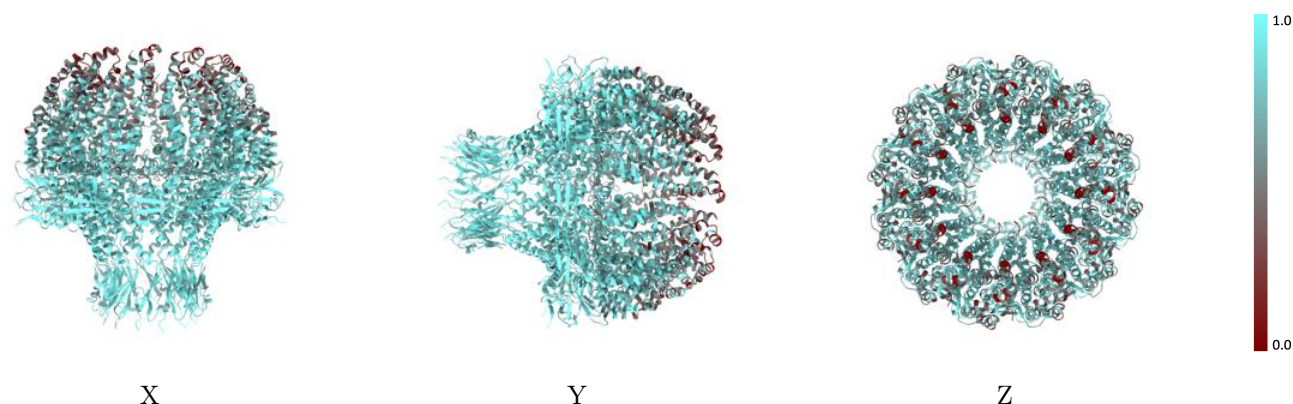
The images above show the 3D surface view of the map at the recommended contour level 0.228 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



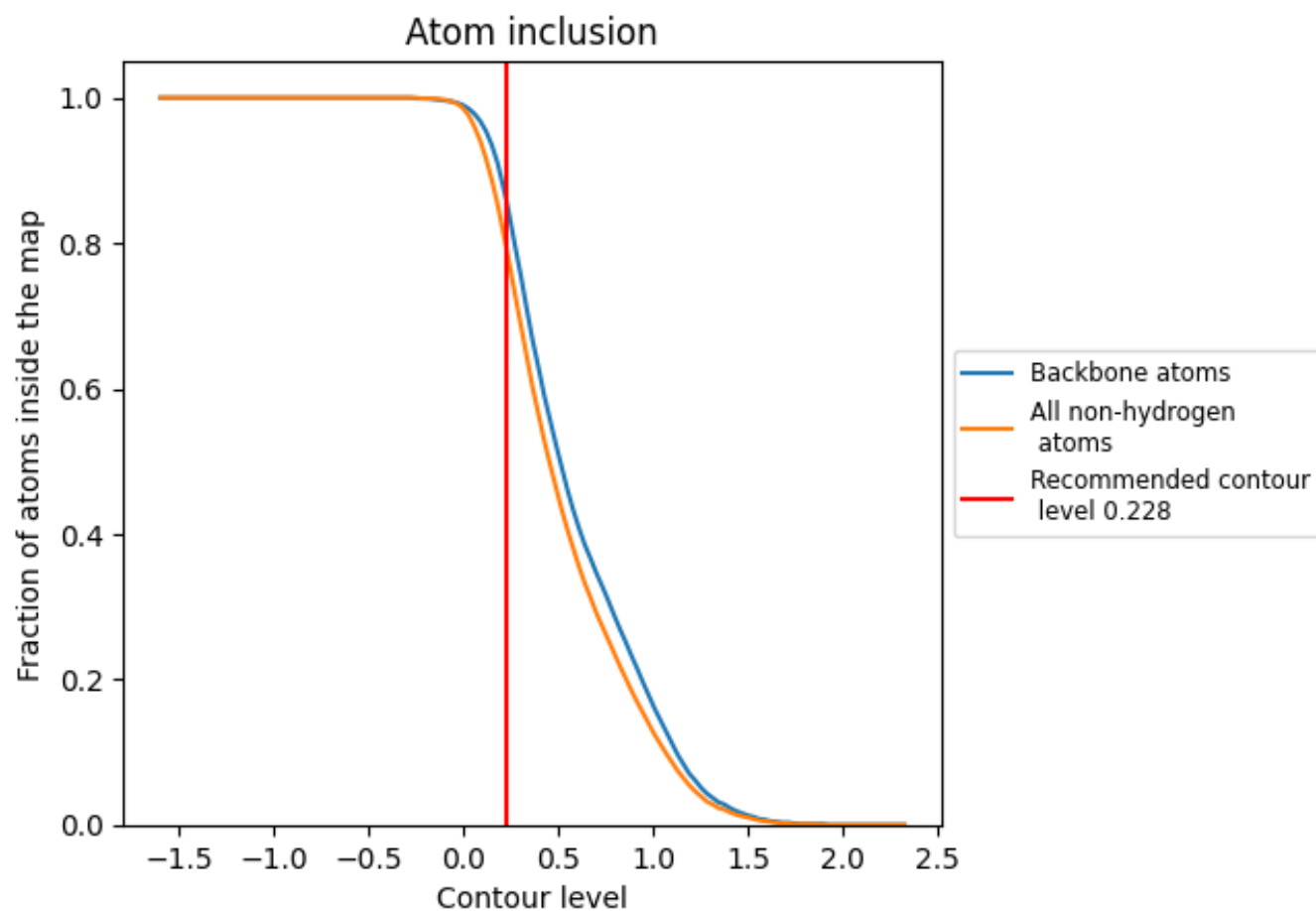
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.228).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.228) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.4320
A	 0.3520	 0.2190
B	 0.3330	 0.2210
C	 0.3150	 0.2690
D	 0.4260	 0.3250
E	 0.2590	 0.2680
F	 0.3700	 0.2580
G	 0.4440	 0.3420
H	 0.2960	 0.2990
I	 0.2410	 0.2050
J	 0.2780	 0.2110
K	 0.4070	 0.3280
L	 0.3700	 0.2620
a	 0.7970	 0.4410
b	 0.7960	 0.4340
c	 0.8040	 0.4350
d	 0.8010	 0.4370
e	 0.7990	 0.4370
f	 0.7980	 0.4340
g	 0.7950	 0.4290
h	 0.7900	 0.4310
i	 0.7990	 0.4300
j	 0.7950	 0.4340
k	 0.7990	 0.4350
l	 0.8070	 0.4340

