



wwPDB EM Validation Summary Report ⓘ

Apr 10, 2025 – 03:12 PM EDT

PDB ID : 9EFK / pdb_00009efk
EMDB ID : EMD-47975
Title : Cryo-EM structure of the portal-tail complex of LME-1 phage
Authors : Deme, J.C.; Lea, S.M.
Deposited on : 2024-11-20
Resolution : 1.90 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.dev117
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) : 2.42

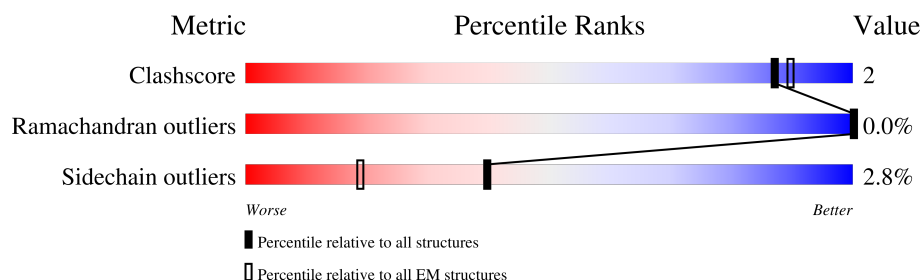
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.90 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	554	<div> <div>7%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	B	554	<div> <div>9%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	C	554	<div> <div>8%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	D	554	<div> <div>10%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	E	554	<div> <div>8%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	F	554	<div> <div>10%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	G	554	<div> <div>9%</div> <div>85%</div> <div>8%</div> <div>6%</div> </div>
1	H	554	<div> <div>10%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>











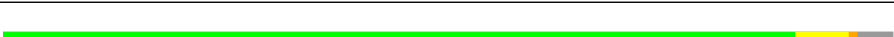


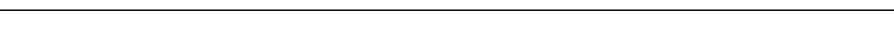
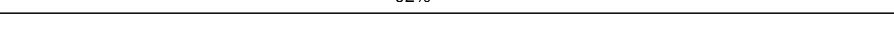
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Mol	Chain	Length	Quality of chain
1	I	554	
1	J	554	
1	K	554	
1	L	554	
2	M	818	
2	N	818	
2	O	818	
2	P	818	
2	Q	818	
2	R	818	
3	AE	658	
3	AF	658	
3	AG	658	
3	AN	658	
3	AO	658	
3	AP	658	
3	AW	658	
3	AX	658	
3	AY	658	
3	BF	658	
3	BG	658	
3	BH	658	
3	BO	658	
3	BP	658	
3	BQ	658	

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Mol	Chain	Length	Quality of chain
3	BX	658	
3	BY	658	
3	BZ	658	
4	AA	201	
4	AB	201	
4	AC	201	
4	AD	201	
4	S	201	
4	T	201	
4	U	201	
4	V	201	
4	W	201	
4	X	201	
4	Y	201	
4	Z	201	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 129576 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 orf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	B	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	C	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	D	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	E	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	F	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	G	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	H	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	I	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	J	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	K	519	Total 4128	C 2626	N 705	O 778	S 19	0	0
1	L	519	Total 4128	C 2626	N 705	O 778	S 19	0	0

- Molecule 2 is a protein called orf18.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	817	Total 6330	C 4003	N 1050	O 1259	S 18	0	0
2	N	817	Total 6330	C 4003	N 1050	O 1259	S 18	0	0
2	O	817	Total 6330	C 4003	N 1050	O 1259	S 18	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	817	Total	C	N	O	S	0	0
			6330	4003	1050	1259	18		
2	Q	817	Total	C	N	O	S	0	0
			6330	4003	1050	1259	18		
2	R	817	Total	C	N	O	S	0	0
			6330	4003	1050	1259	18		

- Molecule 3 is a protein called orf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AE	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AF	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AG	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AN	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AO	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AP	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AW	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AX	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	AY	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BF	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BG	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BH	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BO	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BP	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BQ	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BX	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BY	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		
3	BZ	172	Total	C	N	O	S	0	0
			1320	836	217	262	5		

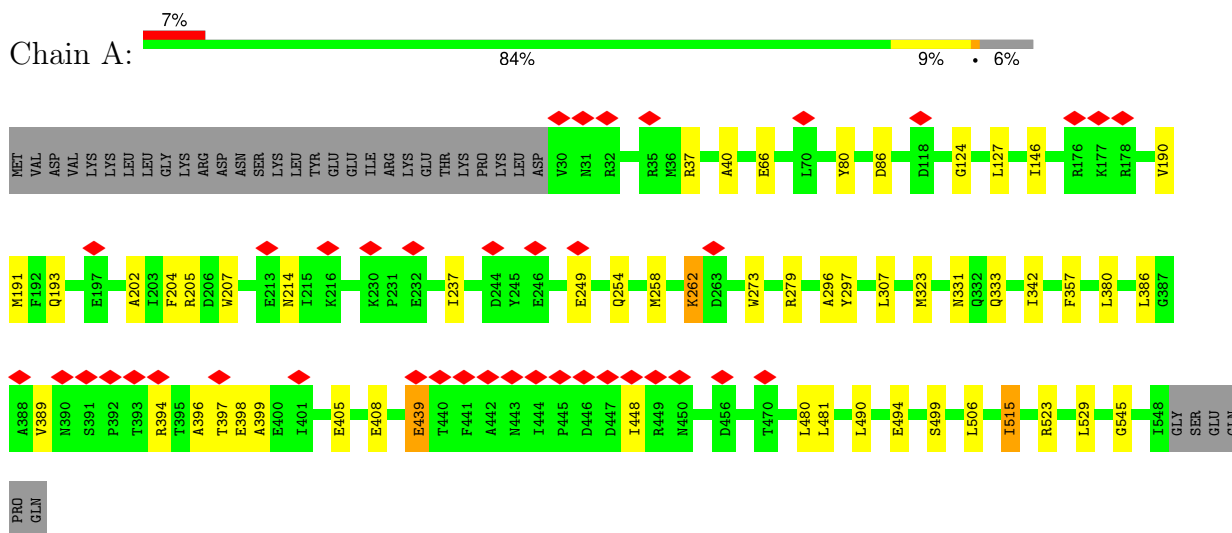
- Molecule 4 is a protein called orf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AC	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AD	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	S	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	X	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	U	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	V	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	W	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	Y	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	Z	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AA	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		
4	AB	193	Total	C	N	O	S	0	0
			1525	982	250	284	9		

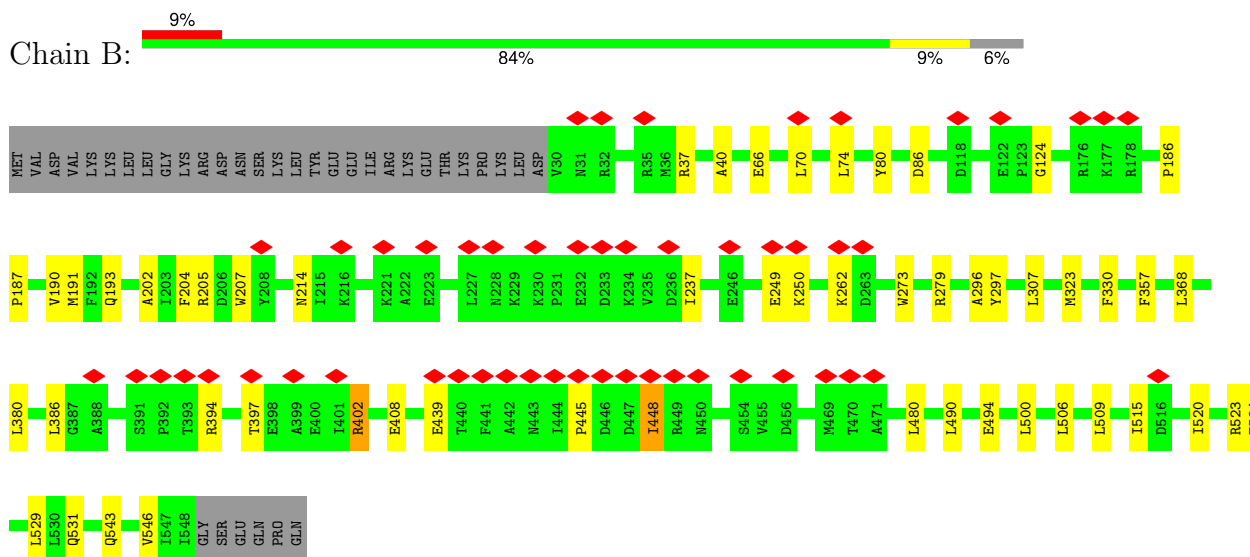
3 Residue-property plots [i](#)

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.

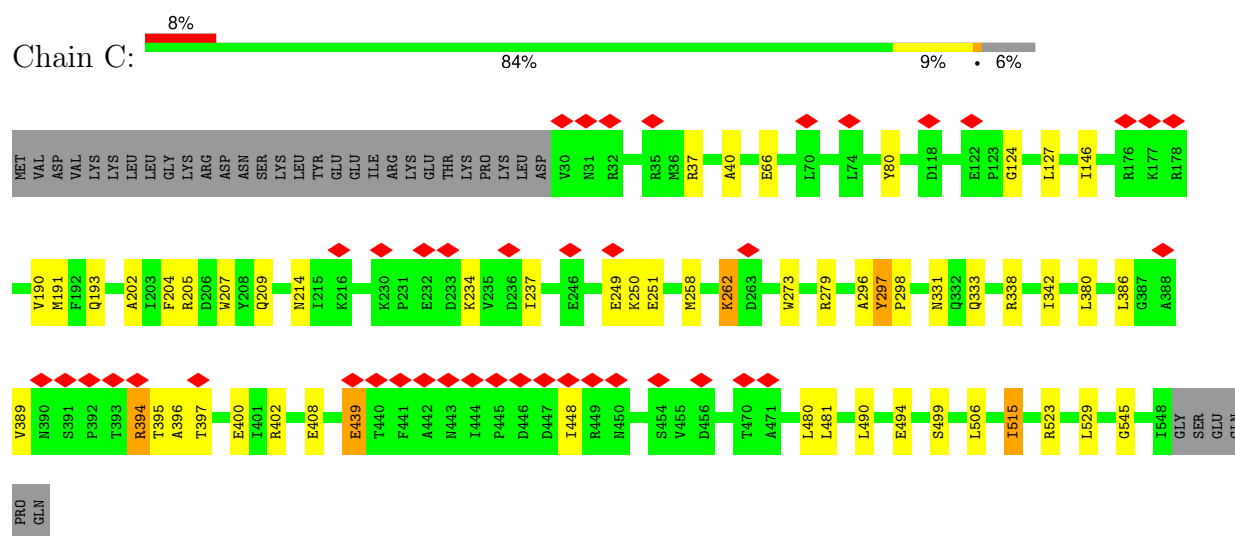
- Molecule 1: orf12



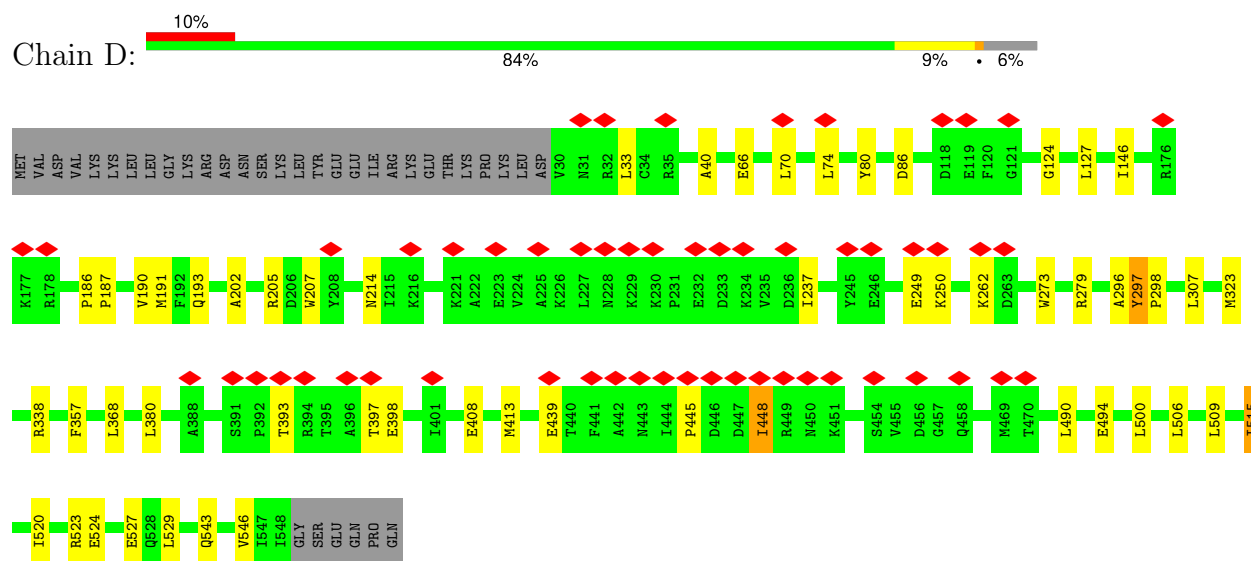
- Molecule 1: orf12



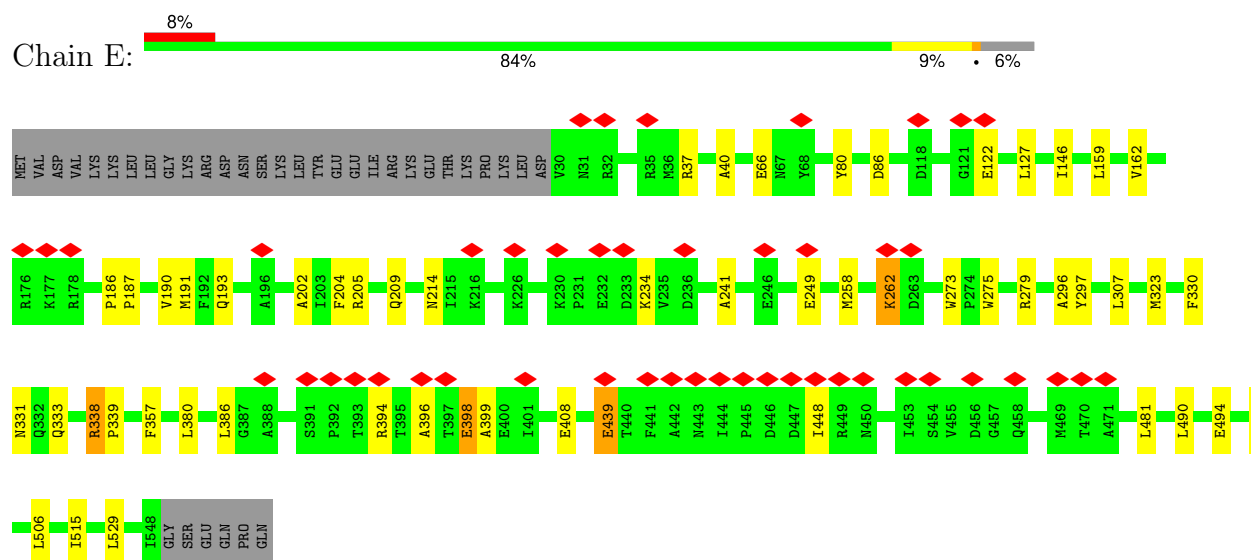
- Molecule 1: orf12



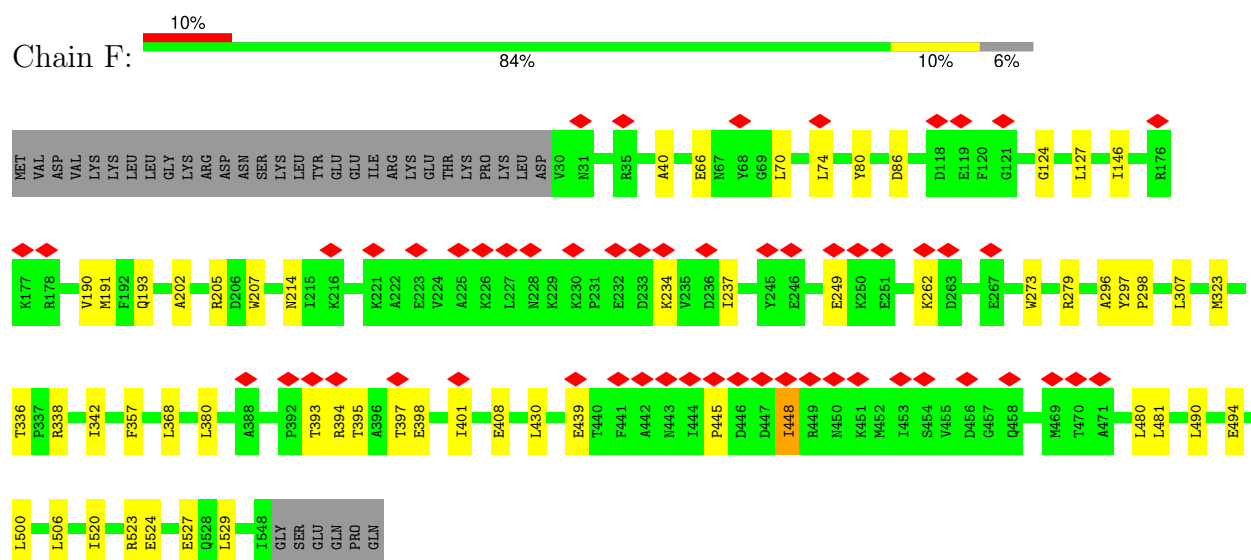
• Molecule 1: orf12



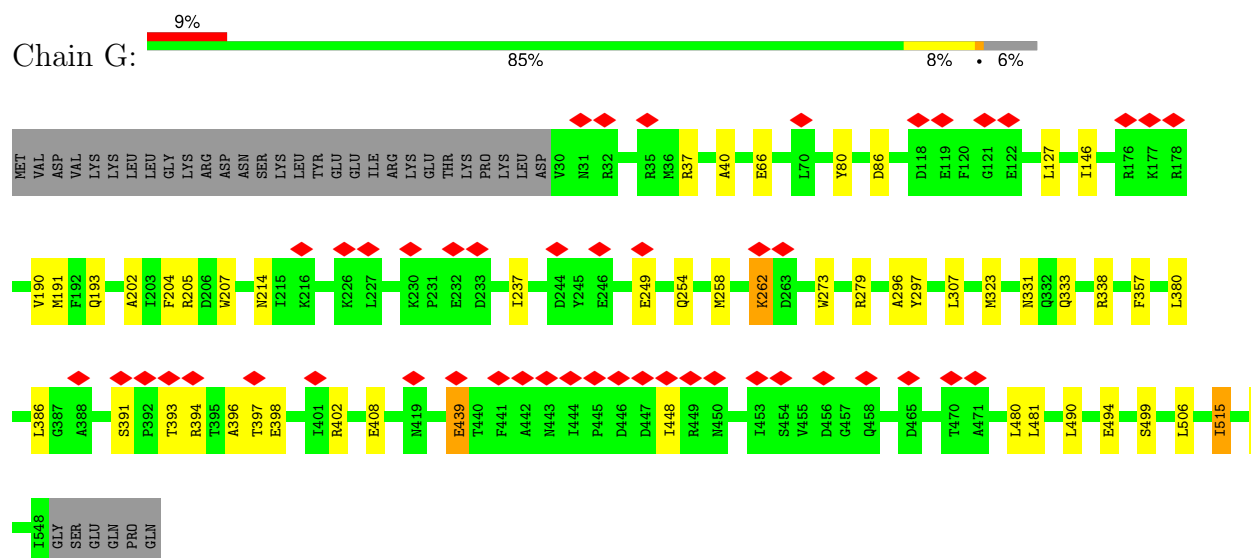
• Molecule 1: orf12



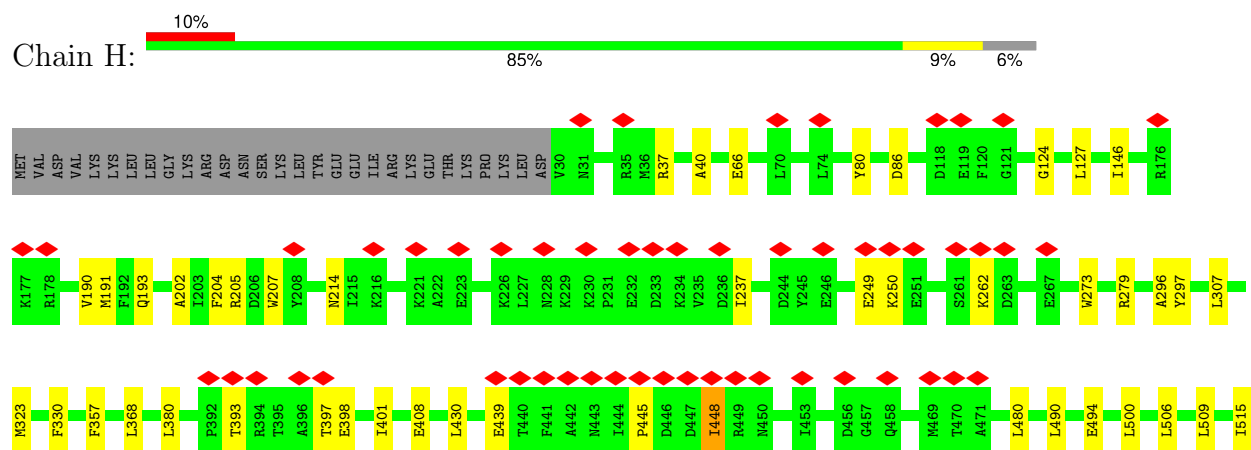
- Molecule 1: orf12

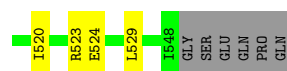


- Molecule 1: orf12



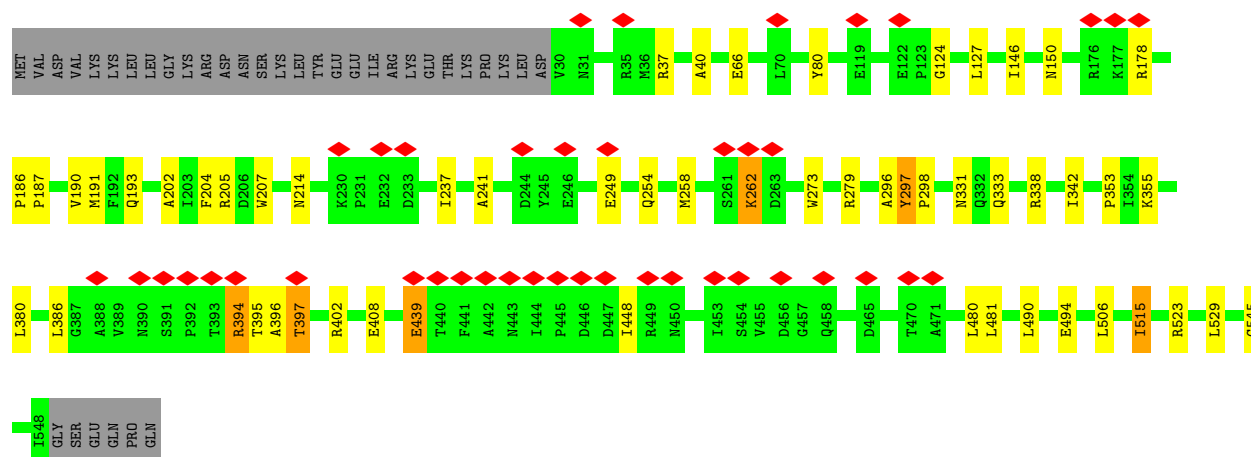
- Molecule 1: orf12





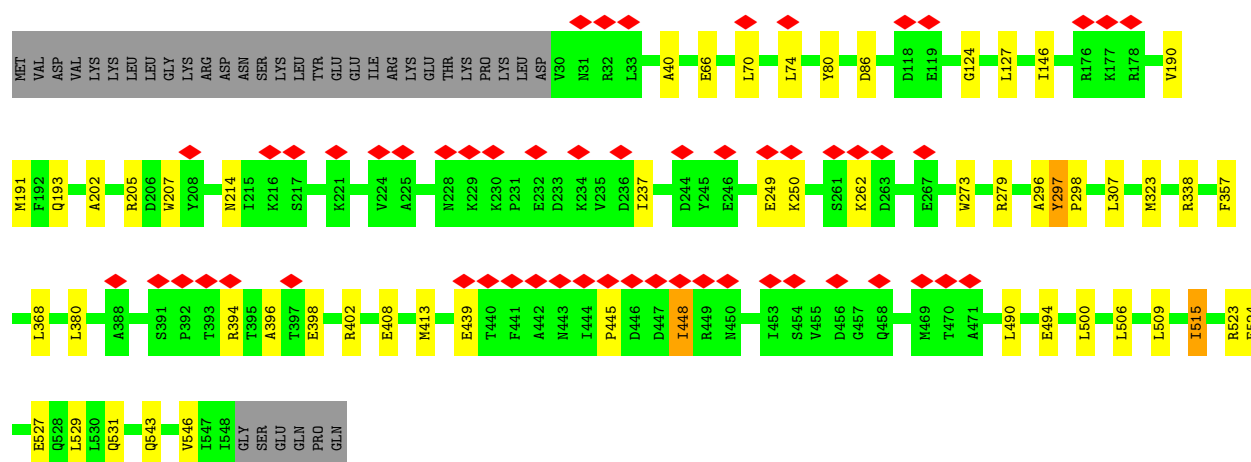
• Molecule 1: orf12

Chain I: 8% 84% 9% • 6%



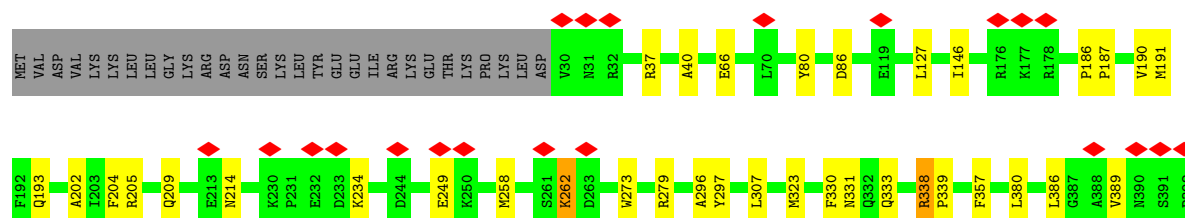
• Molecule 1: orf12

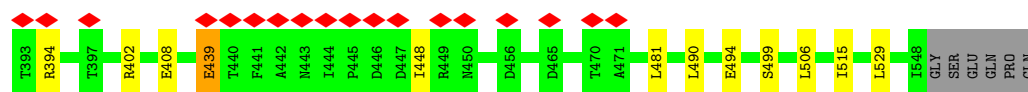
Chain J: 10% 84% 9% • 6%



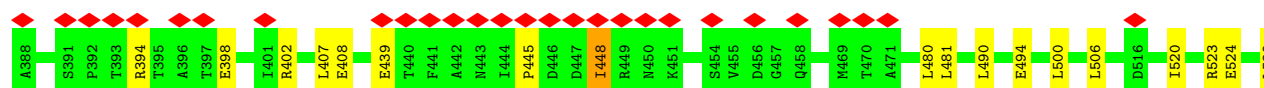
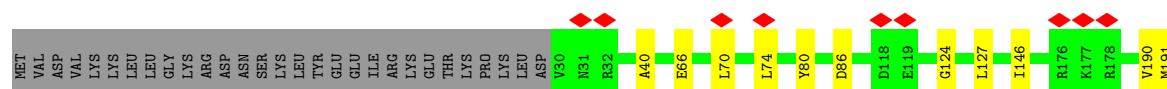
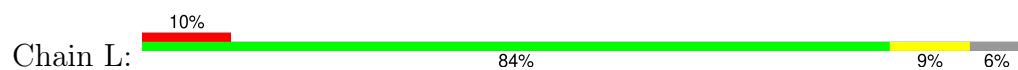
• Molecule 1: orf12

Chain K: 7% 85% 8% • 6%

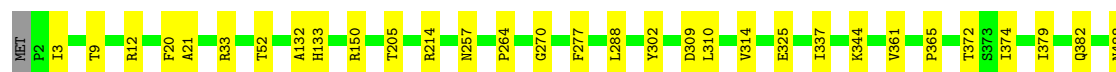




• Molecule 1: orf12



• Molecule 2: orf18



• Molecule 2: orf18



• Molecule 2: orf18



[illegible]

- Molecule 3: orf22

Chain AF:  25% 74%

[illegible]

- Molecule 3: orf22

Chain AG: 25% . 74%

[illegible]

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

- Molecule 3: orf22

Chain AN:  25% 1% 74%

[illegible]

- Molecule 3: orf22

Chain AO:  24% . 74%

MET	S2	I26	I67	S94	S98	QI20	QI23	A131	L134	R146	P149	E167	D172	E173	THR	PRO	ALA	PRO	SER	SER	SER	PRO	PHE	ILE	ILE	TYR	TYR	GLN	ALA	ASP	ALA	THR	LEU	SER	ASV	ASN	GLN	ASN	LEU	GLY	ILE	LEU	THR	SER	GLY	ILE	LEU	ASP
-----	----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



74%

- Molecule 3: orf22

74%



[illegible]

- Molecule 3: orf22

[illegible]

- Molecule 3: orf22



ILE	PHE	GLY	ALA	VAL	MET
ASP	SER	SER	ASN	GLY	S2
LEU	ILE	PRO	PHE	GLY	I26
SER	ILE	ALA	SER	SER	I67
SER	THR	ILE	THR	THR	
SER	ILE	LEU	THR	THR	
GLY	THR	THR	ASN	LEU	S98
LEU	GLY	ARG	ASN	SER	
LEU	ASN	ALA	GLY	ILE	Q120
LEU	GLN	THR	SER	ALA	
GLY	THR	THR	SER	GLN	Q123
ALA	ILE	PHE	GLY	ASN	
ALA	THR	ASP	VAL	ALA	A131
ASN	GLY	GLN	GLY	VAL	
ALA	ASP	PRO	ALA	ASP	L134
ARG	LYS	SER	THR	TYR	
VAL	THR	GLU	LEU	TRP	R446
SER	PHE	ILE	THR	ALA	
THR	THR	GLN	ALA	PRO	P149
ILE	GLY	PRO	SER	GLY	
LEU	THR	GLY	THR	ASP	E167
ASP	THR	ASP	ASN	GLU	
GLU	THR	LEU	GLY	LEU	D172
ASP	LEU	VAL	ALA	THR	E173
ASP	ASP	PRO	PHE	ARG	THR
MET	ASN	VAL	SER	PRO	
ALA	PHE	LEU	LEU	GLN	ALA
SER	ILE	ALA	ASP	ALA	PRO
ASP	PHE	GLY	GLY	PRO	SER
SER	VAL	THR	GLN	VAL	SER
ALA	GLY	VAL	ALA	SER	SER
THR	SER	ASN	GLY	PRO	PHE
ALA	ASN	ASN	VAL	ASP	PHE
LEU	ILE	GLY	LEU	ASP	ILE
ALA	GLN	THR	ASN	VAL	ILE
THR	HIS	LEU	LYS	VAL	TYR
GLN	LEU	TRP	SER	VAL	THR
GLY	GLY	LEU	THR	GLN	ALA
SER	ASP	GLN	LEU	ALA	ASP
ILE	THR	THR	MET	TYR	ALA
LYS	GLY	ASP	LYS	ALA	THR
ALA	ASN	THR	ASP	ASP	LEU
TYR	GLN	VAL	GLN	SER	THR
VAL	ILE	SER	THR	ILE	ASN
ASP	ILE	ALA	ASN	SER	GLN
ASN	PHE	VAL	THR	GLY	ASN
PHE	GLY	GLY	PHE	GLY	ASN
ARG	THR	THR	GLU	PHE	THR
ALA	ALA	ASP	ASN	THR	GLY
ALA	THR	PRO	GLY	PHE	ALA
GLY	GLN	ILE	ILE	ILE	LEU
ALA	ILE	THR	TYR	ASN	THR
ILE	ASN	PHE	ILE	PRO	SER
LEU	THR	ILE	LEU	VAL	THR
GLN	ILE	ALA	THR	ASN	ILE
THR	ASN	PHE	GLN	ALA	LEU
VAL	ASN	LEU	VAL	LYS	THR
SER	THR	ALA	GLY	ALA	GLN

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

- Molecule 3: orf22

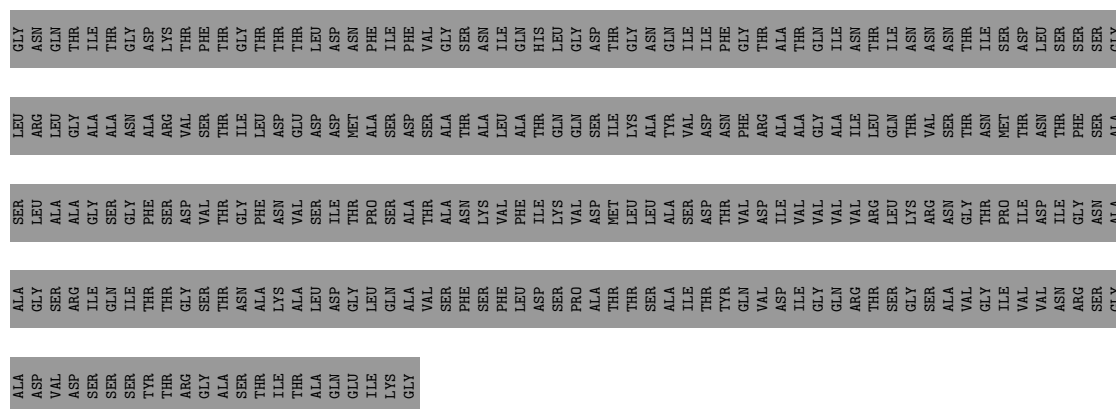
Chain BY: 25% 74%

[illegible]

- Molecule 3: orf22

Chain BZ:  25% 74%

[illegible]



- Molecule 4: orf17



- Molecule 4: orf17



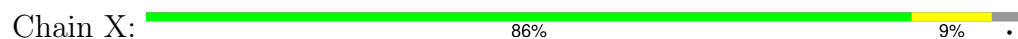
- Molecule 4: orf17



- Molecule 4: orf17



- Molecule 4: orf17



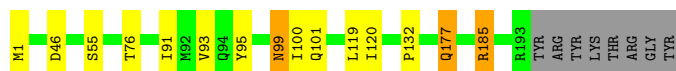
- Molecule 4: orf17





- Molecule 4: orf17

Chain V: 89% 6% . .



- Molecule 4: orf17

Chain W: 89% 7% .



- Molecule 4: orf17

Chain Y: 92% . .



- Molecule 4: orf17

Chain Z: 88% 6% . .



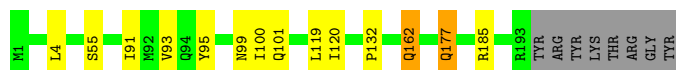
- Molecule 4: orf17

Chain AA: 91% . .



- Molecule 4: orf17

Chain AB: 89% 6% . .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88530	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 ($e^-/\text{\AA}^2$)	52.9	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.337	Depositor
Minimum map value	-0.451	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	702.4, 702.4, 702.4	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.878, 0.878, 0.878	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/4223	0.48	0/5744
1	B	0.29	0/4223	0.47	0/5744
1	C	0.29	0/4223	0.48	0/5744
1	D	0.29	0/4223	0.48	0/5744
1	E	0.29	0/4223	0.48	0/5744
1	F	0.29	0/4223	0.48	0/5744
1	G	0.30	0/4223	0.48	0/5744
1	H	0.29	0/4223	0.48	0/5744
1	I	0.29	0/4223	0.48	0/5744
1	J	0.29	0/4223	0.48	0/5744
1	K	0.29	0/4223	0.48	0/5744
1	L	0.29	0/4223	0.48	0/5744
2	M	0.32	0/6466	0.51	0/8830
2	N	0.32	0/6466	0.51	0/8830
2	O	0.32	0/6466	0.51	0/8830
2	P	0.32	0/6466	0.51	0/8830
2	Q	0.32	0/6466	0.51	0/8830
2	R	0.32	0/6466	0.51	0/8830
3	AE	0.31	0/1347	0.48	0/1837
3	AF	0.30	0/1347	0.48	0/1837
3	AG	0.31	0/1347	0.48	0/1837
3	AN	0.31	0/1347	0.48	0/1837
3	AO	0.30	0/1347	0.48	0/1837
3	AP	0.32	0/1347	0.49	0/1837
3	AW	0.32	0/1347	0.48	0/1837
3	AX	0.31	0/1347	0.48	0/1837
3	AY	0.31	0/1347	0.47	0/1837
3	BF	0.31	0/1347	0.48	0/1837
3	BG	0.30	0/1347	0.48	0/1837
3	BH	0.31	0/1347	0.48	0/1837
3	BO	0.31	0/1347	0.48	0/1837
3	BP	0.30	0/1347	0.48	0/1837
3	BQ	0.32	0/1347	0.48	0/1837
3	BX	0.31	0/1347	0.48	0/1837

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	BY	0.30	0/1347	0.48	0/1837
3	BZ	0.31	0/1347	0.48	0/1837
4	AA	0.32	0/1561	0.48	0/2127
4	AB	0.32	0/1561	0.47	0/2127
4	AC	0.32	0/1561	0.48	0/2127
4	AD	0.32	0/1561	0.48	0/2127
4	S	0.32	0/1561	0.48	0/2127
4	T	0.32	0/1561	0.47	0/2127
4	U	0.32	0/1561	0.48	0/2127
4	V	0.31	0/1561	0.47	0/2127
4	W	0.32	0/1561	0.49	0/2127
4	X	0.32	0/1561	0.47	0/2127
4	Y	0.32	0/1561	0.48	0/2127
4	Z	0.32	0/1561	0.48	0/2127
All	All	0.31	0/132450	0.49	0/180498

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	4128	0	4062	25	0
1	B	4128	0	4062	25	0
1	C	4128	0	4062	27	0
1	D	4128	0	4062	22	0
1	E	4128	0	4062	26	0
1	F	4128	0	4062	22	0
1	G	4128	0	4062	24	0
1	H	4128	0	4062	23	0
1	I	4128	0	4062	28	0
1	J	4128	0	4062	20	0
1	K	4128	0	4062	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	4128	0	4062	21	0
2	M	6330	0	6142	23	0
2	N	6330	0	6142	27	0
2	O	6330	0	6142	25	0
2	P	6330	0	6142	21	0
2	Q	6330	0	6142	27	0
2	R	6330	0	6142	20	0
3	AE	1320	0	1285	2	0
3	AF	1320	0	1285	5	0
3	AG	1320	0	1285	3	0
3	AN	1320	0	1285	5	0
3	AO	1320	0	1285	6	0
3	AP	1320	0	1285	4	0
3	AW	1320	0	1285	4	0
3	AX	1320	0	1285	8	0
3	AY	1320	0	1285	5	0
3	BF	1320	0	1285	5	0
3	BG	1320	0	1285	6	0
3	BH	1320	0	1285	5	0
3	BO	1320	0	1285	2	0
3	BP	1320	0	1285	5	0
3	BQ	1320	0	1285	3	0
3	BX	1320	0	1285	3	0
3	BY	1320	0	1285	4	0
3	BZ	1320	0	1285	3	0
4	AA	1525	0	1526	7	0
4	AB	1525	0	1526	8	0
4	AC	1525	0	1526	8	0
4	AD	1525	0	1526	12	0
4	S	1525	0	1526	4	0
4	T	1525	0	1526	9	0
4	U	1525	0	1526	6	0
4	V	1525	0	1526	10	0
4	W	1525	0	1526	7	0
4	X	1525	0	1526	14	0
4	Y	1525	0	1526	5	0
4	Z	1525	0	1526	10	0
All	All	129576	0	127038	492	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.

The worst 5 of 492 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)
4:V:99:ASN:HB3	4:V:185:ARG:HE	1.44	0.83
4:Z:99:ASN:HB3	4:Z:185:ARG:HE	1.51	0.76
1:I:397:THR:HB	1:J:396:ALA:HA	1.67	0.76
1:B:394:ARG:HH21	1:B:402:ARG:HH12	1.38	0.71
4:AA:132:PRO:HG2	4:AB:91:ILE:HG13	1.73	0.71

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	517/554 (93%)	498 (96%)	19 (4%)	0	100	100
1	B	517/554 (93%)	494 (96%)	23 (4%)	0	100	100
1	C	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	D	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	E	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	F	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
1	G	517/554 (93%)	493 (95%)	24 (5%)	0	100	100
1	H	517/554 (93%)	496 (96%)	21 (4%)	0	100	100
1	I	517/554 (93%)	496 (96%)	21 (4%)	0	100	100
1	J	517/554 (93%)	494 (96%)	23 (4%)	0	100	100
1	K	517/554 (93%)	497 (96%)	20 (4%)	0	100	100
1	L	517/554 (93%)	495 (96%)	22 (4%)	0	100	100
2	M	815/818 (100%)	790 (97%)	24 (3%)	1 (0%)	48	41
2	N	815/818 (100%)	791 (97%)	24 (3%)	0	100	100
2	O	815/818 (100%)	788 (97%)	27 (3%)	0	100	100
2	P	815/818 (100%)	791 (97%)	23 (3%)	1 (0%)	48	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	815/818 (100%)	792 (97%)	23 (3%)	0	100	100
2	R	815/818 (100%)	790 (97%)	25 (3%)	0	100	100
3	AE	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AF	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	AG	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AN	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AO	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AP	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AW	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AX	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	AY	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	BF	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	BG	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	BH	170/658 (26%)	166 (98%)	4 (2%)	0	100	100
3	BO	170/658 (26%)	166 (98%)	4 (2%)	0	100	100
3	BP	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	BQ	170/658 (26%)	166 (98%)	4 (2%)	0	100	100
3	BX	170/658 (26%)	167 (98%)	3 (2%)	0	100	100
3	BY	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
3	BZ	170/658 (26%)	168 (99%)	2 (1%)	0	100	100
4	AA	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	AB	191/201 (95%)	188 (98%)	3 (2%)	0	100	100
4	AC	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	AD	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	S	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	T	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	U	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	V	191/201 (95%)	188 (98%)	3 (2%)	0	100	100
4	W	191/201 (95%)	190 (100%)	1 (0%)	0	100	100
4	X	191/201 (95%)	189 (99%)	2 (1%)	0	100	100
4	Y	191/201 (95%)	190 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Z	191/201 (95%)	189 (99%)	2 (1%)	0	100	100
All	All	16446/25812 (64%)	15967 (97%)	477 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	337	ILE
2	P	337	ILE

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	440/473 (93%)	420 (96%)	20 (4%)	23	16
1	B	440/473 (93%)	420 (96%)	20 (4%)	23	16
1	C	440/473 (93%)	419 (95%)	21 (5%)	21	14
1	D	440/473 (93%)	415 (94%)	25 (6%)	17	9
1	E	440/473 (93%)	421 (96%)	19 (4%)	25	17
1	F	440/473 (93%)	418 (95%)	22 (5%)	20	13
1	G	440/473 (93%)	420 (96%)	20 (4%)	23	16
1	H	440/473 (93%)	421 (96%)	19 (4%)	25	17
1	I	440/473 (93%)	420 (96%)	20 (4%)	23	16
1	J	440/473 (93%)	414 (94%)	26 (6%)	16	9
1	K	440/473 (93%)	423 (96%)	17 (4%)	27	20
1	L	440/473 (93%)	418 (95%)	22 (5%)	20	13
2	M	694/695 (100%)	684 (99%)	10 (1%)	62	62
2	N	694/695 (100%)	685 (99%)	9 (1%)	65	65
2	O	694/695 (100%)	686 (99%)	8 (1%)	67	68
2	P	694/695 (100%)	680 (98%)	14 (2%)	50	47
2	Q	694/695 (100%)	685 (99%)	9 (1%)	65	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	694/695 (100%)	684 (99%)	10 (1%)	62	62
3	AE	144/532 (27%)	142 (99%)	2 (1%)	62	62
3	AF	144/532 (27%)	142 (99%)	2 (1%)	62	62
3	AG	144/532 (27%)	144 (100%)	0	100	100
3	AN	144/532 (27%)	141 (98%)	3 (2%)	48	45
3	AO	144/532 (27%)	142 (99%)	2 (1%)	62	62
3	AP	144/532 (27%)	144 (100%)	0	100	100
3	AW	144/532 (27%)	142 (99%)	2 (1%)	62	62
3	AX	144/532 (27%)	143 (99%)	1 (1%)	81	83
3	AY	144/532 (27%)	143 (99%)	1 (1%)	81	83
3	BF	144/532 (27%)	142 (99%)	2 (1%)	62	62
3	BG	144/532 (27%)	143 (99%)	1 (1%)	81	83
3	BH	144/532 (27%)	143 (99%)	1 (1%)	81	83
3	BO	144/532 (27%)	140 (97%)	4 (3%)	38	33
3	BP	144/532 (27%)	142 (99%)	2 (1%)	62	62
3	BQ	144/532 (27%)	143 (99%)	1 (1%)	81	83
3	BX	144/532 (27%)	143 (99%)	1 (1%)	81	83
3	BY	144/532 (27%)	143 (99%)	1 (1%)	81	83
3	BZ	144/532 (27%)	142 (99%)	2 (1%)	62	62
4	AA	169/176 (96%)	165 (98%)	4 (2%)	44	39
4	AB	169/176 (96%)	164 (97%)	5 (3%)	36	30
4	AC	169/176 (96%)	165 (98%)	4 (2%)	44	39
4	AD	169/176 (96%)	165 (98%)	4 (2%)	44	39
4	S	169/176 (96%)	163 (96%)	6 (4%)	30	23
4	T	169/176 (96%)	166 (98%)	3 (2%)	54	52
4	U	169/176 (96%)	164 (97%)	5 (3%)	36	30
4	V	169/176 (96%)	164 (97%)	5 (3%)	36	30
4	W	169/176 (96%)	164 (97%)	5 (3%)	36	30
4	X	169/176 (96%)	166 (98%)	3 (2%)	54	52
4	Y	169/176 (96%)	165 (98%)	4 (2%)	44	39
4	Z	169/176 (96%)	162 (96%)	7 (4%)	26	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	14064/21534 (65%)	13670 (97%)	394 (3%)	40 33

5 of 394 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	494	GLU
1	J	394	ARG
1	H	205	ARG
1	I	273	TRP
1	K	127	LEU

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	B	543	GLN
1	D	543	GLN
1	J	543	GLN
2	P	133	HIS
2	M	133	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

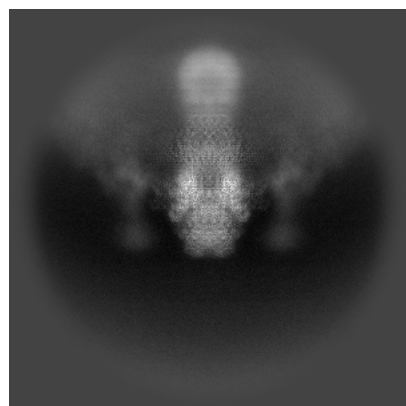
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47975. These allow visual inspection of the internal detail of the map and identification of artifacts.

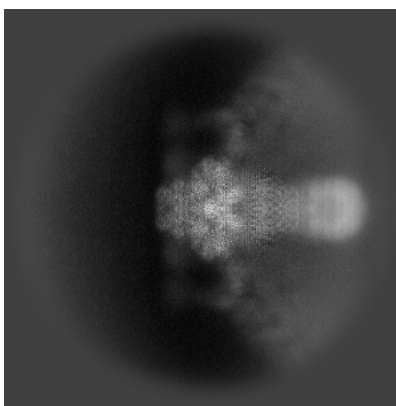
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

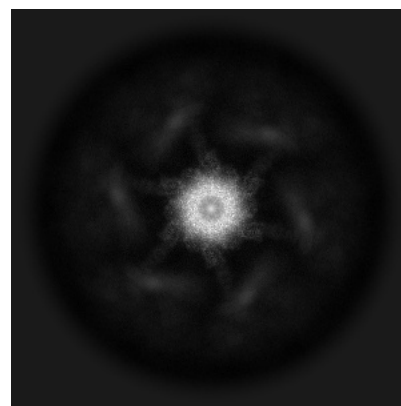
6.1.1 Primary map



X

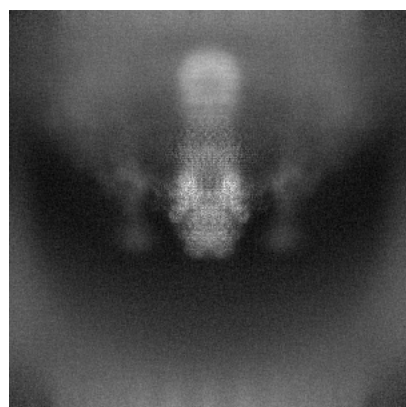


Y

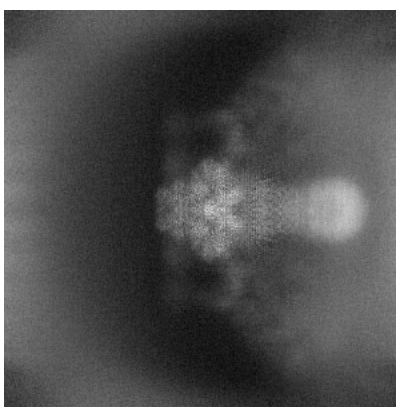


Z

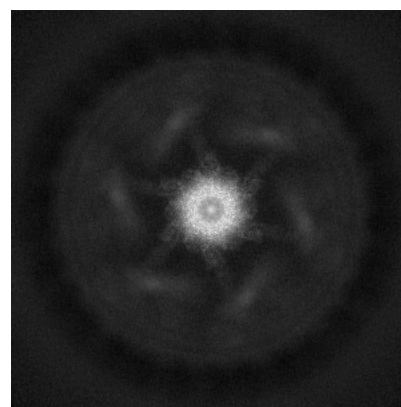
6.1.2 Raw map



X



Y

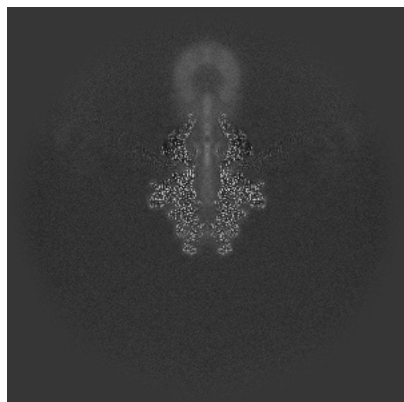


Z

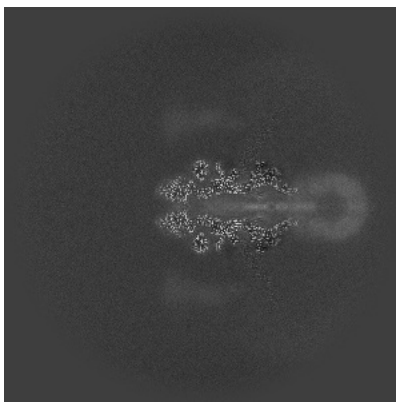
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

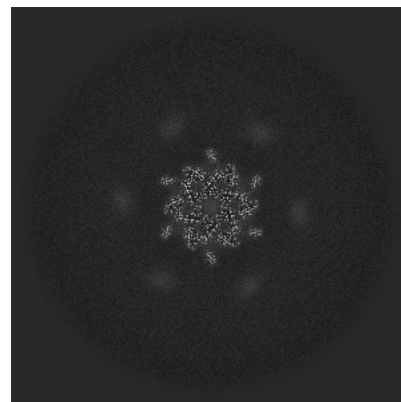
6.2.1 Primary map



X Index: 400

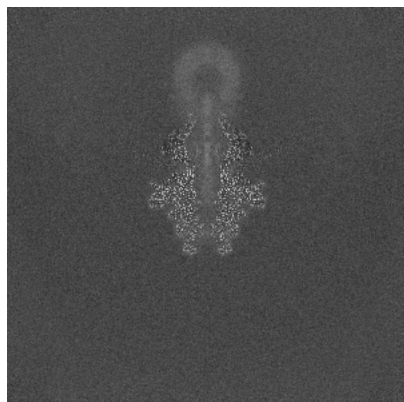


Y Index: 400

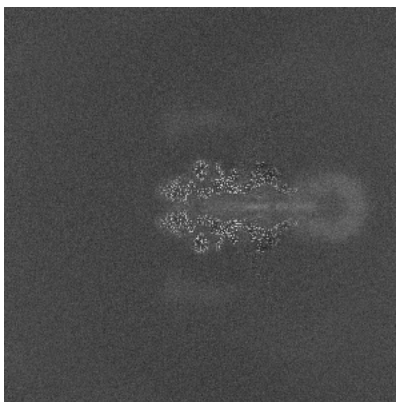


Z Index: 400

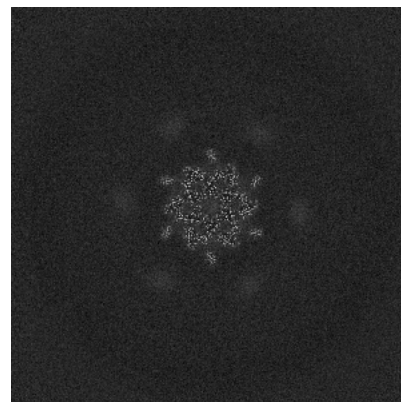
6.2.2 Raw map



X Index: 400



Y Index: 400

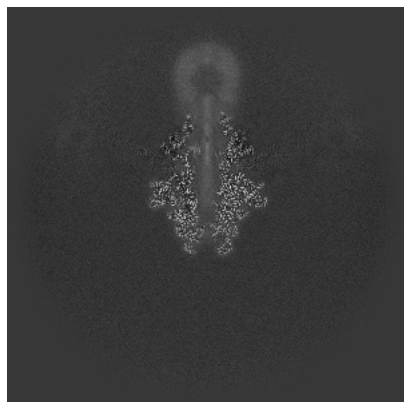


Z Index: 400

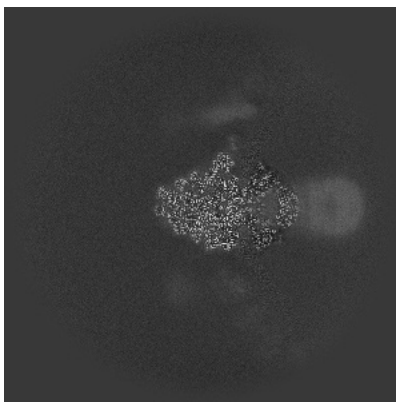
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

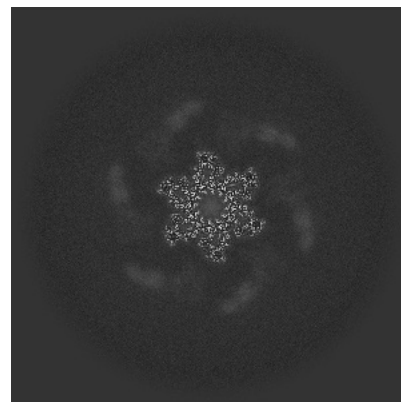
6.3.1 Primary map



X Index: 403

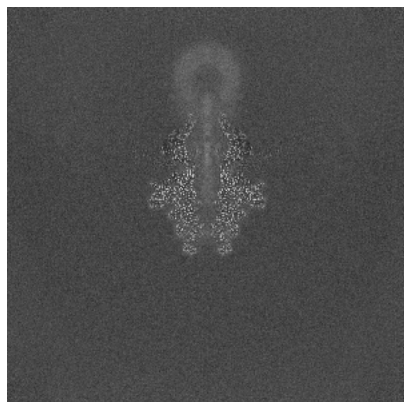


Y Index: 370

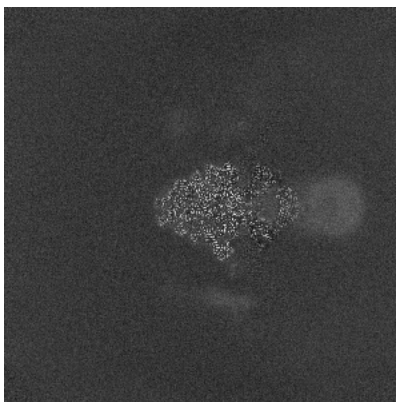


Z Index: 436

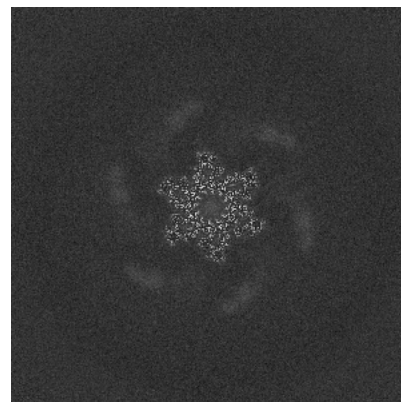
6.3.2 Raw map



X Index: 400



Y Index: 430

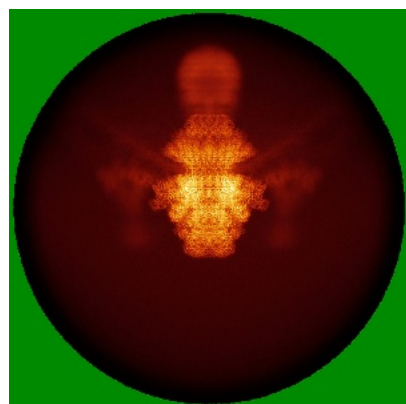


Z Index: 436

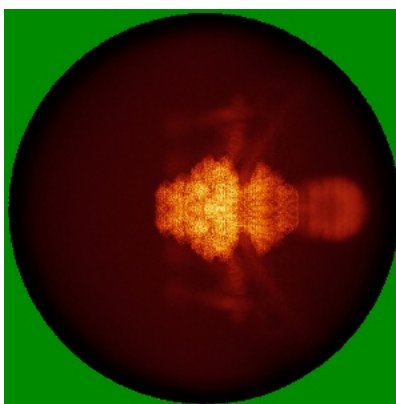
The images above show the largest variance slices of the map in three orthogonal directions.

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

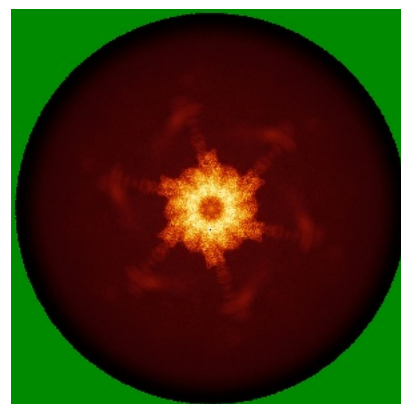
6.4.1 Primary map



X

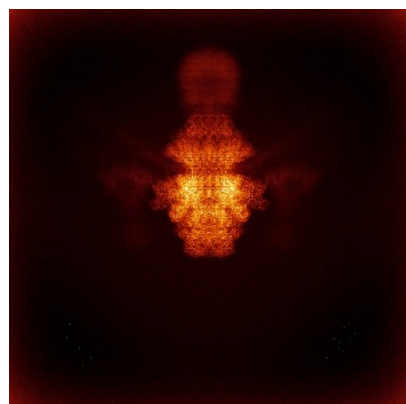


Y

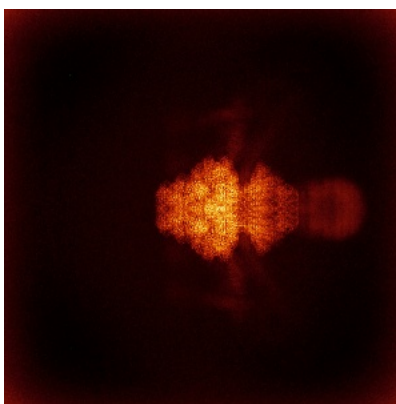


Z

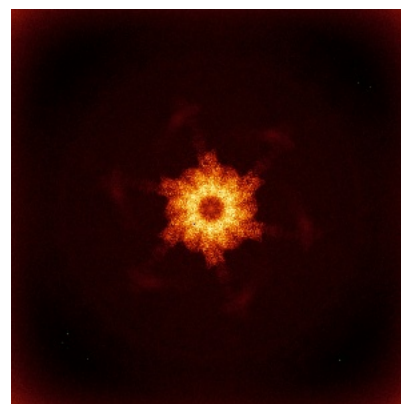
6.4.2 Raw map



X



Y

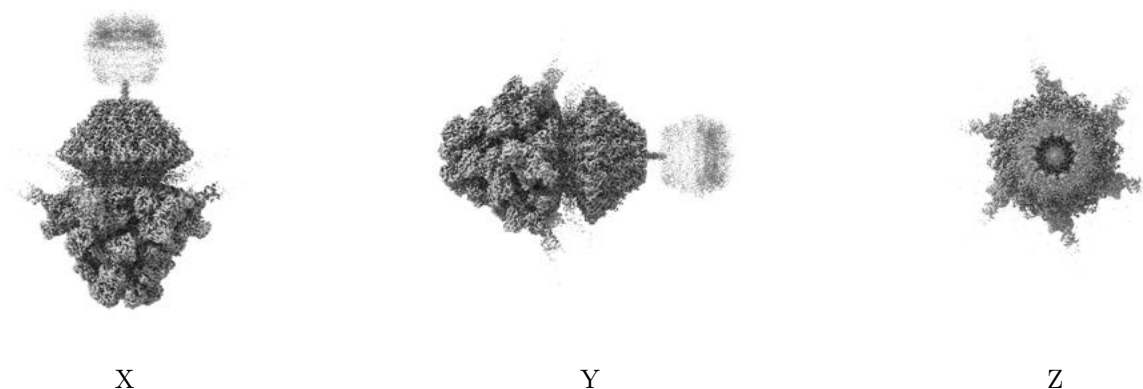


Z

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.

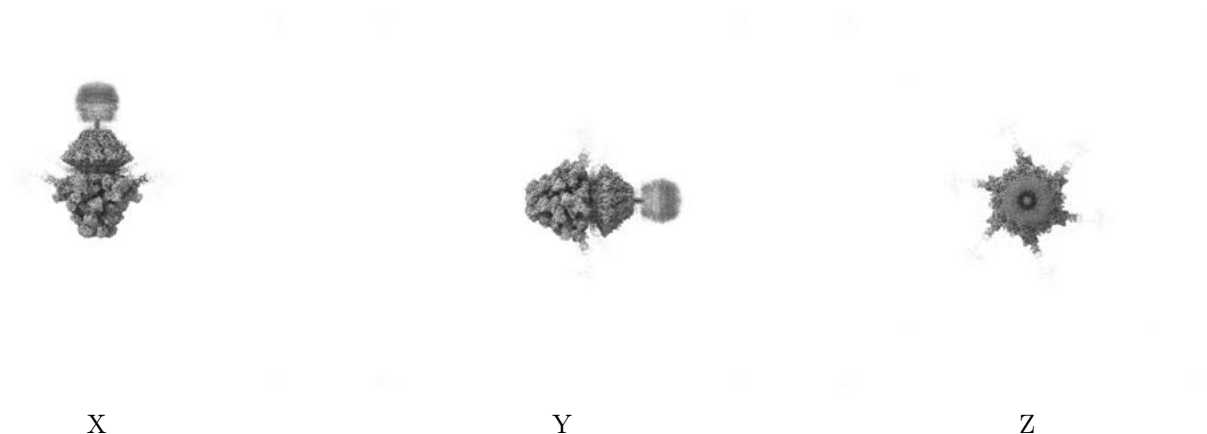
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

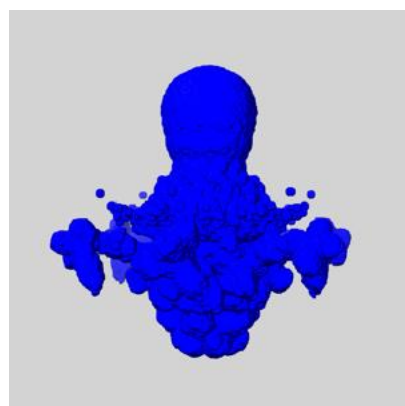
6.6 Mask visualisation [i](#)

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

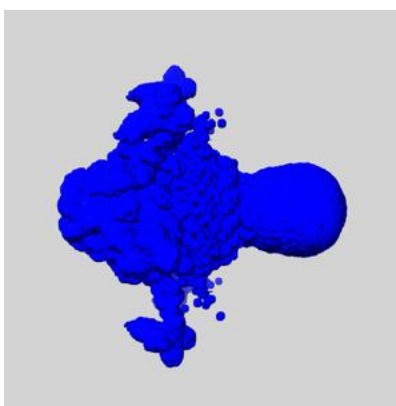
A mask typically either:

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

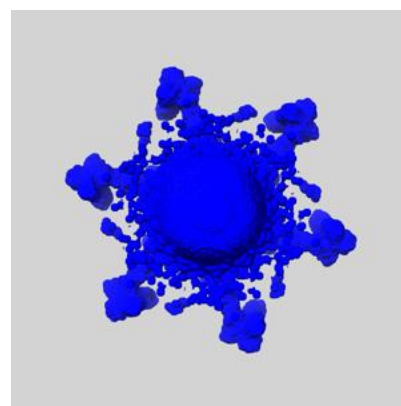
6.6.1 emd_47975_msk_1.map [i](#)



X



Y

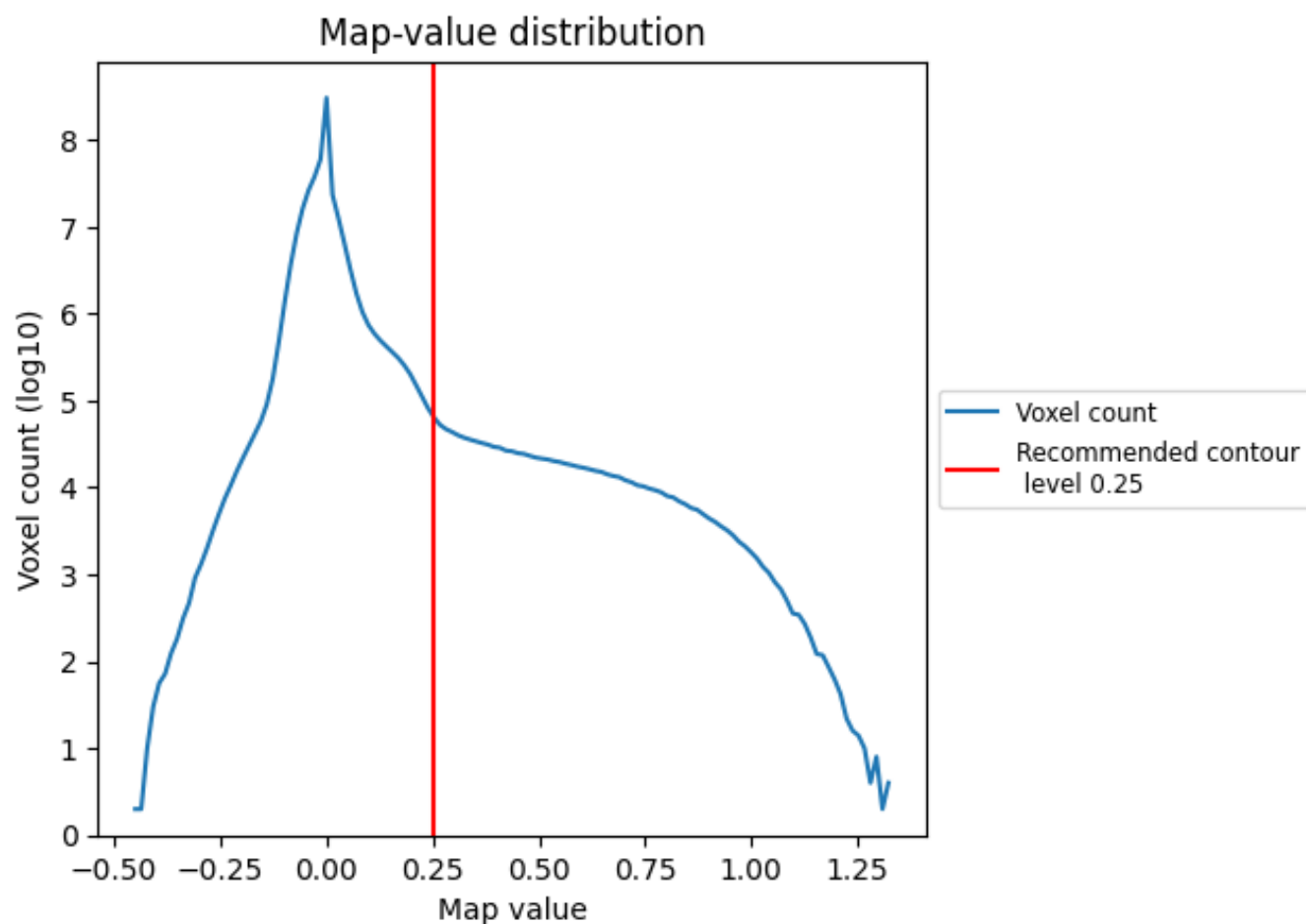


Z

7 Map analysis [i](#)

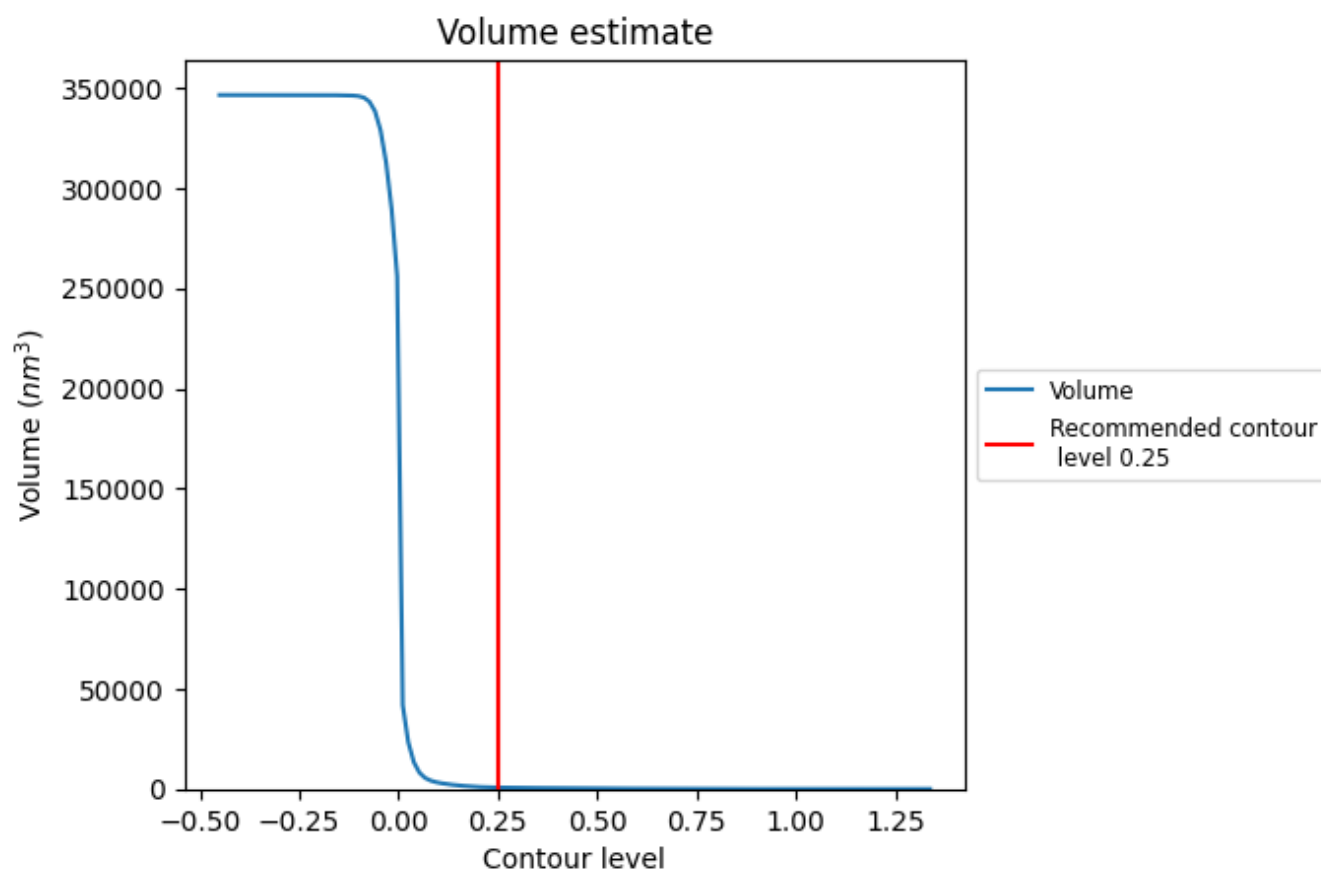
This section contains the results of statistical analysis of the map.

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.

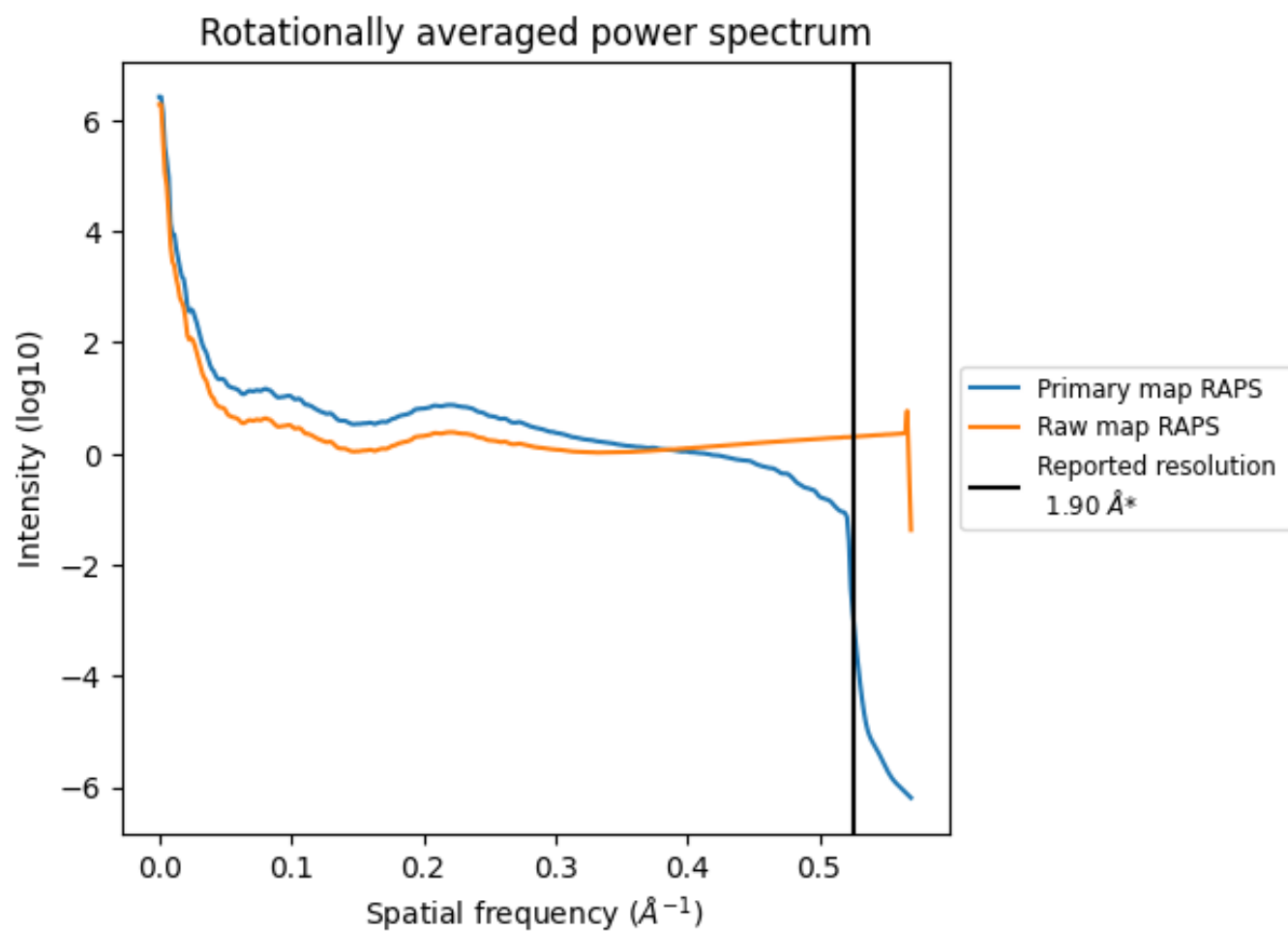
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm^3 ; this corresponds to an approximate mass of 631 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 ⓘ

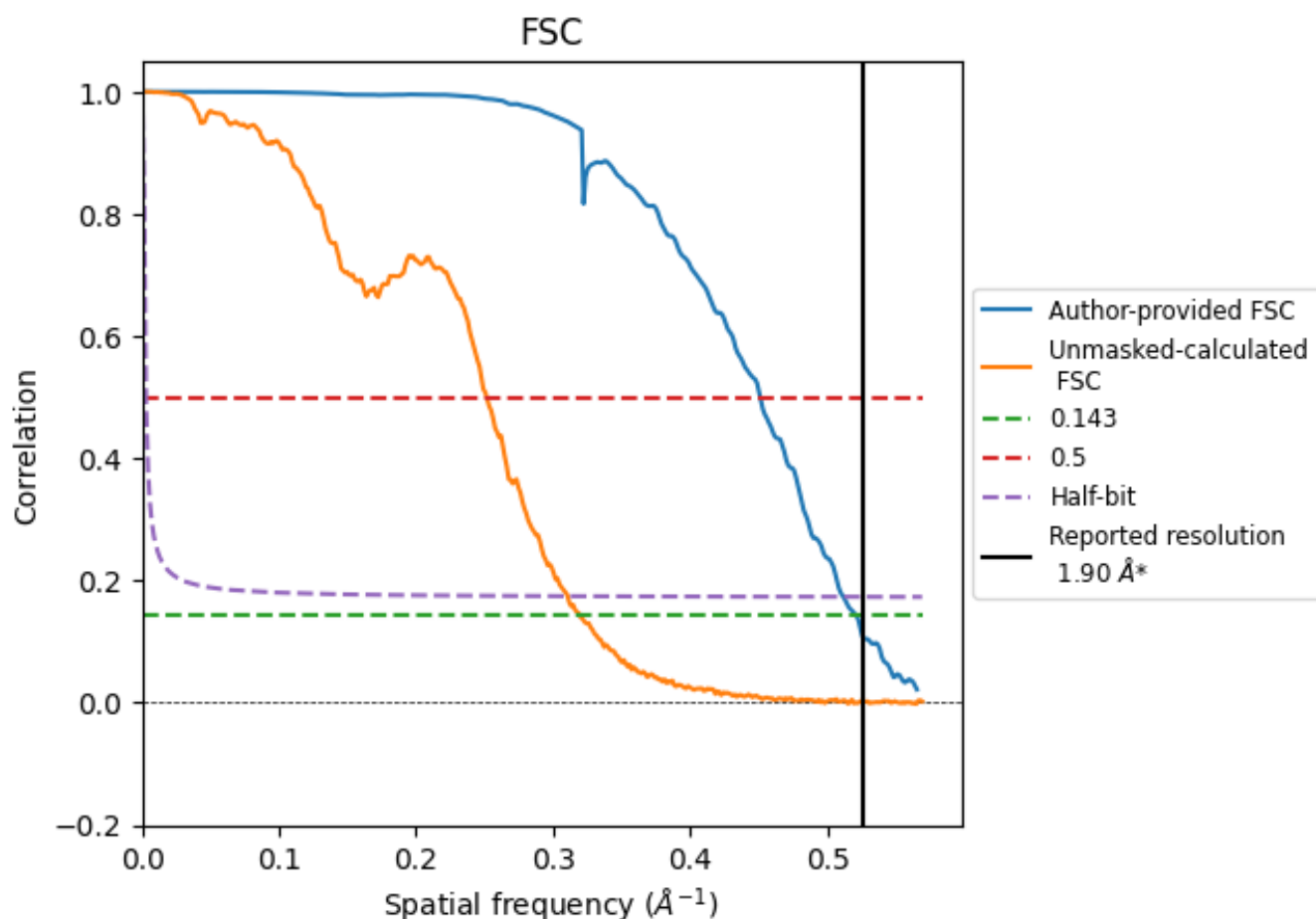


*Reported resolution corresponds to spatial frequency of 0.526 Å⁻¹

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 0.526 \AA^{-1}

8.2 Resolution estimates [i](#)

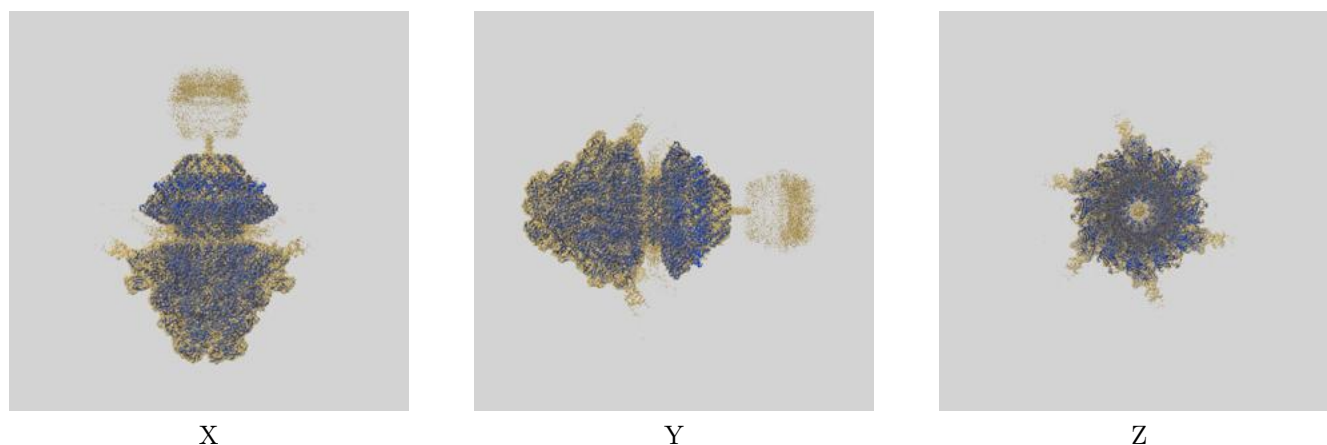
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.90	-	-
Author-provided FSC curve	1.92	2.22	1.95
Unmasked-calculated*	3.13	3.97	3.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 1.9 by more than 10 %

9 Map-model fit [i](#)

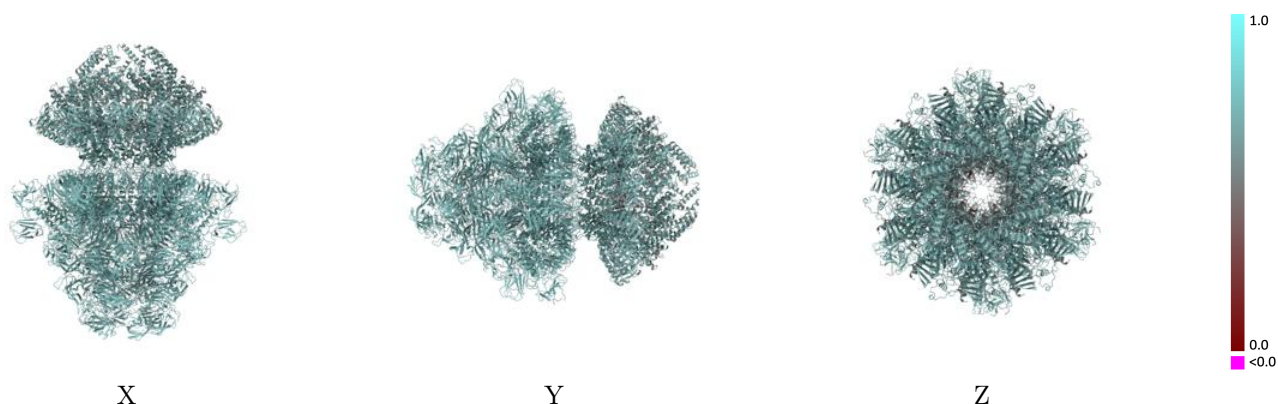
This section contains information regarding the fit between EMDB map EMD-47975 and PDB model 9EFK. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



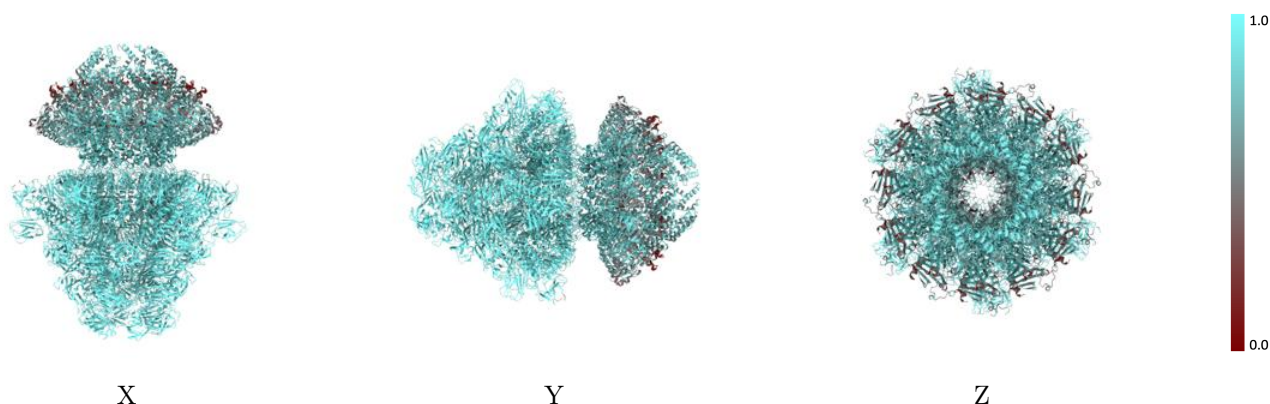
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



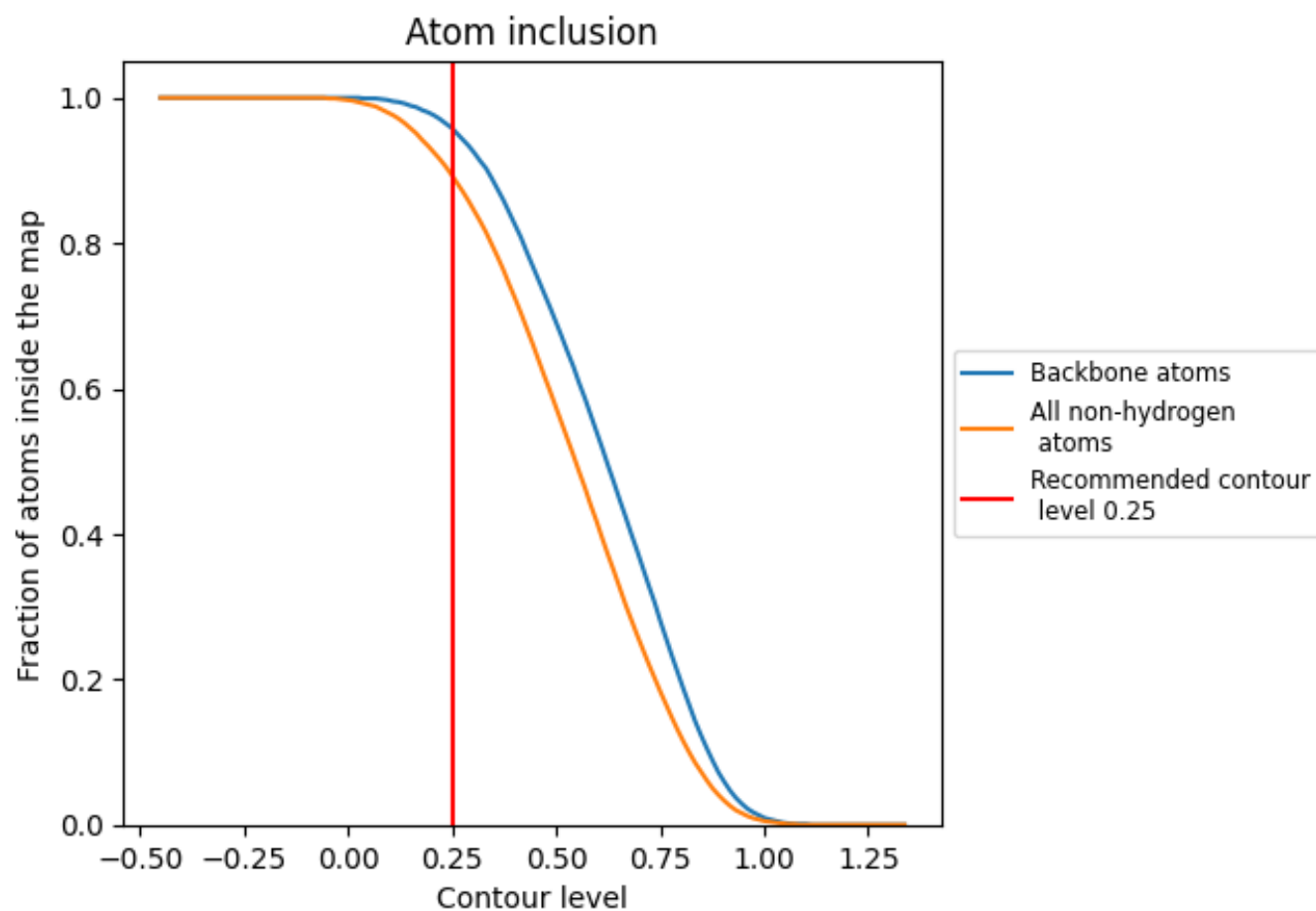
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.6700
A	 0.7890	 0.6500
AA	 0.9660	 0.7020
AB	 0.9600	 0.6950
AC	 0.9650	 0.7000
AD	 0.9550	 0.6940
AE	 0.9630	 0.6890
AF	 0.9570	 0.6770
AG	 0.9620	 0.6910
AN	 0.9600	 0.6920
AO	 0.9580	 0.6780
AP	 0.9590	 0.6940
AW	 0.9610	 0.6850
AX	 0.9530	 0.6740
AY	 0.9580	 0.6860
B	 0.7760	 0.6440
BF	 0.9640	 0.6930
BG	 0.9580	 0.6820
BH	 0.9580	 0.6910
BO	 0.9650	 0.6860
BP	 0.9530	 0.6760
BQ	 0.9590	 0.6880
BX	 0.9650	 0.6910
BY	 0.9550	 0.6820
BZ	 0.9590	 0.6920
C	 0.7860	 0.6470
D	 0.7710	 0.6410
E	 0.7870	 0.6460
F	 0.7740	 0.6410
G	 0.7870	 0.6430
H	 0.7750	 0.6390
I	 0.7850	 0.6420
J	 0.7760	 0.6400
K	 0.7860	 0.6450
L	 0.7730	 0.6430



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Chain	Atom inclusion	Q-score
M	 0.9670	 0.6810
N	 0.9650	 0.6830
O	 0.9640	 0.6830
P	 0.9660	 0.6820
Q	 0.9660	 0.6810
R	 0.9660	 0.6790
S	 0.9680	 0.7010
T	 0.9580	 0.6970
U	 0.9670	 0.7010
V	 0.9570	 0.6950
W	 0.9670	 0.7030
X	 0.9650	 0.7010
Y	 0.9670	 0.7040
Z	 0.9590	 0.6950