



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 06:23 AM UTC

PDB ID : 8B3P / pdb_00008b3p
EMDB ID : EMD-15832
Title : CryoEM structure of the round tip (proteins pVII/pVIII/pIX) from the filamentous bacteriophage
Authors : Conners, R.; McLaren, M.; Gold, V.A.M.
Deposited on : 2022-09-16
Resolution : 2.81 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:

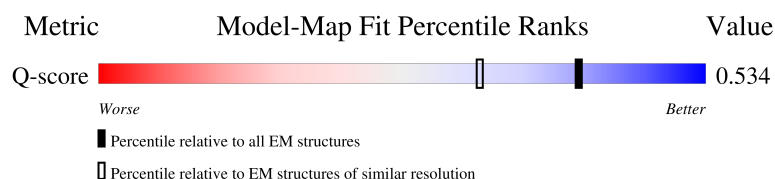
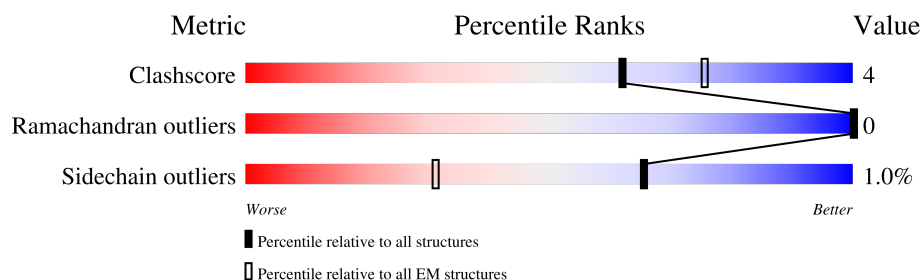
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.81 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	11740 (2.31 - 3.31)

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	AAA	33	9% 67% 18% 15%
1	BBB	33	9% 67% 18% 15%
1	CCC	33	9% 67% 18% 15%
1	DDD	33	9% 67% 18% 15%

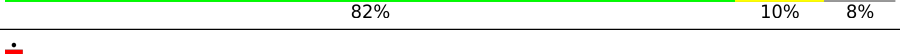
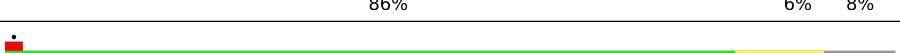
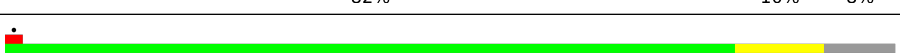
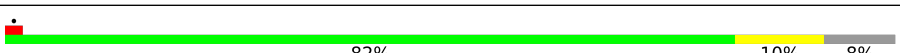
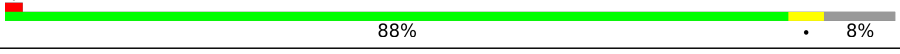
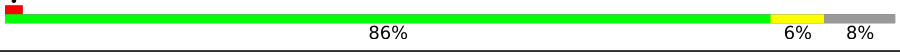
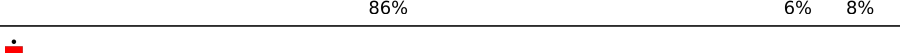
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Mol	Chain	Length	Quality of chain
1	EEE	33	
2	FFF	32	
2	GGG	32	
2	HHH	32	
2	III	32	
2	JJJ	32	
3	111	50	
3	222	50	
3	333	50	
3	KKK	50	
3	LLL	50	
3	MMM	50	
3	NNN	50	
3	OOO	50	
3	PPP	50	
3	QQQ	50	
3	RRR	50	
3	SSS	50	
3	TTT	50	
3	UUU	50	
3	VVV	50	
3	WWW	50	
3	XXX	50	
3	YYY	50	
3	ZZZ	50	

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Mol	Chain	Length	Quality of chain
3	aaa	50	
3	bbb	50	
3	ccc	50	
3	ddd	50	
3	eee	50	
3	fff	50	
3	ggg	50	
3	hhh	50	
3	iii	50	
3	jjj	50	
3	kkk	50	
3	lll	50	
3	mmm	50	
3	nnn	50	
3	ooo	50	
3	ppp	50	
3	qqq	50	
3	rrr	50	
3	sss	50	
3	ttt	50	
3	uuu	50	
3	vvv	50	
3	www	50	
3	xxx	50	
3	yyy	50	

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Mol	Chain	Length	Quality of chain
3	zzz	50	 A horizontal bar chart showing the quality of chain 3. The bar is divided into three segments: a small red segment at the beginning, a large green segment labeled '82%', a small yellow segment labeled '10%', and a small grey segment at the end labeled '8%'. A small red dot is positioned above the start of the bar.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17620 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 virion protein G7P.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AAA	28	Total	C	N	O	S	0	0
			212	138	34	38	2		
1	BBB	28	Total	C	N	O	S	0	0
			212	138	34	38	2		
1	CCC	28	Total	C	N	O	S	0	0
			212	138	34	38	2		
1	DDD	28	Total	C	N	O	S	0	0
			212	138	34	38	2		
1	EEE	28	Total	C	N	O	S	0	0
			212	138	34	38	2		

- Molecule 2 is a protein called Tail virion protein G9P.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FFF	32	Total	C	N	O	S	0	0
			255	168	39	45	3		
2	GGG	32	Total	C	N	O	S	0	0
			255	168	39	45	3		
2	HHH	32	Total	C	N	O	S	0	0
			255	168	39	45	3		
2	III	32	Total	C	N	O	S	0	0
			255	168	39	45	3		
2	JJJ	32	Total	C	N	O	S	0	0
			255	168	39	45	3		

- Molecule 3 is a protein called Capsid protein G8P.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	KKK	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
3	PPP	46	Total	C	N	O	S	0	0
			339	223	53	61	2		
3	UUU	46	Total	C	N	O	S	0	0
			339	223	53	61	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	ZZZ	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	eee	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	jjj	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	ooo	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	ttt	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	yyy	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	LLL	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	QQQ	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	VVV	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	aaa	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	fff	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	kkk	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	ppp	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	uuu	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	222	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	MMM	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	RRR	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	WWW	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	bbb	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	ggg	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	lll	46	Total 340	C 223	N 53	O 62	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	qqq	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	vvv	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	111	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	NNN	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	SSS	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	XXX	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	ccc	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	hhh	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	mmm	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	rrr	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	www	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	zzz	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	OOO	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	TTT	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	YYY	46	Total 339	C 223	N 53	O 61	S 2	0	0
3	ddd	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	iii	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	nnn	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	sss	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	xxx	46	Total 340	C 223	N 53	O 62	S 2	0	0
3	333	46	Total 340	C 223	N 53	O 62	S 2	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
KKK	21	MET	TYR	engineered mutation	UNP P69540
PPP	21	MET	TYR	engineered mutation	UNP P69540
UUU	21	MET	TYR	engineered mutation	UNP P69540
ZZZ	21	MET	TYR	engineered mutation	UNP P69540
eee	21	MET	TYR	engineered mutation	UNP P69540
jjj	21	MET	TYR	engineered mutation	UNP P69540
ooo	21	MET	TYR	engineered mutation	UNP P69540
ttt	21	MET	TYR	engineered mutation	UNP P69540
yyy	21	MET	TYR	engineered mutation	UNP P69540
LLL	21	MET	TYR	engineered mutation	UNP P69540
QQQ	21	MET	TYR	engineered mutation	UNP P69540
VVV	21	MET	TYR	engineered mutation	UNP P69540
aaa	21	MET	TYR	engineered mutation	UNP P69540
fff	21	MET	TYR	engineered mutation	UNP P69540
kkk	21	MET	TYR	engineered mutation	UNP P69540
ppp	21	MET	TYR	engineered mutation	UNP P69540
uuu	21	MET	TYR	engineered mutation	UNP P69540
222	21	MET	TYR	engineered mutation	UNP P69540
MMM	21	MET	TYR	engineered mutation	UNP P69540
RRR	21	MET	TYR	engineered mutation	UNP P69540
WWW	21	MET	TYR	engineered mutation	UNP P69540
bbb	21	MET	TYR	engineered mutation	UNP P69540
ggg	21	MET	TYR	engineered mutation	UNP P69540
lll	21	MET	TYR	engineered mutation	UNP P69540
qqq	21	MET	TYR	engineered mutation	UNP P69540
vvv	21	MET	TYR	engineered mutation	UNP P69540
111	21	MET	TYR	engineered mutation	UNP P69540
NNN	21	MET	TYR	engineered mutation	UNP P69540
SSS	21	MET	TYR	engineered mutation	UNP P69540
XXX	21	MET	TYR	engineered mutation	UNP P69540
ccc	21	MET	TYR	engineered mutation	UNP P69540
hhh	21	MET	TYR	engineered mutation	UNP P69540
mmm	21	MET	TYR	engineered mutation	UNP P69540
rrr	21	MET	TYR	engineered mutation	UNP P69540
www	21	MET	TYR	engineered mutation	UNP P69540
zzz	21	MET	TYR	engineered mutation	UNP P69540
OOO	21	MET	TYR	engineered mutation	UNP P69540
TTT	21	MET	TYR	engineered mutation	UNP P69540
YYY	21	MET	TYR	engineered mutation	UNP P69540
ddd	21	MET	TYR	engineered mutation	UNP P69540
iii	21	MET	TYR	engineered mutation	UNP P69540
nnn	21	MET	TYR	engineered mutation	UNP P69540

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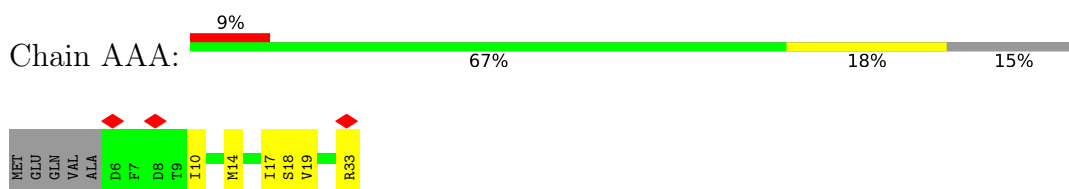
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Chain	Residue	Modelled	Actual	Comment	Reference
sss	21	MET	TYR	engineered mutation	UNP P69540
xxx	21	MET	TYR	engineered mutation	UNP P69540
333	21	MET	TYR	engineered mutation	UNP P69540

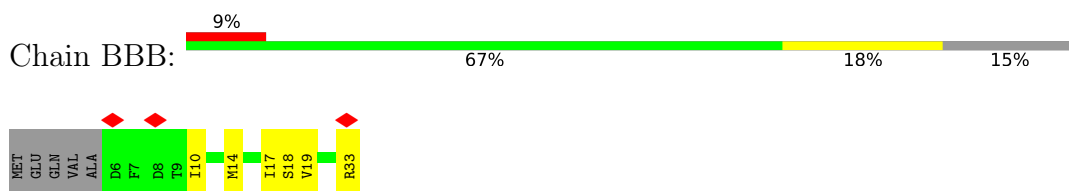
3 Residue-property plots [i](#)

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.

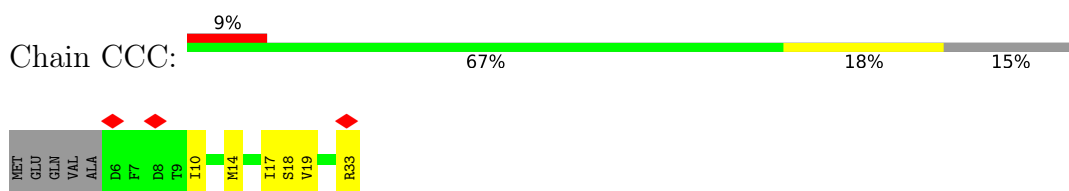
- Molecule 1: Tail virion protein G7P



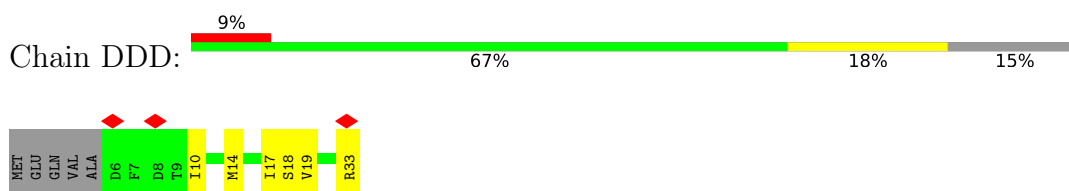
- Molecule 1: Tail virion protein G7P



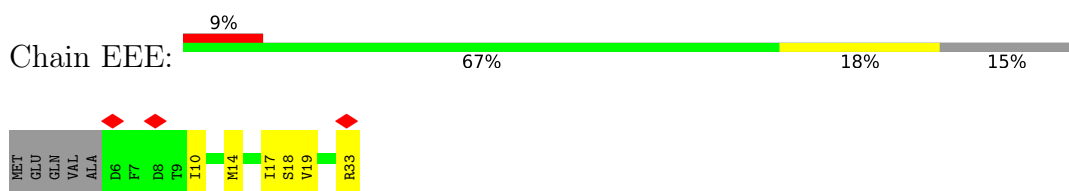
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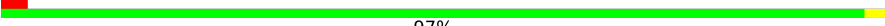
- Molecule 1: Tail virion protein G7P

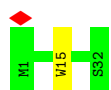


- Molecule 1: Tail virion protein G7P

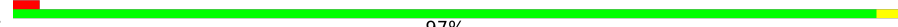


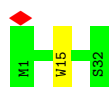
- Molecule 2: Tail virion protein G9P

Chain FFF:  97%



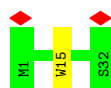
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Chain GGG:  97%



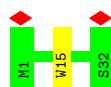
- Molecule 2: Tail virion protein G9P

Chain HHH:  97%



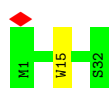
- Molecule 2: Tail virion protein G9P

Chain III:  97%



- Molecule 2: Tail virion protein G9P

Chain JJJ:  97%



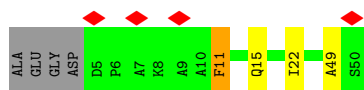
- Molecule 3: Capsid protein G8P

Chain KKK:  76% 16% 8%

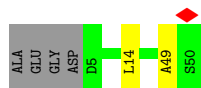


- Molecule 3: Capsid protein G8P

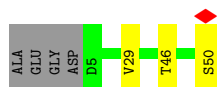
Chain PPP:  84% 6% 8%



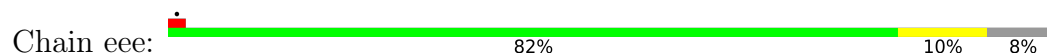
- Molecule 3: Capsid protein G8P



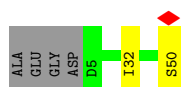
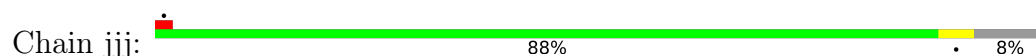
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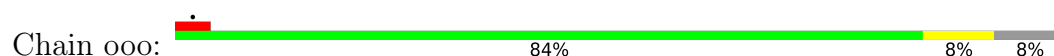
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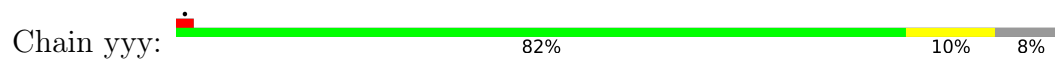
- Molecule 3: Capsid protein G8P



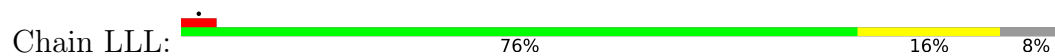
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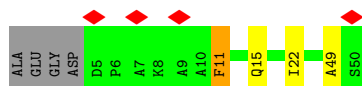
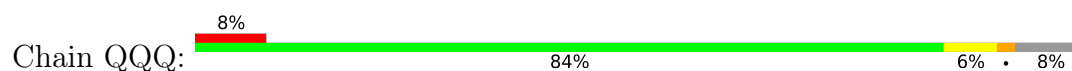
- Molecule 3: Capsid protein G8P



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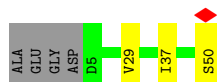
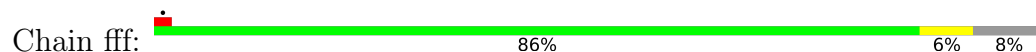
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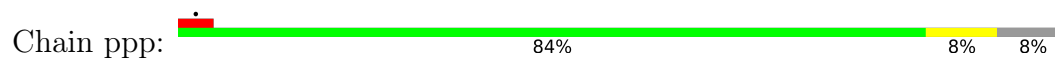


- Molecule 3: Capsid protein G8P

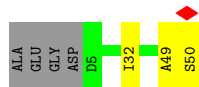




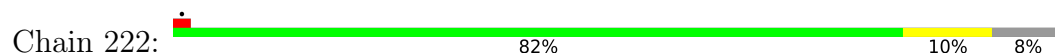
- Molecule 3: Capsid protein G8P



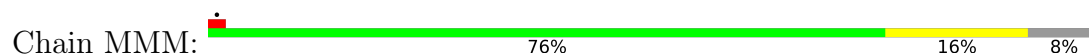
- Molecule 3: Capsid protein G8P



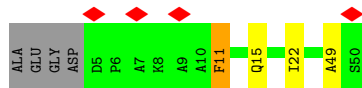
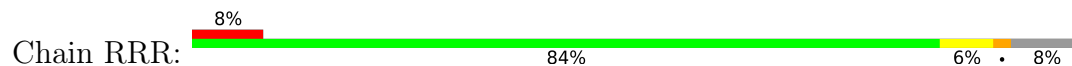
- Molecule 3: Capsid protein G8P



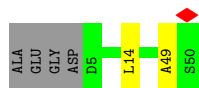
- Molecule 3: Capsid protein G8P



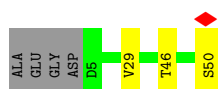
- Molecule 3: Capsid protein G8P



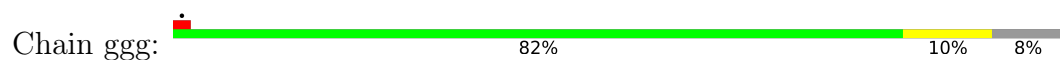
- Molecule 3: Capsid protein G8P



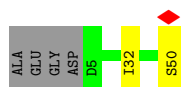
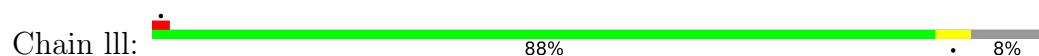
- Molecule 3: Capsid protein G8P



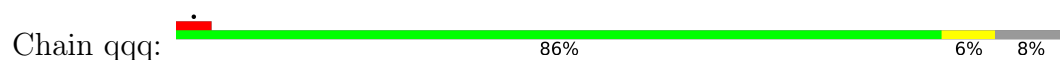
- Molecule 3: Capsid protein G8P



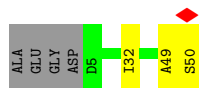
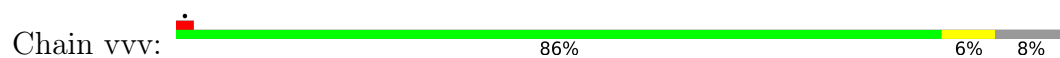
- Molecule 3: Capsid protein G8P



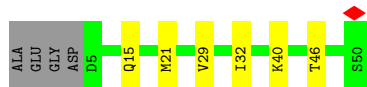
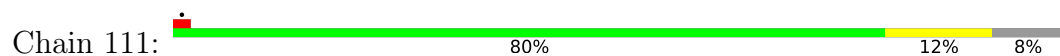
- Molecule 3: Capsid protein G8P



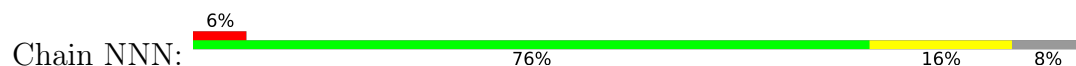
- Molecule 3: Capsid protein G8P

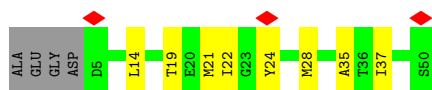


- Molecule 3: Capsid protein G8P

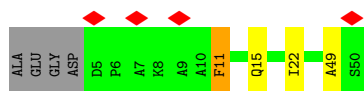
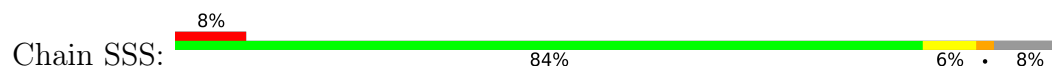


- Molecule 3: Capsid protein G8P

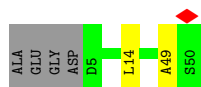




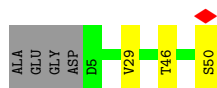
- Molecule 3: Capsid protein G8P



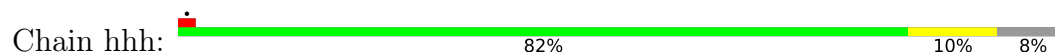
- Molecule 3: Capsid protein G8P



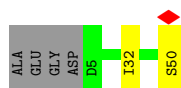
- Molecule 3: Capsid protein G8P



- Molecule 3: Capsid protein G8P



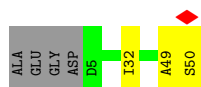
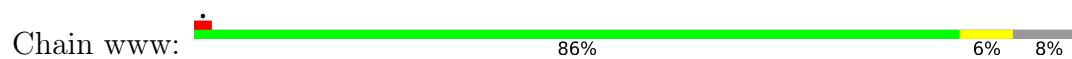
- Molecule 3: Capsid protein G8P



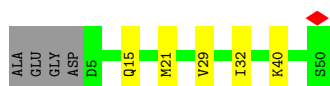
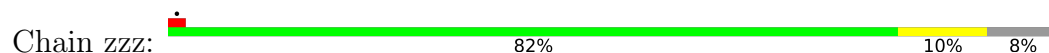
- Molecule 3: Capsid protein G8P



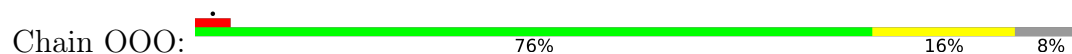
- Molecule 3: Capsid protein G8P



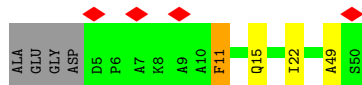
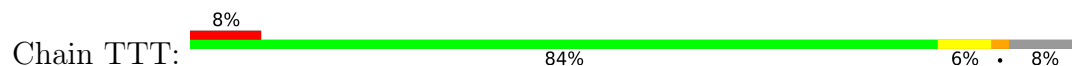
- Molecule 3: Capsid protein G8P



- Molecule 3: Capsid protein G8P



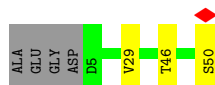
- Molecule 3: Capsid protein G8P



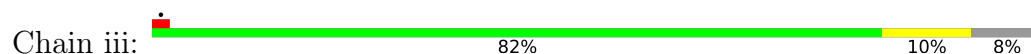
- Molecule 3: Capsid protein G8P



- Molecule 3: Capsid protein G8P

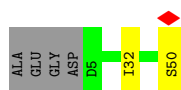


- Molecule 3: Capsid protein G8P



● Molecule 3: Capsid protein G8P

Chain nmh:  88% 8%



● Molecule 3: Capsid protein G8P

Chain sss:  88% 8%



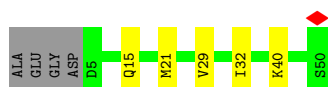
● Molecule 3: Capsid protein G8P

Chain xxx:  86% 6% 8%



● Molecule 3: Capsid protein G8P

Chain 333:  82% 10% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	255372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.838	Depositor
Minimum map value	-0.236	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	422.86078, 422.86078, 422.86078	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1012, 1.1012, 1.1012	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	AAA	0.46	0/214	1.18	0/288
1	BBB	0.46	0/214	1.18	0/288
1	CCC	0.46	0/214	1.18	0/288
1	DDD	0.45	0/214	1.18	0/288
1	EEE	0.46	0/214	1.18	0/288
2	FFF	0.48	0/261	1.13	0/352
2	GGG	0.48	0/261	1.13	0/352
2	HHH	0.47	0/261	1.13	0/352
2	III	0.47	0/261	1.13	0/352
2	JJJ	0.47	0/261	1.13	0/352
3	111	0.49	0/346	1.20	0/465
3	222	0.49	0/346	1.20	0/465
3	333	0.49	0/346	1.21	0/465
3	KKK	0.52	0/345	1.21	0/465
3	LLL	0.52	0/345	1.21	0/465
3	MMM	0.52	0/345	1.21	0/465
3	NNN	0.53	0/345	1.20	0/465
3	OOO	0.52	0/345	1.21	0/465
3	PPP	0.50	0/345	1.23	0/465
3	QQQ	0.49	0/345	1.23	0/465
3	RRR	0.50	0/345	1.23	0/465
3	SSS	0.49	0/345	1.23	0/465
3	TTT	0.50	0/345	1.23	0/465
3	UUU	0.51	0/345	1.21	0/465
3	VVV	0.51	0/345	1.21	0/465
3	WWW	0.50	0/345	1.21	0/465
3	XXX	0.51	0/345	1.21	0/465
3	YYY	0.50	0/345	1.21	0/465
3	ZZZ	0.51	0/346	1.19	0/465
3	aaa	0.51	0/346	1.19	0/465
3	bbb	0.51	0/346	1.19	0/465
3	ccc	0.51	0/346	1.18	0/465
3	ddd	0.51	0/346	1.19	0/465
3	eee	0.51	0/346	1.18	0/465

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	fff	0.50	0/346	1.19	0/465
3	ggg	0.51	0/346	1.18	0/465
3	hhh	0.51	0/346	1.18	0/465
3	iii	0.51	0/346	1.18	0/465
3	jjj	0.50	0/346	1.18	0/465
3	kkk	0.50	0/346	1.18	0/465
3	lll	0.50	0/346	1.18	0/465
3	mmm	0.50	0/346	1.18	0/465
3	nnn	0.50	0/346	1.17	0/465
3	ooo	0.49	0/346	1.17	0/465
3	ppp	0.48	0/346	1.16	0/465
3	qqq	0.49	0/346	1.17	0/465
3	rrr	0.49	0/346	1.16	0/465
3	sss	0.48	0/346	1.16	0/465
3	ttt	0.50	0/346	1.18	0/465
3	uuu	0.50	0/346	1.18	0/465
3	vvv	0.50	0/346	1.18	0/465
3	www	0.50	0/346	1.18	0/465
3	xxx	0.50	0/346	1.18	0/465
3	yyy	0.49	0/346	1.20	0/465
3	zzz	0.49	0/346	1.20	0/465
All	All	0.50	0/17930	1.19	0/24125

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	212	0	216	8	0
1	BBB	212	0	216	8	0
1	CCC	212	0	216	8	0
1	DDD	212	0	216	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EEE	212	0	216	8	0
2	FFF	255	0	256	1	0
2	GGG	255	0	256	1	0
2	HHH	255	0	256	1	0
2	III	255	0	256	1	0
2	JJJ	255	0	256	1	0
3	111	340	0	354	8	0
3	222	340	0	354	10	0
3	333	340	0	354	6	0
3	KKK	339	0	354	9	0
3	LLL	339	0	354	9	0
3	MMM	339	0	354	9	0
3	NNN	339	0	354	10	0
3	OOO	339	0	354	9	0
3	PPP	339	0	354	8	0
3	QQQ	339	0	354	8	0
3	RRR	339	0	354	8	0
3	SSS	339	0	354	8	0
3	TTT	339	0	354	8	0
3	UUU	339	0	354	3	0
3	VVV	339	0	354	4	0
3	WWW	339	0	354	4	0
3	XXX	339	0	354	4	0
3	YYY	339	0	354	4	0
3	ZZZ	340	0	354	4	0
3	aaa	340	0	354	4	0
3	bbb	340	0	354	4	0
3	ccc	340	0	354	4	0
3	ddd	340	0	354	4	0
3	eee	340	0	354	4	0
3	fff	340	0	354	4	0
3	ggg	340	0	354	5	0
3	hhh	340	0	354	5	0
3	iii	340	0	354	5	0
3	jjj	340	0	354	5	0
3	kkk	340	0	354	6	0
3	lll	340	0	354	6	0
3	mmm	340	0	354	6	0
3	nnn	340	0	354	6	0
3	ooo	340	0	354	4	0
3	ppp	340	0	354	4	0
3	qqq	340	0	354	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	rrr	340	0	354	2	0
3	sss	340	0	354	2	0
3	ttt	340	0	354	3	0
3	uuu	340	0	354	3	0
3	vvv	340	0	354	3	0
3	www	340	0	354	3	0
3	xxx	340	0	354	3	0
3	yyy	340	0	354	10	0
3	zzz	340	0	354	8	0
All	All	17620	0	18290	156	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 4.

All (156) 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)
3:jjj:50:SER:HA	3:333:40:LYS:NZ	1.83	0.93
3:zzz:40:LYS:NZ	3:nnn:50:SER:HA	1.84	0.93
3:111:40:LYS:NZ	3:mmm:50:SER:HA	1.83	0.92
3:yyy:40:LYS:NZ	3:kkk:50:SER:HA	1.84	0.92
3:222:40:LYS:NZ	3:lll:50:SER:HA	1.84	0.92
3:111:40:LYS:HZ1	3:mmm:50:SER:HA	1.35	0.88
3:QQQ:15:GLN:NE2	3:MMM:28:MET:SD	2.47	0.86
3:PPP:15:GLN:NE2	3:LLL:28:MET:SD	2.48	0.86
3:yyy:40:LYS:HZ1	3:kkk:50:SER:HA	1.34	0.85
3:zzz:40:LYS:HZ1	3:nnn:50:SER:HA	1.40	0.85
3:KKK:28:MET:SD	3:TTT:15:GLN:NE2	2.50	0.85
3:RRR:15:GLN:NE2	3:NNN:28:MET:SD	2.49	0.85
3:222:40:LYS:HZ1	3:lll:50:SER:HA	1.37	0.83
3:SSS:15:GLN:NE2	3:OOO:28:MET:SD	2.50	0.83
3:jjj:50:SER:HA	3:333:40:LYS:HZ1	1.46	0.81
3:RRR:22:ILE:HD12	3:NNN:35:ALA:HB2	1.65	0.78
3:SSS:22:ILE:HD12	3:OOO:35:ALA:HB2	1.66	0.78
3:KKK:35:ALA:HB2	3:TTT:22:ILE:HD12	1.66	0.77
1:AAA:10:ILE:HG23	1:EEE:14:MET:HE1	1.67	0.77
3:QQQ:22:ILE:HD12	3:MMM:35:ALA:HB2	1.66	0.76
1:CCC:14:MET:HE1	1:DDD:10:ILE:HG23	1.65	0.76
1:BBB:14:MET:HE1	1:CCC:10:ILE:HG23	1.67	0.76
3:PPP:22:ILE:HD12	3:LLL:35:ALA:HB2	1.66	0.76
1:AAA:14:MET:HE1	1:BBB:10:ILE:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:14:MET:HE1	1:EEE:10:ILE:HG23	1.67	0.74
3:ZZZ:50:SER:OXT	3:uuu:32:ILE:HD13	1.89	0.73
1:BBB:18:SER:OG	1:CCC:17:ILE:HD13	1.89	0.73
1:DDD:18:SER:OG	1:EEE:17:ILE:HD13	1.89	0.73
1:AAA:17:ILE:HD13	1:EEE:18:SER:OG	1.88	0.72
1:AAA:18:SER:OG	1:BBB:17:ILE:HD13	1.88	0.72
1:CCC:18:SER:OG	1:DDD:17:ILE:HD13	1.89	0.72
3:aaa:50:SER:OXT	3:vvv:32:ILE:HD13	1.89	0.72
3:ccc:50:SER:OXT	3:xxx:32:ILE:HD13	1.90	0.72
3:bbb:50:SER:OXT	3:www:32:ILE:HD13	1.90	0.71
3:kkk:50:SER:OXT	3:ppp:32:ILE:HD13	1.91	0.70
3:ttt:32:ILE:HD13	3:ddd:50:SER:OXT	1.91	0.70
3:lll:50:SER:OXT	3:qqq:32:ILE:HD13	1.91	0.70
3:nnn:50:SER:OXT	3:sss:32:ILE:HD13	1.92	0.70
3:mmm:50:SER:OXT	3:rrr:32:ILE:HD13	1.91	0.70
3:jjj:50:SER:OXT	3:ooo:32:ILE:HD13	1.92	0.69
3:yyy:32:ILE:HD13	3:uuu:50:SER:OXT	1.92	0.69
3:222:32:ILE:HD13	3:vvv:50:SER:OXT	1.92	0.69
3:ttt:50:SER:OXT	3:333:32:ILE:HD13	1.94	0.68
3:hhh:50:SER:OXT	3:mmm:32:ILE:HD13	1.94	0.68
3:iii:50:SER:OXT	3:nnn:32:ILE:HD13	1.94	0.68
3:111:32:ILE:HD13	3:www:50:SER:OXT	1.94	0.67
3:zzz:32:ILE:HD13	3:xxx:50:SER:OXT	1.94	0.67
3:fff:50:SER:OXT	3:kkk:32:ILE:HD13	1.95	0.67
3:eee:50:SER:OXT	3:jjj:32:ILE:HD13	1.95	0.67
3:RRR:22:ILE:HD12	3:NNN:35:ALA:CB	2.24	0.67
3:jjj:50:SER:HA	3:333:40:LYS:HZ2	1.57	0.66
3:ggg:50:SER:OXT	3:lll:32:ILE:HD13	1.96	0.66
3:KKK:35:ALA:CB	3:TTT:22:ILE:HD12	2.25	0.65
3:SSS:22:ILE:HD12	3:OOO:35:ALA:CB	2.26	0.65
3:PPP:22:ILE:HD12	3:LLL:35:ALA:CB	2.27	0.64
3:QQQ:22:ILE:HD12	3:MMM:35:ALA:CB	2.27	0.64
3:MMM:37:ILE:HG21	3:WWW:14:LEU:HD21	1.82	0.62
3:NNN:37:ILE:HG21	3:XXX:14:LEU:HD21	1.82	0.62
3:KKK:37:ILE:HG21	3:UUU:14:LEU:HD21	1.82	0.62
3:LLL:37:ILE:HG21	3:VVV:14:LEU:HD21	1.82	0.62
3:OOO:37:ILE:HG21	3:YYY:14:LEU:HD21	1.82	0.61
3:KKK:19:THR:O	3:KKK:22:ILE:HG22	2.01	0.61
3:LLL:19:THR:O	3:LLL:22:ILE:HG22	2.02	0.60
3:222:40:LYS:HZ2	3:lll:50:SER:HA	1.67	0.60
3:MMM:19:THR:O	3:MMM:22:ILE:HG22	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:OOO:19:THR:O	3:OOO:22:ILE:HG22	2.02	0.60
3:NNN:19:THR:O	3:NNN:22:ILE:HG22	2.02	0.59
3:zzz:40:LYS:HZ2	3:nnn:50:SER:HA	1.64	0.59
3:rrr:11:PHE:HE2	3:zzz:21:MET:HE2	1.68	0.57
3:qqq:11:PHE:HE2	3:111:21:MET:HE2	1.69	0.57
3:sss:11:PHE:HE2	3:333:21:MET:HE2	1.70	0.56
3:yyy:40:LYS:HZ2	3:kkk:50:SER:HA	1.70	0.55
3:eee:44:LYS:HE3	3:eee:48:LYS:HZ1	1.72	0.54
3:111:40:LYS:HZ1	3:mmm:50:SER:CA	2.15	0.53
3:iii:44:LYS:HE3	3:iii:48:LYS:HZ1	1.74	0.52
3:111:40:LYS:HZ2	3:mmm:50:SER:HA	1.69	0.51
3:yyy:40:LYS:HZ1	3:kkk:50:SER:CA	2.14	0.50
3:222:40:LYS:HZ1	3:lll:50:SER:CA	2.18	0.50
3:ooo:7:ALA:HB1	3:yyy:21:MET:HE3	1.93	0.50
3:hhh:44:LYS:HE3	3:hhh:48:LYS:HZ1	1.76	0.50
1:AAA:10:ILE:HG23	1:EEE:14:MET:CE	2.41	0.49
1:BBB:14:MET:CE	1:CCC:10:ILE:HG23	2.42	0.49
3:PPP:49:ALA:HA	3:ZZZ:29:VAL:HG22	1.95	0.48
3:ppp:7:ALA:HB1	3:222:21:MET:HE3	1.95	0.48
1:CCC:19:VAL:HG12	3:MMM:14:LEU:HD22	1.95	0.48
1:BBB:19:VAL:HG12	3:LLL:14:LEU:HD22	1.95	0.48
3:SSS:49:ALA:HA	3:ccc:29:VAL:HG22	1.96	0.48
1:AAA:19:VAL:HG12	3:KKK:14:LEU:HD22	1.94	0.48
3:QQQ:49:ALA:HA	3:aaa:29:VAL:HG22	1.96	0.48
3:TTT:49:ALA:HA	3:ddd:29:VAL:HG22	1.96	0.47
3:RRR:49:ALA:HA	3:bbb:29:VAL:HG22	1.96	0.47
1:EEE:19:VAL:HG12	3:OOO:14:LEU:HD22	1.95	0.47
1:DDD:19:VAL:HG12	3:NNN:14:LEU:HD22	1.96	0.47
3:SSS:11:PHE:CZ	3:OOO:24:TYR:HB3	2.49	0.47
3:KKK:37:ILE:HG22	3:UUU:14:LEU:HD11	1.97	0.47
1:CCC:14:MET:CE	1:DDD:10:ILE:HG23	2.40	0.47
3:KKK:24:TYR:HB3	3:TTT:11:PHE:CZ	2.49	0.47
3:RRR:11:PHE:CZ	3:NNN:24:TYR:HB3	2.50	0.47
3:222:29:VAL:HG22	3:vvv:49:ALA:HA	1.97	0.46
3:OOO:37:ILE:HG22	3:YYY:14:LEU:HD11	1.97	0.46
3:YYY:49:ALA:HA	3:iii:29:VAL:HG22	1.97	0.46
3:111:29:VAL:HG22	3:www:49:ALA:HA	1.97	0.46
3:PPP:49:ALA:HA	3:ZZZ:29:VAL:CG2	2.46	0.46
3:ttt:49:ALA:HA	3:333:29:VAL:HG22	1.97	0.46
1:DDD:14:MET:CE	1:EEE:10:ILE:HG23	2.41	0.46
3:MMM:37:ILE:HG22	3:WWW:14:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:UUU:49:ALA:HA	3:eee:29:VAL:HG22	1.98	0.46
3:SSS:49:ALA:HA	3:ccc:29:VAL:CG2	2.46	0.46
3:PPP:11:PHE:CZ	3:LLL:24:TYR:HB3	2.51	0.45
3:yyy:29:VAL:HG22	3:uuu:49:ALA:HA	1.97	0.45
3:zzz:29:VAL:HG22	3:xxx:49:ALA:HA	1.97	0.45
3:QQQ:11:PHE:CZ	3:MMM:24:TYR:HB3	2.51	0.45
3:VVV:49:ALA:HA	3:fff:29:VAL:HG22	1.97	0.45
3:QQQ:49:ALA:HA	3:aaa:29:VAL:CG2	2.47	0.45
3:XXX:49:ALA:HA	3:hhh:29:VAL:HG22	1.98	0.45
3:RRR:49:ALA:HA	3:bbb:29:VAL:CG2	2.47	0.45
3:NNN:37:ILE:HG22	3:XXX:14:LEU:HD11	1.98	0.45
1:AAA:14:MET:CE	1:BBB:10:ILE:HG23	2.42	0.45
3:WWW:49:ALA:HA	3:ggg:29:VAL:HG22	1.98	0.45
3:TTT:49:ALA:HA	3:ddd:29:VAL:CG2	2.47	0.45
3:LLL:37:ILE:HG22	3:VVV:14:LEU:HD11	1.98	0.45
2:GGG:15:TRP:HZ3	3:QQQ:11:PHE:CE2	2.35	0.44
3:ppp:11:PHE:HE2	3:222:21:MET:HE2	1.83	0.44
3:ooo:11:PHE:HE2	3:yyy:21:MET:HE2	1.82	0.44
3:ggg:44:LYS:HE3	3:ggg:48:LYS:HZ1	1.82	0.44
2:HHH:15:TRP:HZ3	3:RRR:11:PHE:CE2	2.36	0.44
2:III:15:TRP:HZ3	3:SSS:11:PHE:CE2	2.35	0.43
2:JJJ:15:TRP:HZ3	3:TTT:11:PHE:CE2	2.36	0.43
3:NNN:22:ILE:HD12	3:NNN:22:ILE:HA	1.92	0.43
3:yyy:40:LYS:HB3	3:yyy:40:LYS:HE2	1.79	0.43
3:zzz:40:LYS:HZ1	3:nnn:50:SER:CA	2.20	0.43
3:222:40:LYS:HB3	3:222:40:LYS:HE2	1.79	0.43
2:FFF:15:TRP:HZ3	3:PPP:11:PHE:CE2	2.36	0.43
1:CCC:19:VAL:CG1	3:MMM:14:LEU:HD22	2.50	0.42
1:BBB:19:VAL:CG1	3:LLL:14:LEU:HD22	2.50	0.41
1:AAA:19:VAL:CG1	3:KKK:14:LEU:HD22	2.50	0.41
1:DDD:19:VAL:CG1	3:NNN:14:LEU:HD22	2.50	0.41
3:zzz:40:LYS:HB3	3:zzz:40:LYS:HE2	1.78	0.41
3:QQQ:15:GLN:NE2	3:QQQ:15:GLN:HA	2.36	0.41
3:VVV:49:ALA:HA	3:fff:29:VAL:CG2	2.51	0.41
3:bbb:46:THR:HG22	3:ggg:37:ILE:HG13	2.03	0.41
3:aaa:46:THR:HG22	3:fff:37:ILE:HG13	2.03	0.41
3:qqq:37:ILE:HG13	3:111:46:THR:HG22	2.03	0.41
3:ZZZ:46:THR:HG22	3:eee:37:ILE:HG13	2.03	0.41
3:XXX:49:ALA:HA	3:hhh:29:VAL:CG2	2.51	0.41
3:ccc:46:THR:HG22	3:hhh:37:ILE:HG13	2.03	0.41
3:YYY:49:ALA:HA	3:iii:29:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:ppp:37:ILE:HG13	3:222:46:THR:HG22	2.03	0.41
3:RRR:15:GLN:NE2	3:RRR:15:GLN:HA	2.36	0.41
3:SSS:15:GLN:NE2	3:SSS:15:GLN:HA	2.36	0.41
1:EEE:19:VAL:CG1	3:OOO:14:LEU:HD22	2.51	0.41
3:TTT:15:GLN:NE2	3:TTT:15:GLN:HA	2.36	0.41
3:ddd:46:THR:HG22	3:iii:37:ILE:HG13	2.03	0.41
3:ooo:37:ILE:HG13	3:yyy:46:THR:HG22	2.03	0.40
3:WWW:49:ALA:HA	3:ggg:29:VAL:CG2	2.51	0.40
3:PPP:15:GLN:NE2	3:PPP:15:GLN:HA	2.36	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	AAA	26/33 (79%)	26 (100%)	0	0	100	100
1	BBB	26/33 (79%)	26 (100%)	0	0	100	100
1	CCC	26/33 (79%)	26 (100%)	0	0	100	100
1	DDD	26/33 (79%)	26 (100%)	0	0	100	100
1	EEE	26/33 (79%)	26 (100%)	0	0	100	100
2	FFF	30/32 (94%)	30 (100%)	0	0	100	100
2	GGG	30/32 (94%)	30 (100%)	0	0	100	100
2	HHH	30/32 (94%)	30 (100%)	0	0	100	100
2	III	30/32 (94%)	30 (100%)	0	0	100	100
2	JJJ	30/32 (94%)	30 (100%)	0	0	100	100
3	111	44/50 (88%)	44 (100%)	0	0	100	100
3	222	44/50 (88%)	44 (100%)	0	0	100	100
3	333	44/50 (88%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	KKK	44/50 (88%)	44 (100%)	0	0	100	100
3	LLL	44/50 (88%)	44 (100%)	0	0	100	100
3	MMM	44/50 (88%)	44 (100%)	0	0	100	100
3	NNN	44/50 (88%)	44 (100%)	0	0	100	100
3	OOO	44/50 (88%)	44 (100%)	0	0	100	100
3	PPP	44/50 (88%)	44 (100%)	0	0	100	100
3	QQQ	44/50 (88%)	44 (100%)	0	0	100	100
3	RRR	44/50 (88%)	44 (100%)	0	0	100	100
3	SSS	44/50 (88%)	44 (100%)	0	0	100	100
3	TTT	44/50 (88%)	44 (100%)	0	0	100	100
3	UUU	44/50 (88%)	44 (100%)	0	0	100	100
3	VVV	44/50 (88%)	44 (100%)	0	0	100	100
3	WWW	44/50 (88%)	44 (100%)	0	0	100	100
3	XXX	44/50 (88%)	44 (100%)	0	0	100	100
3	YYY	44/50 (88%)	44 (100%)	0	0	100	100
3	ZZZ	44/50 (88%)	44 (100%)	0	0	100	100
3	aaa	44/50 (88%)	44 (100%)	0	0	100	100
3	bbb	44/50 (88%)	44 (100%)	0	0	100	100
3	ccc	44/50 (88%)	44 (100%)	0	0	100	100
3	ddd	44/50 (88%)	44 (100%)	0	0	100	100
3	eee	44/50 (88%)	44 (100%)	0	0	100	100
3	fff	44/50 (88%)	44 (100%)	0	0	100	100
3	ggg	44/50 (88%)	44 (100%)	0	0	100	100
3	hhh	44/50 (88%)	44 (100%)	0	0	100	100
3	iii	44/50 (88%)	44 (100%)	0	0	100	100
3	jjj	44/50 (88%)	44 (100%)	0	0	100	100
3	kkk	44/50 (88%)	44 (100%)	0	0	100	100
3	lll	44/50 (88%)	44 (100%)	0	0	100	100
3	mmm	44/50 (88%)	44 (100%)	0	0	100	100
3	nnn	44/50 (88%)	44 (100%)	0	0	100	100
3	ooo	44/50 (88%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	ppp	44/50 (88%)	44 (100%)	0	0	100	100
3	qqq	44/50 (88%)	44 (100%)	0	0	100	100
3	rrr	44/50 (88%)	44 (100%)	0	0	100	100
3	sss	44/50 (88%)	44 (100%)	0	0	100	100
3	ttt	44/50 (88%)	44 (100%)	0	0	100	100
3	uuu	44/50 (88%)	44 (100%)	0	0	100	100
3	vvv	44/50 (88%)	44 (100%)	0	0	100	100
3	www	44/50 (88%)	44 (100%)	0	0	100	100
3	xxx	44/50 (88%)	44 (100%)	0	0	100	100
3	yyy	44/50 (88%)	44 (100%)	0	0	100	100
3	zzz	44/50 (88%)	44 (100%)	0	0	100	100
All	All	2260/2575 (88%)	2260 (100%)	0	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	AAA	22/26 (85%)	21 (96%)	1 (4%)	24	57
1	BBB	22/26 (85%)	21 (96%)	1 (4%)	24	57
1	CCC	22/26 (85%)	21 (96%)	1 (4%)	24	57
1	DDD	22/26 (85%)	21 (96%)	1 (4%)	24	57
1	EEE	22/26 (85%)	21 (96%)	1 (4%)	24	57
2	FFF	29/29 (100%)	29 (100%)	0	100	100
2	GGG	29/29 (100%)	29 (100%)	0	100	100
2	HHH	29/29 (100%)	29 (100%)	0	100	100
2	III	29/29 (100%)	29 (100%)	0	100	100
2	JJJ	29/29 (100%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	111	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	222	34/36 (94%)	34 (100%)	0	100	100
3	333	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	KKK	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	LLL	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	MMM	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	NNN	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	OOO	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	PPP	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	QQQ	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	RRR	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	SSS	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	TTT	34/36 (94%)	33 (97%)	1 (3%)	37	71
3	UUU	34/36 (94%)	34 (100%)	0	100	100
3	VVV	34/36 (94%)	34 (100%)	0	100	100
3	WWW	34/36 (94%)	34 (100%)	0	100	100
3	XXX	34/36 (94%)	34 (100%)	0	100	100
3	YYY	34/36 (94%)	34 (100%)	0	100	100
3	ZZZ	34/36 (94%)	34 (100%)	0	100	100
3	aaa	34/36 (94%)	34 (100%)	0	100	100
3	bbb	34/36 (94%)	34 (100%)	0	100	100
3	ccc	34/36 (94%)	34 (100%)	0	100	100
3	ddd	34/36 (94%)	34 (100%)	0	100	100
3	eee	34/36 (94%)	34 (100%)	0	100	100
3	fff	34/36 (94%)	34 (100%)	0	100	100
3	ggg	34/36 (94%)	34 (100%)	0	100	100
3	hhh	34/36 (94%)	34 (100%)	0	100	100
3	iii	34/36 (94%)	34 (100%)	0	100	100
3	jjj	34/36 (94%)	34 (100%)	0	100	100
3	kkk	34/36 (94%)	34 (100%)	0	100	100
3	lll	34/36 (94%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	mmm	34/36 (94%)	34 (100%)	0	100	100
3	nnn	34/36 (94%)	34 (100%)	0	100	100
3	ooo	34/36 (94%)	34 (100%)	0	100	100
3	ppp	34/36 (94%)	34 (100%)	0	100	100
3	qqq	34/36 (94%)	34 (100%)	0	100	100
3	rrr	34/36 (94%)	34 (100%)	0	100	100
3	sss	34/36 (94%)	34 (100%)	0	100	100
3	ttt	34/36 (94%)	34 (100%)	0	100	100
3	uuu	34/36 (94%)	34 (100%)	0	100	100
3	vvv	34/36 (94%)	34 (100%)	0	100	100
3	www	34/36 (94%)	34 (100%)	0	100	100
3	xxx	34/36 (94%)	34 (100%)	0	100	100
3	yyy	34/36 (94%)	34 (100%)	0	100	100
3	zzz	34/36 (94%)	33 (97%)	1 (3%)	37	71
All	All	1785/1895 (94%)	1767 (99%)	18 (1%)	65	88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	33	ARG
3	KKK	21	MET
3	PPP	11	PHE
1	BBB	33	ARG
3	LLL	21	MET
3	QQQ	11	PHE
1	CCC	33	ARG
3	MMM	21	MET
3	RRR	11	PHE
3	111	15	GLN
1	DDD	33	ARG
3	NNN	21	MET
3	SSS	11	PHE
3	zzz	15	GLN
1	EEE	33	ARG
3	OOO	21	MET
3	TTT	11	PHE
3	333	15	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

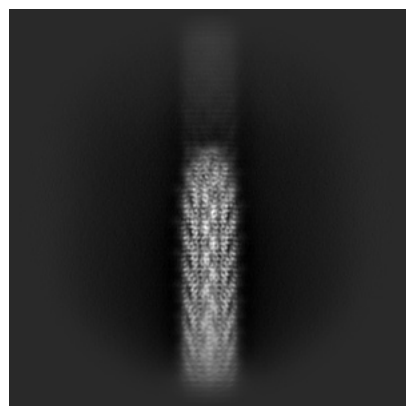
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15832. These allow visual inspection of the internal detail of the map and identification of artifacts.

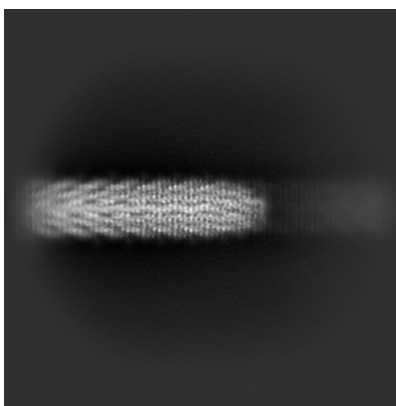
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

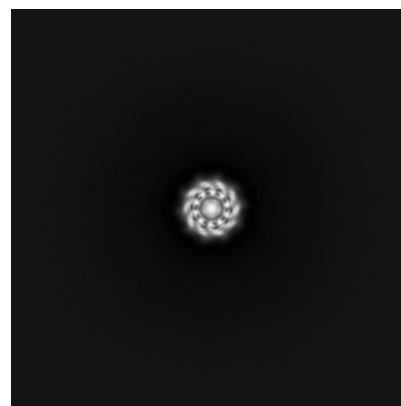
6.1.1 Primary map



X

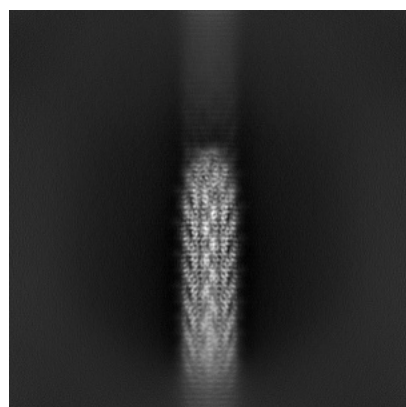


Y

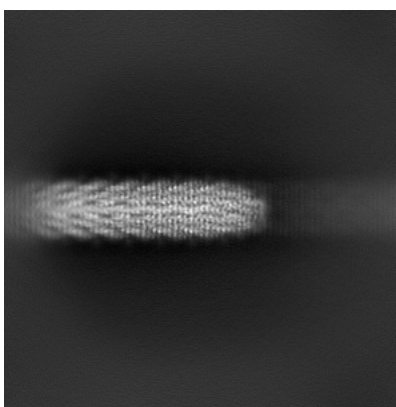


Z

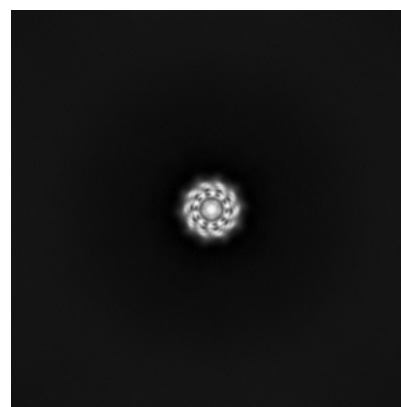
6.1.2 Raw map



X



Y

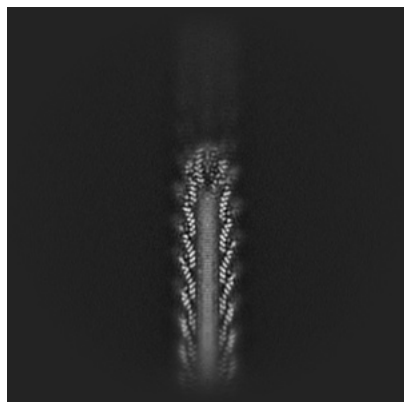


Z

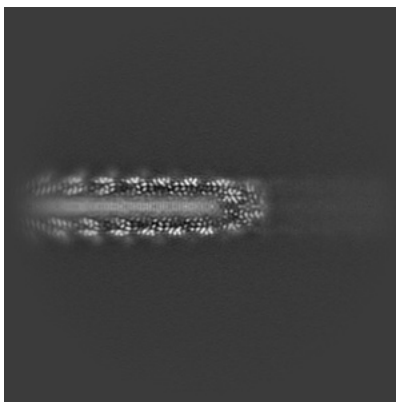
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

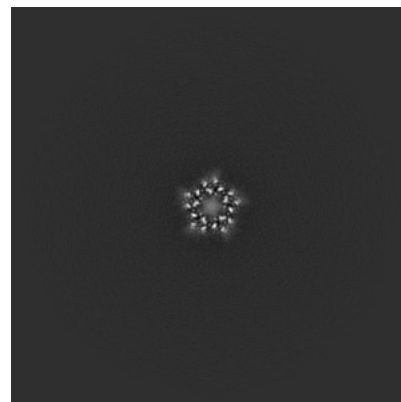
6.2.1 Primary map



X Index: 192

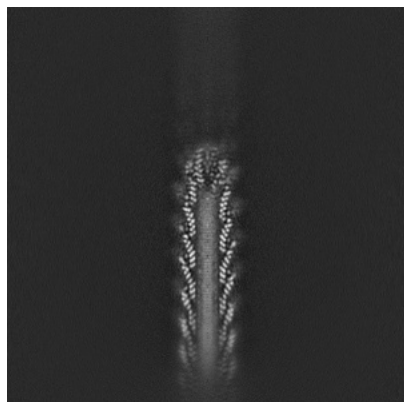


Y Index: 192

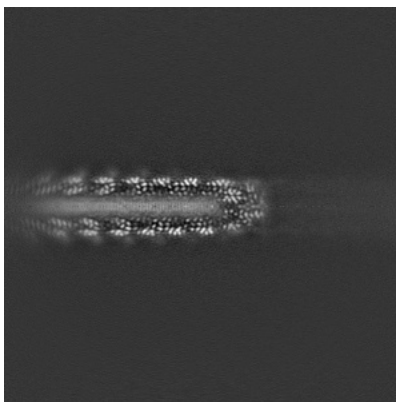


Z Index: 192

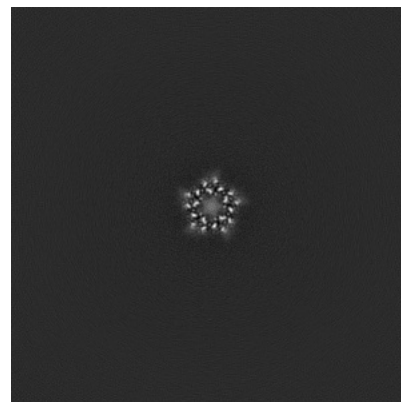
6.2.2 Raw map



X Index: 192



Y Index: 192

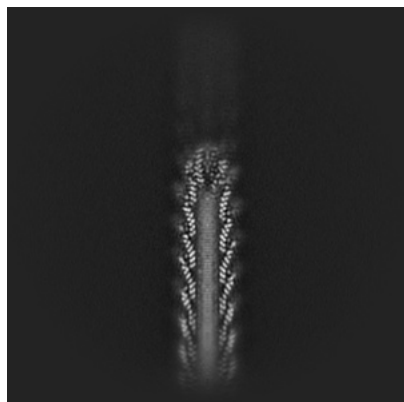


Z Index: 192

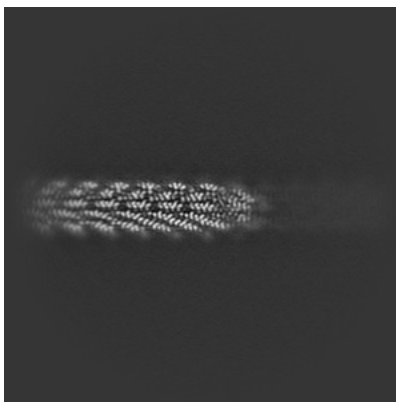
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

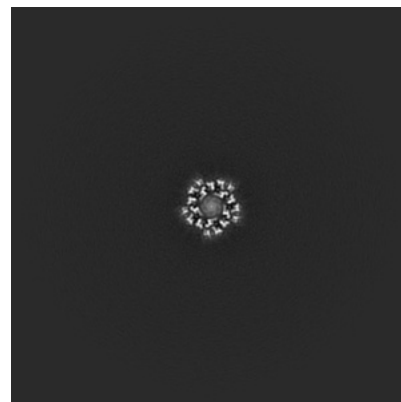
6.3.1 Primary map



X Index: 192

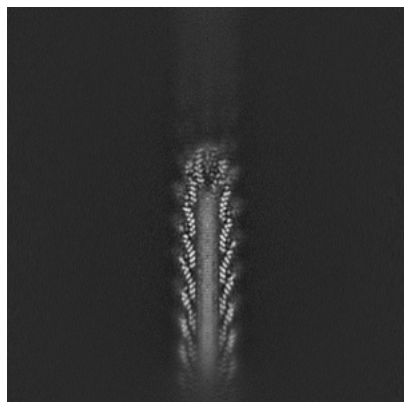


Y Index: 207

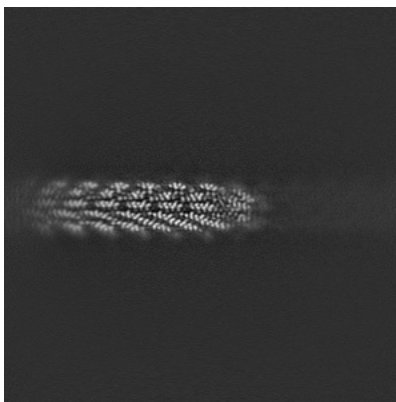


Z Index: 174

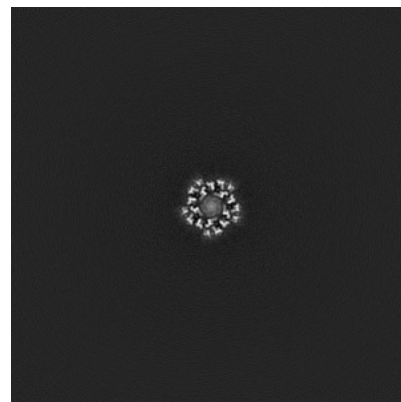
6.3.2 Raw map



X Index: 192



Y Index: 207

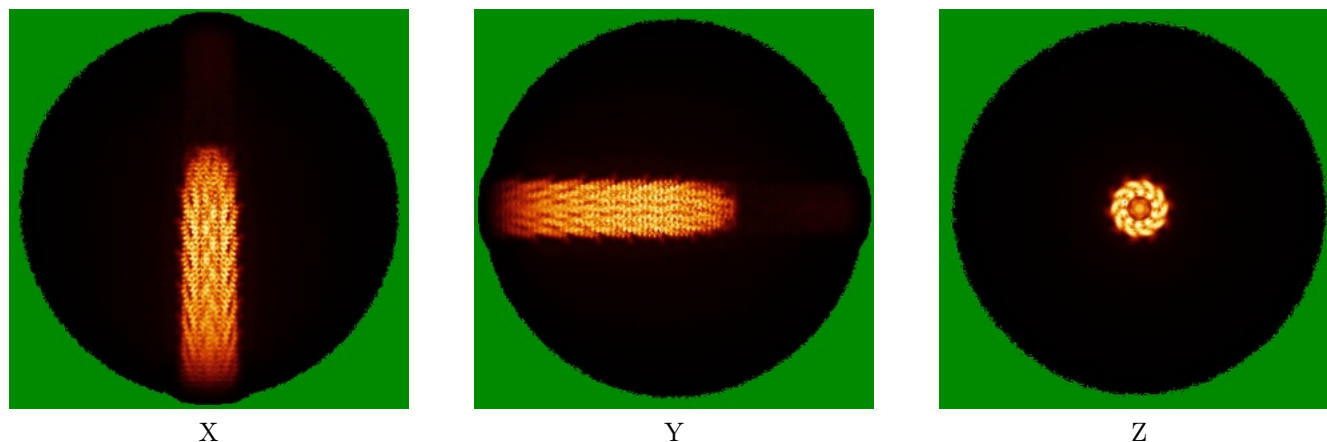


Z Index: 174

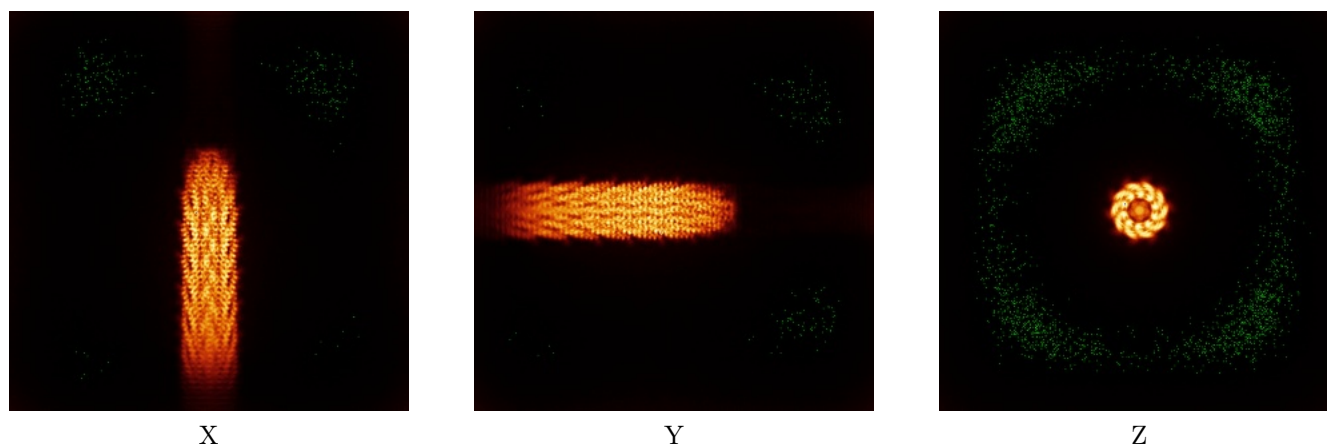
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



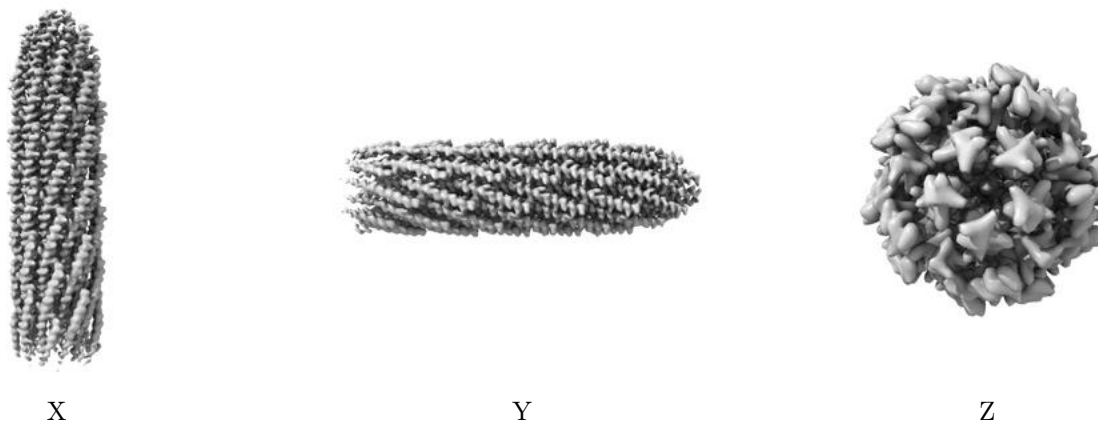
6.4.2 Raw map



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.

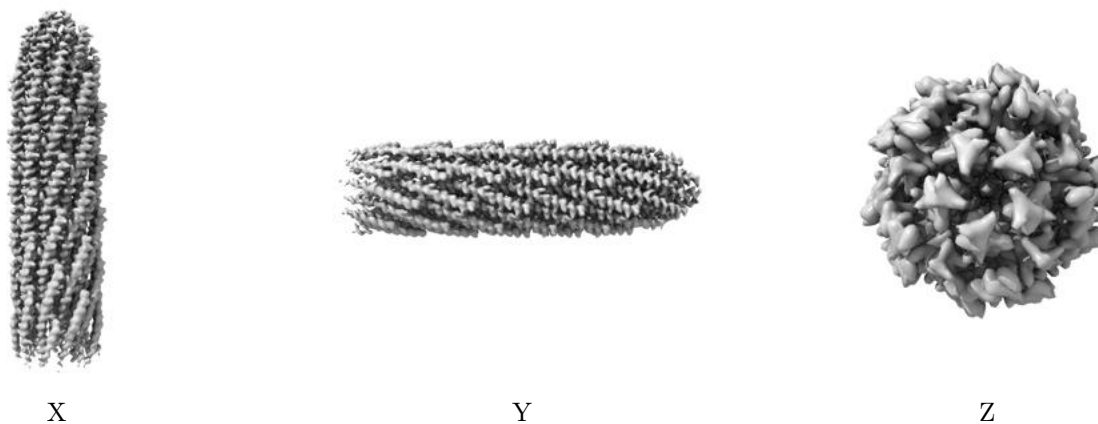
6.5 Orthogonal surface views [i](#)

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.

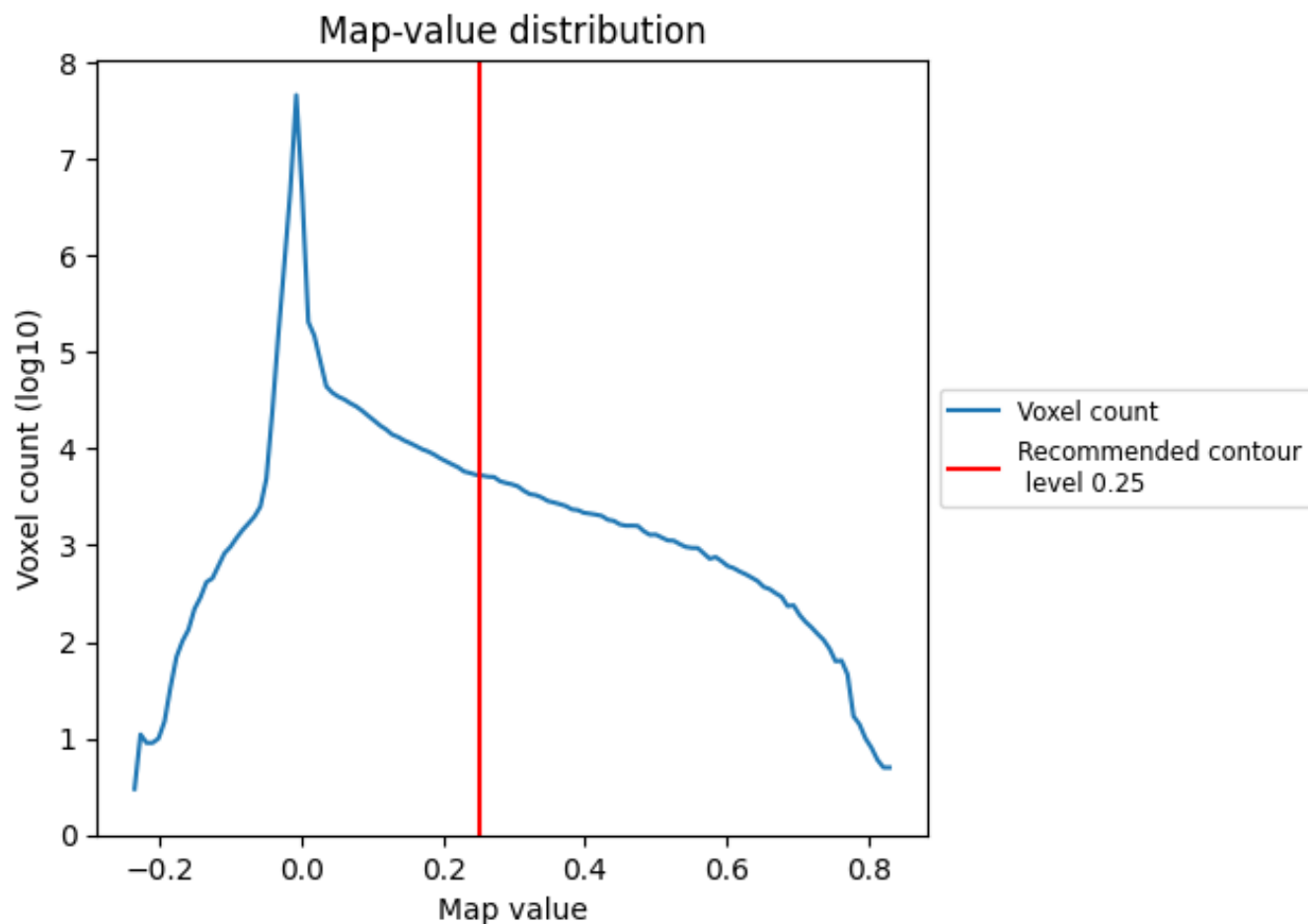
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

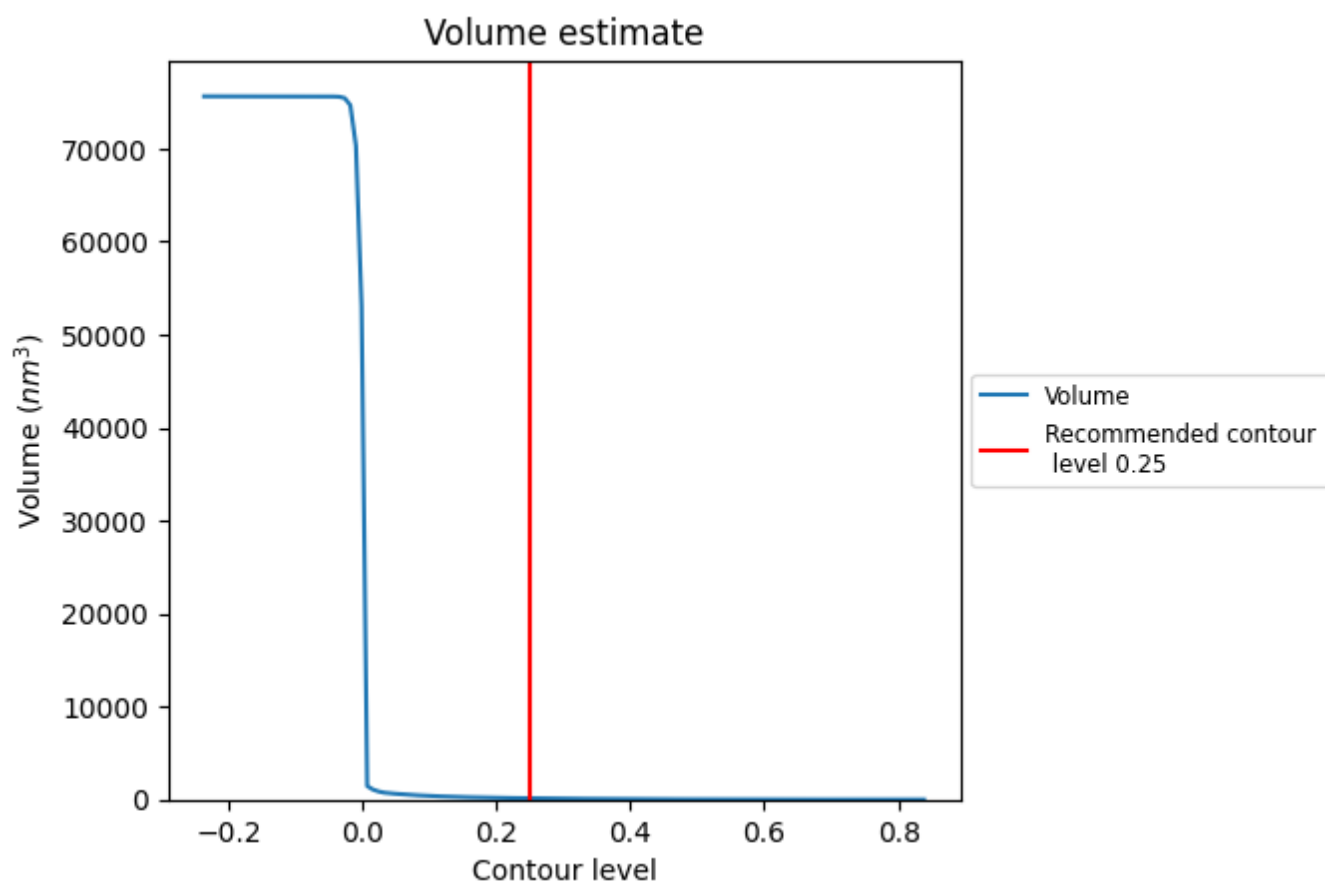
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

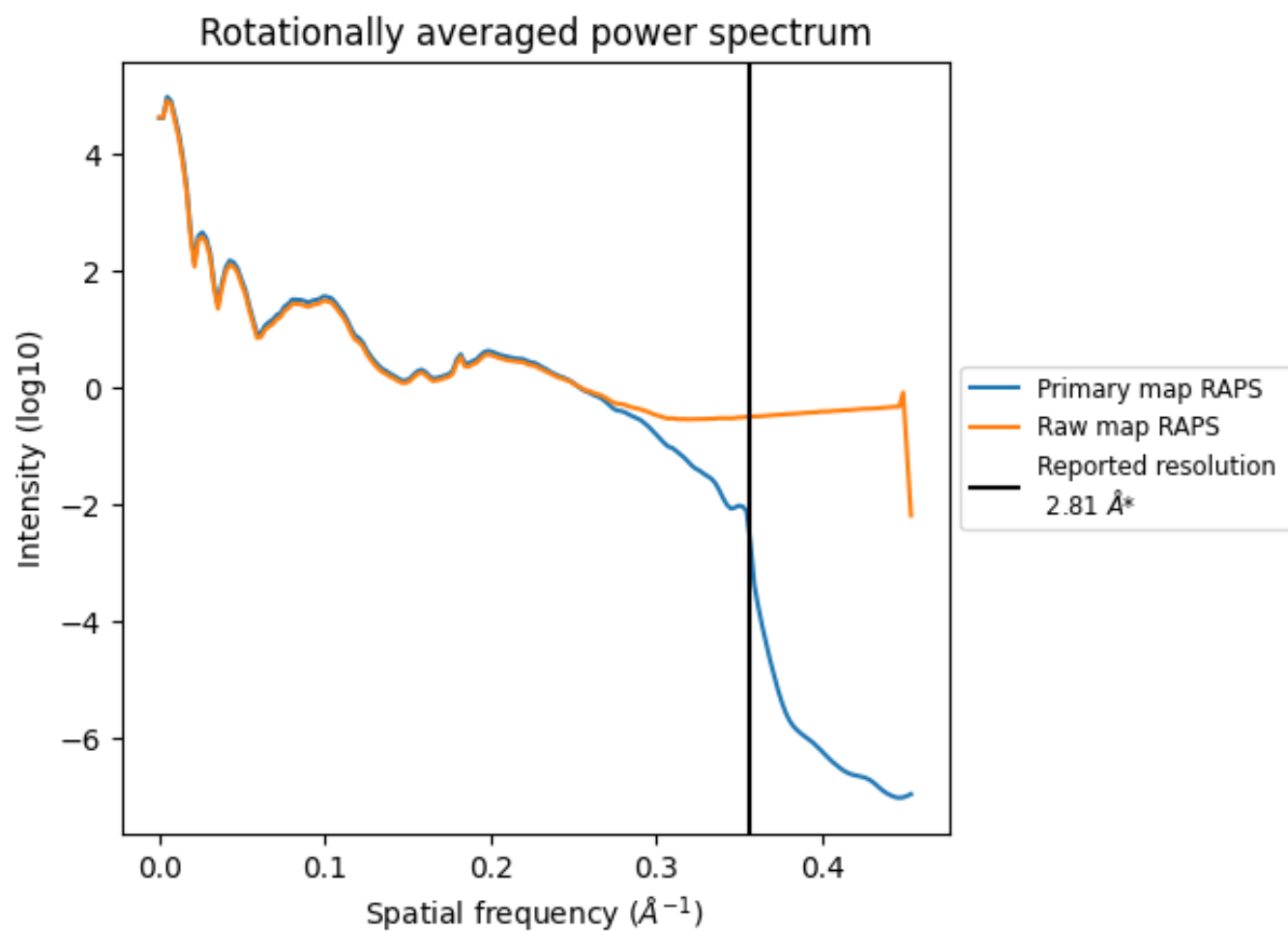
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 125 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 ⓘ

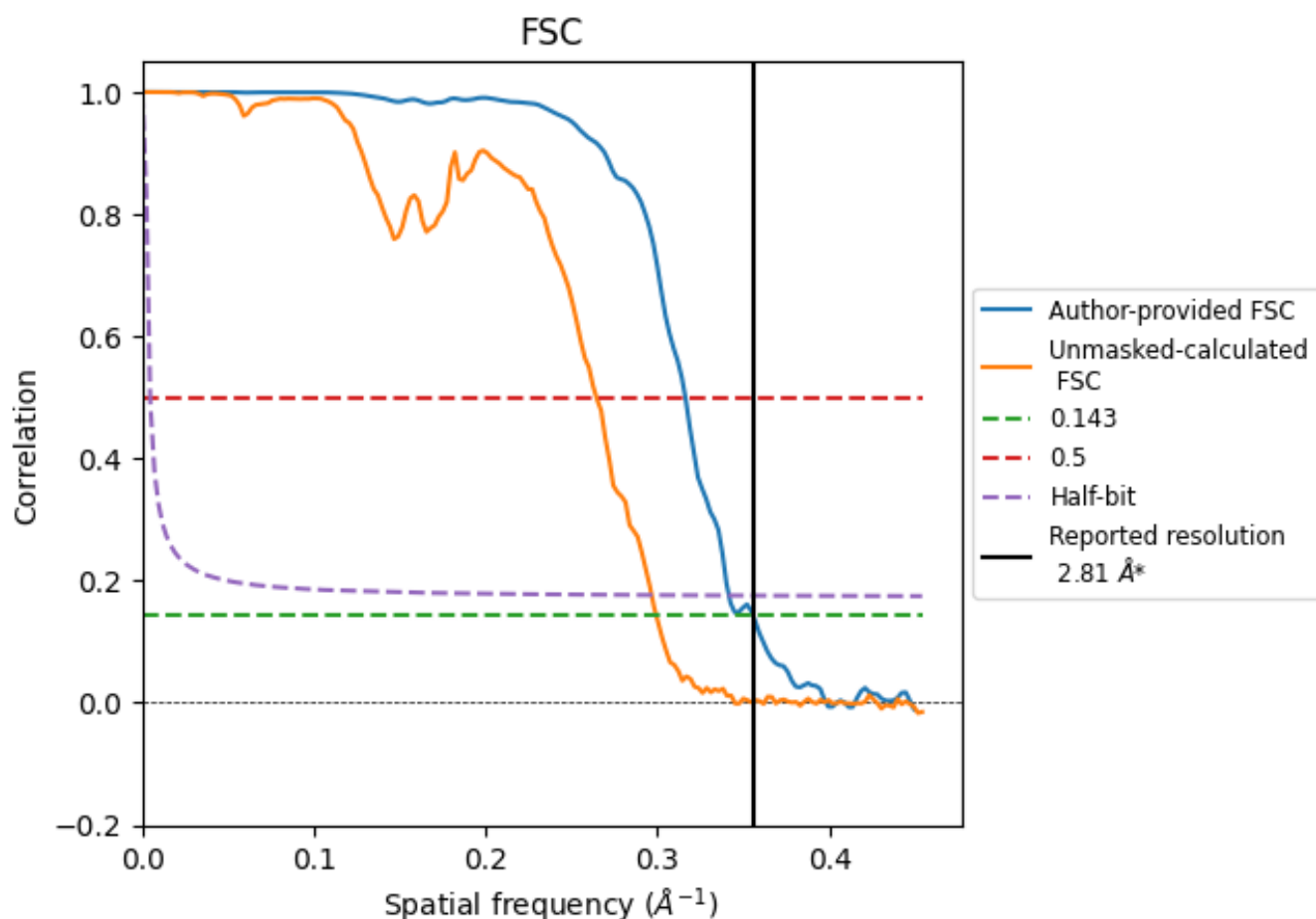


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

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 $0.356 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

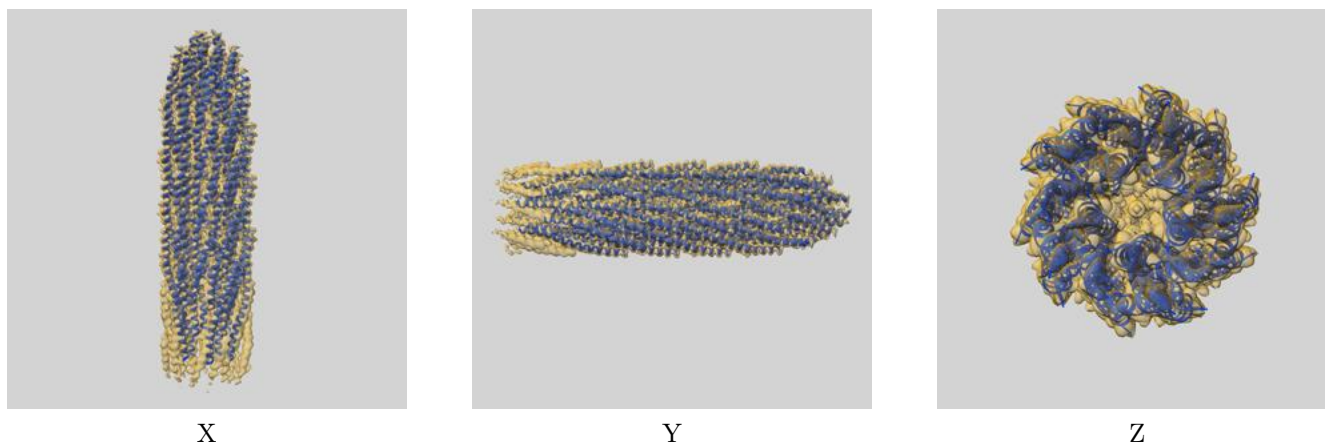
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.16	2.93
Unmasked-calculated*	3.34	3.78	3.37

*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 3.34 differs from the reported value 2.81 by more than 10 %

9 Map-model fit [i](#)

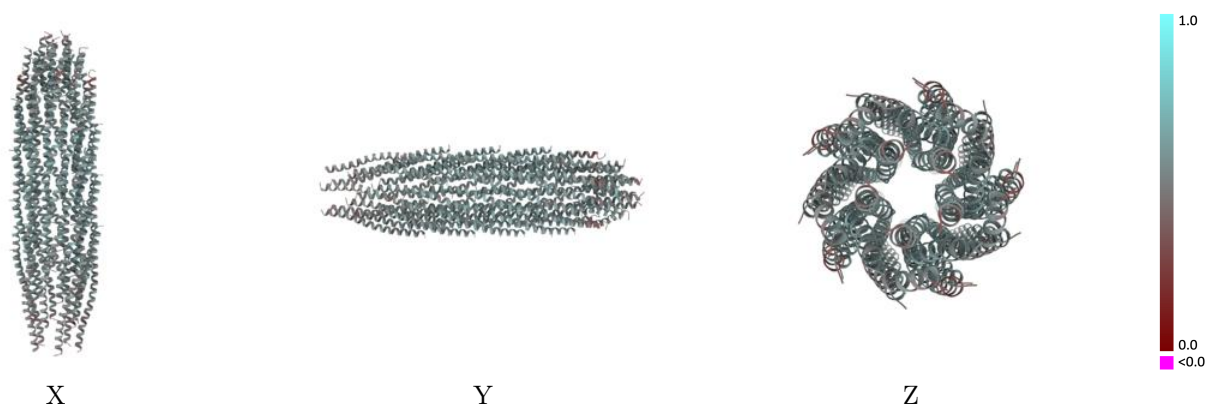
This section contains information regarding the fit between EMDB map EMD-15832 and PDB model 8B3P. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



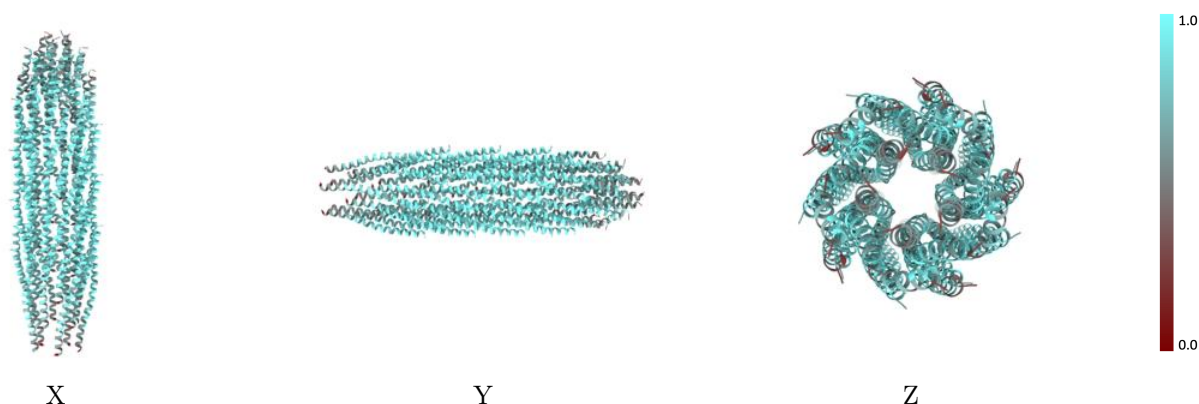
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



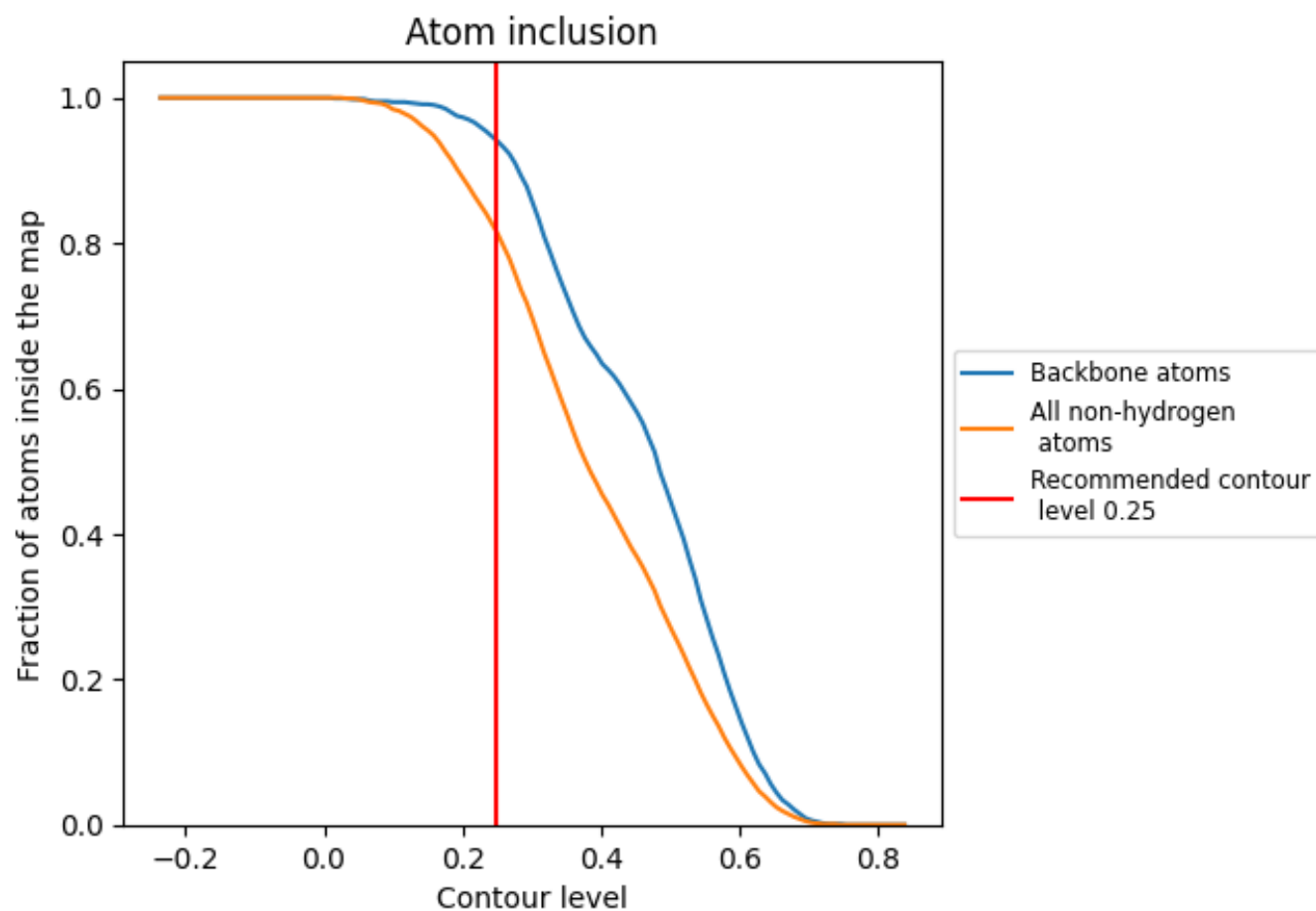
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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	 0.8150	 0.5340
111	 0.7720	 0.5080
222	 0.7690	 0.5090
333	 0.7750	 0.5100
AAA	 0.6790	 0.5250
BBB	 0.6840	 0.5300
CCC	 0.6700	 0.5250
DDD	 0.6700	 0.5220
EEE	 0.6650	 0.5230
FFF	 0.8150	 0.5540
GGG	 0.8190	 0.5510
HHH	 0.8060	 0.5570
III	 0.8230	 0.5600
JJJ	 0.8150	 0.5590
KKK	 0.7480	 0.5200
LLL	 0.7450	 0.5160
MMM	 0.7480	 0.5140
NNN	 0.7360	 0.5210
OOO	 0.7480	 0.5210
PPP	 0.8100	 0.5240
QQQ	 0.8010	 0.5220
RRR	 0.8130	 0.5240
SSS	 0.8130	 0.5240
TTT	 0.8070	 0.5250
UUU	 0.8840	 0.5520
VVV	 0.8840	 0.5540
WWW	 0.8840	 0.5520
XXX	 0.8690	 0.5520
YYY	 0.8810	 0.5530
ZZZ	 0.8900	 0.5610
aaa	 0.8930	 0.5610
bbb	 0.8820	 0.5590
ccc	 0.8930	 0.5610
ddd	 0.8900	 0.5620
eee	 0.8820	 0.5580



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Chain	Atom inclusion	Q-score
fff	 0.8790	 0.5560
ggg	 0.8790	 0.5560
hhh	 0.8850	 0.5570
iii	 0.8850	 0.5570
jjj	 0.8400	 0.5380
kkk	 0.8370	 0.5370
lll	 0.8400	 0.5350
mmm	 0.8310	 0.5360
nnn	 0.8400	 0.5380
ooo	 0.7400	 0.4890
ppp	 0.7370	 0.4850
qqq	 0.7310	 0.4820
rrr	 0.7250	 0.4850
sss	 0.7310	 0.4860
ttt	 0.8670	 0.5540
uuu	 0.8730	 0.5490
vvv	 0.8640	 0.5510
www	 0.8640	 0.5520
xxx	 0.8670	 0.5530
yyy	 0.7780	 0.5070
zzz	 0.7750	 0.5070