



## wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:55 PM UTC

PDB ID : 9DCC / pdb\_00009dcc  
EMDB ID : EMD-46749  
Title : The Structure of AAV5 at 55 Degrees Celsius  
Authors : Bennett, A.B.; McKenna, R.  
Deposited on : 2024-08-25  
Resolution : 3.12 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](mailto: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>.

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

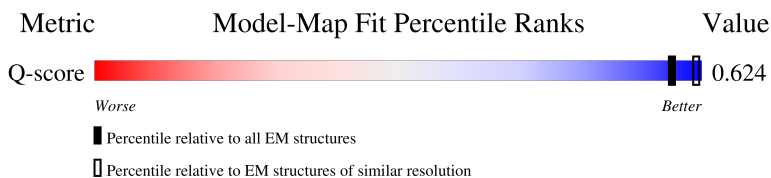
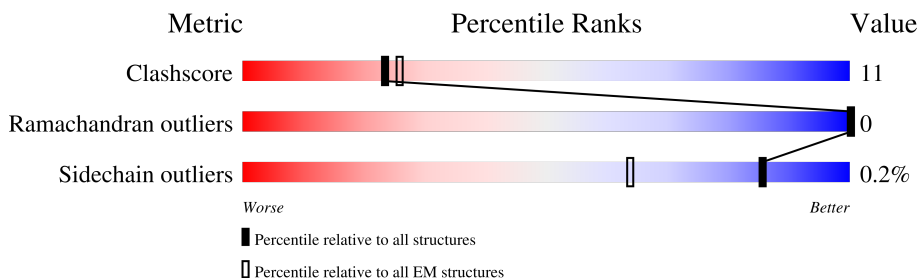
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.12 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.






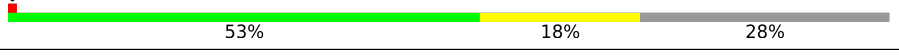
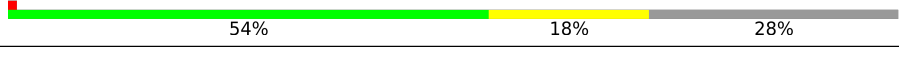



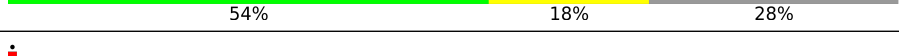
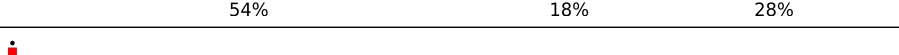
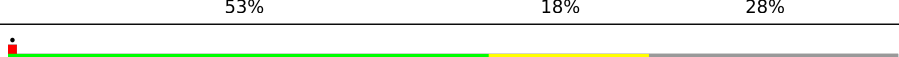
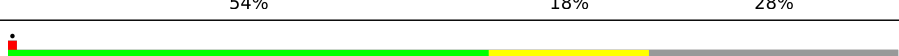

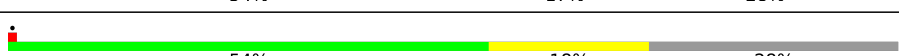
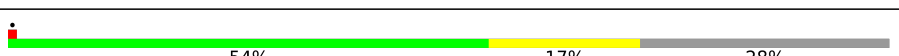
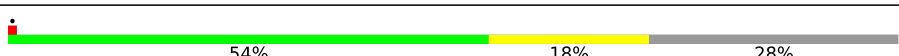





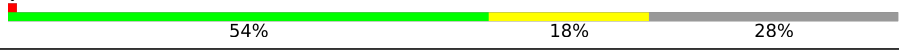

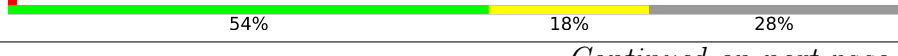

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14478 ( 2.62 - 3.62 )

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  $\geq 3$ , 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	1	724	<p>53% 18% 28%</p>
1	2	724	<p>54% 18% 28%</p>
1	3	724	<p>53% 18% 28%</p>
1	4	724	<p>54% 18% 28%</p>







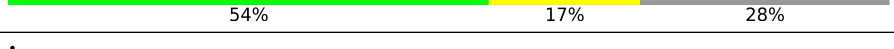
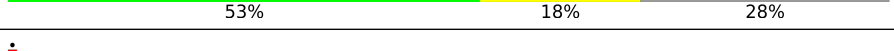
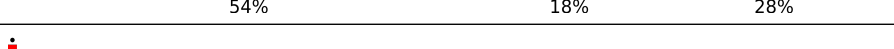
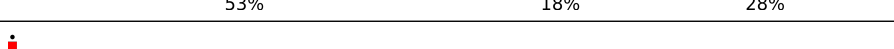
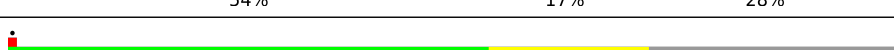

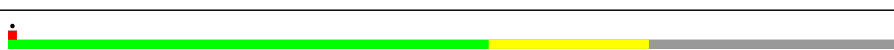

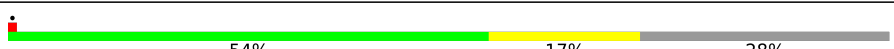





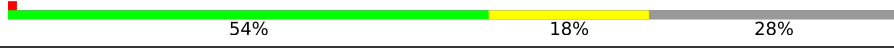
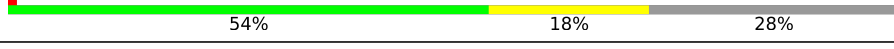



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Mol	Chain	Length	Quality of chain
1	5	724	 54% 18% 28%
1	6	724	 54% 17% 28%
1	7	724	 54% 17% 28%
1	8	724	 53% 18% 28%
1	A	724	 54% 18% 28%
1	B	724	 53% 18% 28%
1	C	724	 54% 18% 28%
1	D	724	 54% 18% 28%
1	E	724	 54% 18% 28%
1	F	724	 54% 18% 28%
1	G	724	 53% 18% 28%
1	H	724	 54% 18% 28%
1	I	724	 54% 18% 28%
1	J	724	 54% 17% 28%
1	K	724	 54% 18% 28%
1	L	724	 54% 17% 28%
1	M	724	 54% 18% 28%
1	N	724	 54% 18% 28%
1	O	724	 54% 17% 28%
1	P	724	 54% 17% 28%
1	Q	724	 54% 18% 28%
1	R	724	 54% 18% 28%
1	S	724	 54% 18% 28%
1	T	724	 54% 17% 28%
1	U	724	 54% 18% 28%







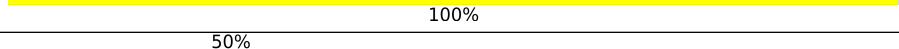
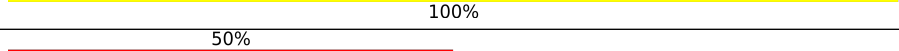
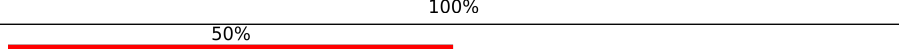
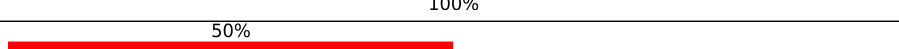
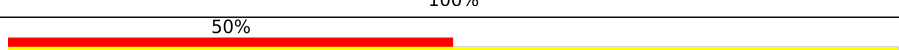
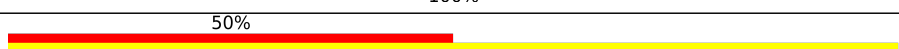
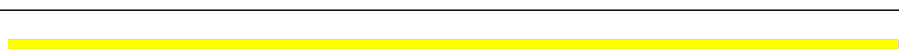
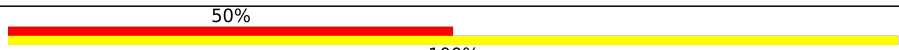
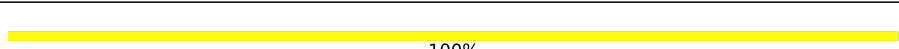


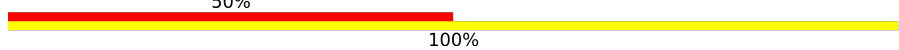
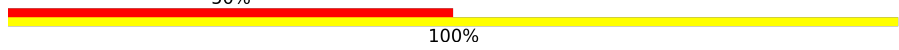

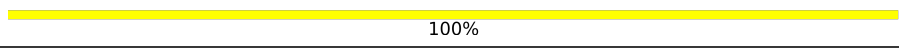
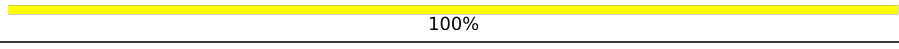
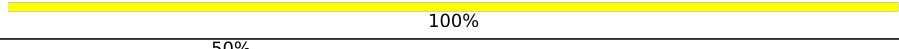
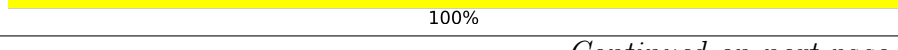

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Mol	Chain	Length	Quality of chain
1	V	724	 53% 18% 28%
1	W	724	 54% 17% 28%
1	X	724	 54% 18% 28%
1	Y	724	 54% 17% 28%
1	Z	724	 53% 18% 28%
1	a	724	 54% 17% 28%
1	b	724	 54% 17% 28%
1	c	724	 53% 18% 28%
1	d	724	 54% 18% 28%
1	e	724	 53% 18% 28%
1	f	724	 54% 17% 28%
1	g	724	 54% 18% 28%
1	h	724	 54% 18% 28%
1	i	724	 54% 18% 28%
1	j	724	 54% 17% 28%
1	k	724	 54% 17% 28%
1	l	724	 54% 17% 28%
1	m	724	 54% 17% 28%
1	n	724	 54% 17% 28%
1	o	724	 54% 18% 28%
1	p	724	 53% 18% 28%
1	q	724	 54% 18% 28%
1	r	724	 54% 18% 28%
1	s	724	 54% 17% 28%
1	t	724	 53% 18% 28%

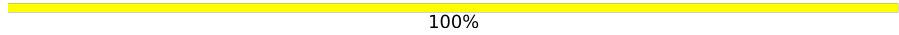



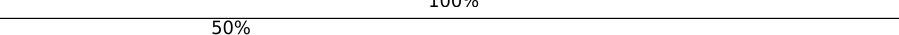
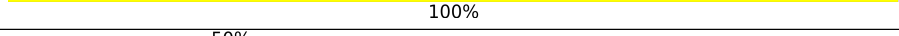
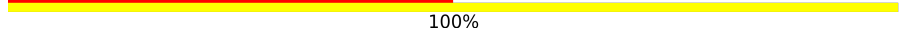



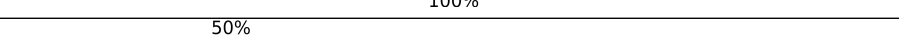
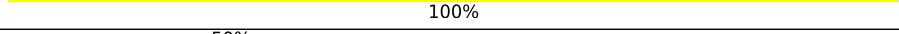
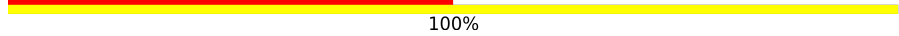



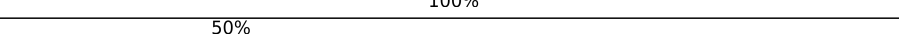
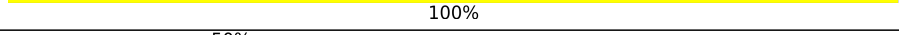
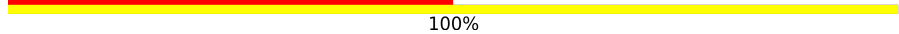



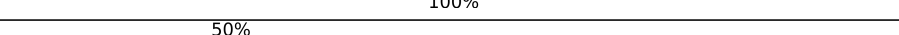
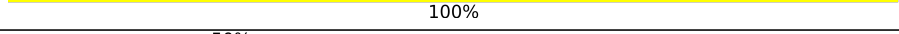
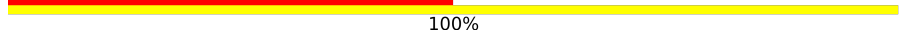
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Mol	Chain	Length	Quality of chain
1	u	724	 54% 18% 28%
1	v	724	 54% 18% 28%
1	w	724	 54% 18% 28%
1	x	724	 54% 17% 28%
1	y	724	 53% 18% 28%
1	z	724	 54% 17% 28%
2	0	2	 50% 100%
2	0A	2	 50% 100%
2	1A	2	 50% 100%
2	2A	2	 50% 100%
2	3A	2	 50% 100%
2	4A	2	 50% 100%
2	5A	2	 50% 100%
2	9	2	 100%
2	AA	2	 50% 100%
2	BA	2	 100%
2	CA	2	 50% 100%
2	DA	2	 50% 100%
2	EA	2	 50% 100%
2	FA	2	 50% 100%
2	GA	2	 50% 100%
2	HA	2	 100%
2	IA	2	 100%
2	JA	2	 100%
2	KA	2	 50% 100%

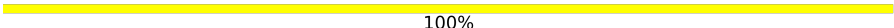
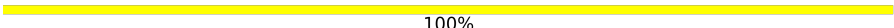

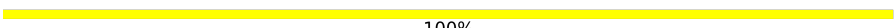


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Mol	Chain	Length	Quality of chain
2	LA	2	 100%
2	MA	2	 50% 100%
2	NA	2	 50% 100%
2	OA	2	 50% 100%
2	PA	2	 50% 100%
2	QA	2	 50% 100%
2	RA	2	 50% 100%
2	SA	2	 50% 100%
2	TA	2	 50% 100%
2	UA	2	 50% 100%
2	VA	2	 50% 100%
2	WA	2	 50% 100%
2	XA	2	 50% 100%
2	YA	2	 50% 100%
2	ZA	2	 50% 100%
2	aA	2	 50% 100%
2	bA	2	 50% 100%
2	cA	2	 50% 100%
2	dA	2	 50% 100%
2	eA	2	 50% 100%
2	fA	2	 50% 100%
2	gA	2	 50% 100%
2	hA	2	 50% 100%
2	iA	2	 50% 100%
2	jA	2	 100%

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Mol	Chain	Length	Quality of chain
2	kA	2	 100%
2	lA	2	 100%
2	mA	2	 50% 100%
2	nA	2	 50% 100%
2	oA	2	 50% 100%
2	pA	2	 50% 100%
2	qA	2	 50% 100%
2	rA	2	 50% 100%
2	sA	2	 50% 100%
2	tA	2	 100%
2	uA	2	 100%
2	vA	2	 100%
2	wA	2	 50% 100%
2	xA	2	 50% 100%
2	yA	2	 50% 100%
2	zA	2	 50% 100%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 249720 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	518	4120	2605	707	792	16	0	0
1	B	518	4120	2605	707	792	16	0	0
1	C	518	4120	2605	707	792	16	0	0
1	D	518	4120	2605	707	792	16	0	0
1	E	518	4120	2605	707	792	16	0	0
1	F	518	4120	2605	707	792	16	0	0
1	G	518	4120	2605	707	792	16	0	0
1	H	518	4120	2605	707	792	16	0	0
1	I	518	4120	2605	707	792	16	0	0
1	J	518	4120	2605	707	792	16	0	0
1	K	518	4120	2605	707	792	16	0	0
1	L	518	4120	2605	707	792	16	0	0
1	M	518	4120	2605	707	792	16	0	0
1	N	518	4120	2605	707	792	16	0	0
1	O	518	4120	2605	707	792	16	0	0
1	P	518	4120	2605	707	792	16	0	0
1	Q	518	4120	2605	707	792	16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	S	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	T	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	U	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	V	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	W	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	X	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	Y	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	Z	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	a	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	b	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	c	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	d	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	e	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	f	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	g	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	h	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	i	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	j	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	k	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		
1	l	518	Total	C	N	O	S	0	0
			4120	2605	707	792	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	n	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	o	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	p	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	q	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	r	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	s	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	t	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	u	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	v	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	w	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	x	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	y	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	z	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	1	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	2	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	3	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	4	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	5	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	6	518	Total 4120	C 2605	N 707	O 792	S 16	0	0
1	7	518	Total 4120	C 2605	N 707	O 792	S 16	0	0

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*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	518	4120	2605	707	792	16	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	0	2	42	20	10	10	2	0	0
2	JA	2	42	20	10	10	2	0	0
2	UA	2	42	20	10	10	2	0	0
2	fA	2	42	20	10	10	2	0	0
2	qA	2	42	20	10	10	2	0	0
2	1A	2	42	20	10	10	2	0	0
2	3A	2	42	20	10	10	2	0	0
2	4A	2	42	20	10	10	2	0	0
2	5A	2	42	20	10	10	2	0	0
2	9	2	42	20	10	10	2	0	0
2	AA	2	42	20	10	10	2	0	0
2	BA	2	42	20	10	10	2	0	0
2	CA	2	42	20	10	10	2	0	0
2	DA	2	42	20	10	10	2	0	0
2	EA	2	42	20	10	10	2	0	0
2	FA	2	42	20	10	10	2	0	0
2	GA	2	42	20	10	10	2	0	0
2	HA	2	42	20	10	10	2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	IA	2	Total 42	20	10	10	2	0	0
2	KA	2	Total 42	20	10	10	2	0	0
2	LA	2	Total 42	20	10	10	2	0	0
2	MA	2	Total 42	20	10	10	2	0	0
2	NA	2	Total 42	20	10	10	2	0	0
2	OA	2	Total 42	20	10	10	2	0	0
2	PA	2	Total 42	20	10	10	2	0	0
2	QA	2	Total 42	20	10	10	2	0	0
2	RA	2	Total 42	20	10	10	2	0	0
2	SA	2	Total 42	20	10	10	2	0	0
2	TA	2	Total 42	20	10	10	2	0	0
2	VA	2	Total 42	20	10	10	2	0	0
2	WA	2	Total 42	20	10	10	2	0	0
2	XA	2	Total 42	20	10	10	2	0	0
2	YA	2	Total 42	20	10	10	2	0	0
2	ZA	2	Total 42	20	10	10	2	0	0
2	aA	2	Total 42	20	10	10	2	0	0
2	bA	2	Total 42	20	10	10	2	0	0
2	cA	2	Total 42	20	10	10	2	0	0
2	dA	2	Total 42	20	10	10	2	0	0
2	eA	2	Total 42	20	10	10	2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	gA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	hA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	iA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	jA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	kA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	lA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	mA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	nA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	oA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	pA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	rA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	sA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	tA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	uA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	vA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	wA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	xA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	yA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	zA	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	0A	2	Total 42	C 20	N 10	O 10	P 2	0	0
2	2A	2	Total 42	C 20	N 10	O 10	P 2	0	0

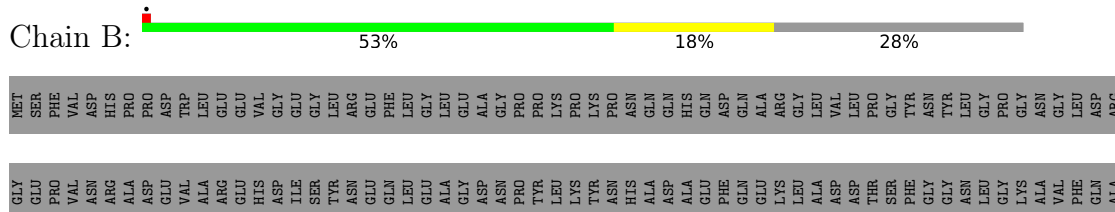
### 3 Residue-property plots

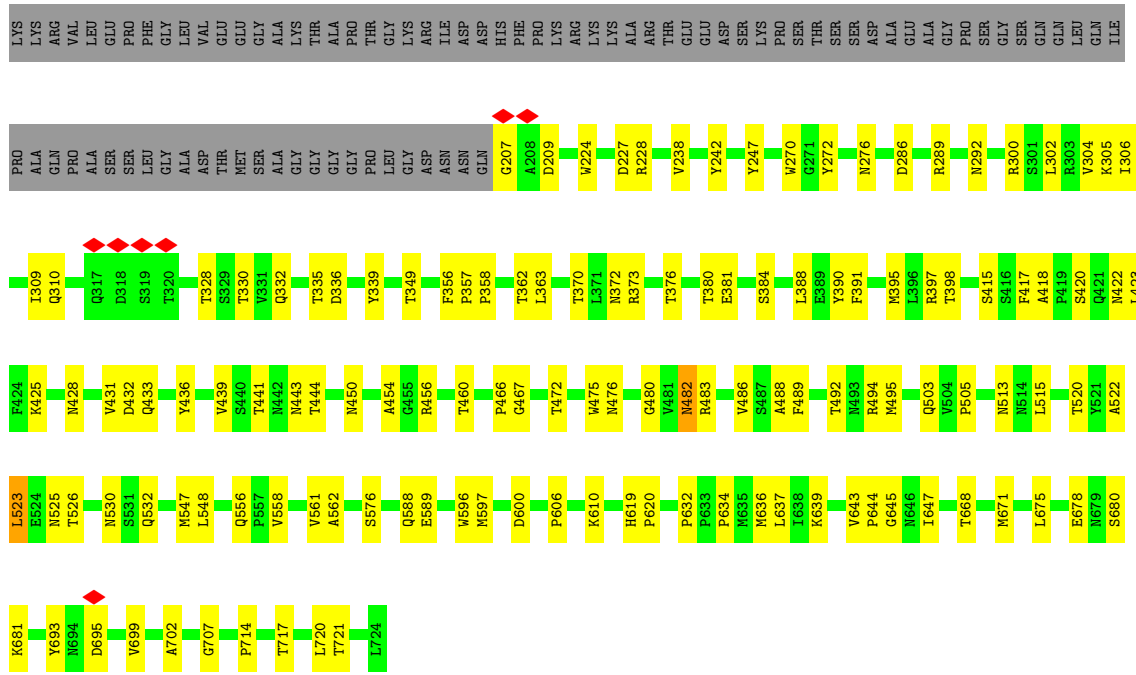
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Capsid protein

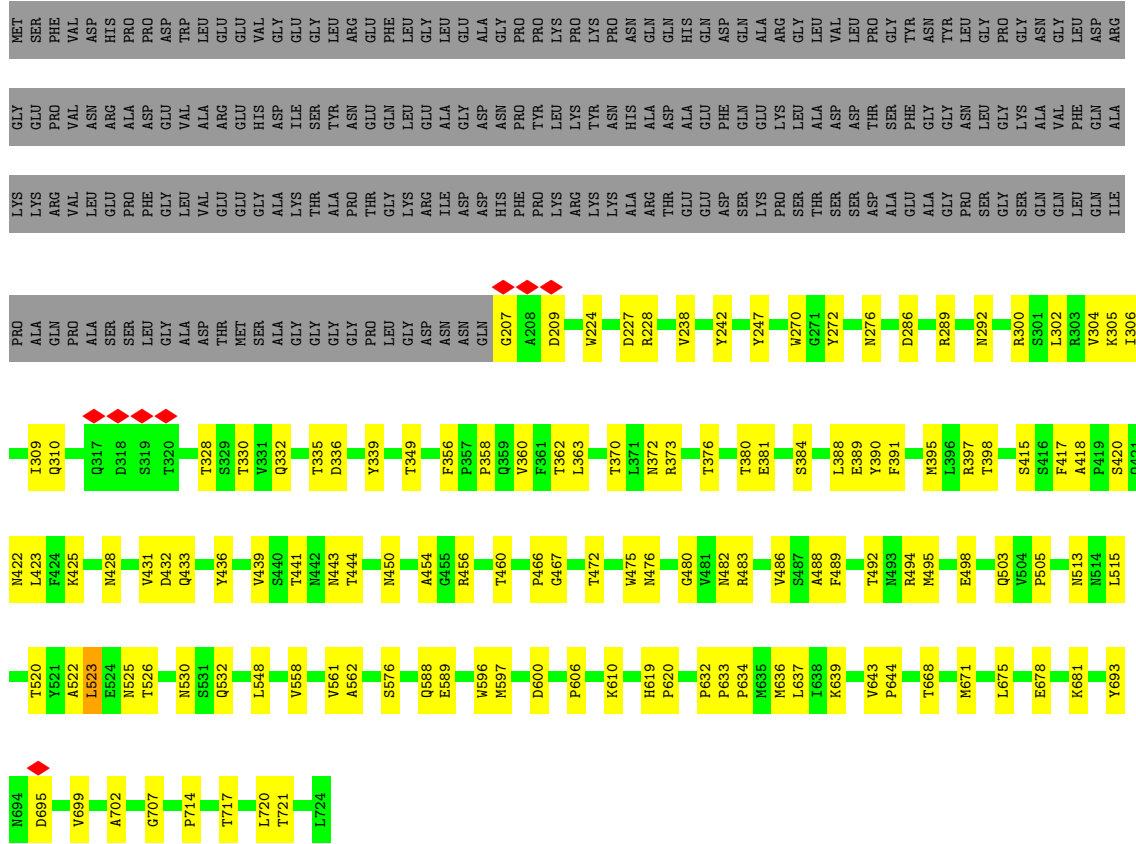


- Molecule 1: Capsid protein





• Molecule 1: Capsid protein

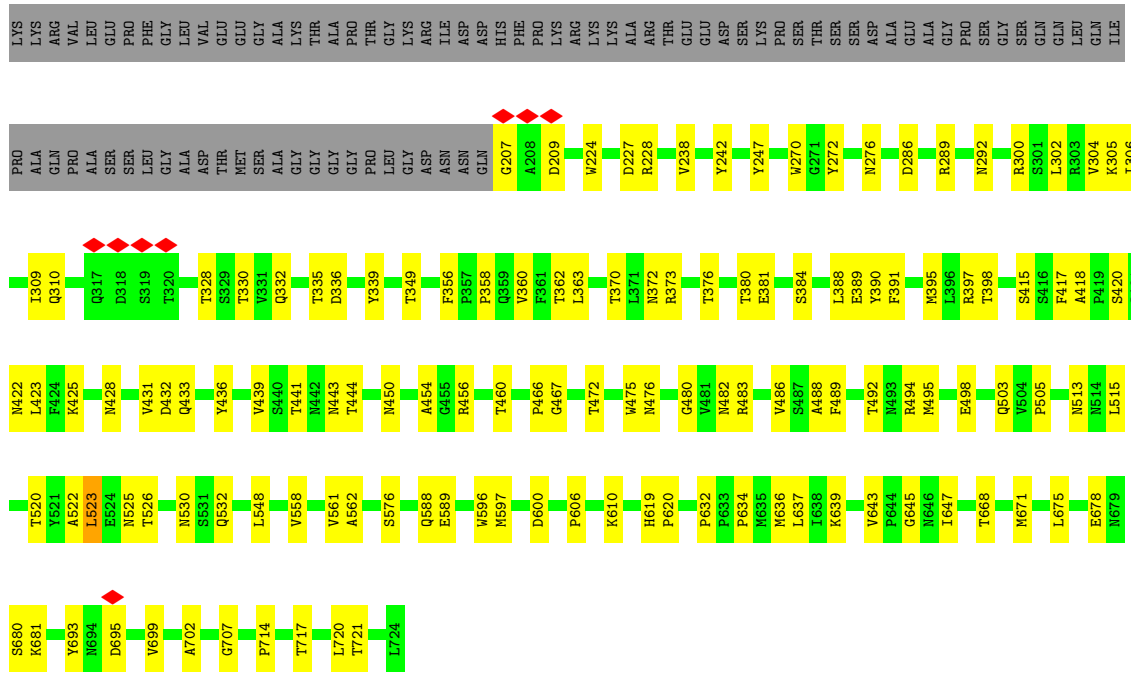


• Molecule 1: Capsid protein









• Molecule 1: Capsid protein



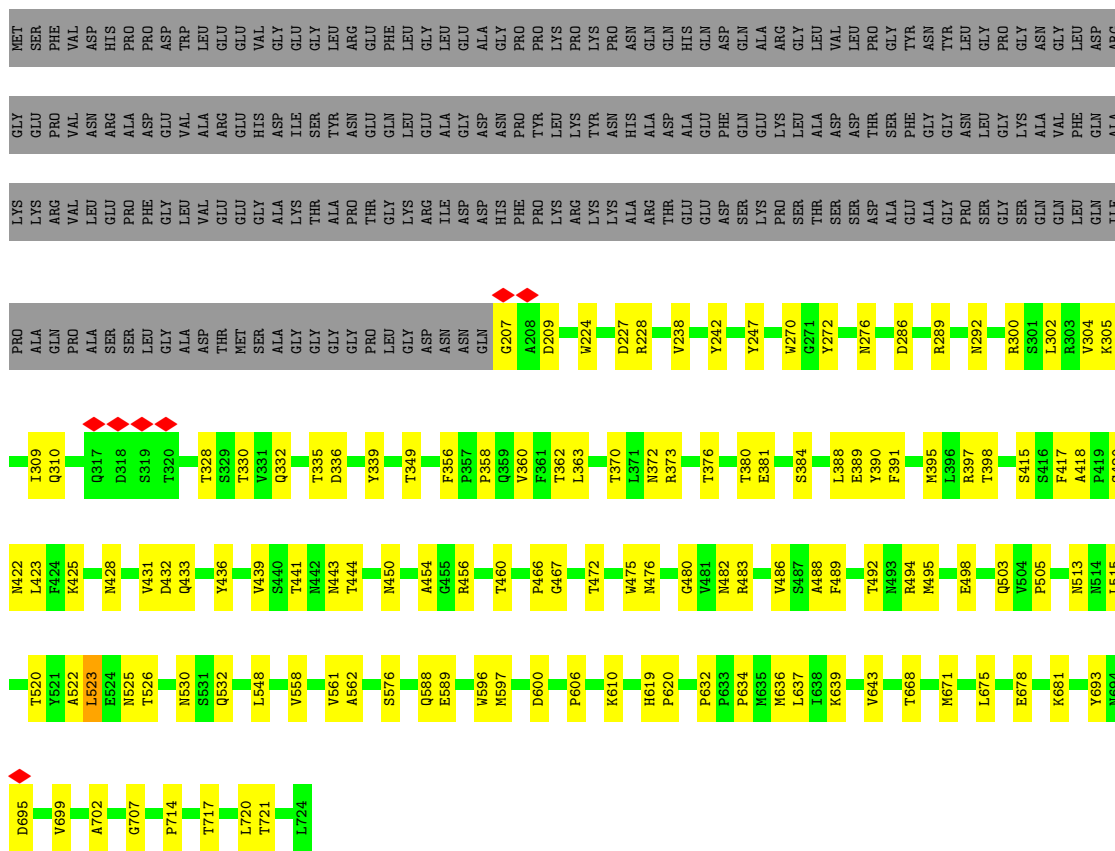
• Molecule 1: Capsid protein



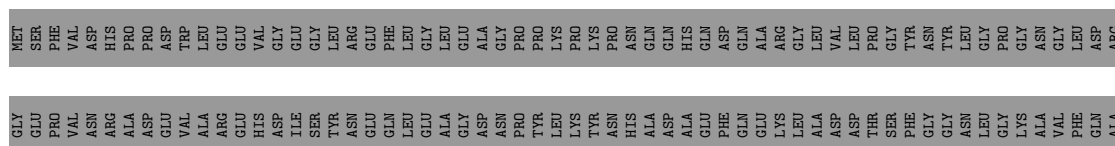


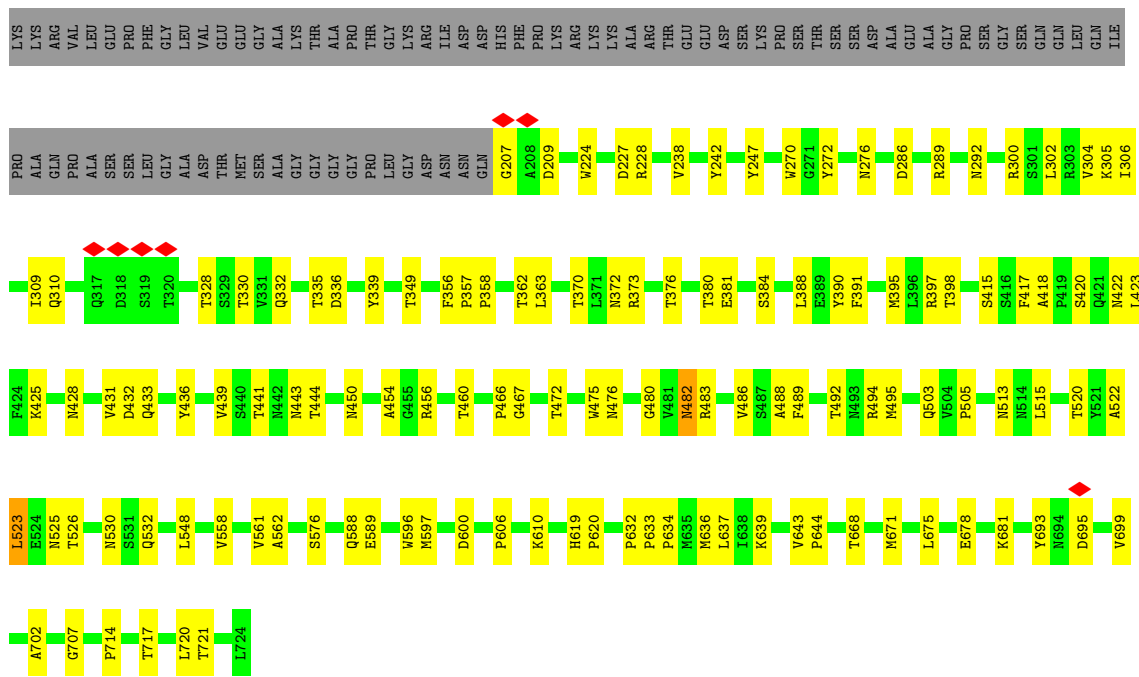


• Molecule 1: Capsid protein



• Molecule 1: Capsid protein





• Molecule 1: Capsid protein

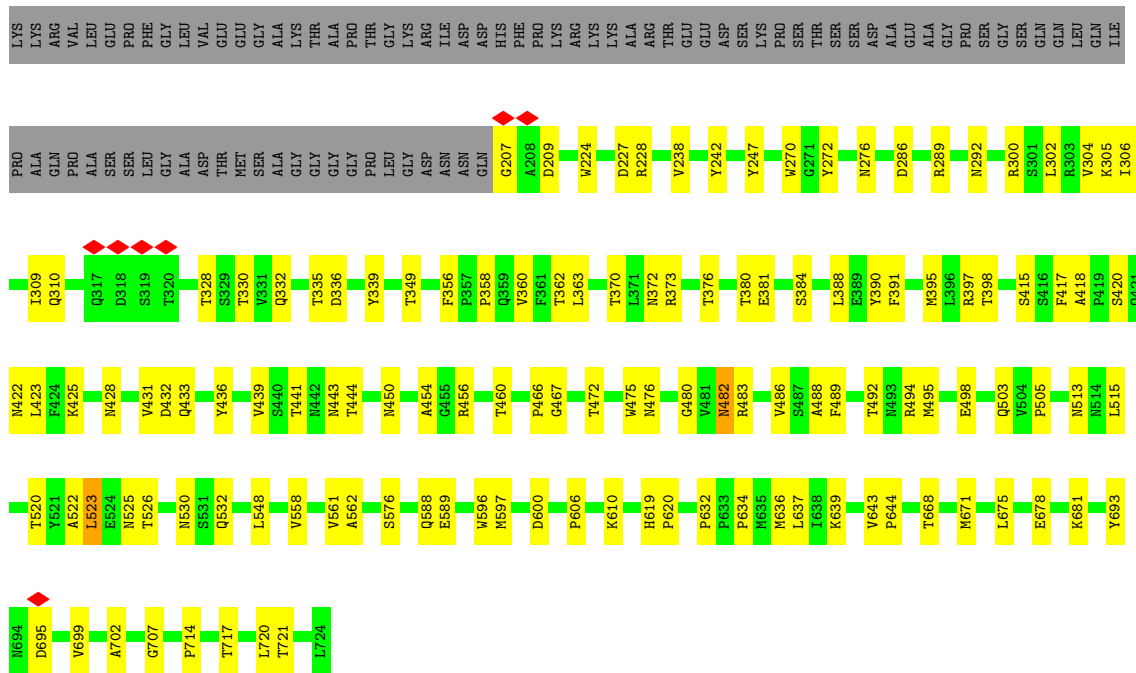


• Molecule 1: Capsid protein







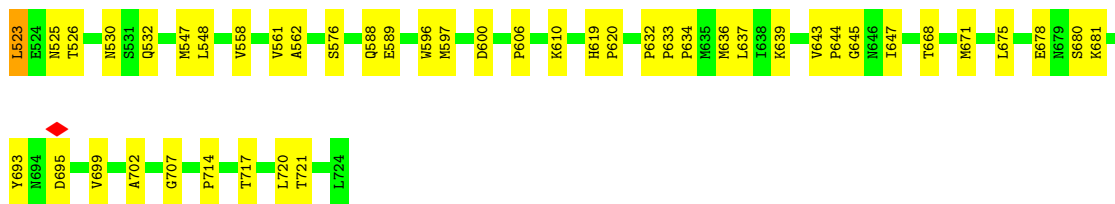


● Molecule 1: Capsid protein



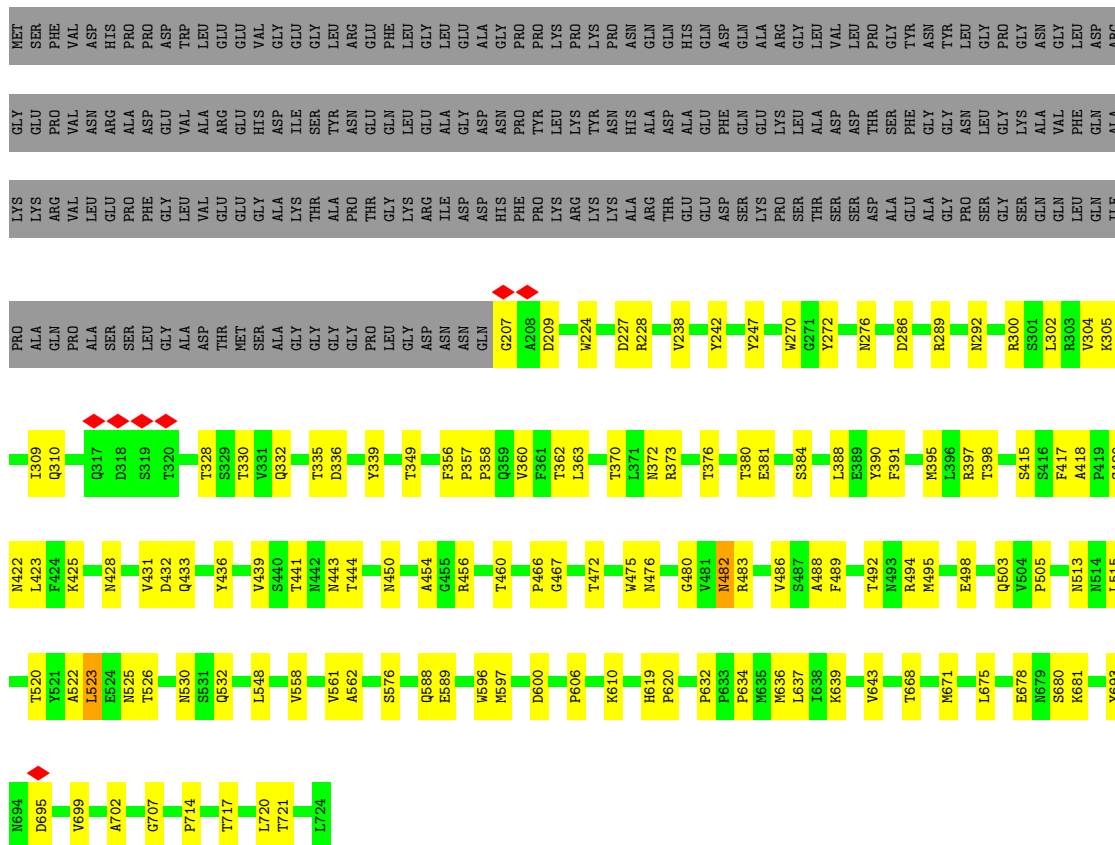
● Molecule 1: Capsid protein





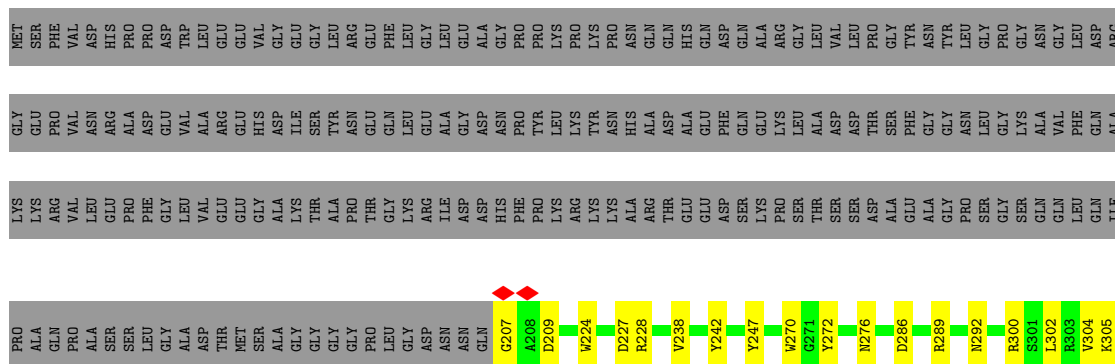
• Molecule 1: Capsid protein

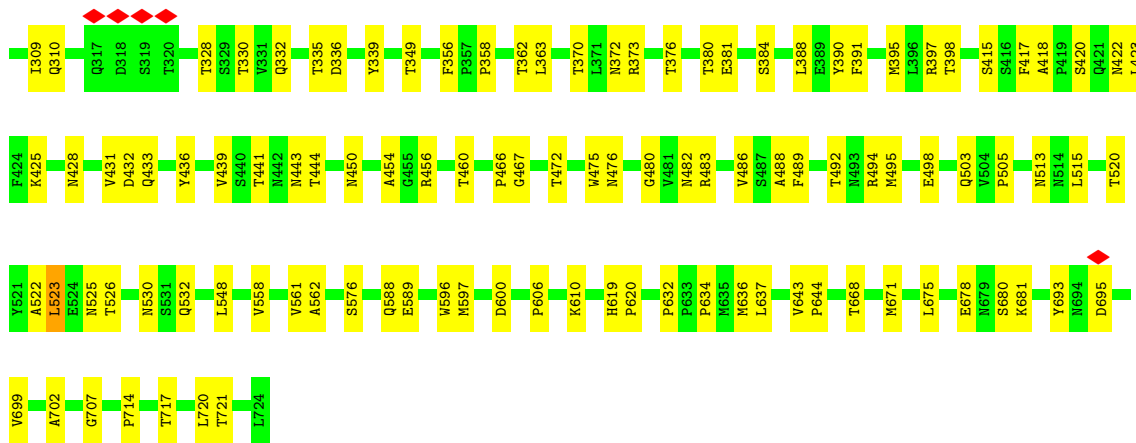
Chain a:



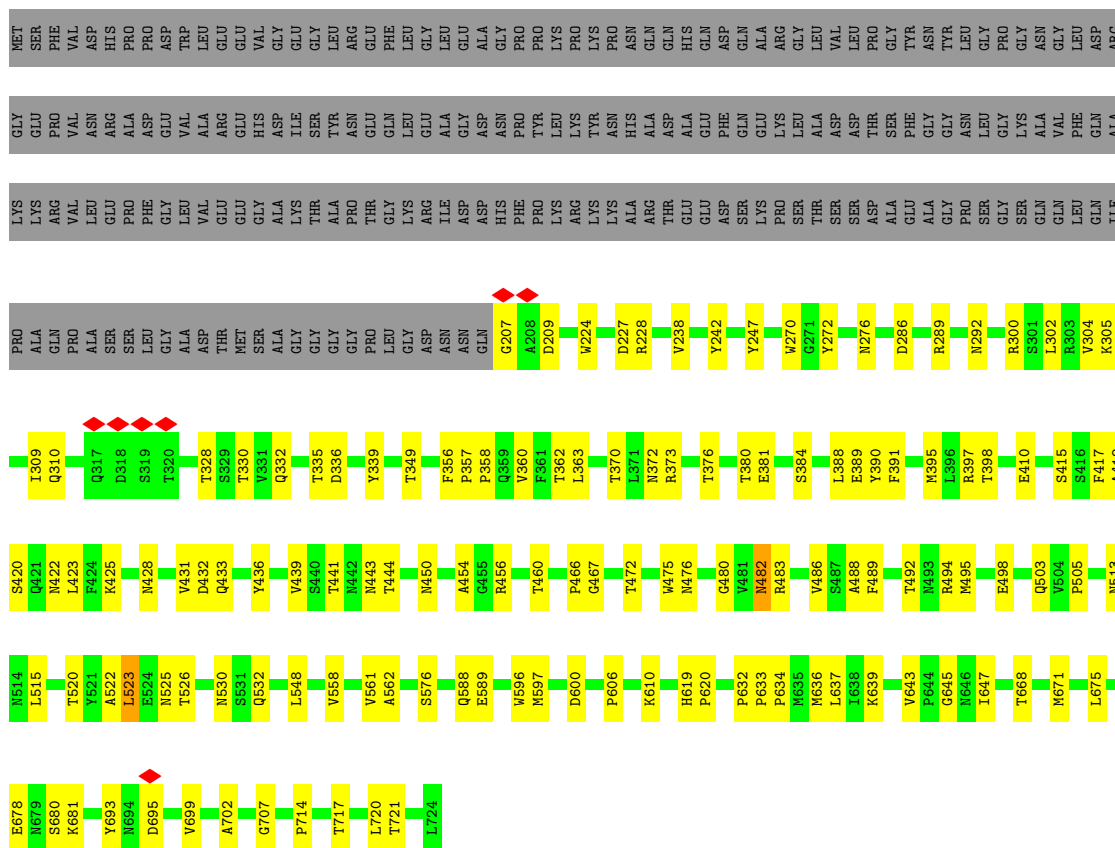
• Molecule 1: Capsid protein

Chain b:

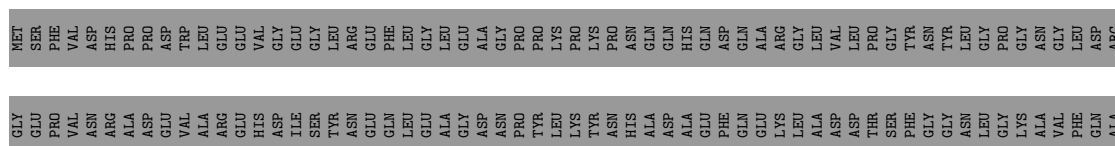


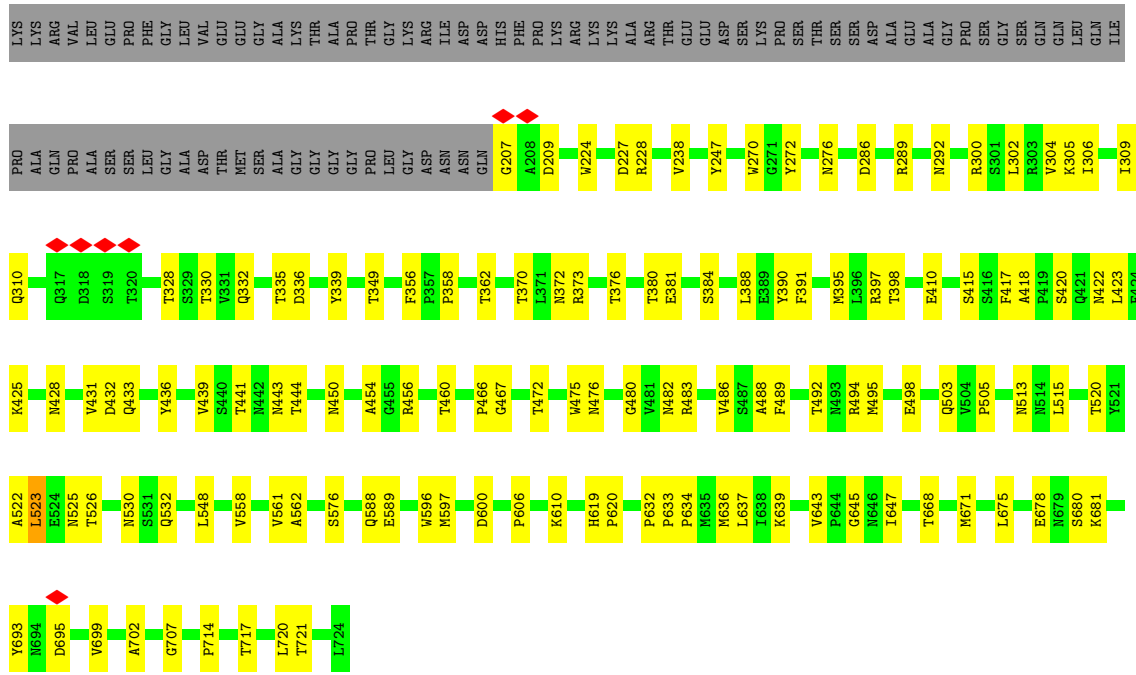


• Molecule 1: Capsid protein

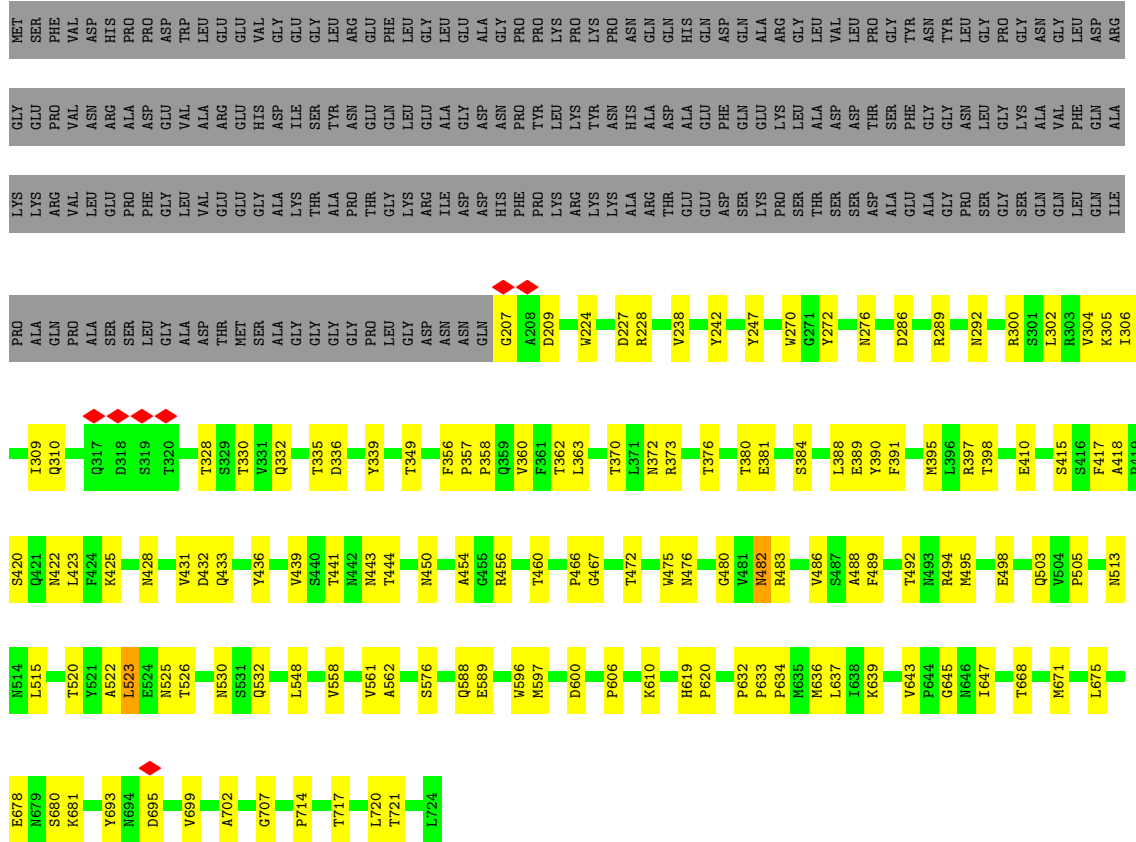


• Molecule 1: Capsid protein





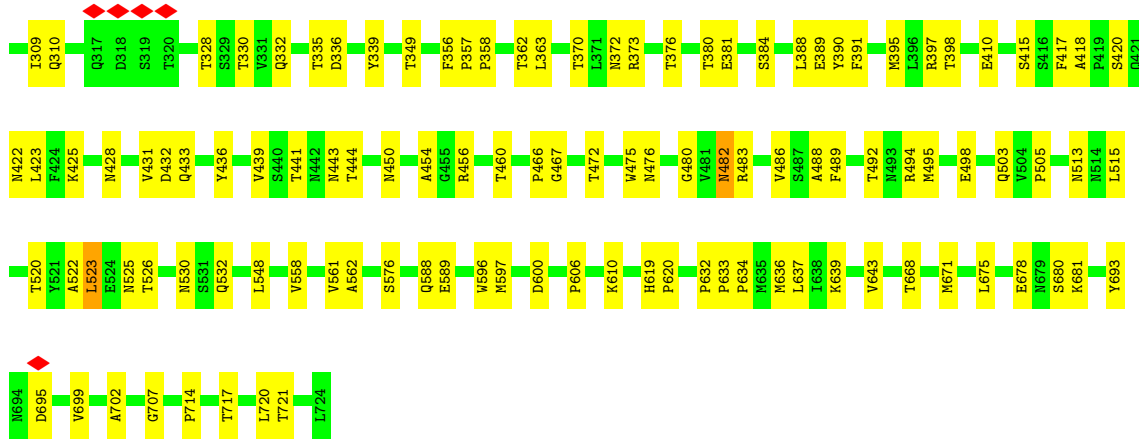
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



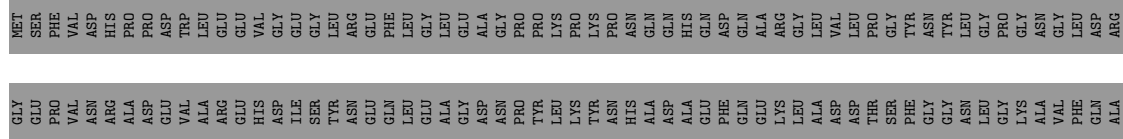


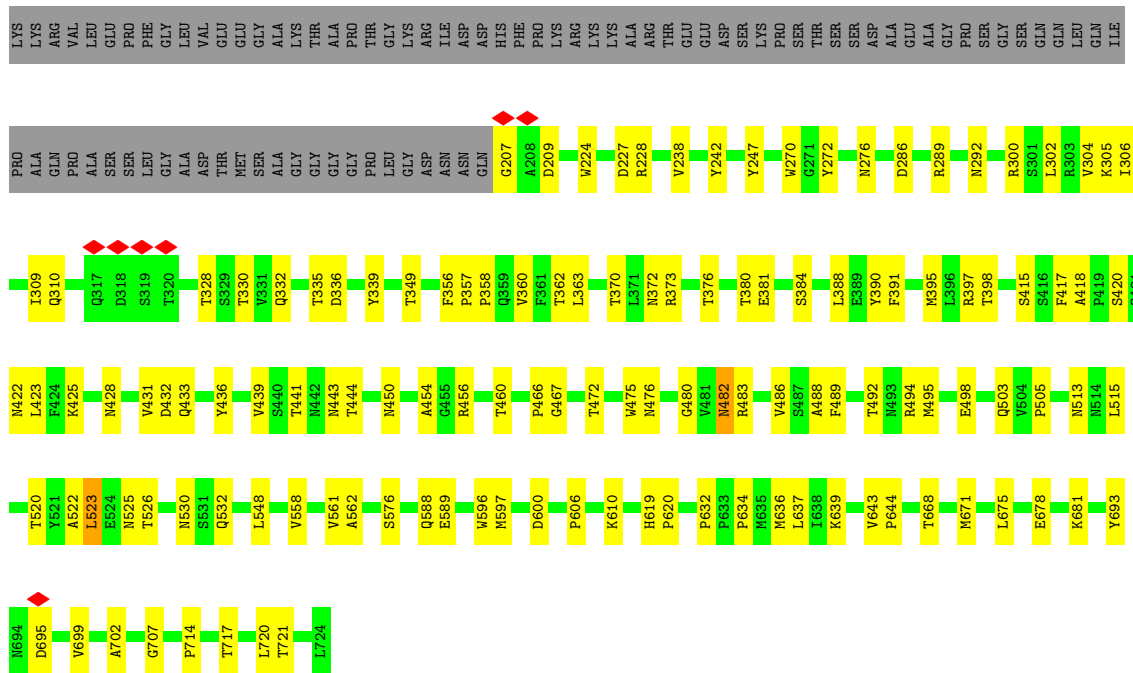


• Molecule 1: Capsid protein



• Molecule 1: Capsid protein





• Molecule 1: Capsid protein



• Molecule 1: Capsid protein





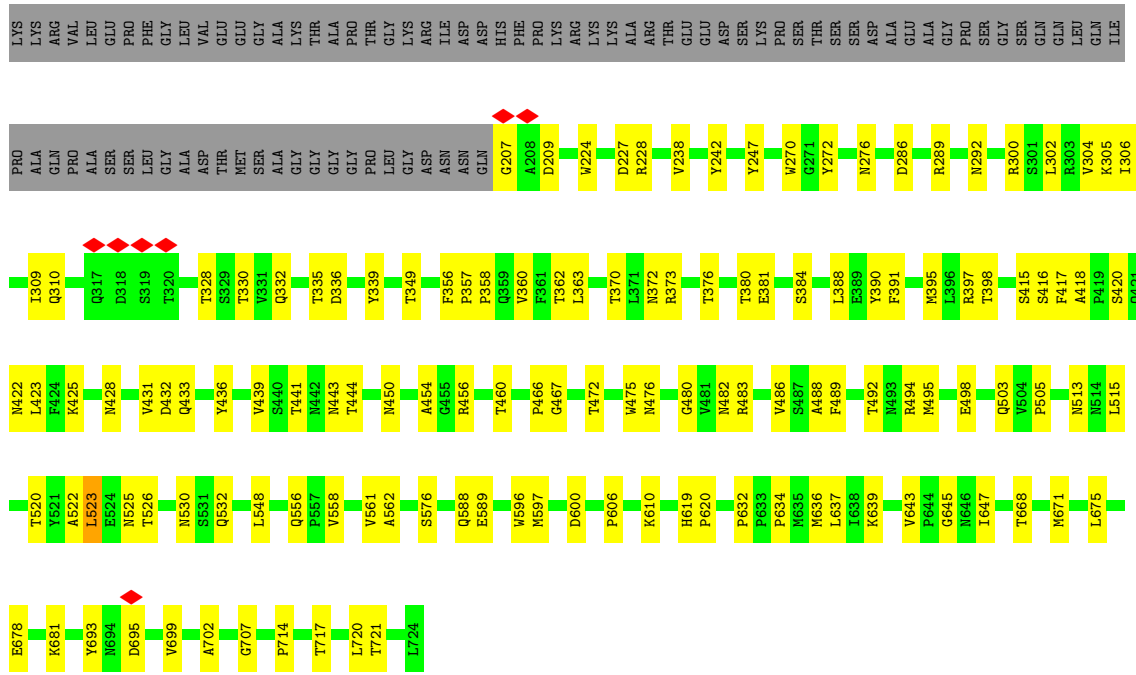












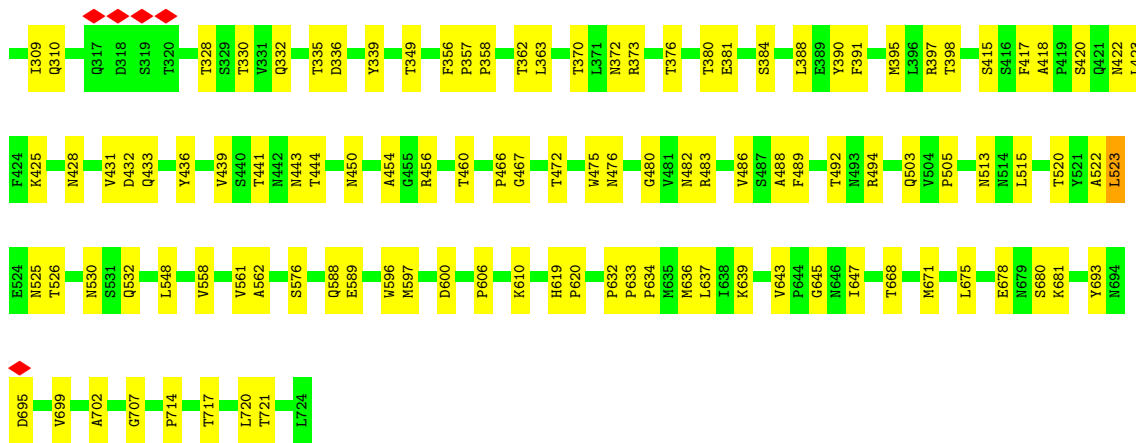
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



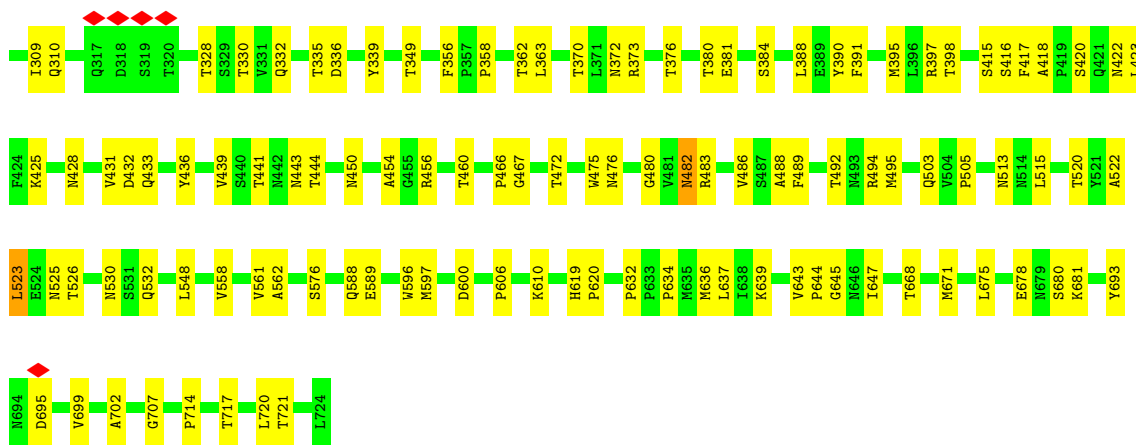




• Molecule 1: Capsid protein



MET	GLY	LYS	PRO	ALA	PRO	GLN	G207	G208	A208	D209	W224	D227	R228	V238	Y242	Y247	W270	G271	Y272	N276	D286	R289	N292	R300	S301	L302	R303	V304	K305	I306	
SER	GLU	ARG	PRO	GLN	ALA	ASP	GLN	GLY	LEU	ASP	PRO	LEU	LEU	ASP	ASN	GLY	LYS	PRO	SER	THR	SER	ALA	GLY	ASN	GLY	LEU	LYS	GLN	LEU	ARG	
PHE	VAL	VAL	VAL	ARG	SER	SER	LEU	GLY	VAL	ASP	THR	GLY	LYS	ALA	THR	GLY	ALA	LEU	LEU	VAL	ASP	THR	PHE	GLY	ASN	TYR	LEU	GLY	LEU	ARG	
VAL	ASN	ARG	GLU	LEU	VAL	VAL	LEU	VAL	VAL	ARG	GLU	GLY	LEU	ARG	GLY	LEU	LYS	THR	SER	SER	ASP	THR	ALA	GLY	ASN	TYR	LEU	GLY	LEU	ARG	
HIS	ASP	ASP	PRO	PRO	ASP	ASP	GLY	ALA	ALA	THR	ALA	ALA	ARG	THR	GLY	LYS	PRO	SER	THR	SER	ASP	THR	ALA	GLY	ASN	TYR	LEU	GLY	LEU	ARG	
PRO	PRO	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG



• Molecule 1: Capsid protein



MET	GLY	LYS	PRO	ALA	PRO	GLN	G207	G208	A208	D209	W224	D227	R228	V238	Y242	Y247	W270	G271	Y272	N276	D286	R289	N292	R300	S301	L302	R303	V304	K305	I306	
SER	GLU	ARG	PRO	GLN	ALA	ASP	GLN	GLY	LEU	ASP	PRO	LEU	LEU	ASP	ASN	GLY	LYS	PRO	SER	THR	SER	ALA	GLY	ASN	GLY	LEU	LYS	GLN	LEU	ARG	
PHE	VAL	VAL	VAL	ARG	SER	SER	LEU	GLY	VAL	ASP	THR	GLY	LYS	ALA	THR	GLY	ALA	LEU	LEU	VAL	ASP	THR	PHE	GLY	ASN	TYR	LEU	GLY	LEU	ARG	
VAL	ASN	ARG	GLU	LEU	VAL	VAL	LEU	VAL	VAL	ARG	GLU	GLY	LEU	ARG	GLY	LEU	LYS	THR	SER	SER	ASP	THR	ALA	GLY	ASN	TYR	LEU	GLY	LEU	ARG	
HIS	ASP	ASP	PRO	PRO	ASP	ASP	GLY	ALA	ALA	THR	ALA	ALA	ARG	THR	GLY	LYS	PRO	SER	THR	SER	ASP	THR	ALA	GLY	ASN	TYR	LEU	GLY	LEU	ARG	
PRO	PRO	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG







A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')




◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain HA:  100%

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain IA:  100%

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain KA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain LA:  100%

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain MA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain NA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain OA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



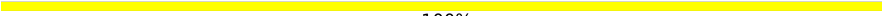
◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain kA:  100%

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain lA:  100%

A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain mA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain nA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain oA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain pA:  50%  
 100%

◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')

Chain rA:  50%  
 100%

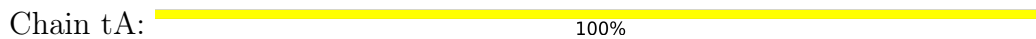
◆  
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



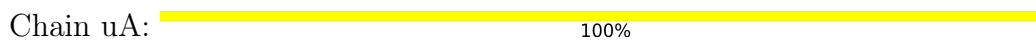
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



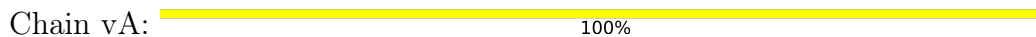
A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

- Molecule 2: DNA (5'-D(P\*AP\*A)-3')



A996  
A997

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42158	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1289	Depositor
Maximum defocus (nm)	3967	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	22.036	Depositor
Minimum map value	-17.362	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	467.5, 467.5, 467.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.935, 0.935, 0.935	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.40	0/4248	0.62	1/5805 (0.0%)
1	2	0.40	0/4248	0.62	1/5805 (0.0%)
1	3	0.40	0/4248	0.62	1/5805 (0.0%)
1	4	0.40	0/4248	0.62	1/5805 (0.0%)
1	5	0.40	0/4248	0.62	1/5805 (0.0%)
1	6	0.40	0/4248	0.62	1/5805 (0.0%)
1	7	0.40	0/4248	0.62	1/5805 (0.0%)
1	8	0.40	0/4248	0.62	1/5805 (0.0%)
1	A	0.40	0/4248	0.62	1/5805 (0.0%)
1	B	0.40	0/4248	0.62	1/5805 (0.0%)
1	C	0.40	0/4248	0.62	1/5805 (0.0%)
1	D	0.40	0/4248	0.62	1/5805 (0.0%)
1	E	0.40	0/4248	0.62	1/5805 (0.0%)
1	F	0.40	0/4248	0.62	1/5805 (0.0%)
1	G	0.40	0/4248	0.62	1/5805 (0.0%)
1	H	0.40	0/4248	0.62	1/5805 (0.0%)
1	I	0.40	0/4248	0.62	1/5805 (0.0%)
1	J	0.40	0/4248	0.62	1/5805 (0.0%)
1	K	0.40	0/4248	0.62	1/5805 (0.0%)
1	L	0.40	0/4248	0.62	1/5805 (0.0%)
1	M	0.40	0/4248	0.62	1/5805 (0.0%)
1	N	0.40	0/4248	0.62	1/5805 (0.0%)
1	O	0.40	0/4248	0.62	1/5805 (0.0%)
1	P	0.40	0/4248	0.62	1/5805 (0.0%)
1	Q	0.40	0/4248	0.62	1/5805 (0.0%)
1	R	0.40	0/4248	0.62	1/5805 (0.0%)
1	S	0.40	0/4248	0.62	1/5805 (0.0%)
1	T	0.40	0/4248	0.62	1/5805 (0.0%)
1	U	0.40	0/4248	0.62	1/5805 (0.0%)
1	V	0.40	0/4248	0.62	1/5805 (0.0%)
1	W	0.40	0/4248	0.62	1/5805 (0.0%)
1	X	0.40	0/4248	0.62	1/5805 (0.0%)
1	Y	0.40	0/4248	0.62	1/5805 (0.0%)
1	Z	0.40	0/4248	0.62	1/5805 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.40	0/4248	0.62	1/5805 (0.0%)
1	b	0.40	0/4248	0.62	1/5805 (0.0%)
1	c	0.40	0/4248	0.62	1/5805 (0.0%)
1	d	0.40	0/4248	0.62	1/5805 (0.0%)
1	e	0.40	0/4248	0.62	1/5805 (0.0%)
1	f	0.40	0/4248	0.62	1/5805 (0.0%)
1	g	0.40	0/4248	0.62	1/5805 (0.0%)
1	h	0.40	0/4248	0.62	1/5805 (0.0%)
1	i	0.40	0/4248	0.62	1/5805 (0.0%)
1	j	0.40	0/4248	0.62	1/5805 (0.0%)
1	k	0.40	0/4248	0.62	1/5805 (0.0%)
1	l	0.40	0/4248	0.62	1/5805 (0.0%)
1	m	0.40	0/4248	0.62	1/5805 (0.0%)
1	n	0.40	0/4248	0.62	1/5805 (0.0%)
1	o	0.40	0/4248	0.62	1/5805 (0.0%)
1	p	0.40	0/4248	0.62	1/5805 (0.0%)
1	q	0.40	0/4248	0.62	1/5805 (0.0%)
1	r	0.40	0/4248	0.62	1/5805 (0.0%)
1	s	0.40	0/4248	0.62	1/5805 (0.0%)
1	t	0.40	0/4248	0.62	1/5805 (0.0%)
1	u	0.40	0/4248	0.62	1/5805 (0.0%)
1	v	0.40	0/4248	0.62	1/5805 (0.0%)
1	w	0.40	0/4248	0.62	1/5805 (0.0%)
1	x	0.40	0/4248	0.62	1/5805 (0.0%)
1	y	0.40	0/4248	0.62	1/5805 (0.0%)
1	z	0.40	0/4248	0.62	1/5805 (0.0%)
2	0	0.26	0/47	0.44	0/70
2	0A	0.26	0/47	0.44	0/70
2	1A	0.26	0/47	0.44	0/70
2	2A	0.26	0/47	0.44	0/70
2	3A	0.26	0/47	0.44	0/70
2	4A	0.26	0/47	0.44	0/70
2	5A	0.26	0/47	0.44	0/70
2	9	0.26	0/47	0.44	0/70
2	AA	0.27	0/47	0.44	0/70
2	BA	0.26	0/47	0.44	0/70
2	CA	0.26	0/47	0.44	0/70
2	DA	0.27	0/47	0.44	0/70
2	EA	0.27	0/47	0.44	0/70
2	FA	0.26	0/47	0.44	0/70
2	GA	0.27	0/47	0.44	0/70
2	HA	0.26	0/47	0.44	0/70
2	IA	0.26	0/47	0.44	0/70

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	JA	0.27	0/47	0.44	0/70
2	KA	0.26	0/47	0.44	0/70
2	LA	0.26	0/47	0.44	0/70
2	MA	0.27	0/47	0.44	0/70
2	NA	0.26	0/47	0.45	0/70
2	OA	0.26	0/47	0.44	0/70
2	PA	0.26	0/47	0.44	0/70
2	QA	0.26	0/47	0.44	0/70
2	RA	0.26	0/47	0.44	0/70
2	SA	0.27	0/47	0.44	0/70
2	TA	0.26	0/47	0.45	0/70
2	UA	0.26	0/47	0.44	0/70
2	VA	0.27	0/47	0.44	0/70
2	WA	0.27	0/47	0.44	0/70
2	XA	0.27	0/47	0.44	0/70
2	YA	0.27	0/47	0.44	0/70
2	ZA	0.27	0/47	0.44	0/70
2	aA	0.26	0/47	0.44	0/70
2	bA	0.26	0/47	0.44	0/70
2	cA	0.26	0/47	0.44	0/70
2	dA	0.26	0/47	0.44	0/70
2	eA	0.26	0/47	0.44	0/70
2	fA	0.27	0/47	0.44	0/70
2	gA	0.27	0/47	0.44	0/70
2	hA	0.26	0/47	0.44	0/70
2	iA	0.27	0/47	0.44	0/70
2	jA	0.26	0/47	0.44	0/70
2	kA	0.26	0/47	0.44	0/70
2	lA	0.26	0/47	0.44	0/70
2	mA	0.26	0/47	0.44	0/70
2	nA	0.26	0/47	0.44	0/70
2	oA	0.27	0/47	0.44	0/70
2	pA	0.26	0/47	0.44	0/70
2	qA	0.27	0/47	0.44	0/70
2	rA	0.26	0/47	0.44	0/70
2	sA	0.27	0/47	0.44	0/70
2	tA	0.26	0/47	0.44	0/70
2	uA	0.26	0/47	0.44	0/70
2	vA	0.26	0/47	0.44	0/70
2	wA	0.27	0/47	0.44	0/70
2	xA	0.27	0/47	0.44	0/70
2	yA	0.26	0/47	0.45	0/70
2	zA	0.26	0/47	0.44	0/70

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.40	0/257700	0.62	60/352500 (0.0%)

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	482	ASN	CB-CA-C	-5.50	108.64	116.34
1	o	482	ASN	CB-CA-C	-5.49	108.65	116.34
1	B	482	ASN	CB-CA-C	-5.49	108.66	116.34
1	L	482	ASN	CB-CA-C	-5.49	108.66	116.34
1	5	482	ASN	CB-CA-C	-5.48	108.66	116.34

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	1	4120	0	3866	114	0
1	2	4120	0	3866	110	0
1	3	4120	0	3866	115	0
1	4	4120	0	3866	113	0
1	5	4120	0	3866	110	0
1	6	4120	0	3866	112	0
1	7	4120	0	3866	109	0
1	8	4120	0	3866	113	0
1	A	4120	0	3866	112	0
1	B	4120	0	3866	113	0
1	C	4120	0	3866	108	0
1	D	4120	0	3866	107	0
1	E	4120	0	3866	113	0
1	F	4120	0	3866	111	0
1	G	4120	0	3866	113	0
1	H	4120	0	3866	110	0
1	I	4120	0	3866	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4120	0	3866	110	0
1	K	4120	0	3866	112	0
1	L	4120	0	3866	113	0
1	M	4120	0	3866	110	0
1	N	4120	0	3866	111	0
1	O	4120	0	3866	109	0
1	P	4120	0	3866	109	0
1	Q	4120	0	3866	111	0
1	R	4120	0	3866	109	0
1	S	4120	0	3866	110	0
1	T	4120	0	3866	108	0
1	U	4120	0	3866	109	0
1	V	4120	0	3866	112	0
1	W	4120	0	3866	111	0
1	X	4120	0	3866	108	0
1	Y	4120	0	3866	109	0
1	Z	4120	0	3866	113	0
1	a	4120	0	3866	112	0
1	b	4120	0	3866	105	0
1	c	4120	0	3866	114	0
1	d	4120	0	3866	111	0
1	e	4120	0	3866	115	0
1	f	4120	0	3866	105	0
1	g	4120	0	3866	108	0
1	h	4120	0	3866	109	0
1	i	4120	0	3866	112	0
1	j	4120	0	3866	109	0
1	k	4120	0	3866	109	0
1	l	4120	0	3866	107	0
1	m	4120	0	3866	108	0
1	n	4120	0	3866	110	0
1	o	4120	0	3866	108	0
1	p	4120	0	3866	114	0
1	q	4120	0	3866	109	0
1	r	4120	0	3866	110	0
1	s	4120	0	3866	107	0
1	t	4120	0	3866	115	0
1	u	4120	0	3866	111	0
1	v	4120	0	3866	114	0
1	w	4120	0	3866	113	0
1	x	4120	0	3866	111	0
1	y	4120	0	3866	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	z	4120	0	3866	112	0
2	0	42	0	23	4	0
2	0A	42	0	23	4	0
2	1A	42	0	23	4	0
2	2A	42	0	23	4	0
2	3A	42	0	23	4	0
2	4A	42	0	23	4	0
2	5A	42	0	23	4	0
2	9	42	0	23	5	0
2	AA	42	0	23	4	0
2	BA	42	0	23	4	0
2	CA	42	0	23	4	0
2	DA	42	0	23	5	0
2	EA	42	0	23	4	0
2	FA	42	0	23	4	0
2	GA	42	0	23	4	0
2	HA	42	0	23	4	0
2	IA	42	0	23	5	0
2	JA	42	0	23	4	0
2	KA	42	0	23	4	0
2	LA	42	0	23	4	0
2	MA	42	0	23	4	0
2	NA	42	0	23	4	0
2	OA	42	0	23	4	0
2	PA	42	0	23	4	0
2	QA	42	0	23	4	0
2	RA	42	0	23	4	0
2	SA	42	0	23	4	0
2	TA	42	0	23	5	0
2	UA	42	0	23	4	0
2	VA	42	0	23	5	0
2	WA	42	0	23	6	0
2	XA	42	0	23	4	0
2	YA	42	0	23	4	0
2	ZA	42	0	23	4	0
2	aA	42	0	23	5	0
2	bA	42	0	23	4	0
2	cA	42	0	23	5	0
2	dA	42	0	23	4	0
2	eA	42	0	23	4	0
2	fA	42	0	23	4	0
2	gA	42	0	23	4	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	hA	42	0	23	4	0
2	iA	42	0	23	4	0
2	jA	42	0	23	4	0
2	kA	42	0	23	5	0
2	lA	42	0	23	4	0
2	mA	42	0	23	5	0
2	nA	42	0	23	4	0
2	oA	42	0	23	5	0
2	pA	42	0	23	4	0
2	qA	42	0	23	4	0
2	rA	42	0	23	4	0
2	sA	42	0	23	4	0
2	tA	42	0	23	4	0
2	uA	42	0	23	4	0
2	vA	42	0	23	5	0
2	wA	42	0	23	4	0
2	xA	42	0	23	4	0
2	yA	42	0	23	4	0
2	zA	42	0	23	4	0
All	All	249720	0	233340	5333	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 11.

The worst 5 of 5333 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ASN:HD22	1:A:526:THR:HG22	1.21	1.06
1:v:513:ASN:HD22	1:v:526:THR:HG22	1.21	1.06
1:B:513:ASN:HD22	1:B:526:THR:HG22	1.21	1.06
1:1:513:ASN:HD22	1:1:526:THR:HG22	1.21	1.06
1:5:513:ASN:HD22	1:5:526:THR:HG22	1.21	1.06

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	1	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	2	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	3	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	4	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	5	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	6	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	7	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	8	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	A	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	B	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	C	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	D	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	E	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	F	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	G	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	H	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	I	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	J	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	K	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	L	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	M	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	N	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	O	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	P	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	Q	516/724 (71%)	503 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	S	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	T	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	U	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	V	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	W	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	X	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	Y	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	Z	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	a	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	b	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	c	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	d	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	e	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	f	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	g	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	h	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	i	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	j	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	k	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	l	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	m	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	n	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	o	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	p	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	q	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	r	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	s	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	t	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	u	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	v	516/724 (71%)	503 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	x	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	y	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
1	z	516/724 (71%)	503 (98%)	13 (2%)	0	100	100
All	All	30960/43440 (71%)	30180 (98%)	780 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	1	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	2	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	3	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	4	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	5	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	6	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	7	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	8	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	A	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	B	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	C	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	D	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	E	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	F	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	G	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	H	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	I	451/613 (74%)	450 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	K	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	L	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	M	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	N	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	O	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	P	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	Q	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	R	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	S	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	T	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	U	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	V	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	W	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	X	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	Y	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	Z	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	a	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	b	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	c	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	d	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	e	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	f	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	g	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	h	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	i	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	j	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	k	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	l	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	m	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	n	451/613 (74%)	450 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	p	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	q	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	r	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	s	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	t	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	u	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	v	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	w	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	x	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	y	451/613 (74%)	450 (100%)	1 (0%)	87	87
1	z	451/613 (74%)	450 (100%)	1 (0%)	87	87
All	All	27060/36780 (74%)	27000 (100%)	60 (0%)	85	87

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	523	LEU
1	4	523	LEU
1	j	523	LEU
1	3	523	LEU
1	8	523	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 802 such sidechains are listed below:

Mol	Chain	Res	Type
1	i	525	ASN
1	r	332	GLN
1	8	574	GLN
1	j	535	ASN
1	i	509	ASN

### 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.

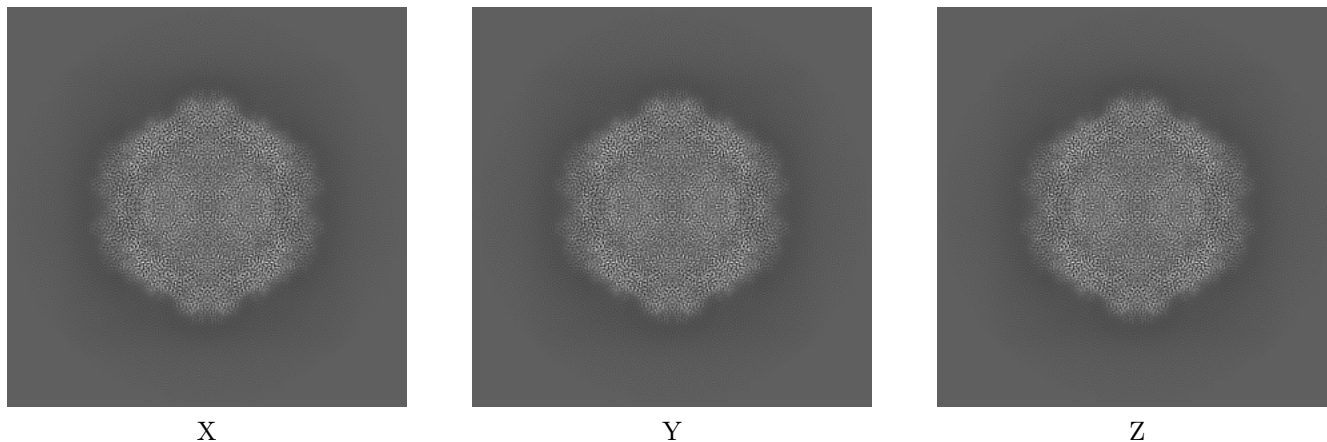
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46749. These allow visual inspection of the internal detail of the map and identification of artifacts.

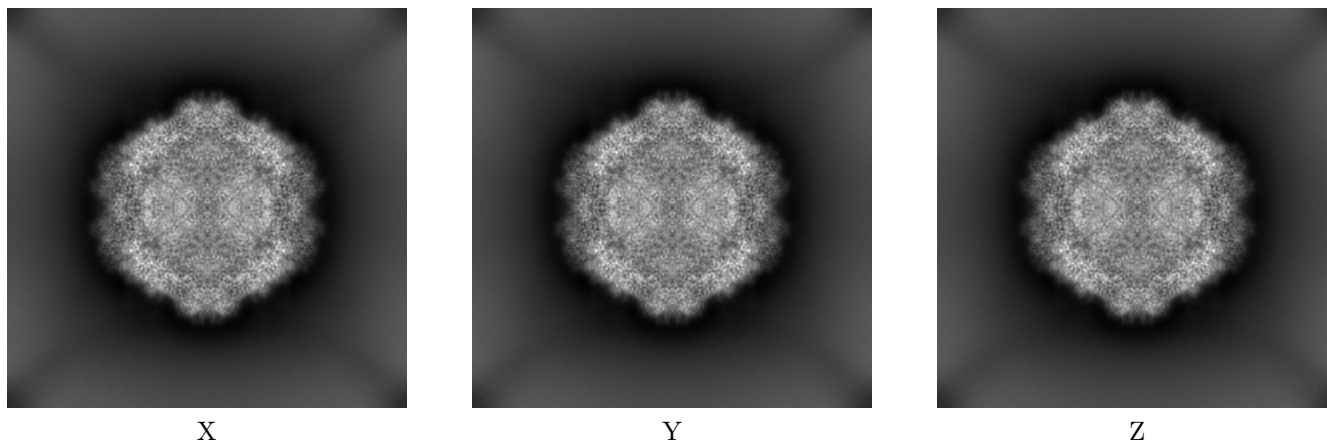
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



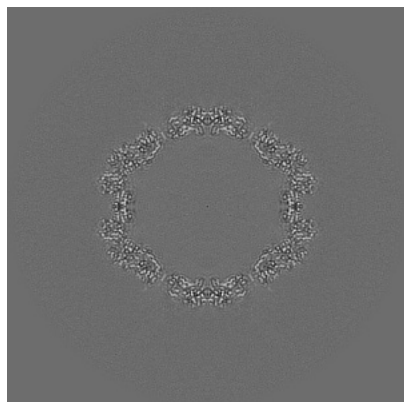
#### 6.1.2 Raw map



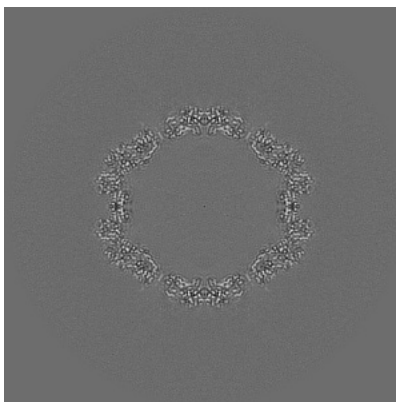
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

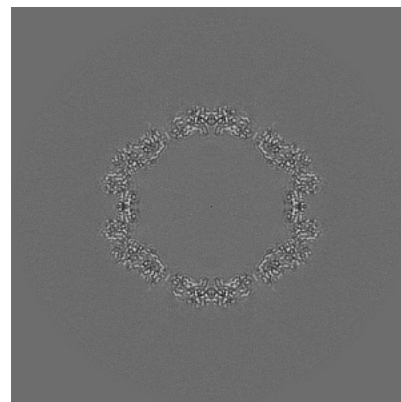
### 6.2.1 Primary map



X Index: 250

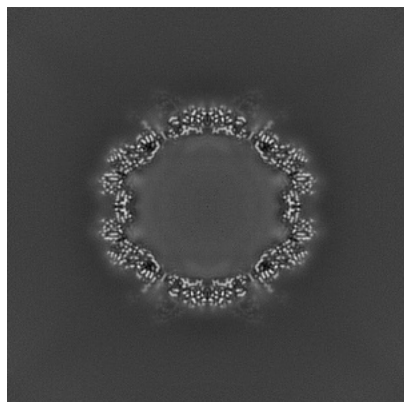


Y Index: 250

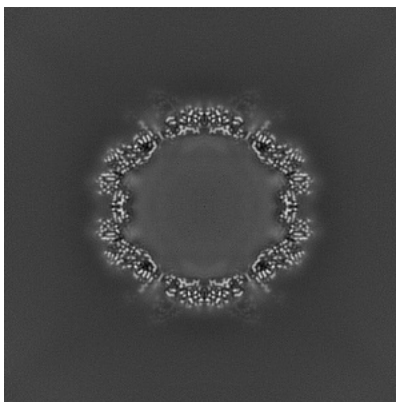


Z Index: 250

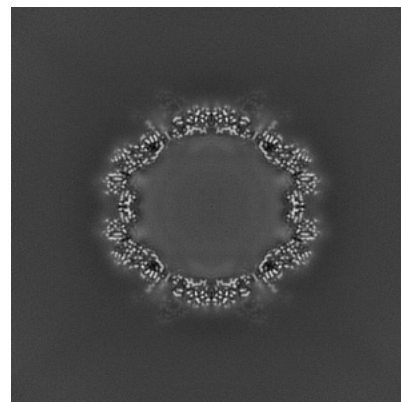
### 6.2.2 Raw map



X Index: 250



Y Index: 250

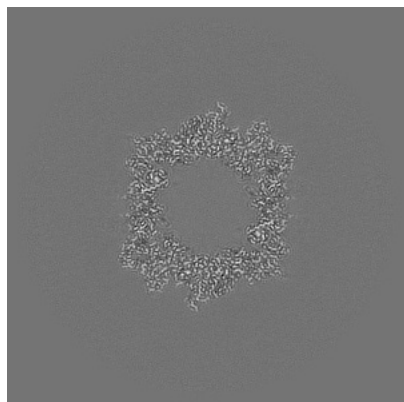


Z Index: 250

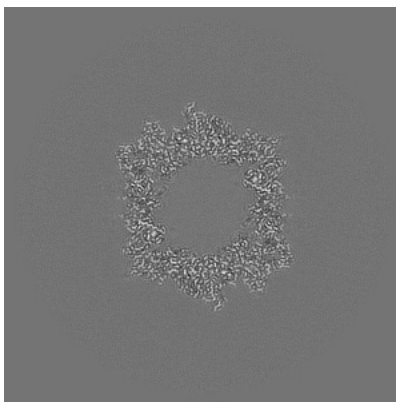
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

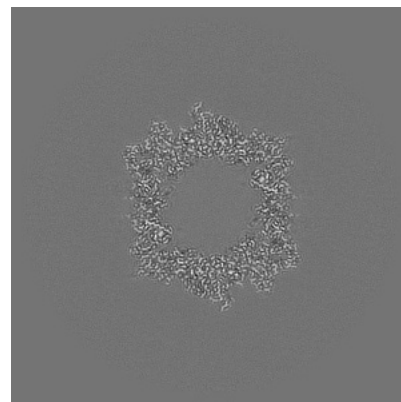
### 6.3.1 Primary map



X Index: 320

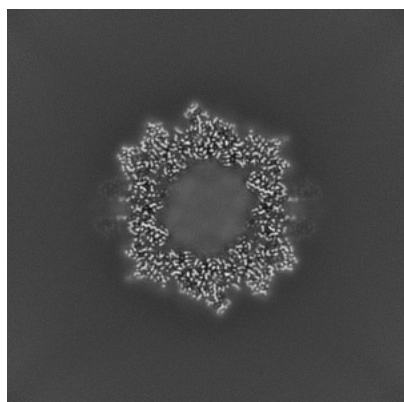


Y Index: 180

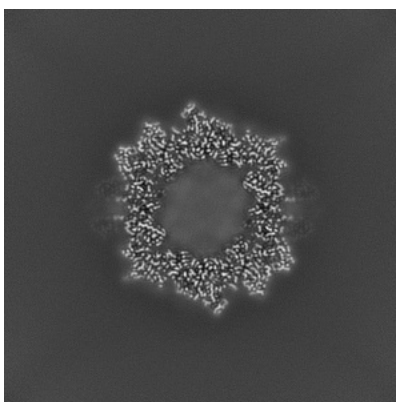


Z Index: 180

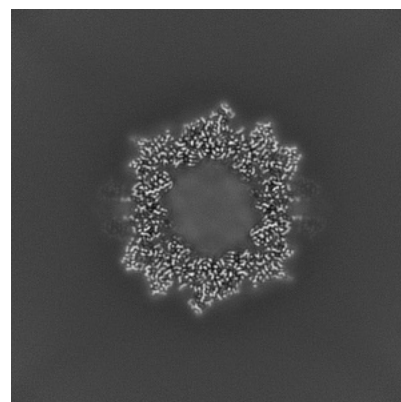
### 6.3.2 Raw map



X Index: 180



Y Index: 180

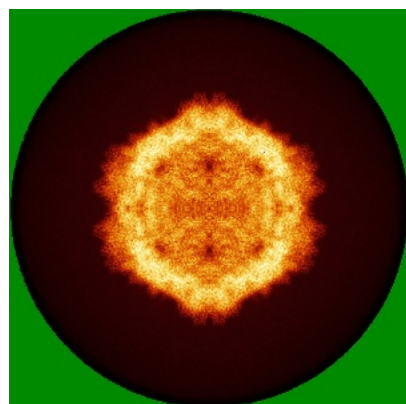


Z Index: 320

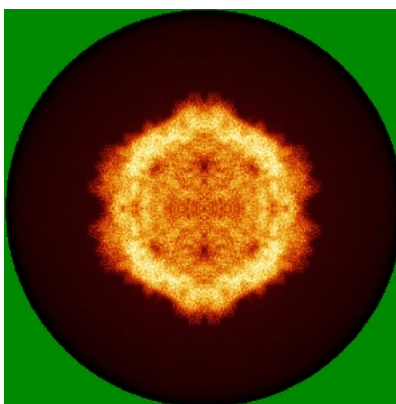
The images above show the largest variance slices of the map in three orthogonal directions.

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

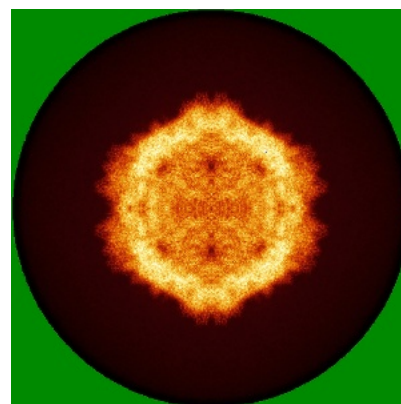
### 6.4.1 Primary map



X

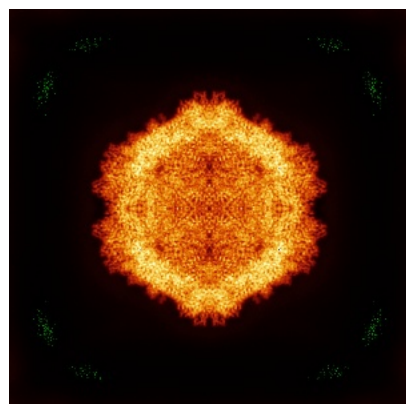


Y

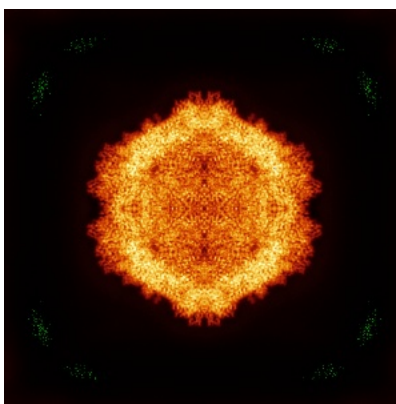


Z

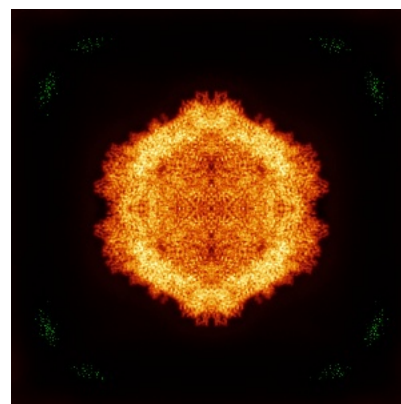
### 6.4.2 Raw map



X



Y

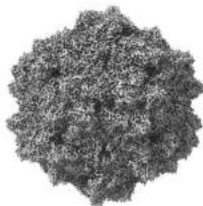


Z

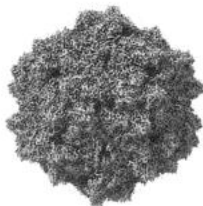
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

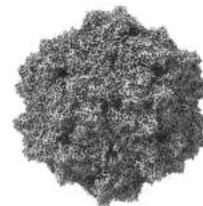
### 6.5.1 Primary map



X



Y



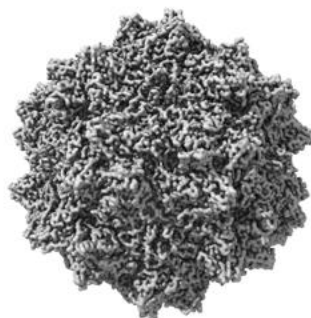
Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. 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



X



Y



Z

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.

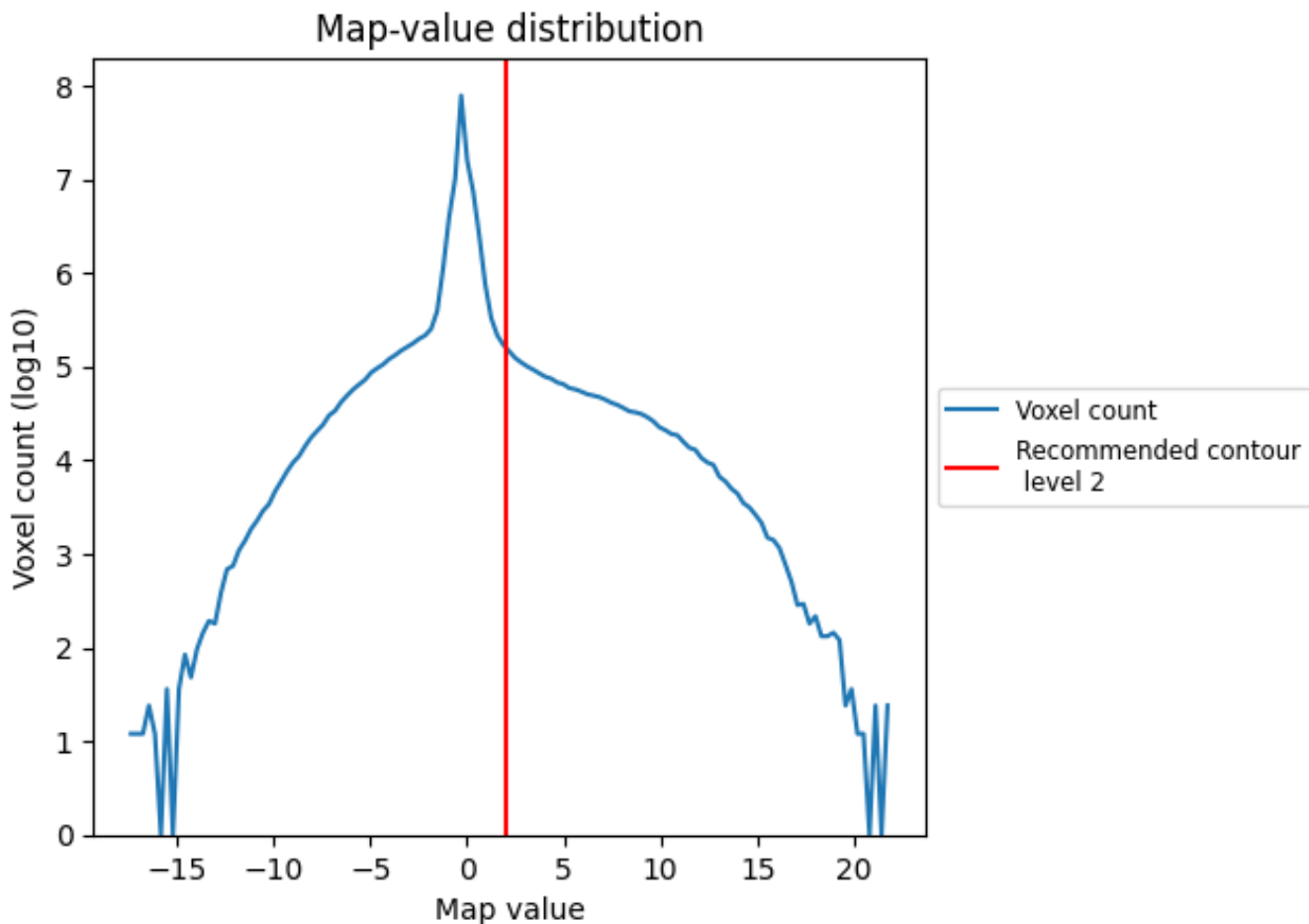
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

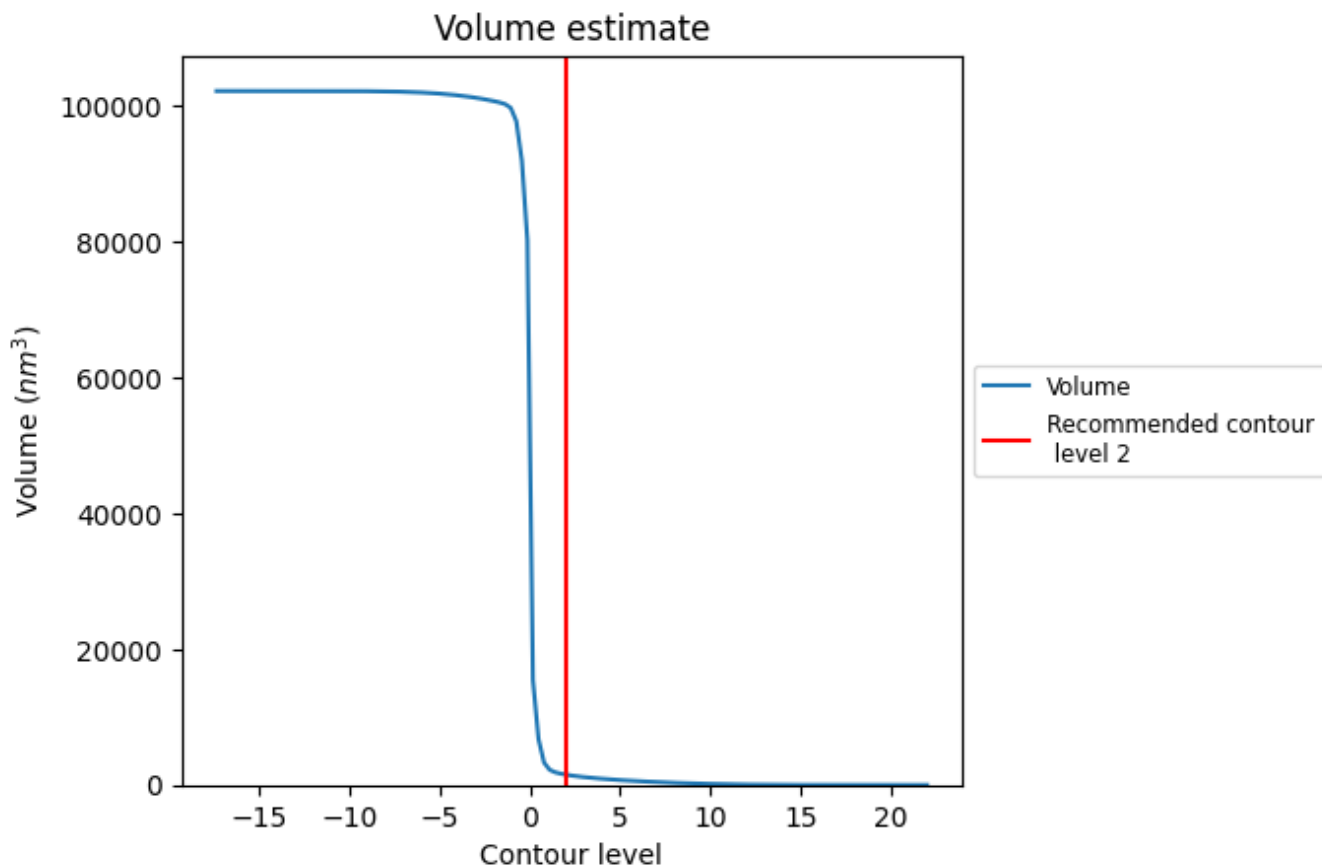
This section contains the results of statistical analysis of the map.

### 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.

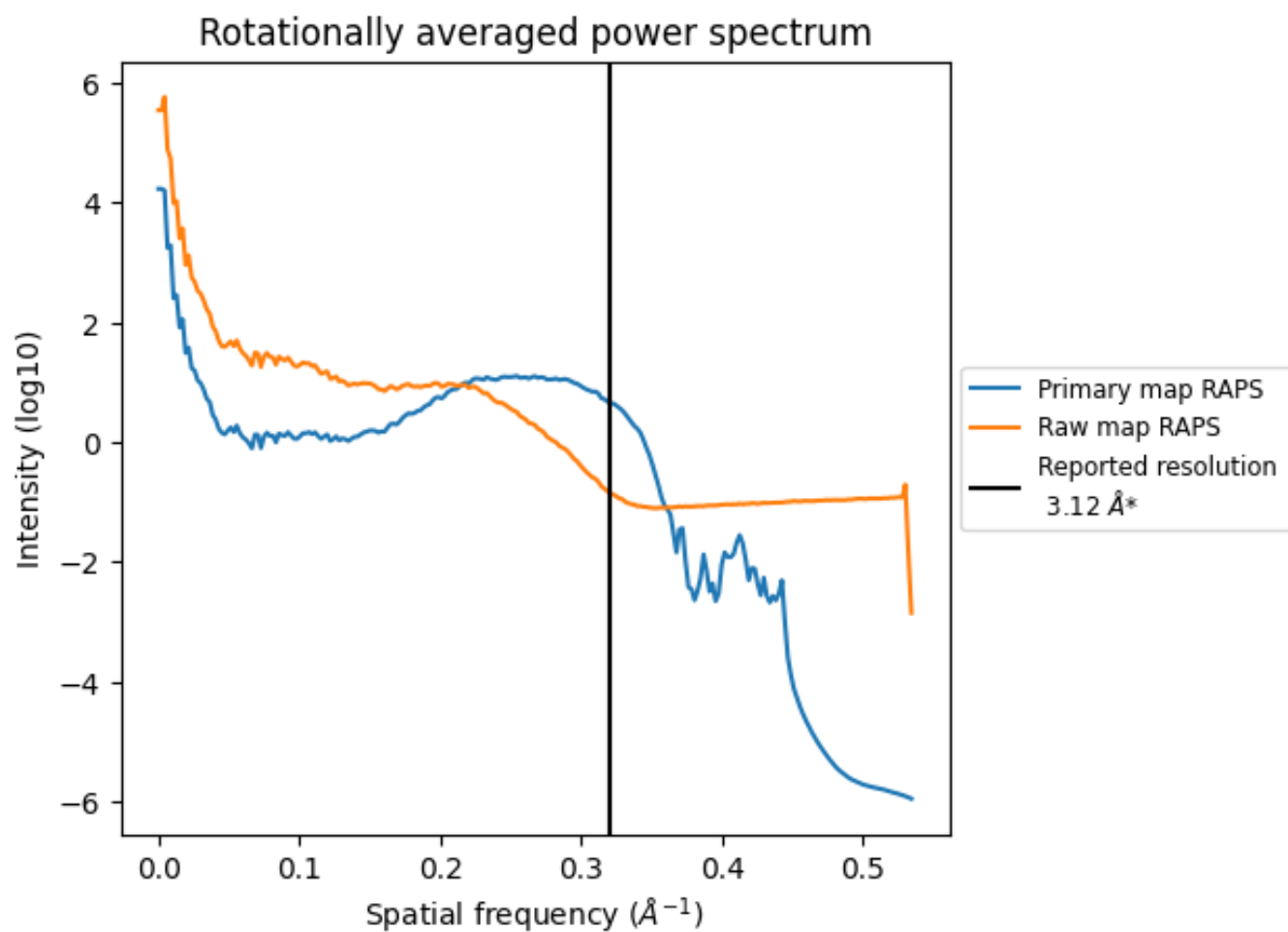
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $1520 \text{ nm}^3$ ; this corresponds to an approximate mass of 1373 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 i

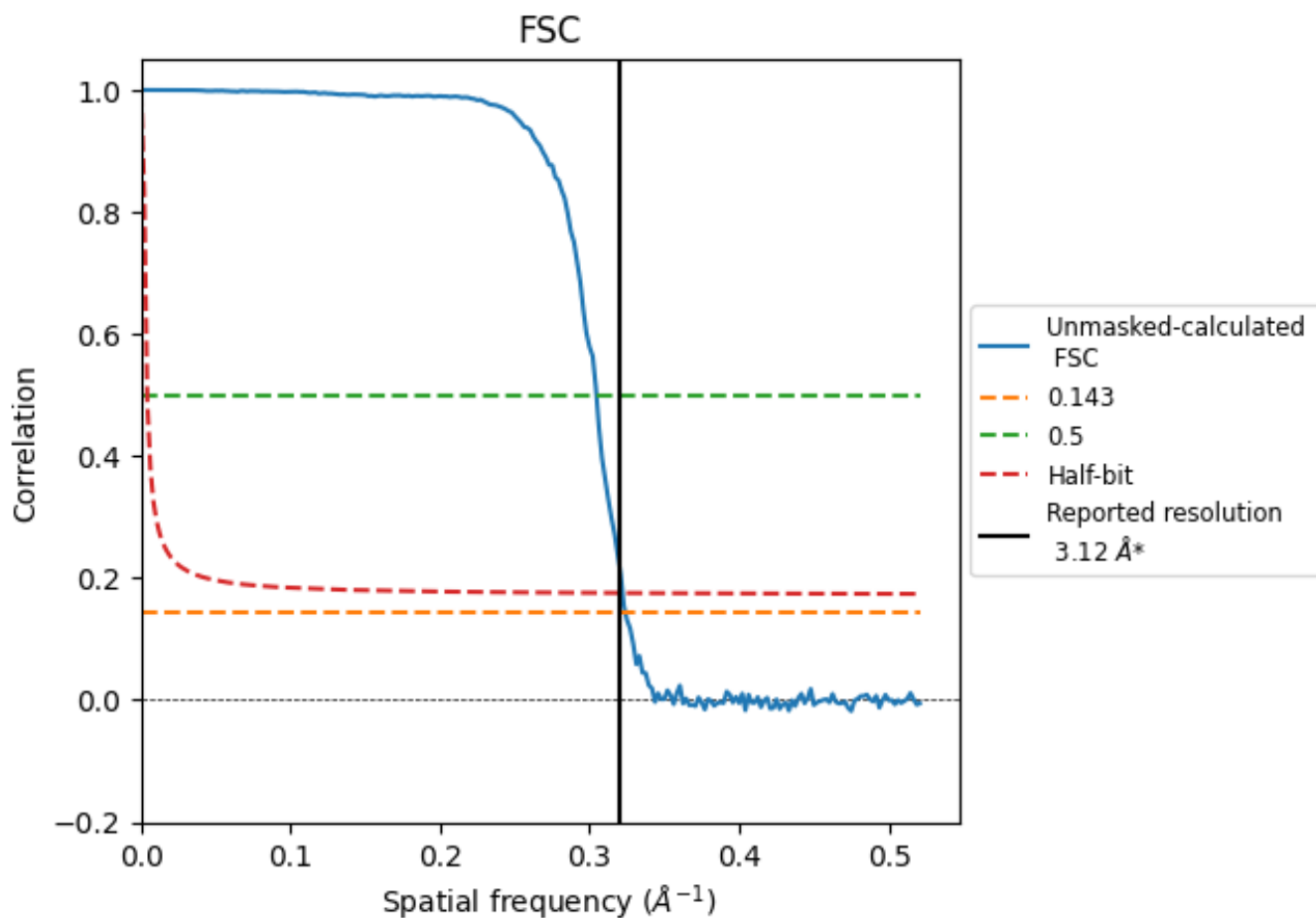


\*Reported resolution corresponds to spatial frequency of 0.321 Å<sup>-1</sup>

## 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  $0.321 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

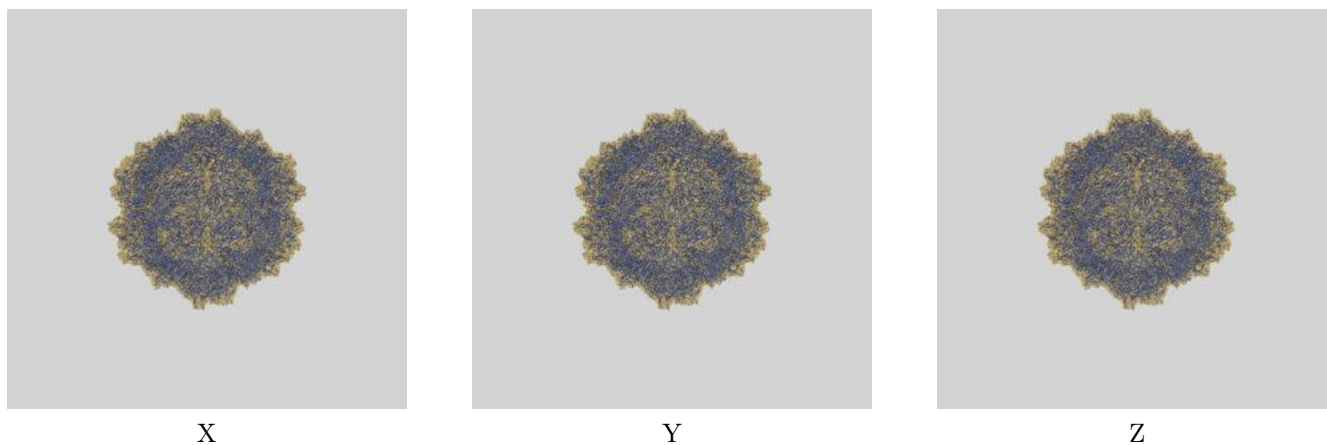
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.12	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.09	3.28	3.10

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

## 9 Map-model fit [i](#)

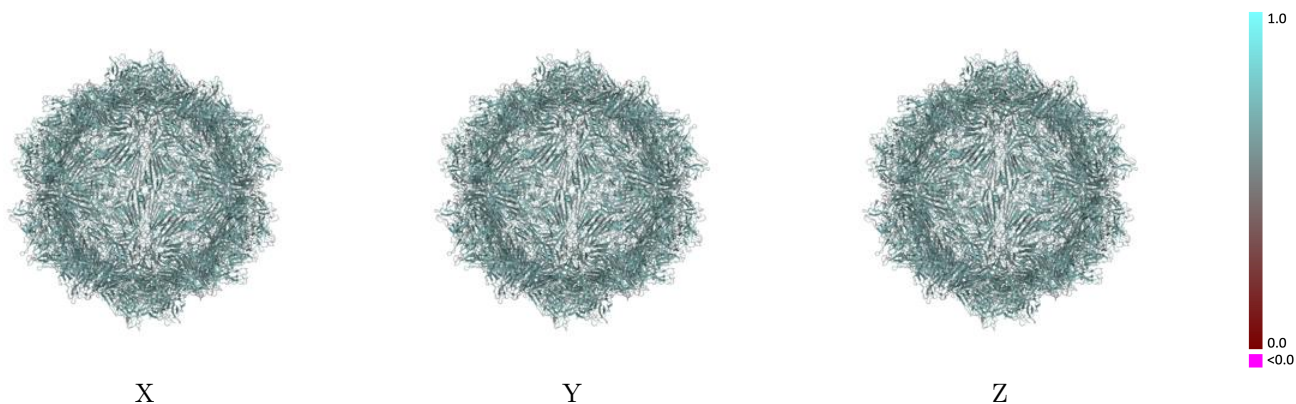
This section contains information regarding the fit between EMDB map EMD-46749 and PDB model 9DCC. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



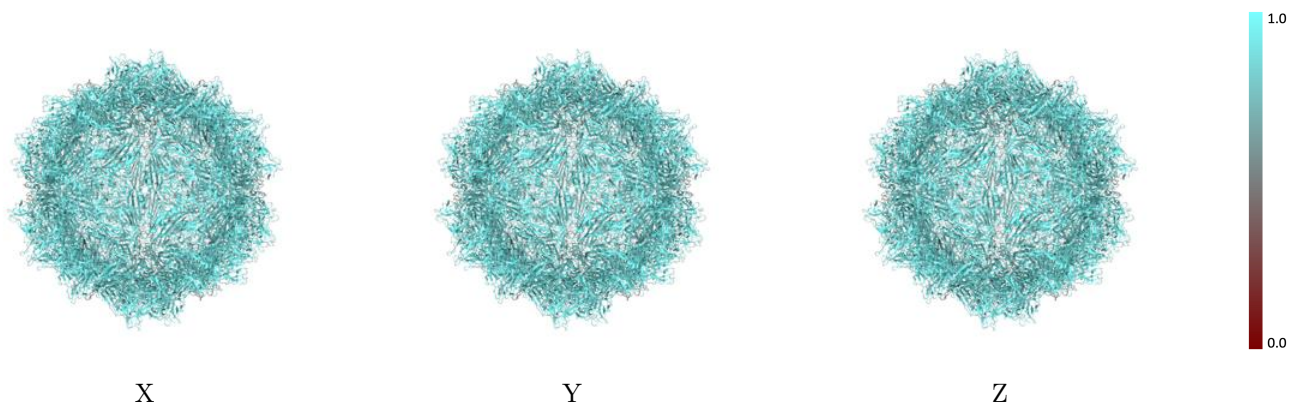
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



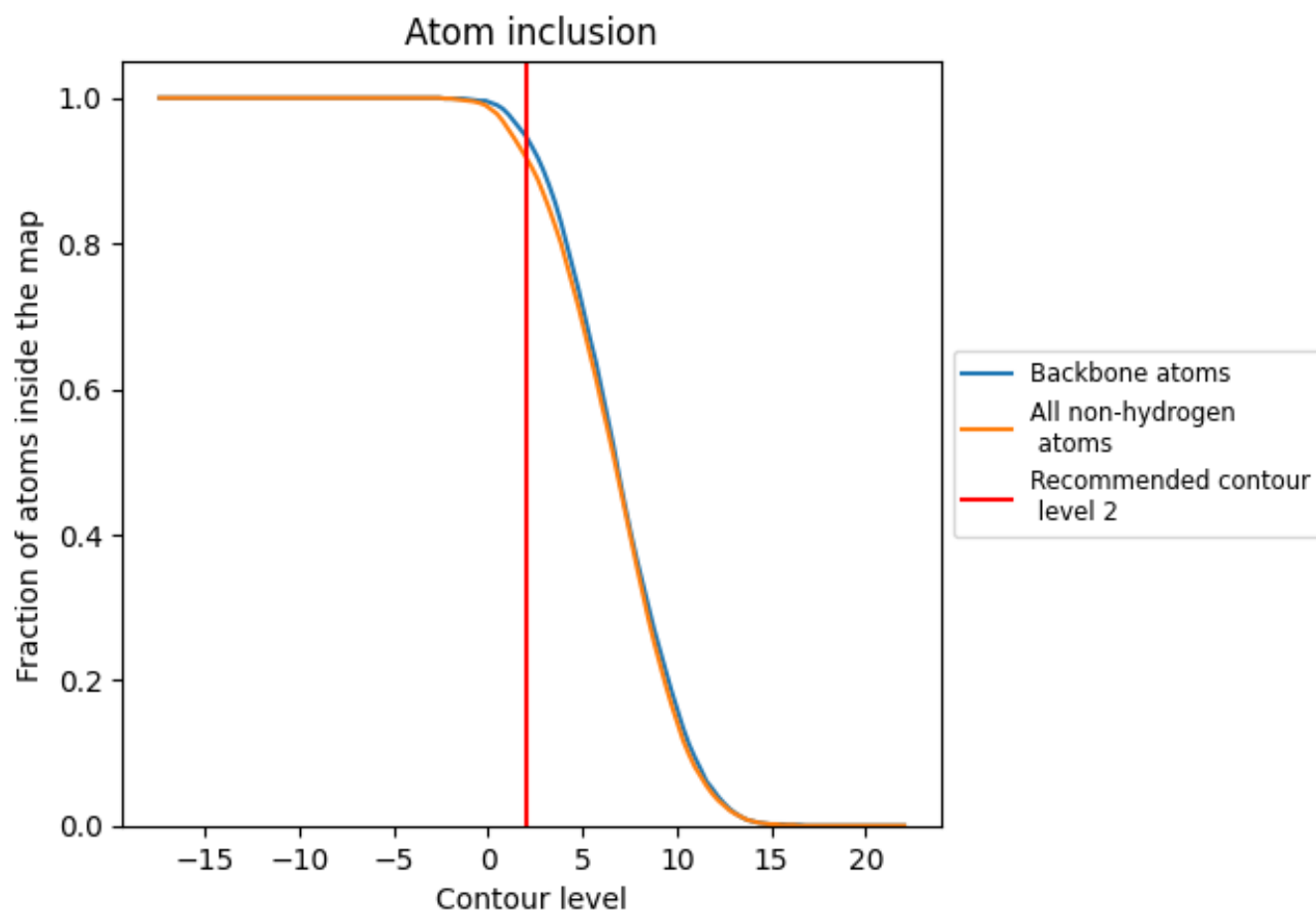
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.6240
0	 0.5480	 0.5410
0A	 0.5480	 0.5400
1	 0.9230	 0.6250
1A	 0.5480	 0.5460
2	 0.9230	 0.6250
2A	 0.5710	 0.5480
3	 0.9230	 0.6250
3A	 0.5710	 0.5540
4	 0.9220	 0.6250
4A	 0.5480	 0.5490
5	 0.9230	 0.6250
5A	 0.5480	 0.5420
6	 0.9230	 0.6250
7	 0.9230	 0.6250
8	 0.9240	 0.6260
9	 0.5950	 0.5400
A	 0.9240	 0.6260
AA	 0.5480	 0.5340
B	 0.9230	 0.6250
BA	 0.5950	 0.5370
C	 0.9220	 0.6240
CA	 0.5710	 0.5560
D	 0.9230	 0.6250
DA	 0.5480	 0.5380
E	 0.9240	 0.6260
EA	 0.5710	 0.5510
F	 0.9240	 0.6250
FA	 0.5480	 0.5420
G	 0.9230	 0.6250
GA	 0.5480	 0.5430
H	 0.9230	 0.6250
HA	 0.5950	 0.5370
I	 0.9220	 0.6250
IA	 0.5950	 0.5400























































































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Chain	Atom inclusion	Q-score
J	 0.9230	 0.6250
JA	 0.5950	 0.5400
K	 0.9220	 0.6240
KA	 0.5480	 0.5400
L	 0.9230	 0.6250
LA	 0.5950	 0.5360
M	 0.9240	 0.6250
MA	 0.5480	 0.5390
N	 0.9230	 0.6250
NA	 0.5480	 0.5470
O	 0.9240	 0.6250
OA	 0.5710	 0.5550
P	 0.9230	 0.6250
PA	 0.5480	 0.5380
Q	 0.9220	 0.6250
QA	 0.5710	 0.5610
R	 0.9230	 0.6250
RA	 0.5480	 0.5440
S	 0.9230	 0.6250
SA	 0.5480	 0.5380
T	 0.9220	 0.6250
TA	 0.5480	 0.5370
U	 0.9230	 0.6260
UA	 0.5480	 0.5390
V	 0.9220	 0.6250
VA	 0.5480	 0.5390
W	 0.9230	 0.6260
WA	 0.5480	 0.5450
X	 0.9240	 0.6250
XA	 0.5480	 0.5420
Y	 0.9230	 0.6250
YA	 0.5480	 0.5430
Z	 0.9240	 0.6260
ZA	 0.5710	 0.5580
a	 0.9240	 0.6250
aA	 0.5480	 0.5310
b	 0.9240	 0.6250
bA	 0.5480	 0.5460
c	 0.9240	 0.6260
cA	 0.5480	 0.5440
d	 0.9240	 0.6250
dA	 0.5710	 0.5590


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Chain	Atom inclusion	Q-score
e	 0.9240	 0.6260
eA	 0.5480	 0.5380
f	 0.9240	 0.6250
fA	 0.5480	 0.5420
g	 0.9220	 0.6250
gA	 0.5480	 0.5460
h	 0.9240	 0.6260
hA	 0.5710	 0.5520
i	 0.9230	 0.6240
iA	 0.5480	 0.5370
j	 0.9230	 0.6250
jA	 0.5950	 0.5350
k	 0.9230	 0.6260
kA	 0.5950	 0.5440
l	 0.9240	 0.6250
lA	 0.5950	 0.5400
m	 0.9220	 0.6250
mA	 0.5710	 0.5530
n	 0.9240	 0.6250
nA	 0.5480	 0.5450
o	 0.9240	 0.6250
oA	 0.5480	 0.5470
p	 0.9220	 0.6250
pA	 0.5710	 0.5540
q	 0.9230	 0.6250
qA	 0.5710	 0.5550
r	 0.9230	 0.6250
rA	 0.5480	 0.5460
s	 0.9230	 0.6250
sA	 0.5480	 0.5390
t	 0.9240	 0.6250
tA	 0.5950	 0.5340
u	 0.9220	 0.6240
uA	 0.5950	 0.5430
v	 0.9240	 0.6250
vA	 0.5950	 0.5340
w	 0.9240	 0.6250
wA	 0.5480	 0.5400
x	 0.9220	 0.6240
xA	 0.5480	 0.5340
y	 0.9240	 0.6250
yA	 0.5480	 0.5380

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Chain	Atom inclusion	Q-score
z	 0.9230	 0.6250
zA	 0.5480	 0.5340