



Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 02:53 AM EDT

PDB ID : 8FZ0
EMDB ID : EMD-29600
Title : Cryo-EM Structure of empty AAV2 capsid
Authors : Bennett, A.D.; McKenna, R.
Deposited on : 2023-01-27
Resolution : 2.94 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:

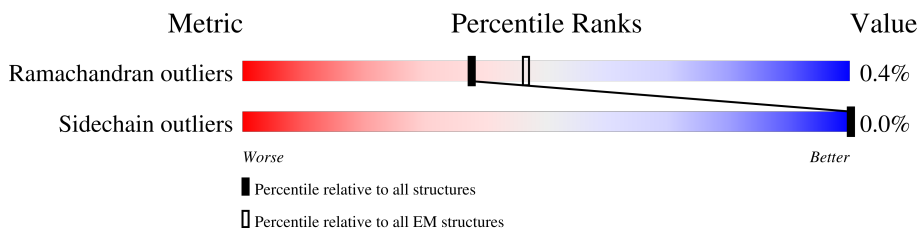
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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 2.94 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.




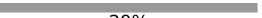






















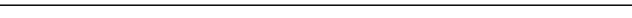
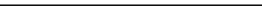




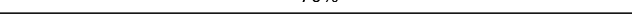
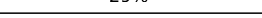
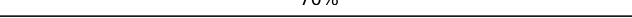
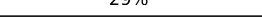


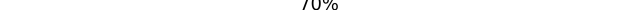
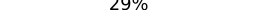
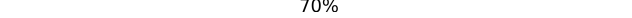
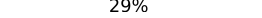
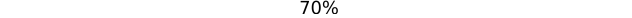
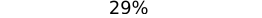
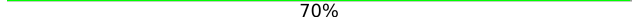

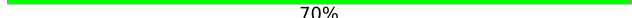
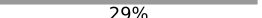
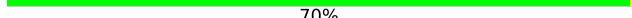
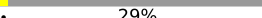
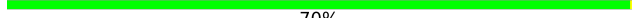

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1	735	70% 29%
1	2	735	70% 29%
1	3	735	70% 29%
1	4	735	70% 29%
1	5	735	70% 29%
1	6	735	70% 29%
1	7	735	70% 29%
1	8	735	70% 29%
1	A	735	70% 29%


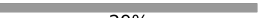






















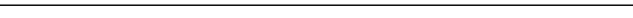
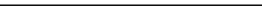




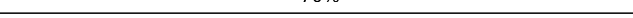
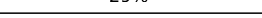
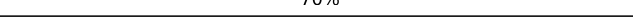
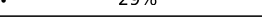

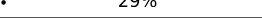
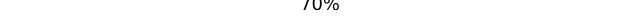
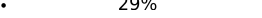
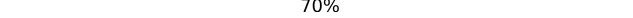
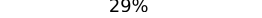
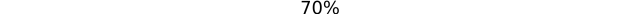
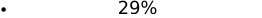
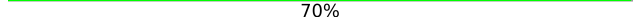

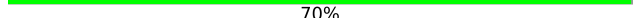
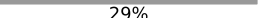
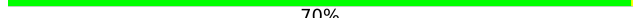
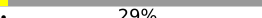
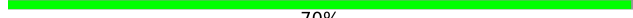
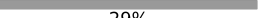
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	B	735	 70%	 29%
1	C	735	 70%	 29%
1	D	735	 70%	 29%
1	E	735	 70%	 29%
1	F	735	 70%	 29%
1	G	735	 70%	 29%
1	H	735	 70%	 29%
1	I	735	 70%	 29%
1	J	735	 70%	 29%
1	K	735	 70%	 29%
1	L	735	 70%	 29%
1	M	735	 70%	 29%
1	N	735	 70%	 29%
1	O	735	 70%	 29%
1	P	735	 70%	 29%
1	Q	735	 70%	 29%
1	R	735	 70%	 29%
1	S	735	 70%	 29%
1	T	735	 70%	 29%
1	U	735	 70%	 29%
1	V	735	 70%	 29%
1	W	735	 70%	 29%
1	X	735	 70%	 29%
1	Y	735	 70%	 29%
1	Z	735	 70%	 29%


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	a	735	 70%	 29%
1	b	735	 70%	 29%
1	c	735	 70%	 29%
1	d	735	 70%	 29%
1	e	735	 70%	 29%
1	f	735	 70%	 29%
1	g	735	 70%	 29%
1	h	735	 70%	 29%
1	i	735	 70%	 29%
1	j	735	 70%	 29%
1	k	735	 70%	 29%
1	l	735	 70%	 29%
1	m	735	 70%	 29%
1	n	735	 70%	 29%
1	o	735	 70%	 29%
1	p	735	 70%	 29%
1	q	735	 70%	 29%
1	r	735	 70%	 29%
1	s	735	 70%	 29%
1	t	735	 70%	 29%
1	u	735	 70%	 29%
1	v	735	 70%	 29%
1	w	735	 70%	 29%
1	x	735	 70%	 29%
1	y	735	 70%	 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	z	735	 70% 29%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 250080 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	519	4168	2621	732	802	13	3	0
1	B	519	4168	2621	732	802	13	3	0
1	C	519	4168	2621	732	802	13	3	0
1	D	519	4168	2621	732	802	13	3	0
1	E	519	4168	2621	732	802	13	3	0
1	F	519	4168	2621	732	802	13	3	0
1	G	519	4168	2621	732	802	13	3	0
1	H	519	4168	2621	732	802	13	3	0
1	I	519	4168	2621	732	802	13	3	0
1	J	519	4168	2621	732	802	13	3	0
1	K	519	4168	2621	732	802	13	3	0
1	L	519	4168	2621	732	802	13	3	0
1	M	519	4168	2621	732	802	13	3	0
1	N	519	4168	2621	732	802	13	3	0
1	O	519	4168	2621	732	802	13	3	0
1	P	519	4168	2621	732	802	13	3	0
1	Q	519	4168	2621	732	802	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	S	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	T	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	U	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	V	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	W	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	X	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	Y	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	Z	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	a	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	b	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	c	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	d	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	e	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	f	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	g	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	h	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	i	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	j	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	k	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	l	519	Total 4168	C 2621	N 732	O 802	S 13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	n	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	o	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	p	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	q	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	r	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	s	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	t	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	u	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	v	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	w	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	x	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	y	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	z	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	1	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	2	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	3	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	4	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	5	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	6	519	Total 4168	C 2621	N 732	O 802	S 13	3	0
1	7	519	Total 4168	C 2621	N 732	O 802	S 13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	519	4168	2621	732	802	13	3	0

Chain b:  70% 29%

Sequence listing for Chain b showing amino acid residues and highlighted mutations: G217 (green), V221 (yellow), R298 (red), I470 (yellow), V600 (yellow), H629 (yellow), and L735 (green).

• Molecule 1: Capsid protein VP1

Chain c:  70% 29%

Sequence listing for Chain c showing amino acid residues and highlighted mutations: G217 (green), V221 (yellow), I470 (yellow), V600 (yellow), and L735 (green).

• Molecule 1: Capsid protein VP1

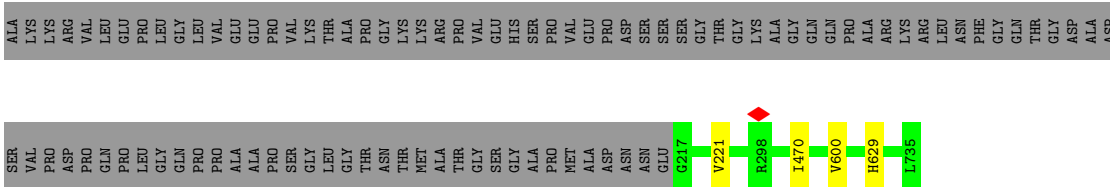
Chain d:  70% 29%

Sequence listing for Chain d showing amino acid residues and highlighted mutations: G217 (green), V221 (yellow), I470 (yellow), V600 (yellow), and L735 (green).

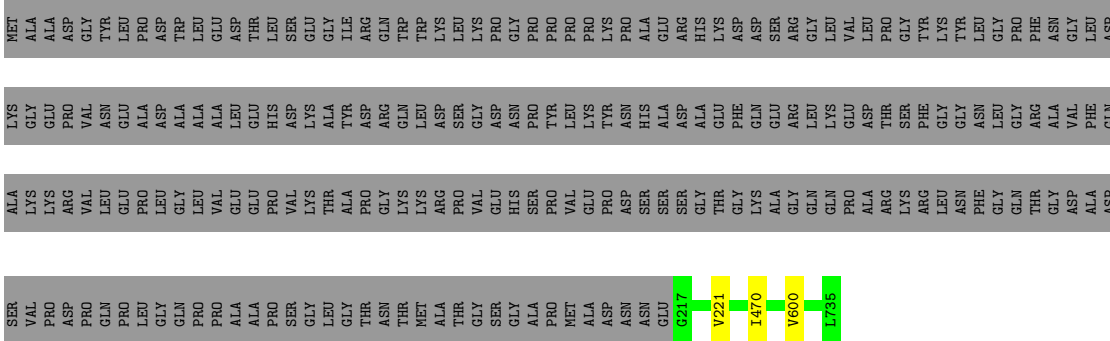
• Molecule 1: Capsid protein VP1

Chain e:  70% 29%

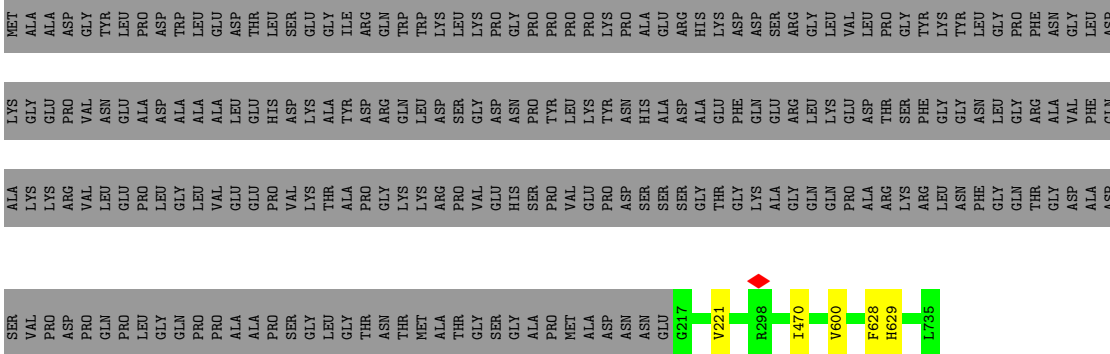
Sequence listing for Chain e showing amino acid residues and highlighted mutations: G217 (green), V221 (yellow), I470 (yellow), V600 (yellow), and L735 (green).



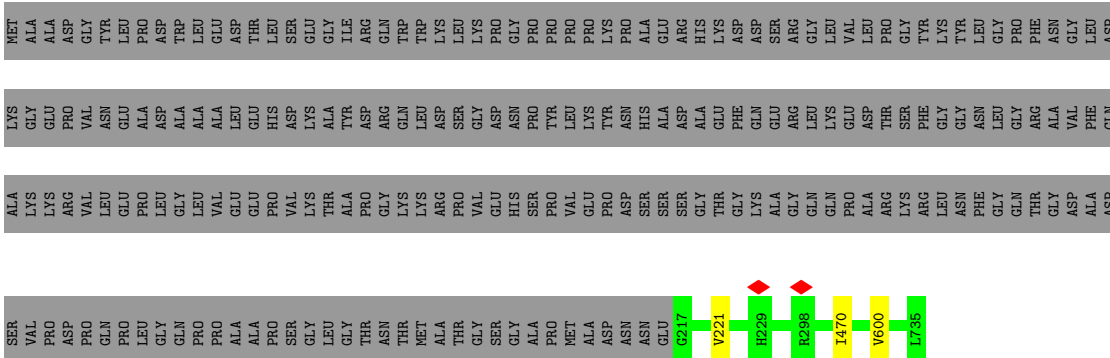
● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



MET	ALA	ALA	ASP	ASP	TRP	LEU	ASP	THR	GLU	ASP	THR	ILE	ARG	GLN	TRP	TRP	LYS	LYS	PRO	LYS	PRO	PRO	ALA	GLU	ARG	HIS	LYS	ASP	ASP	GLY	VAL	LEU	LEU	PRO	VAL	LEU	GLY	LEU	LEU	LEU	TYR	LYS	GLY	LEU	LEU	ASP	ASP	ASP	
LYS	GLY	PRO	ASP	ASP	ALA	GLU	ALA	GLU	GLY	HIS	ASP	ALA	TYR	ASP	ARG	GLN	LYS	TRP	LYS	LYS	PRO	PRO	PRO	PRO	LEU	ALA	GLY	THR	LEU	VAL	VAL	VAL	GLY	LEU	GLY	LEU	LEU	LEU	GLY	TYR	LEU	LEU	ASP	PHE	ARG	GLY	VAL	PHE	GLN
ALA	LYS	LYS	ARG	VAL	GLY	PRO	LEU	GLU	VAL	PRO	GLU	THR	ALA	PRO	GLY	LYS	ARG	VAL	VAL	VAL	PRO	PRO	PRO	VAL	VAL	GLY	THR	LEU	GLY	GLN	PRO	VAL	ARG	ALA	ALA	ARG	LYS	LYS	ARG	LEU	ASN	ASN	GLY	VAL	PHE	ARG	ASP	ASP	
SER	VAL	PRO	PRO	GLN	LEU	LEU	GLY	PRO	PRO	PRO	PRO	GLY	THR	ASP	ASN	THR	MET	LYS	ALA	ALA	THR	GLY	THR	VAL	GLY	SER	GLY	THR	THR	G217	V221	I470	V600	L735															

- Molecule 1: Capsid protein VP1



MET	ALA	ALA	ASP	ASP	TRP	LEU	ASP	THR	GLU	ASP	THR	ILE	ARG	GLN	TRP	TRP	LYS	LYS	PRO	LYS	PRO	PRO	ALA	GLU	ARG	HIS	LYS	ASP	ASP	GLY	VAL	LEU	LEU	PRO	VAL	LEU	LEU	LEU	GLY	TYR	LYS	GLY	LEU	LEU	ASP	ASP	ASP				
LYS	GLY	PRO	ASP	ASP	ALA	GLU	ALA	GLU	GLY	HIS	ASP	ALA	TYR	ASP	ARG	GLN	LYS	TRP	LYS	LYS	PRO	PRO	PRO	PRO	LEU	ALA	GLY	THR	LEU	VAL	VAL	VAL	GLY	LEU	GLY	LEU	LEU	LEU	GLY	TYR	LEU	LEU	ASP	PHE	ARG	GLY	VAL	PHE	GLN		
ALA	LYS	LYS	ARG	VAL	GLY	PRO	LEU	GLU	VAL	PRO	GLU	THR	ALA	PRO	GLY	LYS	ARG	VAL	VAL	VAL	PRO	PRO	PRO	VAL	VAL	GLY	THR	LEU	GLY	GLN	PRO	VAL	ARG	ALA	ALA	ARG	LYS	LYS	ARG	LEU	ASN	ASN	GLY	VAL	PHE	ARG	ASP	ASP			
SER	VAL	PRO	PRO	GLN	LEU	LEU	GLY	PRO	PRO	PRO	PRO	GLY	THR	ASP	ASN	THR	MET	LYS	ALA	ALA	THR	GLY	THR	VAL	GLY	SER	GLY	THR	THR	G217	V221	R298	I470	V600	F628	H629	L735														

- Molecule 1: Capsid protein VP1

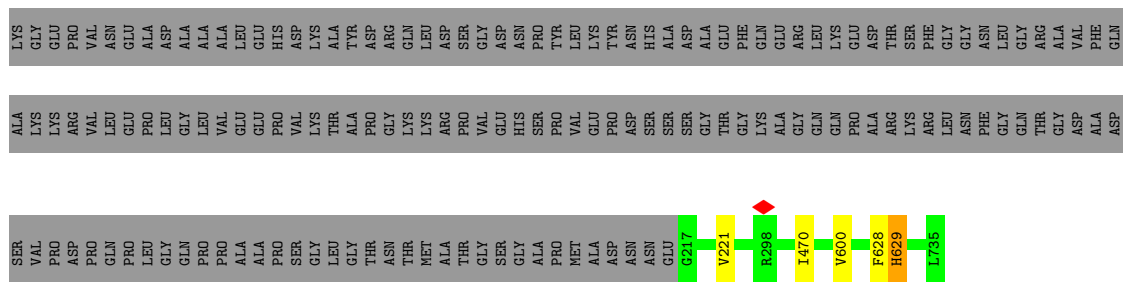


MET	ALA	ALA	ASP	ASP	TRP	LEU	ASP	THR	GLU	ASP	THR	ILE	ARG	GLN	TRP	TRP	LYS	LYS	PRO	LYS	PRO	PRO	ALA	GLU	ARG	HIS	LYS	ASP	ASP	GLY	VAL	LEU	LEU	PRO	VAL	LEU	LEU	LEU	GLY	TYR	LYS	GLY	LEU	LEU	ASP	ASP	ASP							
LYS	GLY	PRO	ASP	ASP	ALA	GLU	ALA	GLU	GLY	HIS	ASP	ALA	TYR	ASP	ARG	GLN	LYS	TRP	LYS	LYS	PRO	PRO	PRO	PRO	LEU	ALA	GLY	THR	LEU	VAL	VAL	VAL	GLY	LEU	GLY	LEU	LEU	LEU	GLY	TYR	LEU	LEU	ASP	PHE	ARG	GLY	VAL	PHE	GLN					
ALA	LYS	LYS	ARG	VAL	GLY	PRO	LEU	GLU	VAL	PRO	GLU	THR	ALA	PRO	GLY	LYS	ARG	VAL	VAL	VAL	PRO	PRO	PRO	VAL	VAL	GLY	THR	LEU	GLY	GLN	PRO	VAL	ARG	ALA	ALA	ARG	LYS	LYS	ARG	LEU	ASN	ASN	GLY	VAL	PHE	ARG	ASP	ASP						
SER	VAL	PRO	PRO	GLN	LEU	LEU	GLY	PRO	PRO	PRO	PRO	GLY	THR	ASP	ASN	THR	MET	LYS	ALA	ALA	THR	GLY	THR	VAL	GLY	SER	GLY	THR	THR	G217	V221	R298	I470	V600	H629	L735																		

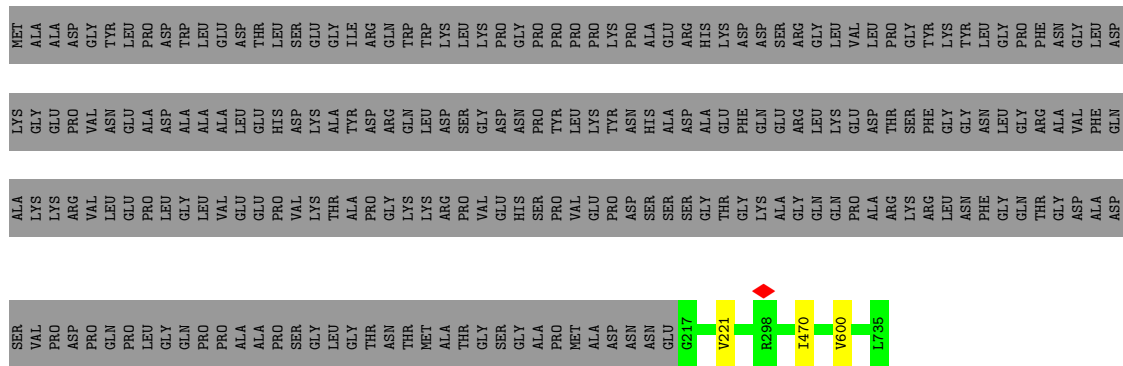
- Molecule 1: Capsid protein VP1



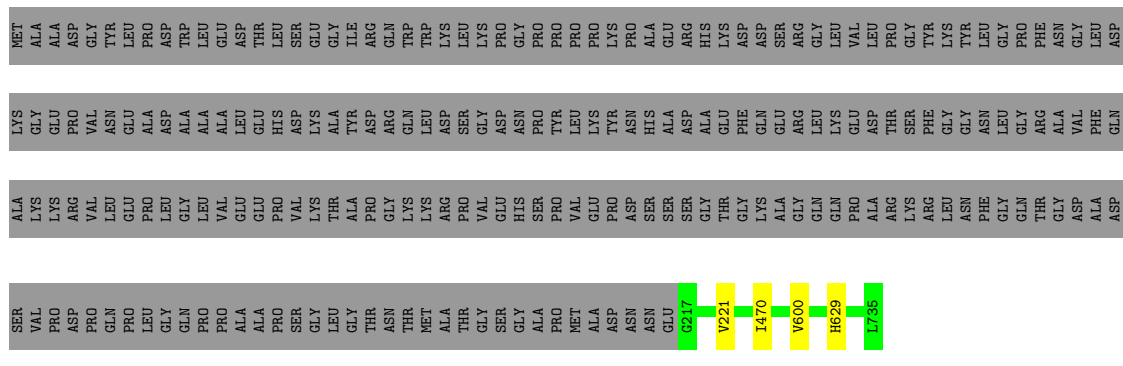
MET	ALA	ALA	ASP	ASP	TRP	LEU	ASP	THR	GLU	ASP	THR	ILE	ARG	GLN	TRP	TRP	LYS	LYS	PRO	LYS	PRO	PRO	ALA	GLU	ARG	HIS	LYS	ASP	ASP	GLY	VAL	LEU	LEU	PRO	VAL	LEU	LEU	LEU	GLY	TYR	LYS	GLY	LEU	LEU	ASP	ASP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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



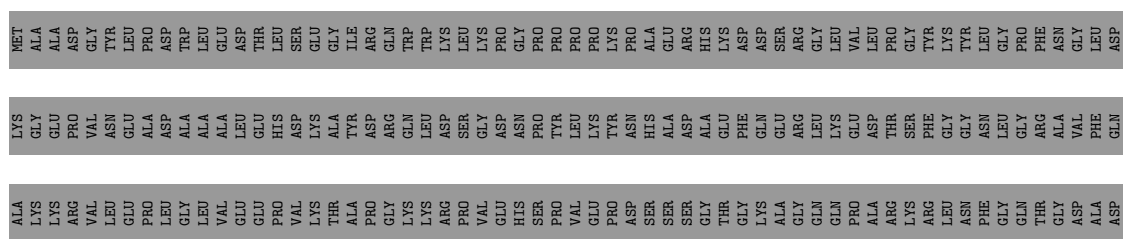
● Molecule 1: Capsid protein VP1

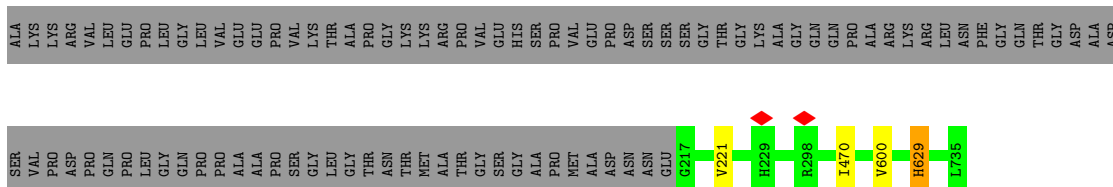


● Molecule 1: Capsid protein VP1

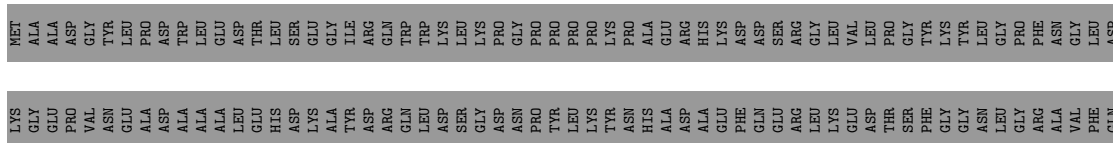


● Molecule 1: Capsid protein VP1

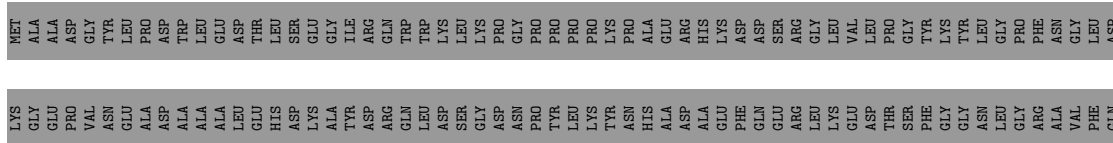




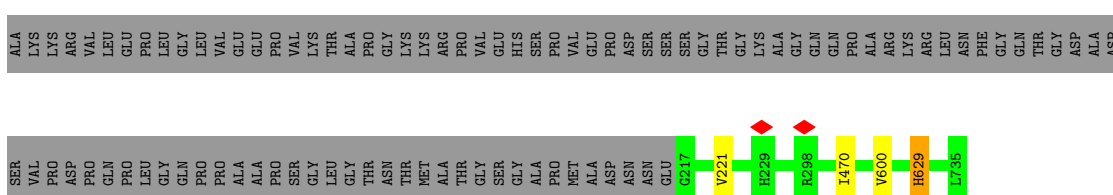
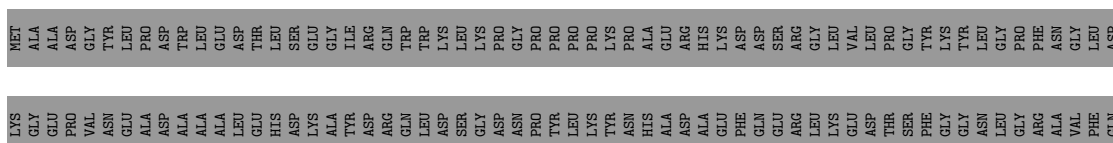
● Molecule 1: Capsid protein VP1

Chain w:  70% 29%

● Molecule 1: Capsid protein VP1

Chain x:  70% 29%

● Molecule 1: Capsid protein VP1

Chain y:  70% 29%

LYS GLY LEU PRO ARG VAL ASN GLU ALA ASP LEU ALA LEU VAL GLU GLU HIS PRO VAL SER LYS LYS ALA TYR ASP ARG GLY LEU GLY SER VAL SER GLY LEU GLY ALA GLY THR	ALA LYS LYS ARG VAL VAL LEU PRO GLU LEU ALA LEU VAL VAL GLU GLU HIS PRO VAL SER VAL SER LYS LYS ALA TYR ASP ARG GLY LEU GLY SER VAL SER GLY LEU GLY ALA GLY THR	SER VAL PRO ASP PRO GLN PRO LEU GLY PRO PRO ALA ALA GLU THR
--	--	---

● Molecule 1: Capsid protein VP1



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

● Molecule 1: Capsid protein VP1

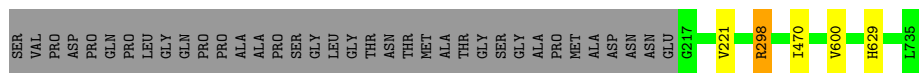


MET ALA LYS LYS ASP GLY TYR LEU PRO LEU ASP GLY TRP LEU TRP GLU GLU HIS PRO VAL SER VAL SER GLY GLY ILE ARG GLY GLN TRP TRP LYS LYS LEU SER LEU LYS LEU SER THR	LYS GLY GLU PRO VAL ASN GLU ALA LEU TRP ALA LEU VAL VAL GLU GLU HIS PRO VAL SER VAL SER GLY GLY ILE ARG GLY GLN TRP TRP LYS LYS LEU SER LEU LYS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

● Molecule 1: Capsid protein VP1

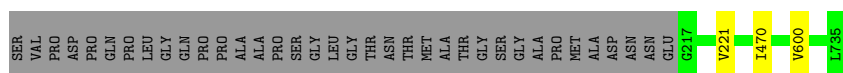
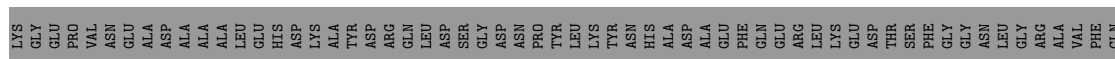


MET ALA LYS LYS ASP GLY TYR LEU PRO LEU ASP GLY TRP LEU TRP GLU GLU HIS PRO VAL SER VAL SER GLY GLY ILE ARG GLY GLN TRP TRP LYS LYS LEU SER LEU LYS LEU SER THR	LYS GLY GLU PRO VAL ASN GLU ALA LEU TRP ALA LEU VAL VAL GLU GLU HIS PRO VAL SER VAL SER GLY GLY ILE ARG GLY GLN TRP TRP LYS LYS LEU SER LEU LYS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



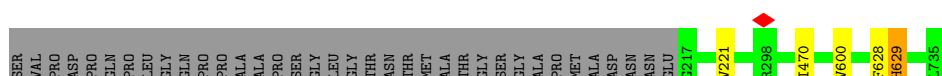
• Molecule 1: Capsid protein VP1

Chain 7: 70% 29%



• Molecule 1: Capsid protein VP1

Chain 8: 70% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	11.436	Depositor
Minimum map value	-7.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (\AA)	351.68, 351.68, 351.68	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.099, 1.099, 1.099	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	0.46	1/4308 (0.0%)	0.61	1/5872 (0.0%)
1	2	0.45	2/4308 (0.0%)	0.59	1/5872 (0.0%)
1	3	0.46	0/4308	0.59	1/5872 (0.0%)
1	4	0.45	0/4308	0.59	1/5872 (0.0%)
1	5	0.46	0/4308	0.61	4/5872 (0.1%)
1	6	0.47	2/4308 (0.0%)	0.60	1/5872 (0.0%)
1	7	0.45	0/4308	0.59	1/5872 (0.0%)
1	8	0.47	3/4308 (0.1%)	0.60	1/5872 (0.0%)
1	A	0.44	0/4308	0.59	1/5872 (0.0%)
1	B	0.43	0/4308	0.58	1/5872 (0.0%)
1	C	0.44	0/4308	0.58	1/5872 (0.0%)
1	D	0.45	0/4308	0.59	1/5872 (0.0%)
1	E	0.44	0/4308	0.59	2/5872 (0.0%)
1	F	0.44	0/4308	0.59	2/5872 (0.0%)
1	G	0.44	0/4308	0.59	2/5872 (0.0%)
1	H	0.43	0/4308	0.58	1/5872 (0.0%)
1	I	0.44	0/4308	0.59	1/5872 (0.0%)
1	J	0.45	0/4308	0.59	1/5872 (0.0%)
1	K	0.44	0/4308	0.59	1/5872 (0.0%)
1	L	0.44	0/4308	0.59	1/5872 (0.0%)
1	M	0.44	0/4308	0.58	1/5872 (0.0%)
1	N	0.46	3/4308 (0.1%)	0.59	1/5872 (0.0%)
1	O	0.44	0/4308	0.59	1/5872 (0.0%)
1	P	0.43	0/4308	0.58	1/5872 (0.0%)
1	Q	0.44	0/4308	0.59	1/5872 (0.0%)
1	R	0.43	0/4308	0.58	1/5872 (0.0%)
1	S	0.45	0/4308	0.59	1/5872 (0.0%)
1	T	0.44	0/4308	0.58	1/5872 (0.0%)
1	U	0.44	0/4308	0.59	1/5872 (0.0%)
1	V	0.44	0/4308	0.58	1/5872 (0.0%)
1	W	0.45	0/4308	0.59	1/5872 (0.0%)
1	X	0.44	0/4308	0.58	1/5872 (0.0%)
1	Y	0.46	3/4308 (0.1%)	0.59	1/5872 (0.0%)
1	Z	0.44	0/4308	0.59	1/5872 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.45	0/4308	0.59	1/5872 (0.0%)
1	b	0.46	0/4308	0.60	1/5872 (0.0%)
1	c	0.45	0/4308	0.60	1/5872 (0.0%)
1	d	0.45	0/4308	0.59	1/5872 (0.0%)
1	e	0.46	0/4308	0.60	1/5872 (0.0%)
1	f	0.45	0/4308	0.60	1/5872 (0.0%)
1	g	0.47	1/4308 (0.0%)	0.60	1/5872 (0.0%)
1	h	0.45	0/4308	0.59	1/5872 (0.0%)
1	i	0.45	0/4308	0.59	1/5872 (0.0%)
1	j	0.46	0/4308	0.61	4/5872 (0.1%)
1	k	0.47	2/4308 (0.0%)	0.60	1/5872 (0.0%)
1	l	0.47	3/4308 (0.1%)	0.60	1/5872 (0.0%)
1	m	0.45	0/4308	0.59	1/5872 (0.0%)
1	n	0.46	0/4308	0.59	1/5872 (0.0%)
1	o	0.45	0/4308	0.59	1/5872 (0.0%)
1	p	0.47	1/4308 (0.0%)	0.60	1/5872 (0.0%)
1	q	0.46	1/4308 (0.0%)	0.61	1/5872 (0.0%)
1	r	0.45	2/4308 (0.0%)	0.60	1/5872 (0.0%)
1	s	0.45	0/4308	0.59	1/5872 (0.0%)
1	t	0.46	2/4308 (0.0%)	0.60	3/5872 (0.1%)
1	u	0.45	0/4308	0.60	1/5872 (0.0%)
1	v	0.46	0/4308	0.61	3/5872 (0.1%)
1	w	0.46	2/4308 (0.0%)	0.60	3/5872 (0.1%)
1	x	0.45	0/4308	0.60	1/5872 (0.0%)
1	y	0.46	0/4308	0.61	3/5872 (0.1%)
1	z	0.45	0/4308	0.59	1/5872 (0.0%)
All	All	0.45	28/258480 (0.0%)	0.59	77/352320 (0.0%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8	628	PHE	C-N	-5.82	1.20	1.34
1	l	628	PHE	C-N	-5.82	1.20	1.34
1	2	298[A]	ARG	CB-CG	-5.41	1.38	1.52
1	2	298[B]	ARG	CB-CG	-5.41	1.38	1.52
1	r	298[A]	ARG	CB-CG	-5.40	1.38	1.52
1	r	298[B]	ARG	CB-CG	-5.40	1.38	1.52
1	t	298[A]	ARG	CB-CG	-5.36	1.38	1.52
1	t	298[B]	ARG	CB-CG	-5.36	1.38	1.52
1	w	298[A]	ARG	CB-CG	-5.36	1.38	1.52
1	w	298[B]	ARG	CB-CG	-5.36	1.38	1.52
1	g	628	PHE	C-N	-5.33	1.21	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	p	628	PHE	C-N	-5.33	1.21	1.34
1	6	298[A]	ARG	CB-CG	-5.12	1.38	1.52
1	6	298[B]	ARG	CB-CG	-5.12	1.38	1.52
1	k	298[A]	ARG	CB-CG	-5.11	1.38	1.52
1	k	298[B]	ARG	CB-CG	-5.11	1.38	1.52
1	N	628	PHE	C-N	-5.09	1.22	1.34
1	Y	628	PHE	C-N	-5.09	1.22	1.34
1	1	628	PHE	C-N	-5.06	1.22	1.34
1	q	628	PHE	C-N	-5.05	1.22	1.34
1	Y	629[A]	HIS	C-N	-5.04	1.24	1.34
1	Y	629[B]	HIS	C-N	-5.04	1.24	1.34
1	l	629[A]	HIS	C-N	-5.03	1.24	1.34
1	l	629[B]	HIS	C-N	-5.03	1.24	1.34
1	8	629[A]	HIS	C-N	-5.03	1.24	1.34
1	8	629[B]	HIS	C-N	-5.03	1.24	1.34
1	N	629[A]	HIS	C-N	-5.01	1.24	1.34
1	N	629[B]	HIS	C-N	-5.01	1.24	1.34

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	629[A]	HIS	N-CA-C	-5.86	95.18	111.00
1	j	629[B]	HIS	N-CA-C	-5.86	95.18	111.00
1	5	629[A]	HIS	N-CA-C	-5.86	95.18	111.00
1	5	629[B]	HIS	N-CA-C	-5.86	95.18	111.00
1	v	629[A]	HIS	N-CA-C	-5.78	95.40	111.00
1	v	629[B]	HIS	N-CA-C	-5.78	95.40	111.00
1	y	629[A]	HIS	N-CA-C	-5.78	95.40	111.00
1	y	629[B]	HIS	N-CA-C	-5.78	95.40	111.00
1	s	600	VAL	C-N-CA	5.62	135.76	121.70
1	Q	600	VAL	C-N-CA	5.62	135.76	121.70
1	v	600	VAL	C-N-CA	5.62	135.74	121.70
1	y	600	VAL	C-N-CA	5.62	135.74	121.70
1	R	600	VAL	C-N-CA	5.62	135.74	121.70
1	L	600	VAL	C-N-CA	5.62	135.74	121.70
1	T	600	VAL	C-N-CA	5.61	135.73	121.70
1	f	600	VAL	C-N-CA	5.61	135.73	121.70
1	D	600	VAL	C-N-CA	5.61	135.72	121.70
1	W	600	VAL	C-N-CA	5.61	135.72	121.70
1	I	600	VAL	C-N-CA	5.61	135.72	121.70
1	O	600	VAL	C-N-CA	5.61	135.72	121.70
1	o	600	VAL	C-N-CA	5.61	135.72	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	600	VAL	C-N-CA	5.61	135.72	121.70
1	M	600	VAL	C-N-CA	5.61	135.72	121.70
1	A	600	VAL	C-N-CA	5.60	135.71	121.70
1	C	600	VAL	C-N-CA	5.60	135.71	121.70
1	U	600	VAL	C-N-CA	5.60	135.71	121.70
1	b	600	VAL	C-N-CA	5.60	135.71	121.70
1	e	600	VAL	C-N-CA	5.60	135.71	121.70
1	H	600	VAL	C-N-CA	5.60	135.70	121.70
1	P	600	VAL	C-N-CA	5.60	135.70	121.70
1	3	600	VAL	C-N-CA	5.60	135.70	121.70
1	B	600	VAL	C-N-CA	5.60	135.69	121.70
1	E	600	VAL	C-N-CA	5.60	135.69	121.70
1	X	600	VAL	C-N-CA	5.60	135.69	121.70
1	Z	600	VAL	C-N-CA	5.60	135.70	121.70
1	i	600	VAL	C-N-CA	5.60	135.69	121.70
1	j	600	VAL	C-N-CA	5.60	135.69	121.70
1	5	600	VAL	C-N-CA	5.60	135.69	121.70
1	7	600	VAL	C-N-CA	5.60	135.69	121.70
1	N	600	VAL	C-N-CA	5.60	135.69	121.70
1	z	600	VAL	C-N-CA	5.60	135.69	121.70
1	g	600	VAL	C-N-CA	5.59	135.69	121.70
1	p	600	VAL	C-N-CA	5.59	135.69	121.70
1	r	600	VAL	C-N-CA	5.59	135.68	121.70
1	t	600	VAL	C-N-CA	5.59	135.69	121.70
1	c	600	VAL	C-N-CA	5.59	135.68	121.70
1	l	600	VAL	C-N-CA	5.59	135.68	121.70
1	8	600	VAL	C-N-CA	5.59	135.68	121.70
1	k	600	VAL	C-N-CA	5.59	135.68	121.70
1	u	600	VAL	C-N-CA	5.59	135.68	121.70
1	x	600	VAL	C-N-CA	5.59	135.68	121.70
1	G	600	VAL	C-N-CA	5.59	135.67	121.70
1	h	600	VAL	C-N-CA	5.59	135.67	121.70
1	V	600	VAL	C-N-CA	5.59	135.67	121.70
1	a	600	VAL	C-N-CA	5.59	135.67	121.70
1	d	600	VAL	C-N-CA	5.59	135.67	121.70
1	J	600	VAL	C-N-CA	5.59	135.67	121.70
1	m	600	VAL	C-N-CA	5.59	135.67	121.70
1	n	600	VAL	C-N-CA	5.59	135.67	121.70
1	q	600	VAL	C-N-CA	5.59	135.67	121.70
1	w	600	VAL	C-N-CA	5.59	135.66	121.70
1	1	600	VAL	C-N-CA	5.59	135.67	121.70
1	4	600	VAL	C-N-CA	5.59	135.67	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	600	VAL	C-N-CA	5.58	135.66	121.70
1	F	600	VAL	C-N-CA	5.58	135.66	121.70
1	S	600	VAL	C-N-CA	5.58	135.66	121.70
1	2	600	VAL	C-N-CA	5.58	135.66	121.70
1	K	600	VAL	C-N-CA	5.58	135.65	121.70
1	E	228	TRP	C-N-CA	-5.51	107.92	121.70
1	G	228	TRP	C-N-CA	-5.51	107.92	121.70
1	t	298[A]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	t	298[B]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	w	298[A]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	w	298[B]	ARG	CG-CD-NE	-5.32	100.64	111.80
1	j	628	PHE	C-N-CA	5.20	134.69	121.70
1	5	628	PHE	C-N-CA	5.20	134.69	121.70
1	F	228	TRP	C-N-CA	-5.06	109.06	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19 49
1	2	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34 64
1	3	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19 49
1	4	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34 64
1	5	520/735 (71%)	492 (95%)	24 (5%)	4 (1%)	19 49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	7	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	8	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	A	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	B	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	C	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	D	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	E	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	F	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	G	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	H	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	I	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	J	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	K	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	L	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	M	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	N	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	O	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	P	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	Q	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	R	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	S	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	T	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	U	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	V	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	W	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	X	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	Y	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	Z	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	a	520/735 (71%)	491 (94%)	27 (5%)	2 (0%)	34	64
1	b	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	d	520/735 (71%)	491 (94%)	27 (5%)	2 (0%)	34	64
1	e	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	f	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	g	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	h	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34	64
1	i	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	j	520/735 (71%)	492 (95%)	24 (5%)	4 (1%)	19	49
1	k	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	l	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	m	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34	64
1	n	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	o	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34	64
1	p	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	q	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	r	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	s	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34	64
1	t	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	u	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34	64
1	v	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	w	520/735 (71%)	490 (94%)	28 (5%)	2 (0%)	34	64
1	x	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34	64
1	y	520/735 (71%)	490 (94%)	26 (5%)	4 (1%)	19	49
1	z	520/735 (71%)	492 (95%)	26 (5%)	2 (0%)	34	64
All	All	31200/44100 (71%)	29422 (94%)	1622 (5%)	156 (0%)	38	60

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	470	ILE
1	B	470	ILE
1	C	470	ILE
1	D	470	ILE
1	E	470	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	470	ILE
1	G	470	ILE
1	H	470	ILE
1	I	470	ILE
1	J	470	ILE
1	K	470	ILE
1	L	470	ILE
1	M	470	ILE
1	N	470	ILE
1	O	470	ILE
1	P	470	ILE
1	Q	470	ILE
1	R	470	ILE
1	S	470	ILE
1	T	470	ILE
1	U	470	ILE
1	V	470	ILE
1	W	470	ILE
1	X	470	ILE
1	Y	470	ILE
1	Z	470	ILE
1	a	470	ILE
1	b	470	ILE
1	c	470	ILE
1	d	470	ILE
1	e	470	ILE
1	f	470	ILE
1	g	470	ILE
1	h	470	ILE
1	i	470	ILE
1	j	470	ILE
1	k	470	ILE
1	l	470	ILE
1	m	470	ILE
1	n	470	ILE
1	o	470	ILE
1	p	470	ILE
1	q	470	ILE
1	r	470	ILE
1	s	470	ILE
1	t	470	ILE
1	u	470	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	v	470	ILE
1	w	470	ILE
1	x	470	ILE
1	y	470	ILE
1	z	470	ILE
1	1	470	ILE
1	2	470	ILE
1	3	470	ILE
1	4	470	ILE
1	5	470	ILE
1	6	470	ILE
1	7	470	ILE
1	8	470	ILE
1	b	629[A]	HIS
1	b	629[B]	HIS
1	e	629[A]	HIS
1	e	629[B]	HIS
1	j	629[A]	HIS
1	j	629[B]	HIS
1	5	629[A]	HIS
1	5	629[B]	HIS
1	N	629[A]	HIS
1	N	629[B]	HIS
1	Y	629[A]	HIS
1	Y	629[B]	HIS
1	k	629[A]	HIS
1	k	629[B]	HIS
1	l	629[A]	HIS
1	l	629[B]	HIS
1	q	629[A]	HIS
1	q	629[B]	HIS
1	v	629[A]	HIS
1	v	629[B]	HIS
1	y	629[A]	HIS
1	y	629[B]	HIS
1	1	629[A]	HIS
1	1	629[B]	HIS
1	6	629[A]	HIS
1	6	629[B]	HIS
1	8	629[A]	HIS
1	8	629[B]	HIS
1	g	629[A]	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	g	629[B]	HIS
1	n	629[A]	HIS
1	n	629[B]	HIS
1	p	629[A]	HIS
1	p	629[B]	HIS
1	3	629[A]	HIS
1	3	629[B]	HIS
1	A	221	VAL
1	B	221	VAL
1	C	221	VAL
1	D	221	VAL
1	E	221	VAL
1	F	221	VAL
1	G	221	VAL
1	H	221	VAL
1	I	221	VAL
1	J	221	VAL
1	K	221	VAL
1	L	221	VAL
1	M	221	VAL
1	N	221	VAL
1	O	221	VAL
1	P	221	VAL
1	Q	221	VAL
1	R	221	VAL
1	S	221	VAL
1	T	221	VAL
1	U	221	VAL
1	V	221	VAL
1	W	221	VAL
1	X	221	VAL
1	Y	221	VAL
1	Z	221	VAL
1	a	221	VAL
1	b	221	VAL
1	c	221	VAL
1	d	221	VAL
1	e	221	VAL
1	f	221	VAL
1	g	221	VAL
1	h	221	VAL
1	i	221	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	j	221	VAL
1	k	221	VAL
1	l	221	VAL
1	m	221	VAL
1	n	221	VAL
1	o	221	VAL
1	p	221	VAL
1	q	221	VAL
1	r	221	VAL
1	s	221	VAL
1	t	221	VAL
1	u	221	VAL
1	v	221	VAL
1	w	221	VAL
1	x	221	VAL
1	y	221	VAL
1	z	221	VAL
1	1	221	VAL
1	2	221	VAL
1	3	221	VAL
1	4	221	VAL
1	5	221	VAL
1	6	221	VAL
1	7	221	VAL
1	8	221	VAL

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	462/630 (73%)	462 (100%)	0	100	100
1	2	462/630 (73%)	462 (100%)	0	100	100
1	3	462/630 (73%)	462 (100%)	0	100	100
1	4	462/630 (73%)	462 (100%)	0	100	100
1	5	462/630 (73%)	462 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	462/630 (73%)	460 (100%)	2 (0%)	91	97
1	7	462/630 (73%)	462 (100%)	0	100	100
1	8	462/630 (73%)	462 (100%)	0	100	100
1	A	462/630 (73%)	462 (100%)	0	100	100
1	B	462/630 (73%)	462 (100%)	0	100	100
1	C	462/630 (73%)	462 (100%)	0	100	100
1	D	462/630 (73%)	462 (100%)	0	100	100
1	E	462/630 (73%)	462 (100%)	0	100	100
1	F	462/630 (73%)	462 (100%)	0	100	100
1	G	462/630 (73%)	462 (100%)	0	100	100
1	H	462/630 (73%)	462 (100%)	0	100	100
1	I	462/630 (73%)	462 (100%)	0	100	100
1	J	462/630 (73%)	462 (100%)	0	100	100
1	K	462/630 (73%)	462 (100%)	0	100	100
1	L	462/630 (73%)	462 (100%)	0	100	100
1	M	462/630 (73%)	460 (100%)	2 (0%)	91	97
1	N	462/630 (73%)	462 (100%)	0	100	100
1	O	462/630 (73%)	462 (100%)	0	100	100
1	P	462/630 (73%)	462 (100%)	0	100	100
1	Q	462/630 (73%)	462 (100%)	0	100	100
1	R	462/630 (73%)	462 (100%)	0	100	100
1	S	462/630 (73%)	462 (100%)	0	100	100
1	T	462/630 (73%)	462 (100%)	0	100	100
1	U	462/630 (73%)	462 (100%)	0	100	100
1	V	462/630 (73%)	462 (100%)	0	100	100
1	W	462/630 (73%)	462 (100%)	0	100	100
1	X	462/630 (73%)	460 (100%)	2 (0%)	91	97
1	Y	462/630 (73%)	462 (100%)	0	100	100
1	Z	462/630 (73%)	462 (100%)	0	100	100
1	a	462/630 (73%)	462 (100%)	0	100	100
1	b	462/630 (73%)	462 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	462/630 (73%)	462 (100%)	0	100	100
1	d	462/630 (73%)	462 (100%)	0	100	100
1	e	462/630 (73%)	462 (100%)	0	100	100
1	f	462/630 (73%)	462 (100%)	0	100	100
1	g	462/630 (73%)	462 (100%)	0	100	100
1	h	462/630 (73%)	462 (100%)	0	100	100
1	i	462/630 (73%)	462 (100%)	0	100	100
1	j	462/630 (73%)	462 (100%)	0	100	100
1	k	462/630 (73%)	462 (100%)	0	100	100
1	l	462/630 (73%)	462 (100%)	0	100	100
1	m	462/630 (73%)	462 (100%)	0	100	100
1	n	462/630 (73%)	462 (100%)	0	100	100
1	o	462/630 (73%)	462 (100%)	0	100	100
1	p	462/630 (73%)	462 (100%)	0	100	100
1	q	462/630 (73%)	462 (100%)	0	100	100
1	r	462/630 (73%)	462 (100%)	0	100	100
1	s	462/630 (73%)	462 (100%)	0	100	100
1	t	462/630 (73%)	462 (100%)	0	100	100
1	u	462/630 (73%)	462 (100%)	0	100	100
1	v	462/630 (73%)	462 (100%)	0	100	100
1	w	462/630 (73%)	462 (100%)	0	100	100
1	x	462/630 (73%)	462 (100%)	0	100	100
1	y	462/630 (73%)	462 (100%)	0	100	100
1	z	462/630 (73%)	462 (100%)	0	100	100
All	All	27720/37800 (73%)	27714 (100%)	6 (0%)	100	100

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	298[A]	ARG
1	M	298[B]	ARG
1	X	298[A]	ARG
1	X	298[B]	ARG
1	6	298[A]	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6	298[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (595) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	A	334	ASN
1	A	407	ASN
1	A	426	HIS
1	A	428	GLN
1	A	526	HIS
1	A	584	GLN
1	A	627	HIS
1	A	645	GLN
1	A	699	GLN
1	A	709	ASN
1	B	334	ASN
1	B	407	ASN
1	B	426	HIS
1	B	428	GLN
1	B	584	GLN
1	B	627	HIS
1	B	645	GLN
1	B	699	GLN
1	B	709	ASN
1	C	334	ASN
1	C	407	ASN
1	C	426	HIS
1	C	428	GLN
1	C	584	GLN
1	C	627	HIS
1	C	645	GLN
1	C	699	GLN
1	C	709	ASN
1	D	302	ASN
1	D	334	ASN
1	D	407	ASN
1	D	426	HIS
1	D	428	GLN
1	D	584	GLN
1	D	627	HIS
1	D	645	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	699	GLN
1	D	709	ASN
1	E	302	ASN
1	E	334	ASN
1	E	407	ASN
1	E	426	HIS
1	E	428	GLN
1	E	526	HIS
1	E	584	GLN
1	E	627	HIS
1	E	645	GLN
1	E	699	GLN
1	E	709	ASN
1	F	302	ASN
1	F	334	ASN
1	F	407	ASN
1	F	426	HIS
1	F	428	GLN
1	F	485	GLN
1	F	584	GLN
1	F	627	HIS
1	F	645	GLN
1	F	699	GLN
1	F	709	ASN
1	G	302	ASN
1	G	334	ASN
1	G	407	ASN
1	G	426	HIS
1	G	428	GLN
1	G	584	GLN
1	G	627	HIS
1	G	645	GLN
1	G	699	GLN
1	G	709	ASN
1	H	302	ASN
1	H	334	ASN
1	H	407	ASN
1	H	426	HIS
1	H	428	GLN
1	H	584	GLN
1	H	627	HIS
1	H	645	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	699	GLN
1	H	709	ASN
1	I	302	ASN
1	I	334	ASN
1	I	407	ASN
1	I	426	HIS
1	I	428	GLN
1	I	584	GLN
1	I	627	HIS
1	I	645	GLN
1	I	699	GLN
1	I	709	ASN
1	J	302	ASN
1	J	334	ASN
1	J	407	ASN
1	J	426	HIS
1	J	428	GLN
1	J	526	HIS
1	J	584	GLN
1	J	627	HIS
1	J	645	GLN
1	J	699	GLN
1	J	709	ASN
1	K	334	ASN
1	K	407	ASN
1	K	426	HIS
1	K	428	GLN
1	K	584	GLN
1	K	627	HIS
1	K	645	GLN
1	K	699	GLN
1	K	709	ASN
1	L	302	ASN
1	L	334	ASN
1	L	407	ASN
1	L	426	HIS
1	L	428	GLN
1	L	584	GLN
1	L	627	HIS
1	L	645	GLN
1	L	699	GLN
1	L	709	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	302	ASN
1	M	334	ASN
1	M	407	ASN
1	M	426	HIS
1	M	428	GLN
1	M	584	GLN
1	M	627	HIS
1	M	645	GLN
1	M	699	GLN
1	M	709	ASN
1	N	302	ASN
1	N	334	ASN
1	N	407	ASN
1	N	426	HIS
1	N	428	GLN
1	N	526	HIS
1	N	584	GLN
1	N	627	HIS
1	N	645	GLN
1	N	699	GLN
1	N	709	ASN
1	O	334	ASN
1	O	407	ASN
1	O	426	HIS
1	O	428	GLN
1	O	584	GLN
1	O	627	HIS
1	O	645	GLN
1	O	699	GLN
1	O	709	ASN
1	P	334	ASN
1	P	407	ASN
1	P	426	HIS
1	P	428	GLN
1	P	485	GLN
1	P	584	GLN
1	P	627	HIS
1	P	645	GLN
1	P	699	GLN
1	P	709	ASN
1	Q	302	ASN
1	Q	334	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	407	ASN
1	Q	426	HIS
1	Q	428	GLN
1	Q	584	GLN
1	Q	627	HIS
1	Q	645	GLN
1	Q	699	GLN
1	Q	709	ASN
1	R	334	ASN
1	R	407	ASN
1	R	426	HIS
1	R	428	GLN
1	R	485	GLN
1	R	584	GLN
1	R	627	HIS
1	R	645	GLN
1	R	699	GLN
1	R	709	ASN
1	S	302	ASN
1	S	334	ASN
1	S	407	ASN
1	S	426	HIS
1	S	428	GLN
1	S	584	GLN
1	S	627	HIS
1	S	645	GLN
1	S	699	GLN
1	S	709	ASN
1	T	334	ASN
1	T	407	ASN
1	T	426	HIS
1	T	428	GLN
1	T	584	GLN
1	T	627	HIS
1	T	645	GLN
1	T	699	GLN
1	T	709	ASN
1	U	302	ASN
1	U	334	ASN
1	U	407	ASN
1	U	426	HIS
1	U	428	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	584	GLN
1	U	627	HIS
1	U	645	GLN
1	U	699	GLN
1	U	709	ASN
1	V	334	ASN
1	V	407	ASN
1	V	426	HIS
1	V	428	GLN
1	V	526	HIS
1	V	584	GLN
1	V	627	HIS
1	V	645	GLN
1	V	699	GLN
1	V	709	ASN
1	W	302	ASN
1	W	334	ASN
1	W	407	ASN
1	W	426	HIS
1	W	428	GLN
1	W	584	GLN
1	W	627	HIS
1	W	645	GLN
1	W	699	GLN
1	W	709	ASN
1	X	302	ASN
1	X	334	ASN
1	X	407	ASN
1	X	426	HIS
1	X	428	GLN
1	X	526	HIS
1	X	584	GLN
1	X	627	HIS
1	X	645	GLN
1	X	699	GLN
1	X	709	ASN
1	Y	302	ASN
1	Y	334	ASN
1	Y	407	ASN
1	Y	426	HIS
1	Y	428	GLN
1	Y	526	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Y	584	GLN
1	Y	627	HIS
1	Y	645	GLN
1	Y	699	GLN
1	Y	709	ASN
1	Z	334	ASN
1	Z	407	ASN
1	Z	426	HIS
1	Z	428	GLN
1	Z	584	GLN
1	Z	627	HIS
1	Z	645	GLN
1	Z	699	GLN
1	Z	709	ASN
1	a	334	ASN
1	a	407	ASN
1	a	426	HIS
1	a	428	GLN
1	a	584	GLN
1	a	627	HIS
1	a	645	GLN
1	a	699	GLN
1	a	709	ASN
1	b	302	ASN
1	b	334	ASN
1	b	407	ASN
1	b	426	HIS
1	b	428	GLN
1	b	485	GLN
1	b	526	HIS
1	b	584	GLN
1	b	627	HIS
1	b	645	GLN
1	b	699	GLN
1	b	709	ASN
1	c	334	ASN
1	c	407	ASN
1	c	426	HIS
1	c	428	GLN
1	c	584	GLN
1	c	627	HIS
1	c	645	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	c	699	GLN
1	c	709	ASN
1	d	334	ASN
1	d	407	ASN
1	d	426	HIS
1	d	428	GLN
1	d	584	GLN
1	d	627	HIS
1	d	645	GLN
1	d	699	GLN
1	d	709	ASN
1	e	302	ASN
1	e	334	ASN
1	e	407	ASN
1	e	426	HIS
1	e	428	GLN
1	e	485	GLN
1	e	584	GLN
1	e	627	HIS
1	e	645	GLN
1	e	699	GLN
1	e	709	ASN
1	f	334	ASN
1	f	407	ASN
1	f	428	GLN
1	f	485	GLN
1	f	584	GLN
1	f	627	HIS
1	f	645	GLN
1	f	699	GLN
1	f	709	ASN
1	g	302	ASN
1	g	334	ASN
1	g	407	ASN
1	g	426	HIS
1	g	428	GLN
1	g	584	GLN
1	g	627	HIS
1	g	645	GLN
1	g	699	GLN
1	g	709	ASN
1	h	302	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	h	334	ASN
1	h	407	ASN
1	h	426	HIS
1	h	428	GLN
1	h	584	GLN
1	h	627	HIS
1	h	645	GLN
1	h	699	GLN
1	h	709	ASN
1	i	334	ASN
1	i	407	ASN
1	i	426	HIS
1	i	428	GLN
1	i	526	HIS
1	i	584	GLN
1	i	627	HIS
1	i	645	GLN
1	i	699	GLN
1	i	709	ASN
1	j	302	ASN
1	j	334	ASN
1	j	407	ASN
1	j	426	HIS
1	j	428	GLN
1	j	584	GLN
1	j	627	HIS
1	j	645	GLN
1	j	699	GLN
1	j	709	ASN
1	k	334	ASN
1	k	407	ASN
1	k	426	HIS
1	k	428	GLN
1	k	584	GLN
1	k	627	HIS
1	k	645	GLN
1	k	699	GLN
1	k	709	ASN
1	l	302	ASN
1	l	334	ASN
1	l	407	ASN
1	l	426	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	l	428	GLN
1	l	584	GLN
1	l	627	HIS
1	l	645	GLN
1	l	699	GLN
1	l	709	ASN
1	m	302	ASN
1	m	334	ASN
1	m	407	ASN
1	m	426	HIS
1	m	428	GLN
1	m	584	GLN
1	m	627	HIS
1	m	645	GLN
1	m	699	GLN
1	m	709	ASN
1	n	302	ASN
1	n	334	ASN
1	n	407	ASN
1	n	426	HIS
1	n	428	GLN
1	n	584	GLN
1	n	627	HIS
1	n	645	GLN
1	n	699	GLN
1	n	709	ASN
1	o	302	ASN
1	o	334	ASN
1	o	407	ASN
1	o	426	HIS
1	o	428	GLN
1	o	526	HIS
1	o	584	GLN
1	o	627	HIS
1	o	645	GLN
1	o	699	GLN
1	o	709	ASN
1	p	302	ASN
1	p	334	ASN
1	p	407	ASN
1	p	426	HIS
1	p	428	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	p	584	GLN
1	p	627	HIS
1	p	645	GLN
1	p	699	GLN
1	p	709	ASN
1	q	302	ASN
1	q	334	ASN
1	q	407	ASN
1	q	426	HIS
1	q	428	GLN
1	q	485	GLN
1	q	584	GLN
1	q	627	HIS
1	q	645	GLN
1	q	699	GLN
1	q	709	ASN
1	r	334	ASN
1	r	407	ASN
1	r	428	GLN
1	r	584	GLN
1	r	627	HIS
1	r	645	GLN
1	r	699	GLN
1	r	709	ASN
1	s	334	ASN
1	s	407	ASN
1	s	426	HIS
1	s	428	GLN
1	s	485	GLN
1	s	518	ASN
1	s	584	GLN
1	s	627	HIS
1	s	645	GLN
1	s	699	GLN
1	s	709	ASN
1	t	334	ASN
1	t	407	ASN
1	t	426	HIS
1	t	428	GLN
1	t	584	GLN
1	t	627	HIS
1	t	645	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	t	699	GLN
1	t	709	ASN
1	u	334	ASN
1	u	407	ASN
1	u	426	HIS
1	u	428	GLN
1	u	485	GLN
1	u	584	GLN
1	u	627	HIS
1	u	645	GLN
1	u	699	GLN
1	u	709	ASN
1	v	334	ASN
1	v	407	ASN
1	v	426	HIS
1	v	428	GLN
1	v	584	GLN
1	v	627	HIS
1	v	645	GLN
1	v	699	GLN
1	v	709	ASN
1	w	334	ASN
1	w	407	ASN
1	w	426	HIS
1	w	428	GLN
1	w	526	HIS
1	w	584	GLN
1	w	627	HIS
1	w	645	GLN
1	w	699	GLN
1	w	709	ASN
1	x	334	ASN
1	x	407	ASN
1	x	426	HIS
1	x	428	GLN
1	x	584	GLN
1	x	627	HIS
1	x	645	GLN
1	x	699	GLN
1	x	709	ASN
1	y	334	ASN
1	y	407	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	y	426	HIS
1	y	428	GLN
1	y	485	GLN
1	y	584	GLN
1	y	627	HIS
1	y	645	GLN
1	y	699	GLN
1	y	709	ASN
1	z	334	ASN
1	z	407	ASN
1	z	426	HIS
1	z	428	GLN
1	z	584	GLN
1	z	627	HIS
1	z	645	GLN
1	z	699	GLN
1	z	709	ASN
1	1	302	ASN
1	1	334	ASN
1	1	407	ASN
1	1	426	HIS
1	1	428	GLN
1	1	584	GLN
1	1	627	HIS
1	1	645	GLN
1	1	699	GLN
1	1	709	ASN
1	2	334	ASN
1	2	407	ASN
1	2	428	GLN
1	2	526	HIS
1	2	584	GLN
1	2	627	HIS
1	2	645	GLN
1	2	699	GLN
1	2	709	ASN
1	3	302	ASN
1	3	334	ASN
1	3	407	ASN
1	3	426	HIS
1	3	428	GLN
1	3	584	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	627	HIS
1	3	645	GLN
1	3	699	GLN
1	3	709	ASN
1	4	302	ASN
1	4	334	ASN
1	4	407	ASN
1	4	426	HIS
1	4	428	GLN
1	4	584	GLN
1	4	627	HIS
1	4	645	GLN
1	4	699	GLN
1	4	709	ASN
1	5	302	ASN
1	5	334	ASN
1	5	407	ASN
1	5	426	HIS
1	5	428	GLN
1	5	584	GLN
1	5	627	HIS
1	5	645	GLN
1	5	699	GLN
1	5	709	ASN
1	6	302	ASN
1	6	334	ASN
1	6	407	ASN
1	6	426	HIS
1	6	428	GLN
1	6	584	GLN
1	6	627	HIS
1	6	645	GLN
1	6	699	GLN
1	6	709	ASN
1	7	334	ASN
1	7	407	ASN
1	7	426	HIS
1	7	428	GLN
1	7	526	HIS
1	7	584	GLN
1	7	627	HIS
1	7	645	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7	699	GLN
1	7	709	ASN
1	8	302	ASN
1	8	334	ASN
1	8	407	ASN
1	8	426	HIS
1	8	428	GLN
1	8	584	GLN
1	8	627	HIS
1	8	645	GLN
1	8	699	GLN
1	8	709	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 monosaccharides 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.

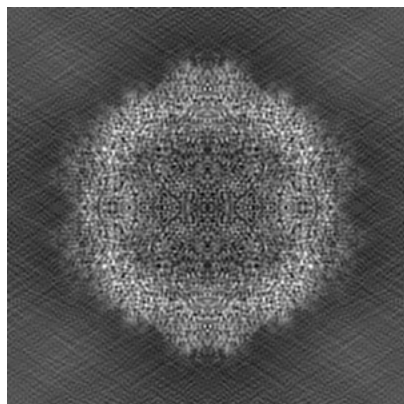
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29600. These allow visual inspection of the internal detail of the map and identification of artifacts.

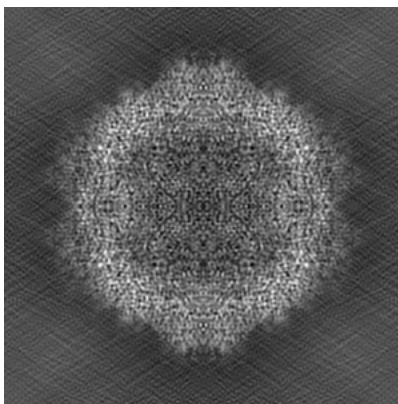
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

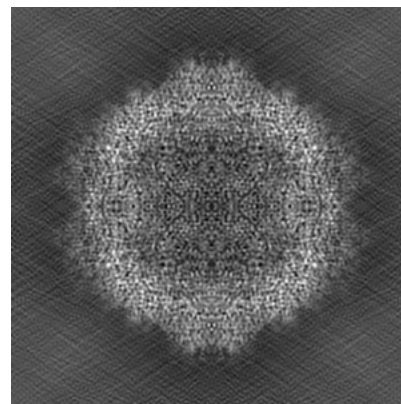
6.1.1 Primary map



X

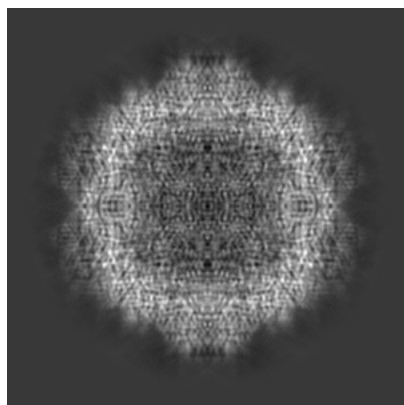


Y

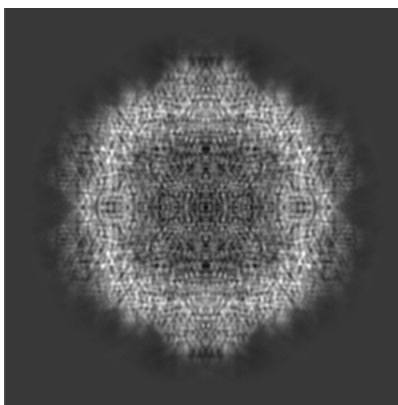


Z

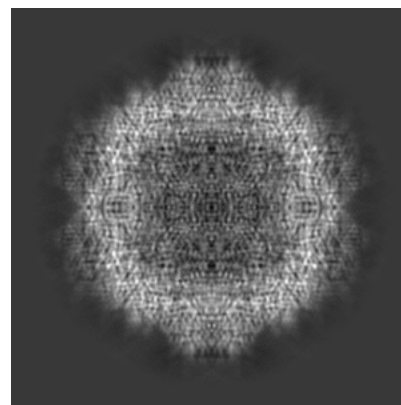
6.1.2 Raw map



X



Y

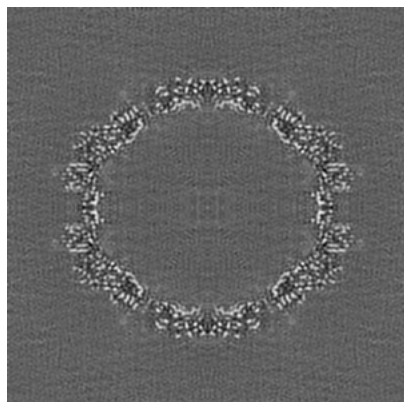


Z

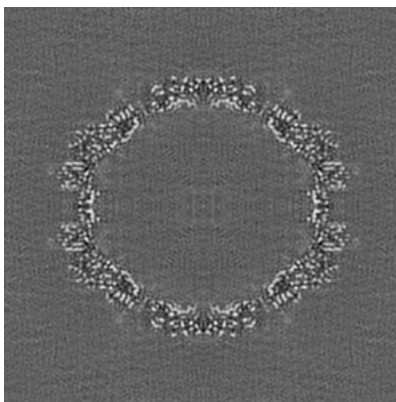
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

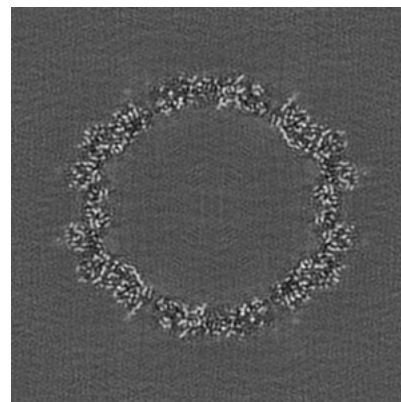
6.2.1 Primary map



X Index: 160

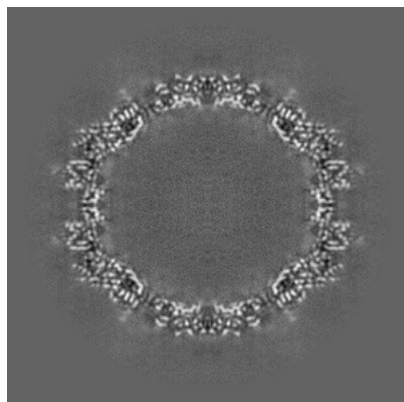


Y Index: 160

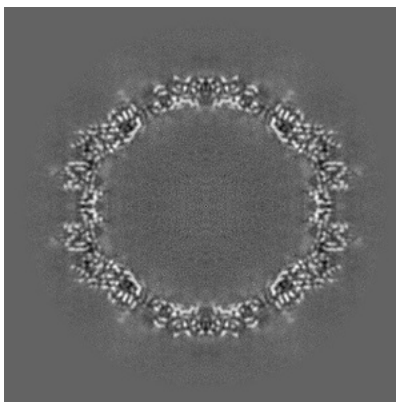


Z Index: 160

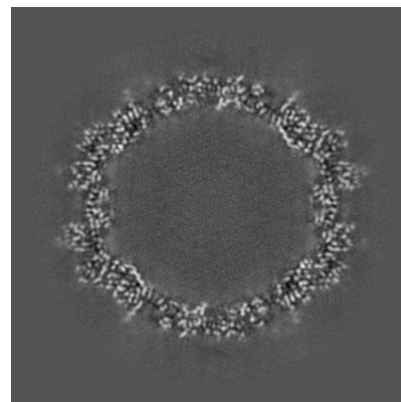
6.2.2 Raw map



X Index: 160



Y Index: 160

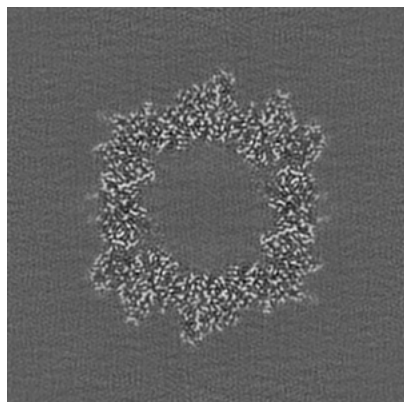


Z Index: 160

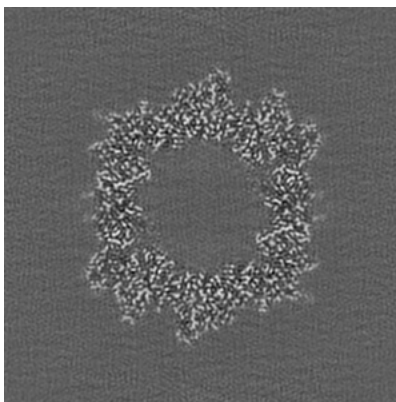
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

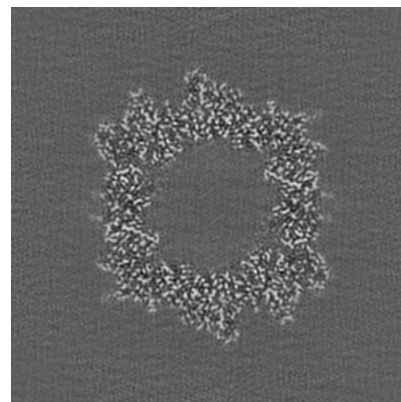
6.3.1 Primary map



X Index: 221

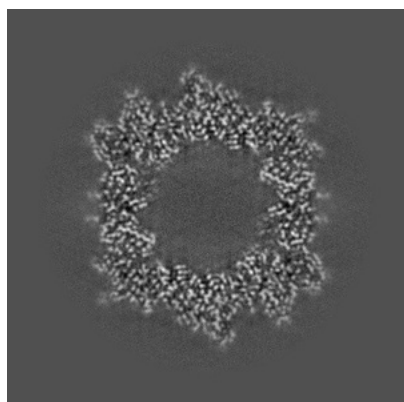


Y Index: 221

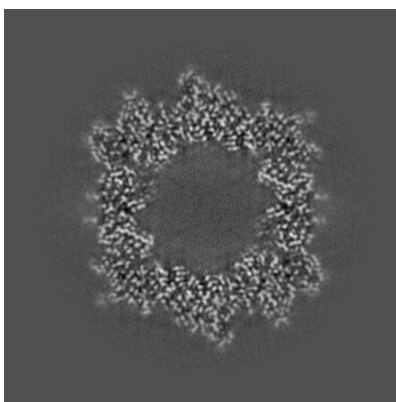


Z Index: 98

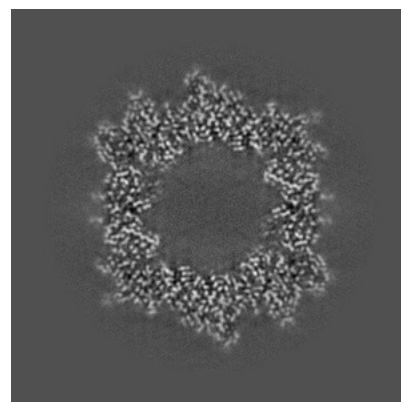
6.3.2 Raw map



X Index: 221



Y Index: 221

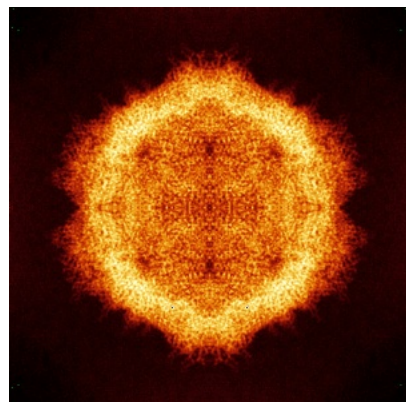


Z Index: 222

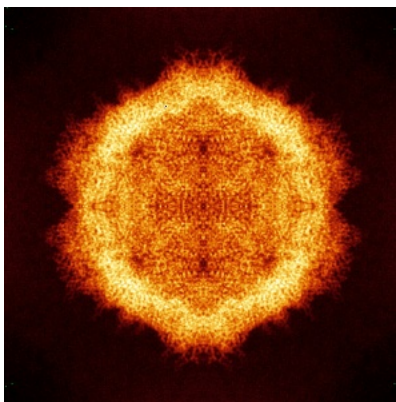
The images above show the largest variance slices of the map in three orthogonal directions.

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

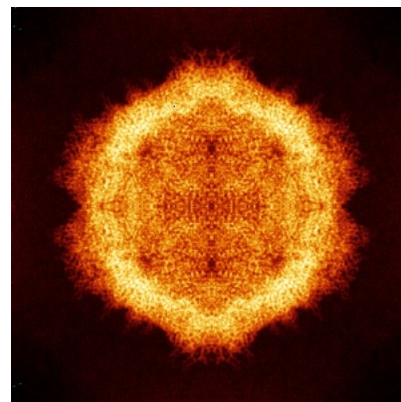
6.4.1 Primary map



X

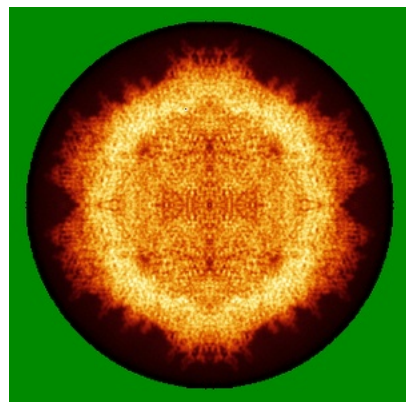


Y

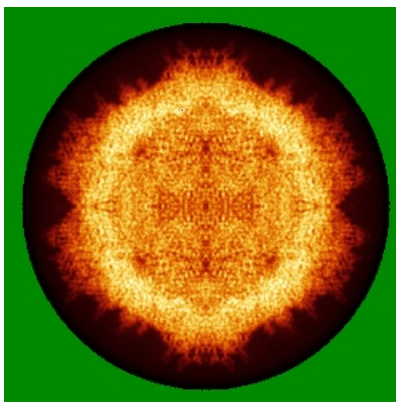


Z

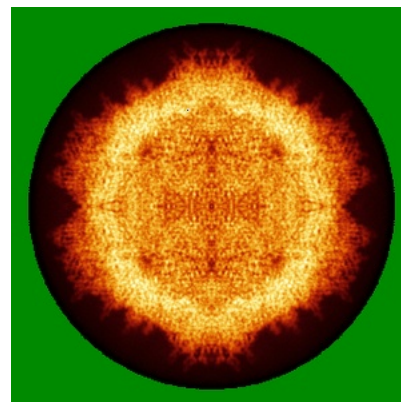
6.4.2 Raw map



X



Y

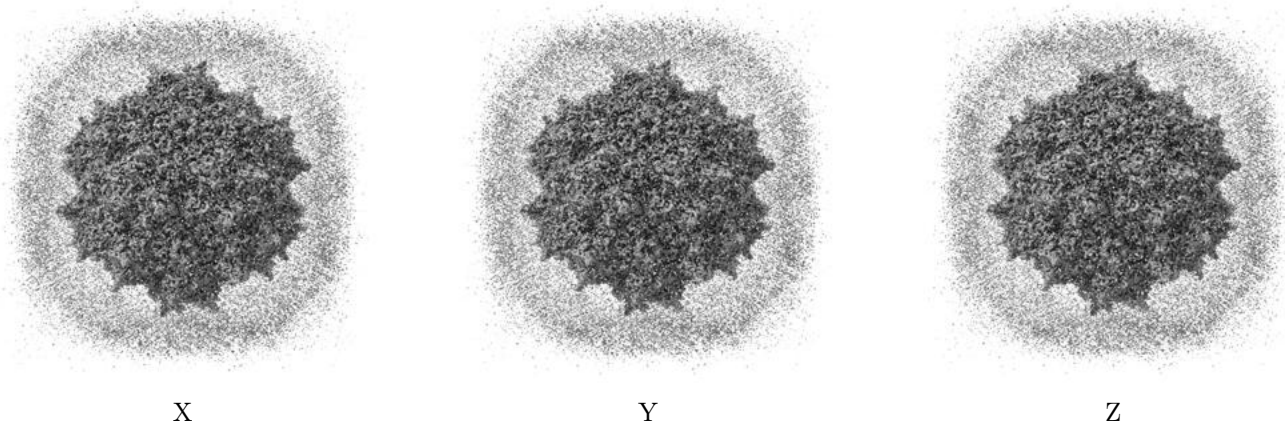


Z

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

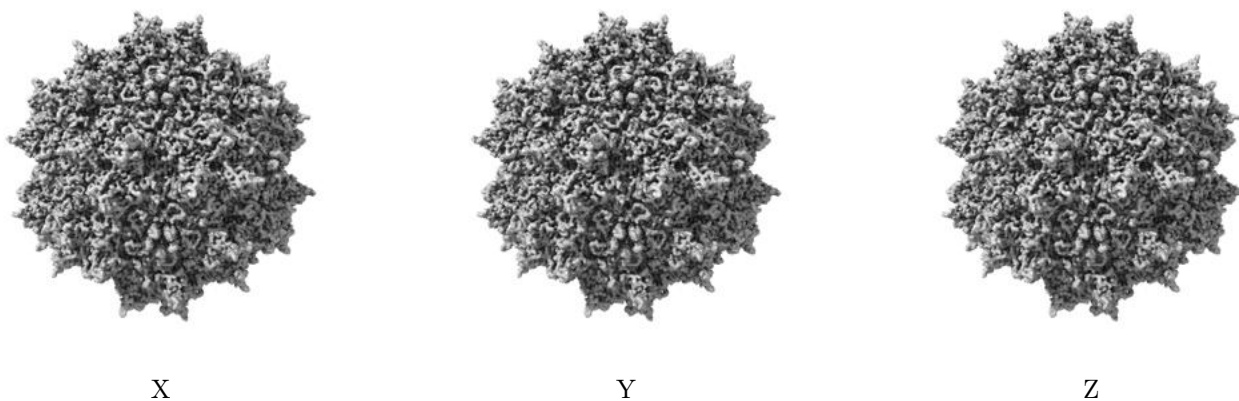
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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



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.

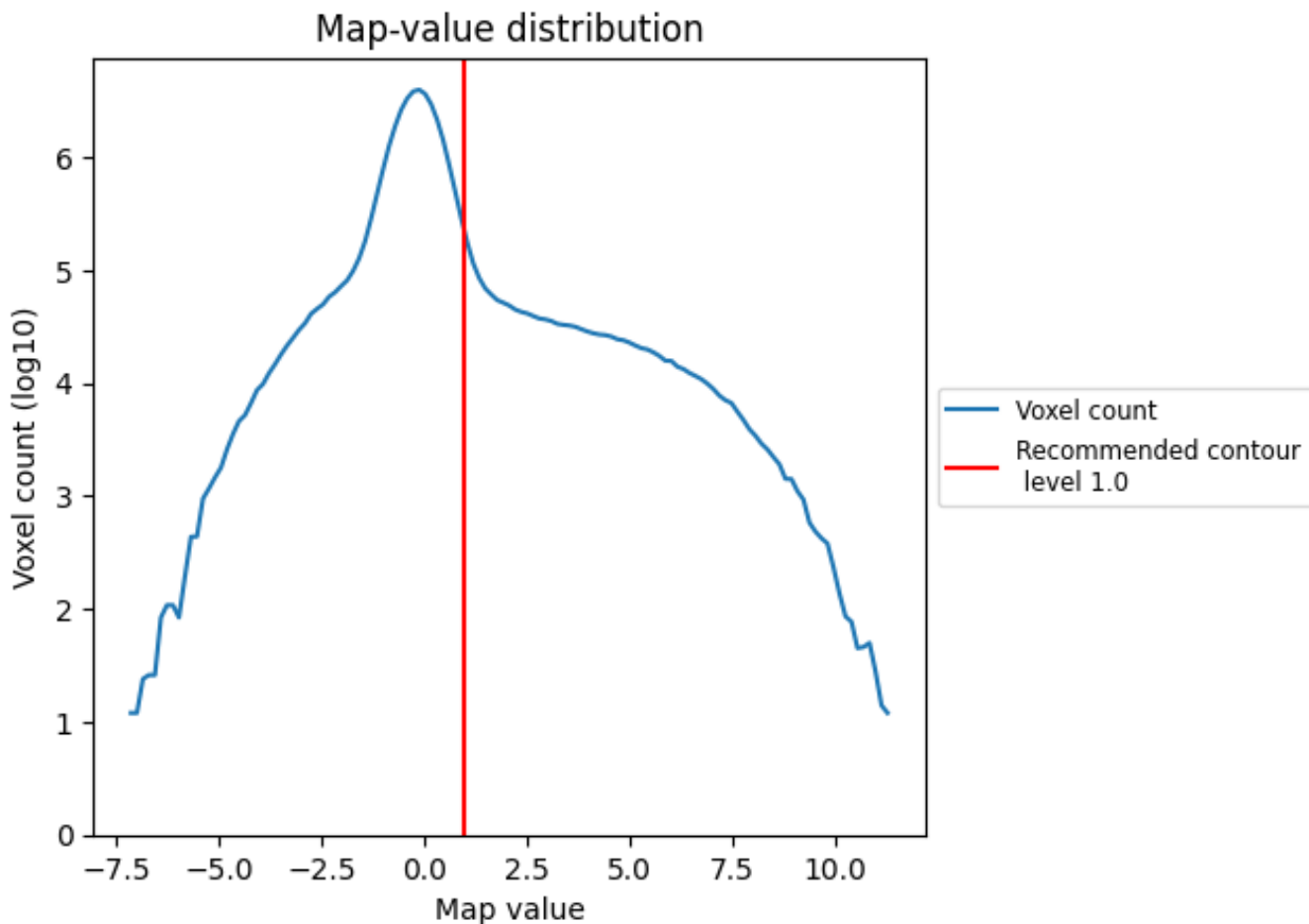
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

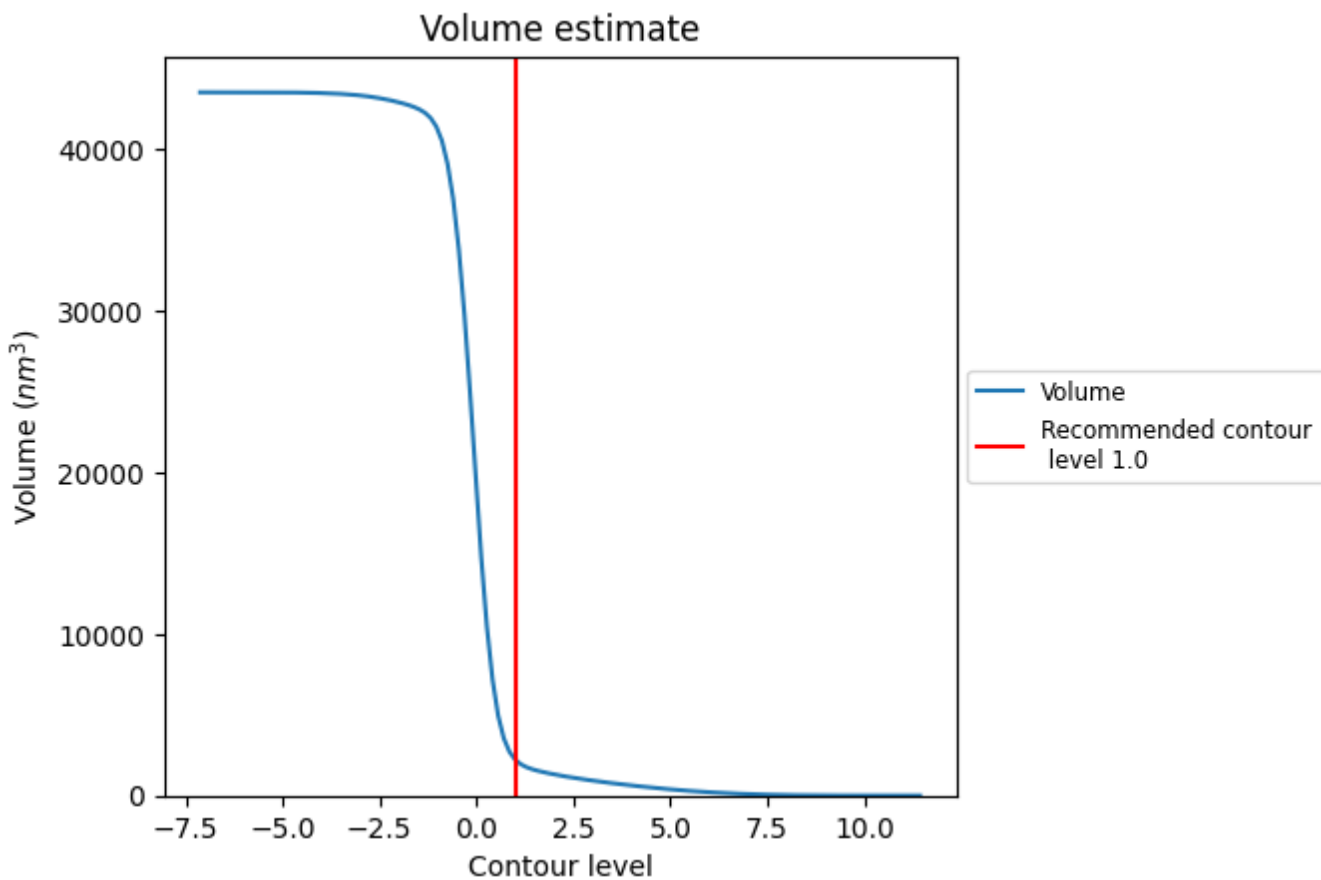
This section contains the results of statistical analysis of the map.

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.

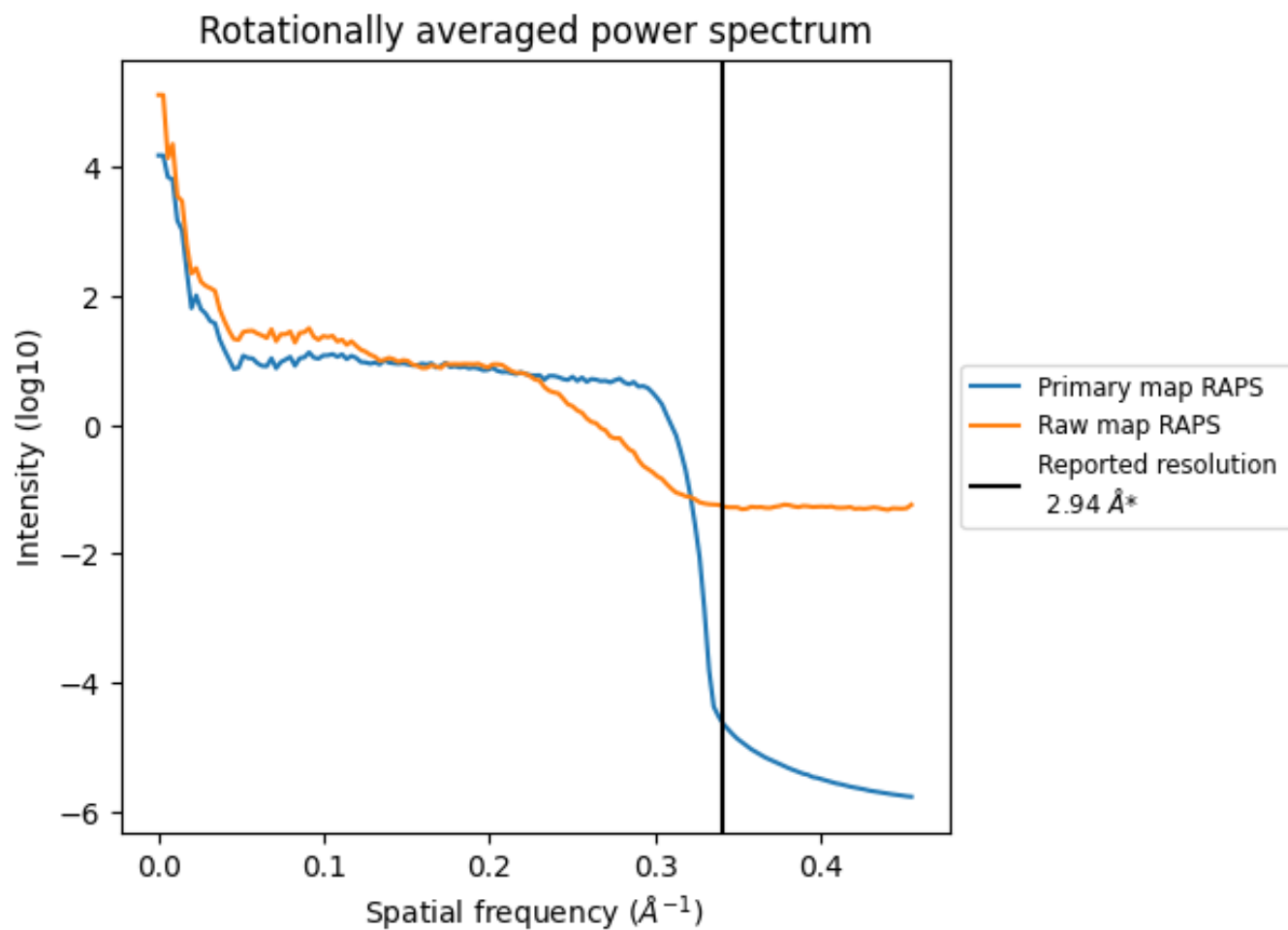
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2221 nm³; this corresponds to an approximate mass of 2007 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

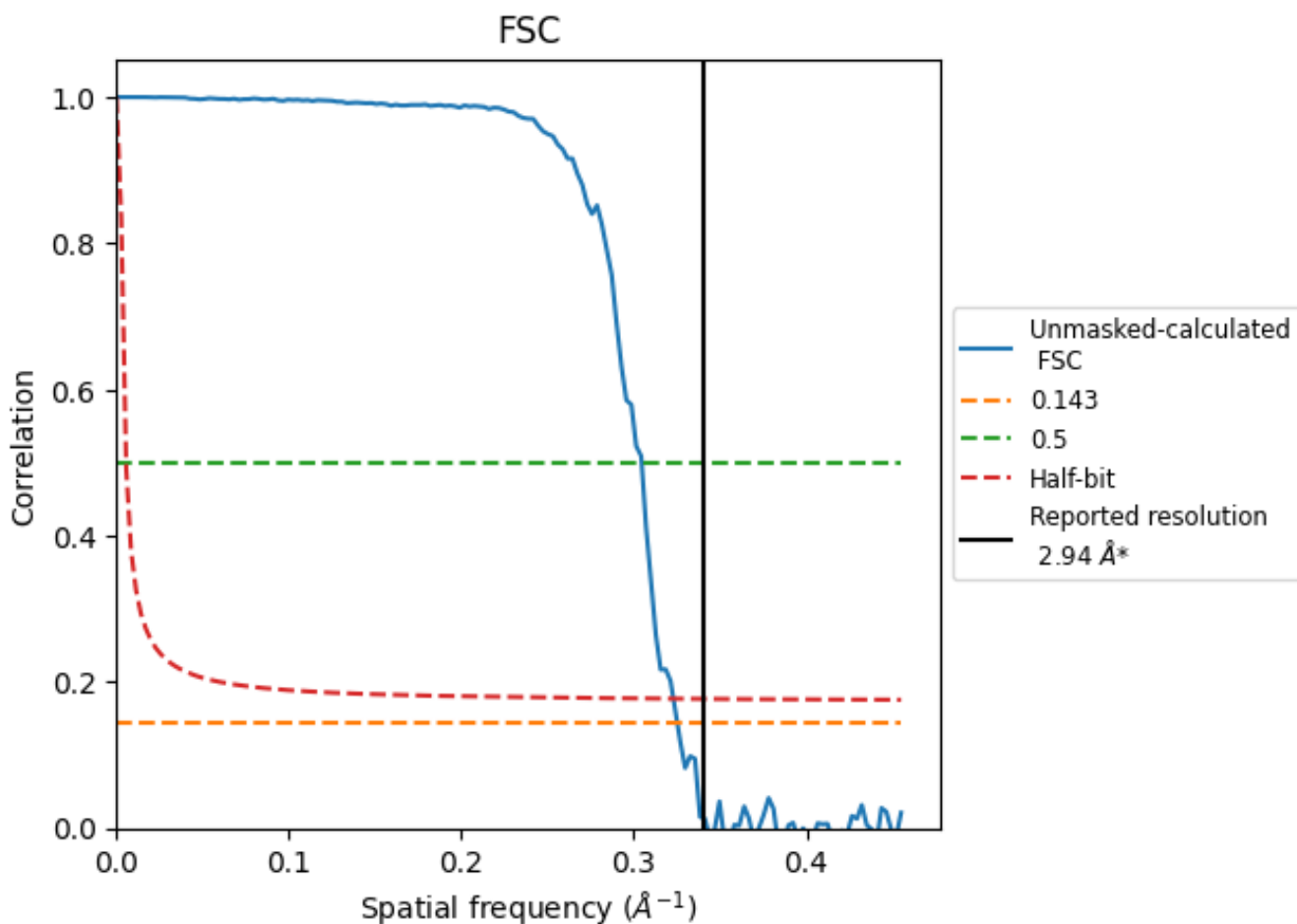


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

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 0.340 \AA^{-1}

8.2 Resolution estimates [i](#)

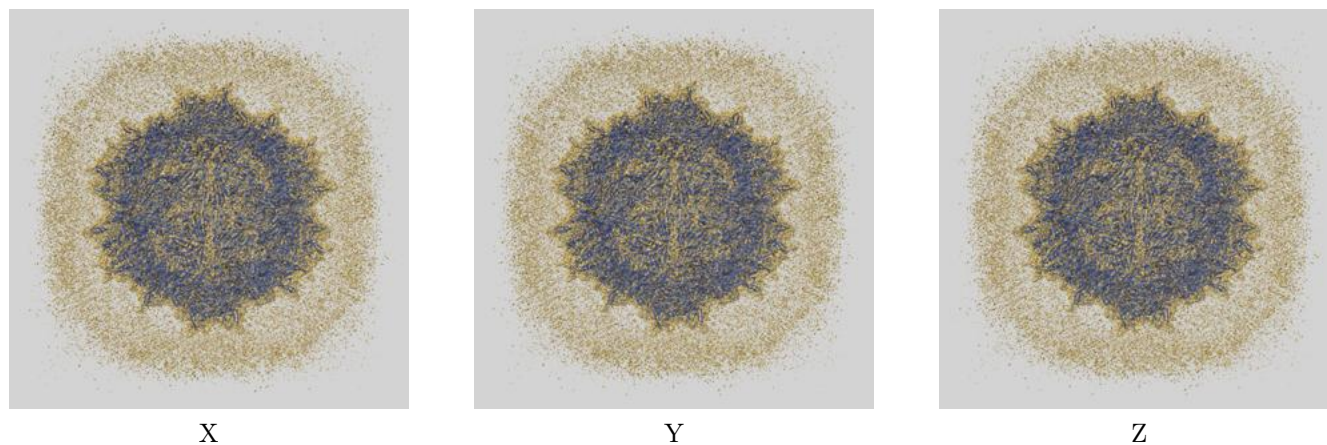
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.08	3.28	3.10

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

9 Map-model fit [i](#)

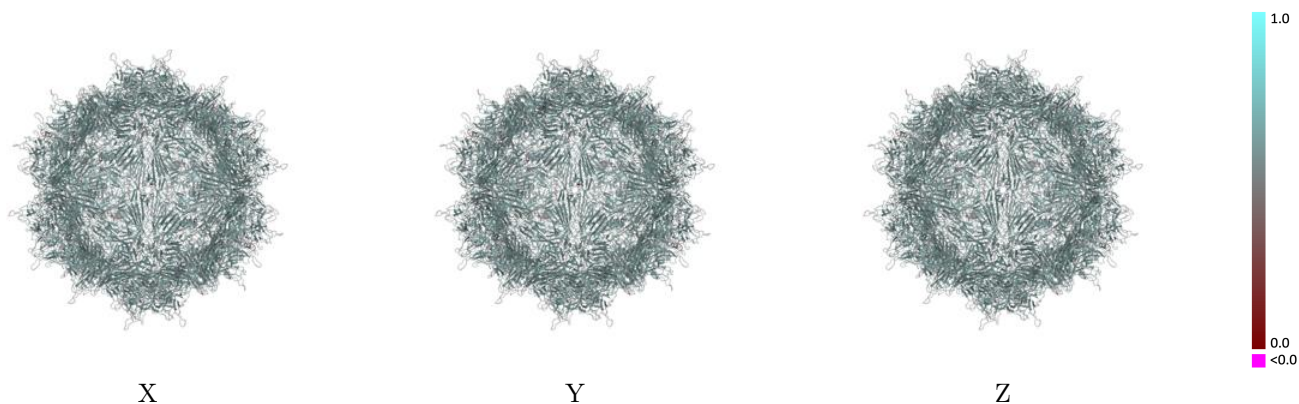
This section contains information regarding the fit between EMDB map EMD-29600 and PDB model 8FZ0. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



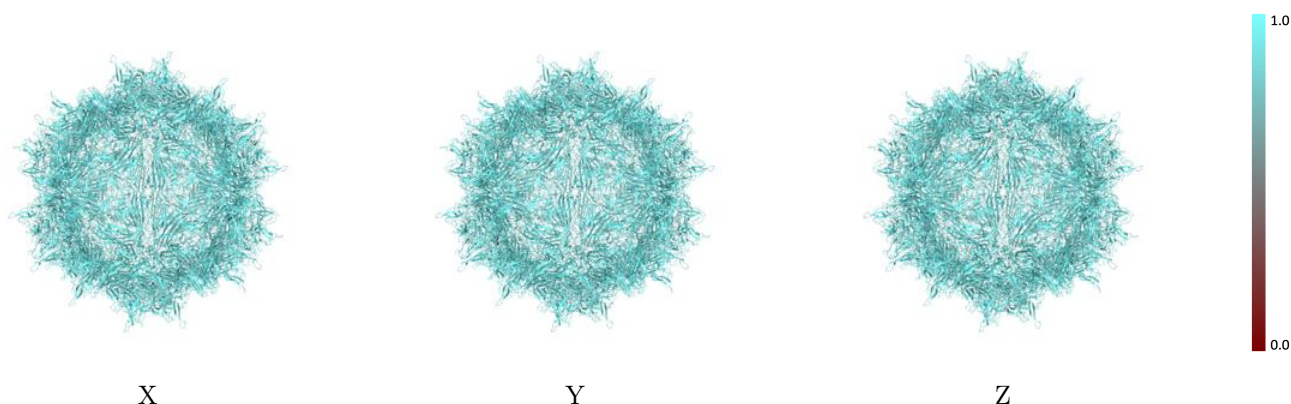
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



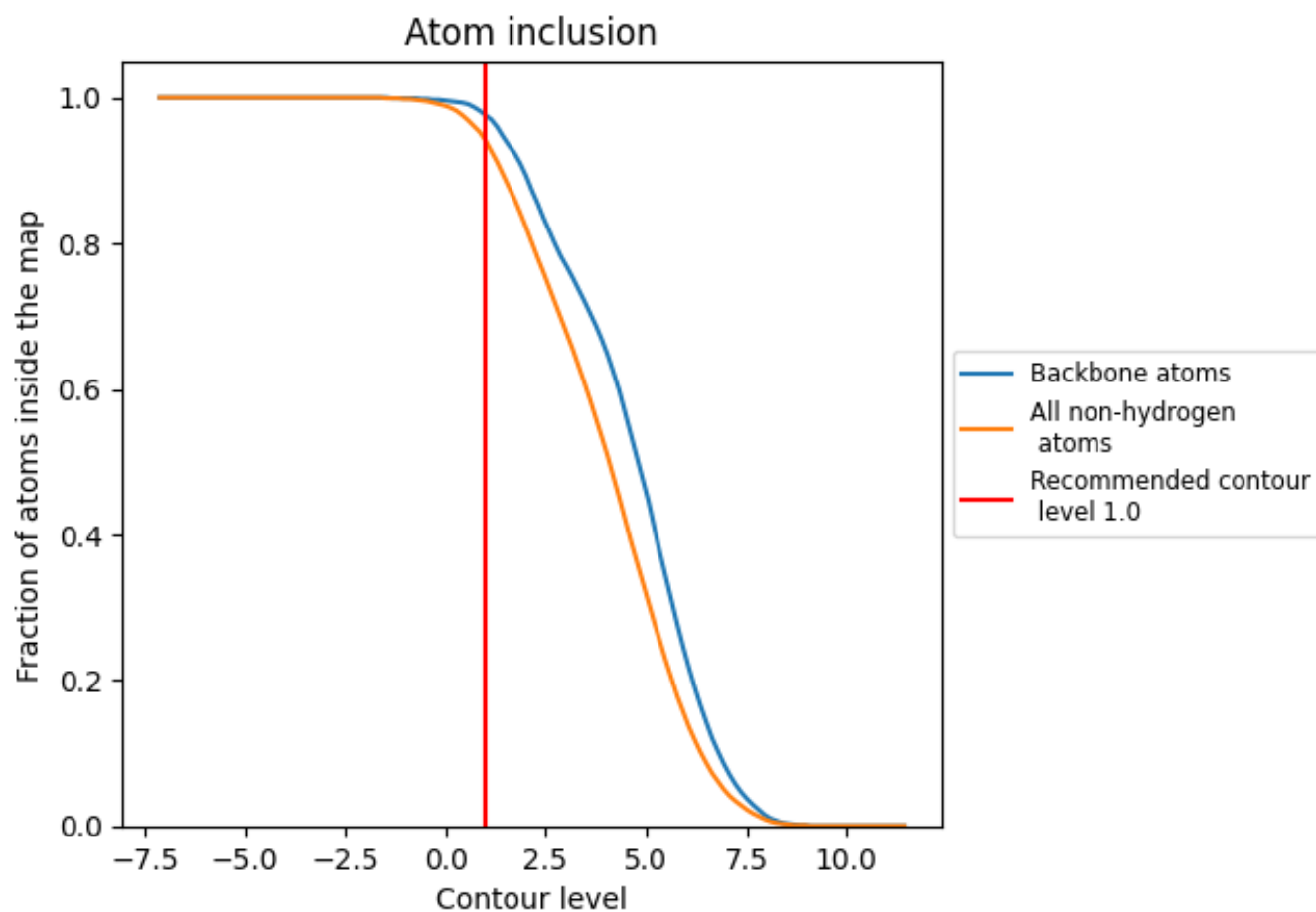
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.5640
1	 0.9420	 0.5620
2	 0.9420	 0.5650
3	 0.9410	 0.5650
4	 0.9410	 0.5640
5	 0.9390	 0.5620
6	 0.9380	 0.5640
7	 0.9390	 0.5640
8	 0.9400	 0.5620
A	 0.9410	 0.5670
B	 0.9410	 0.5660
C	 0.9420	 0.5650
D	 0.9400	 0.5650
E	 0.9410	 0.5650
F	 0.9400	 0.5660
G	 0.9410	 0.5650
H	 0.9370	 0.5660
I	 0.9410	 0.5670
J	 0.9400	 0.5640
K	 0.9410	 0.5660
L	 0.9410	 0.5650
M	 0.9410	 0.5650
N	 0.9380	 0.5650
O	 0.9410	 0.5640
P	 0.9370	 0.5660
Q	 0.9410	 0.5670
R	 0.9430	 0.5640
S	 0.9400	 0.5630
T	 0.9420	 0.5660
U	 0.9400	 0.5650
V	 0.9420	 0.5660
W	 0.9400	 0.5650
X	 0.9410	 0.5640
Y	 0.9380	 0.5640
Z	 0.9410	 0.5640



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.9440	 0.5640
b	 0.9410	 0.5640
c	 0.9420	 0.5660
d	 0.9440	 0.5640
e	 0.9410	 0.5640
f	 0.9420	 0.5660
g	 0.9400	 0.5640
h	 0.9410	 0.5620
i	 0.9390	 0.5640
j	 0.9390	 0.5620
k	 0.9380	 0.5640
l	 0.9400	 0.5620
m	 0.9410	 0.5630
n	 0.9400	 0.5660
o	 0.9410	 0.5620
p	 0.9400	 0.5640
q	 0.9420	 0.5620
r	 0.9420	 0.5640
s	 0.9420	 0.5620
t	 0.9410	 0.5640
u	 0.9410	 0.5640
v	 0.9420	 0.5620
w	 0.9410	 0.5630
x	 0.9420	 0.5640
y	 0.9420	 0.5640
z	 0.9420	 0.5630