



Full wwPDB EM Validation Report ⓘ

Jan 27, 2025 – 03:39 PM EST

PDB ID : 9ME0
EMDB ID : EMD-48181
Title : Goose Parvovirus Capsid
Authors : Jabbari, K.; Mietzsch, M.; McKenna, R.
Deposited on : 2024-12-05
Resolution : 2.43 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:

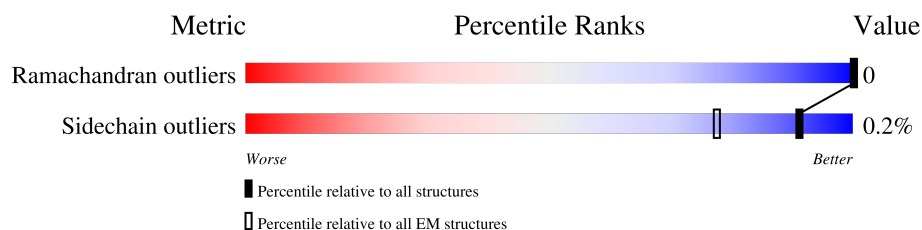
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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










The reported resolution of this entry is 2.43 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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	1	732		
1	2	732		
1	3	732		
1	4	732		
1	5	732		
1	6	732		
1	7	732		
1	8	732		
1	A	732		

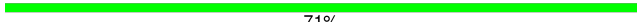
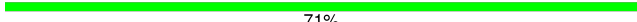
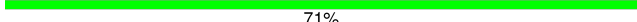
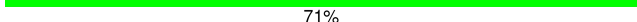
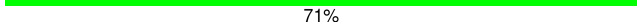
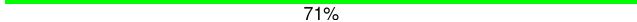

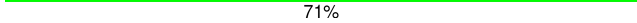
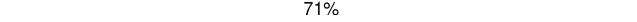
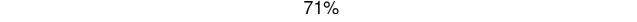
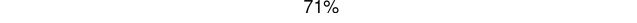
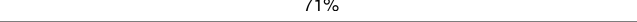
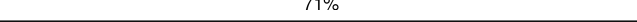
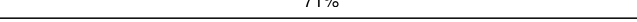
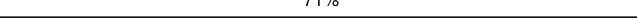
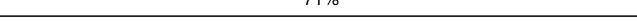
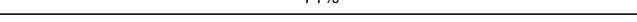
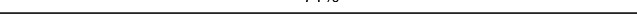







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Mol	Chain	Length	Quality of chain	
1	B	732		29%
1	C	732		29%
1	D	732		29%
1	E	732		29%
1	F	732		29%
1	G	732		29%
1	H	732		29%
1	I	732		29%
1	J	732		29%
1	K	732		29%
1	L	732		29%
1	M	732		29%
1	N	732		29%
1	O	732		29%
1	P	732		29%
1	Q	732		29%
1	R	732		29%
1	S	732		29%
1	T	732		29%
1	U	732		29%
1	V	732		29%
1	W	732		29%
1	X	732		29%
1	Y	732		29%
1	Z	732		29%

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Mol	Chain	Length	Quality of chain	
1	a	732		29%
1	b	732		29%
1	c	732		29%
1	d	732		29%
1	e	732		29%
1	f	732		29%
1	g	732		29%
1	h	732		29%
1	i	732		29%
1	j	732		29%
1	k	732		29%
1	l	732		29%
1	m	732		29%
1	n	732		29%
1	o	732		29%
1	p	732		29%
1	q	732		29%
1	r	732		29%
1	s	732		29%
1	t	732		29%
1	u	732		29%
1	v	732		29%
1	w	732		29%
1	x	732		29%
1	y	732		29%

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Mol	Chain	Length	Quality of chain
1	z	732	<div><div></div><div>71%</div><div>29%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 249900 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	B	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	C	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	D	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	E	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	F	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	G	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	H	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	I	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	J	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	K	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	L	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	M	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	N	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	O	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	P	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	Q	519	Total 4165	C 2640	N 719	O 790	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	S	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	T	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	U	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	V	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	W	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	X	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	Y	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	Z	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	a	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	b	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	c	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	d	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	e	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	f	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	g	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	h	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	i	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	j	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	k	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	l	519	Total 4165	C 2640	N 719	O 790	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	n	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	o	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	p	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	q	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	r	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	s	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	t	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	u	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	v	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	w	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	x	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	y	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	z	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	1	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	2	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	3	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	4	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	5	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	6	519	Total 4165	C 2640	N 719	O 790	S 16	0	0
1	7	519	Total 4165	C 2640	N 719	O 790	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	519	Total	C	N	O	S	0	0
			4165	2640	719	790	16		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	TRP	GLY	conflict	UNP Q67666
B	615	TRP	GLY	conflict	UNP Q67666
C	615	TRP	GLY	conflict	UNP Q67666
D	615	TRP	GLY	conflict	UNP Q67666
E	615	TRP	GLY	conflict	UNP Q67666
F	615	TRP	GLY	conflict	UNP Q67666
G	615	TRP	GLY	conflict	UNP Q67666
H	615	TRP	GLY	conflict	UNP Q67666
I	615	TRP	GLY	conflict	UNP Q67666
J	615	TRP	GLY	conflict	UNP Q67666
K	615	TRP	GLY	conflict	UNP Q67666
L	615	TRP	GLY	conflict	UNP Q67666
M	615	TRP	GLY	conflict	UNP Q67666
N	615	TRP	GLY	conflict	UNP Q67666
O	615	TRP	GLY	conflict	UNP Q67666
P	615	TRP	GLY	conflict	UNP Q67666
Q	615	TRP	GLY	conflict	UNP Q67666
R	615	TRP	GLY	conflict	UNP Q67666
S	615	TRP	GLY	conflict	UNP Q67666
T	615	TRP	GLY	conflict	UNP Q67666
U	615	TRP	GLY	conflict	UNP Q67666
V	615	TRP	GLY	conflict	UNP Q67666
W	615	TRP	GLY	conflict	UNP Q67666
X	615	TRP	GLY	conflict	UNP Q67666
Y	615	TRP	GLY	conflict	UNP Q67666
Z	615	TRP	GLY	conflict	UNP Q67666
a	615	TRP	GLY	conflict	UNP Q67666
b	615	TRP	GLY	conflict	UNP Q67666
c	615	TRP	GLY	conflict	UNP Q67666
d	615	TRP	GLY	conflict	UNP Q67666
e	615	TRP	GLY	conflict	UNP Q67666
f	615	TRP	GLY	conflict	UNP Q67666
g	615	TRP	GLY	conflict	UNP Q67666
h	615	TRP	GLY	conflict	UNP Q67666
i	615	TRP	GLY	conflict	UNP Q67666
j	615	TRP	GLY	conflict	UNP Q67666

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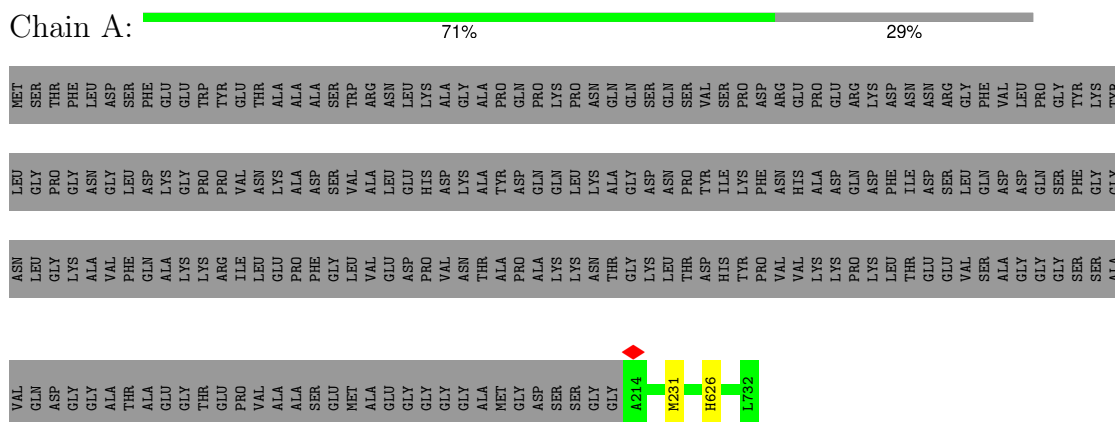
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Chain	Residue	Modelled	Actual	Comment	Reference
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l	615	TRP	GLY	conflict	UNP Q67666
m	615	TRP	GLY	conflict	UNP Q67666
n	615	TRP	GLY	conflict	UNP Q67666
o	615	TRP	GLY	conflict	UNP Q67666
p	615	TRP	GLY	conflict	UNP Q67666
q	615	TRP	GLY	conflict	UNP Q67666
r	615	TRP	GLY	conflict	UNP Q67666
s	615	TRP	GLY	conflict	UNP Q67666
t	615	TRP	GLY	conflict	UNP Q67666
u	615	TRP	GLY	conflict	UNP Q67666
v	615	TRP	GLY	conflict	UNP Q67666
w	615	TRP	GLY	conflict	UNP Q67666
x	615	TRP	GLY	conflict	UNP Q67666
y	615	TRP	GLY	conflict	UNP Q67666
z	615	TRP	GLY	conflict	UNP Q67666
1	615	TRP	GLY	conflict	UNP Q67666
2	615	TRP	GLY	conflict	UNP Q67666
3	615	TRP	GLY	conflict	UNP Q67666
4	615	TRP	GLY	conflict	UNP Q67666
5	615	TRP	GLY	conflict	UNP Q67666
6	615	TRP	GLY	conflict	UNP Q67666
7	615	TRP	GLY	conflict	UNP Q67666
8	615	TRP	GLY	conflict	UNP Q67666

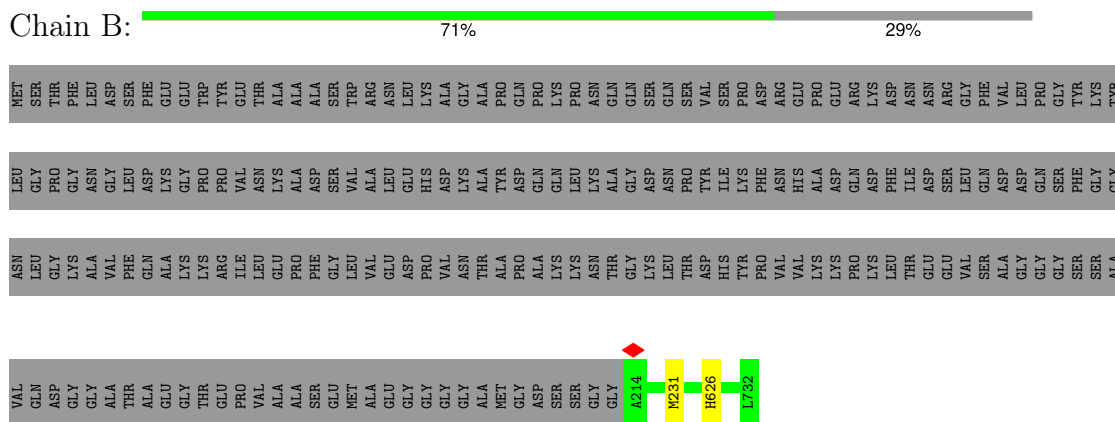
3 Residue-property plots

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.

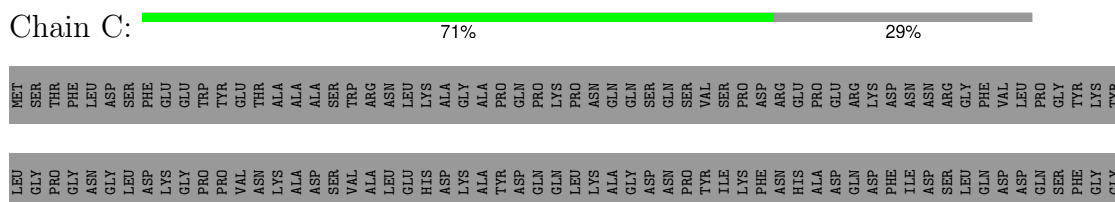
• Molecule 1: VP1

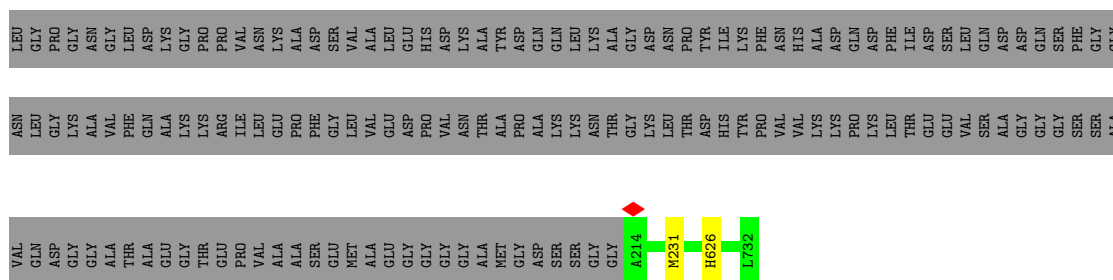


• Molecule 1: VP1



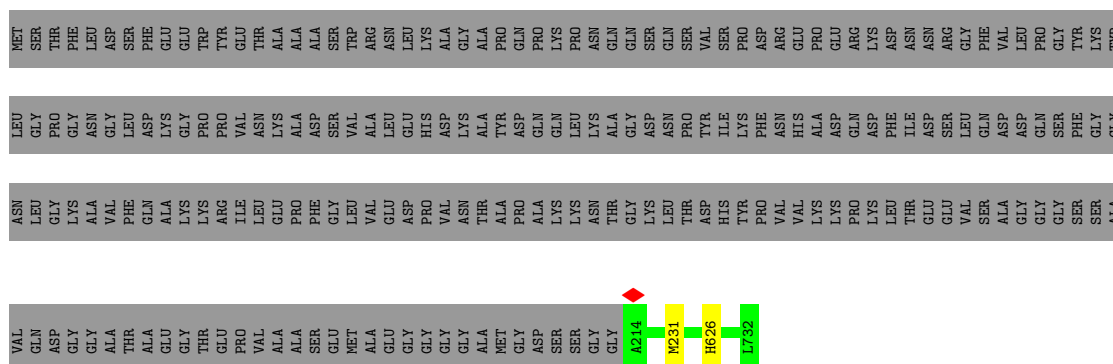
• Molecule 1: VP1





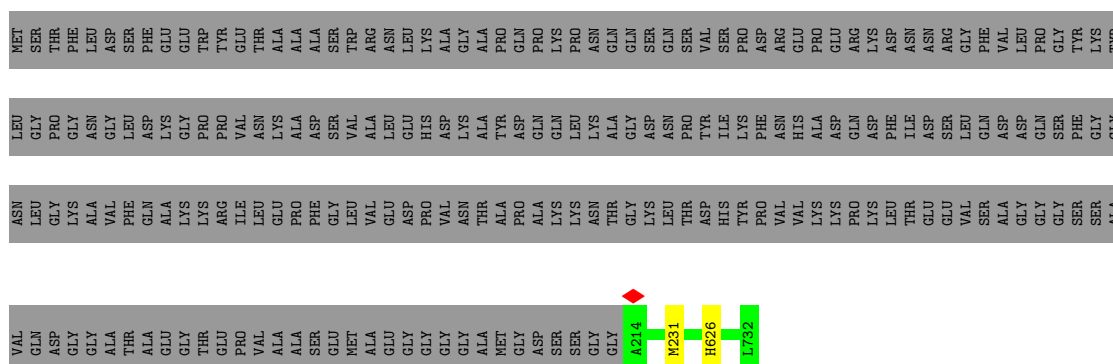
- Molecule 1: VP1

Chain K: 71% 29%



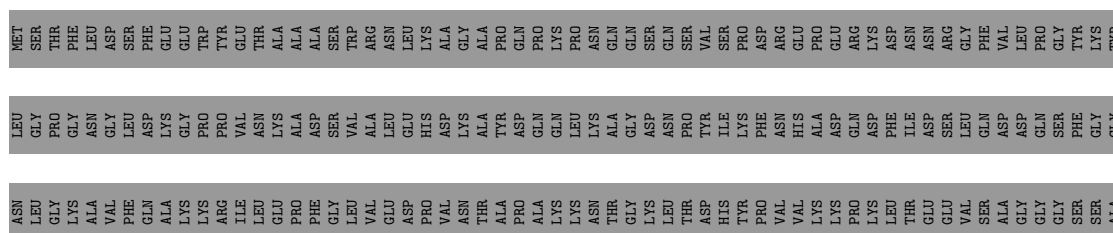
- Molecule 1: VP1

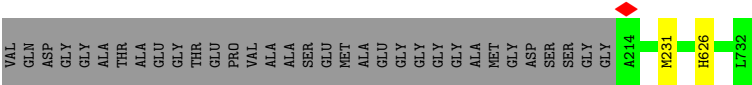
Chain L: 71% 29%



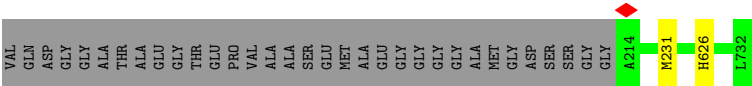
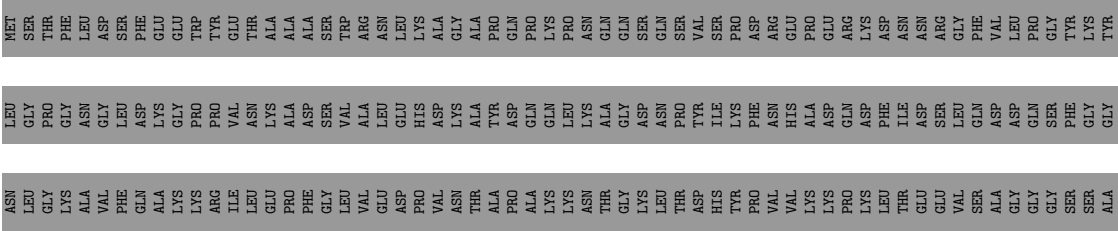
- Molecule 1: VP1

Chain M:  71% 29%

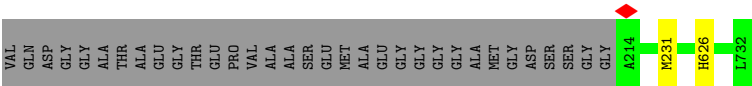
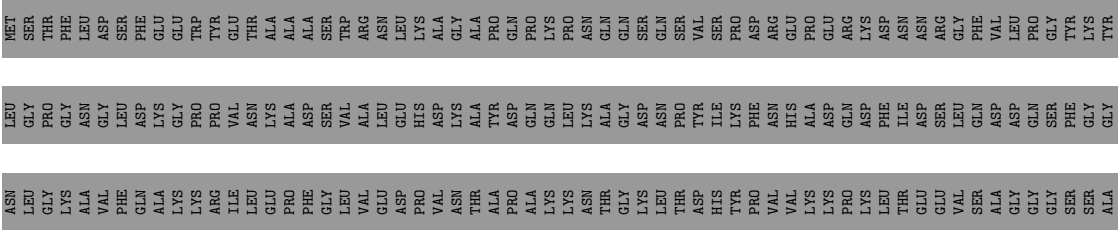




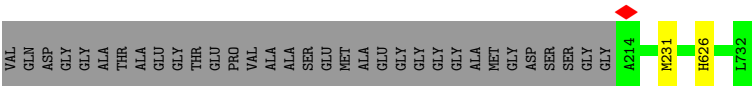
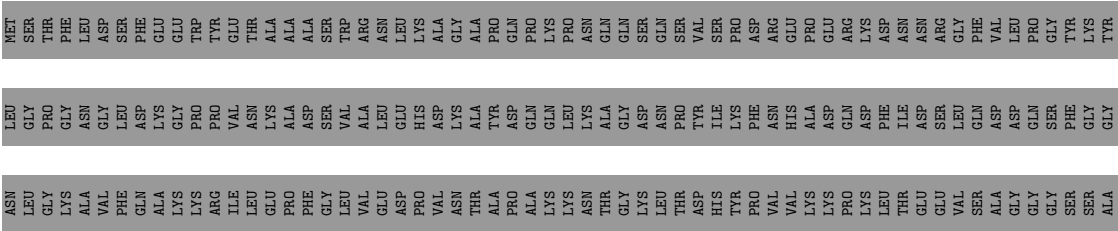
• Molecule 1: VP1



• Molecule 1: VP1



• Molecule 1: VP1



• Molecule 1: VP1

Opinion	Percentage
Doing a good job	71%
Doing a bad job	29%

- Molecule 1: VP1

Response	Percentage
Satisfied	71%
Not Satisfied	29%

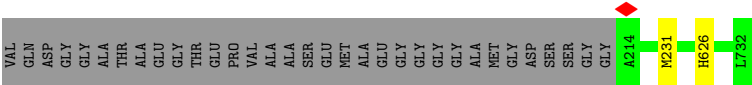
- Molecule 1: VP1

71% 29%

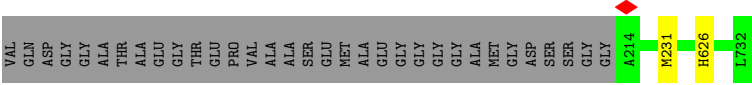
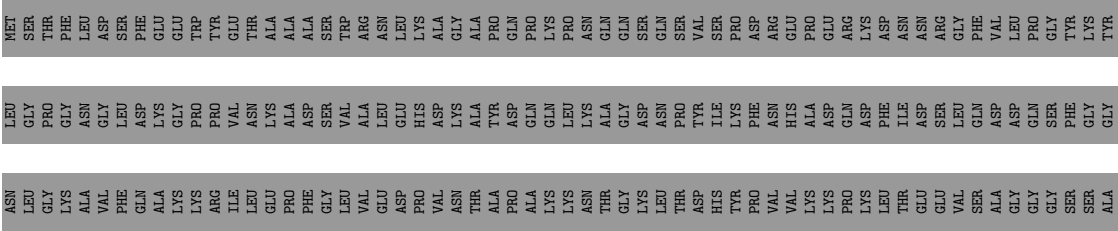
- Molecule 1: VP1

Opinion	Percentage
Doing a good job	71%
Doing a bad job	29%

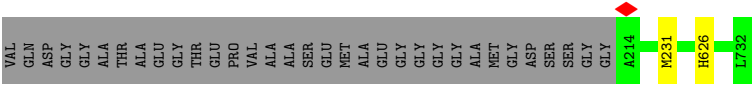
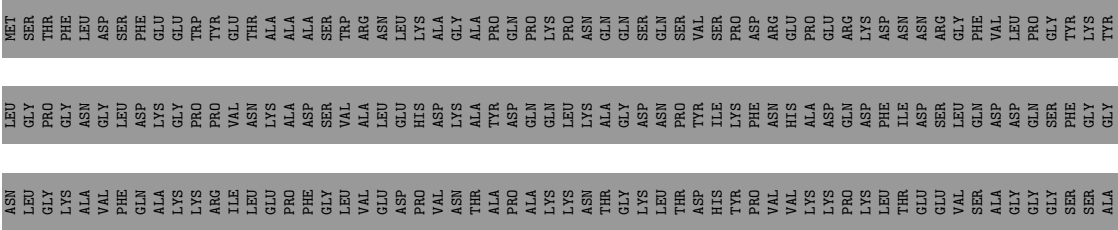
MET
 SER
 THR
 PHE
 LEU
 ASP
 SER
 PHE
 GLU
 GLY
 TRP
 TYR
 GLU
 THR
 ALA
 ALA
 ALA
 SER
 TRP
 ARG
 ASN
 LEU
 LYS
 ALA
 GLY
 ALA
 PRO
 GLN
 PRO
 LYS
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 ASP
 ARG
 GLU
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 ASP
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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



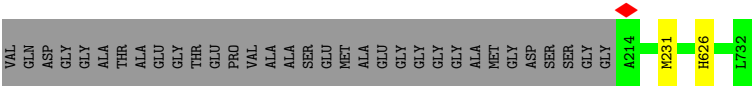
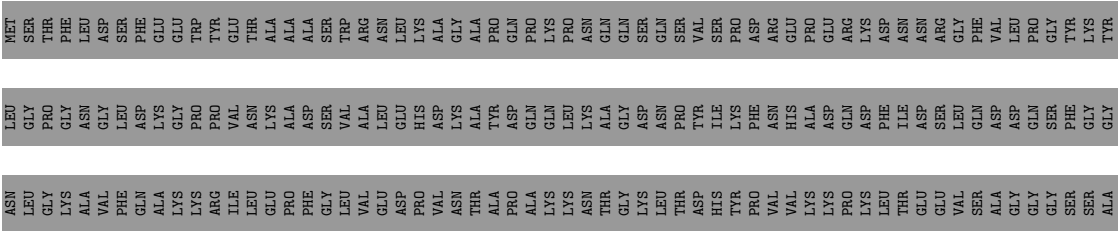
• Molecule 1: VP1



• Molecule 1: VP1



• Molecule 1: VP1



• Molecule 1: VP1

71% 29%

VAL	GLN	ASP	GLY	GLY	ALA	THR	ALA	GLU	GLY	THR	GLU	PRO	VAL	ALA	ALA	SER	GLU	MET	ALA	GLU	GLY	GLY	GLY	ALA	MET	GLY	ASP	SER	SER	GLY	GLY	GLY	A214	M231	H626	L732
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- Molecule 1: VP1

71% 29%

VAL
GLN
ASP
GLY
GLY
ALA
THR
ALA
ALA
GLU
GLY
THR
GLU
PRO
VAL
ALA
ALA
SER
SER
GLU
MET
ALA
GLU
GLY
GLY
GLY
ALA
ALA
MET
GLY
ASP
SER
SER
GLY
GLY
GLY
A214
M231
H626
L732

- Molecule 1: VP1

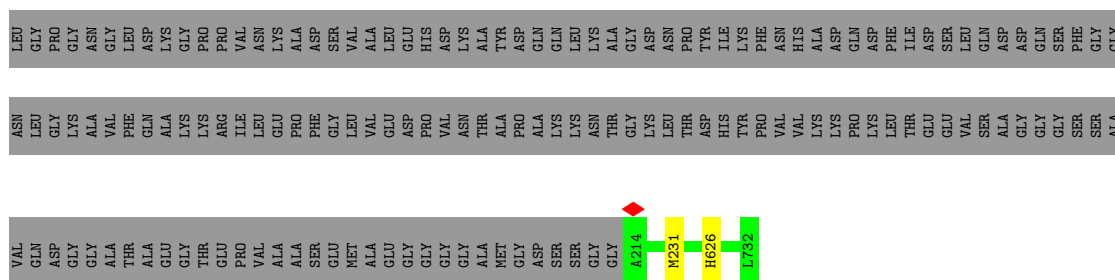
Response	Percentage
Doing a good job	71%
Doing a bad job	29%

VAL GLN ASP GLY GLY GLY GLY ALA THR ALA VAL GLY GLY THR GLU PRO VAL VAL ALA SER ALA GLU MET MET GLU GLY GLY GLY GLY ALA MET GLY ASP SER SER SER GLY GLY GLY A214 M231 H626 L732

- Molecule 1: VP1

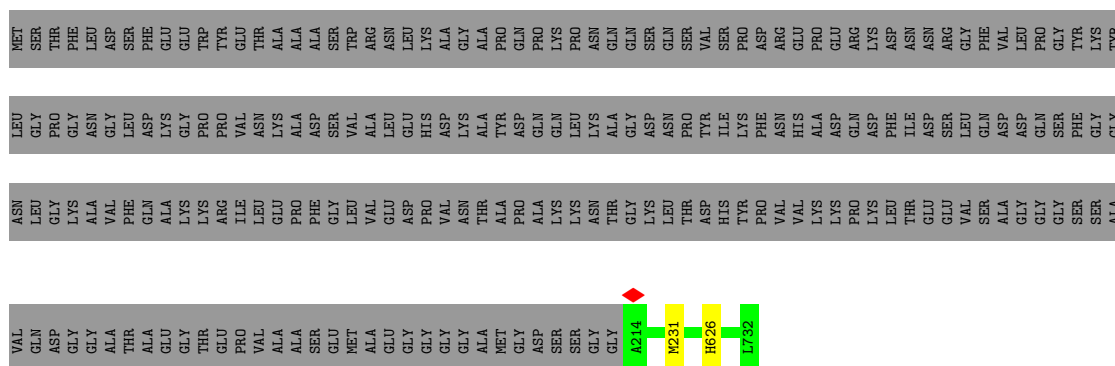
71% 29%

LEU GLY PRO PRO GLY ASN GLY LEU LEU ASP GLY LYS GLY PRO PRO VAL ASN LYS ALA ALA SER ASP VAL VAL ALA ALA LEU LEU GLU GLN GLN LEU LYS LYS ALA ALA GLY GLY ASP ASN PRO PRO TYR ILE PHE PHE ASN HIS ALA ASP ASP GLN GLN LEU LEU SER SER PHE GLY GLY



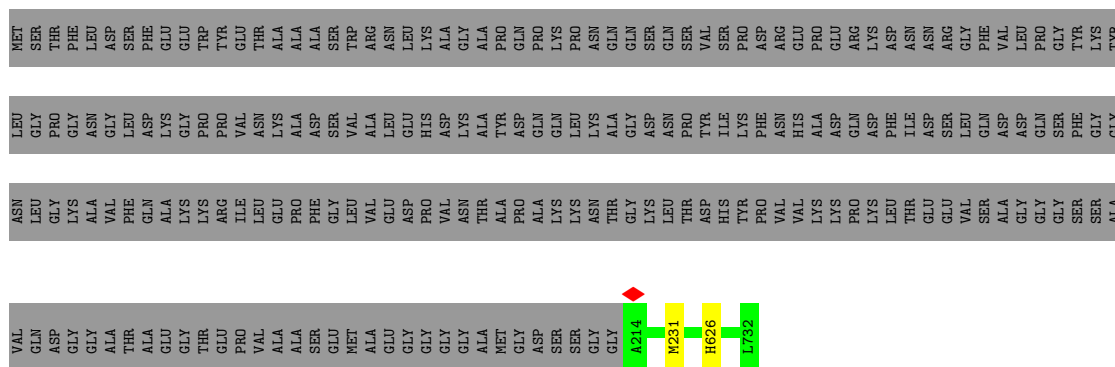
- Molecule 1: VP1

Chain 1: 71% 29%



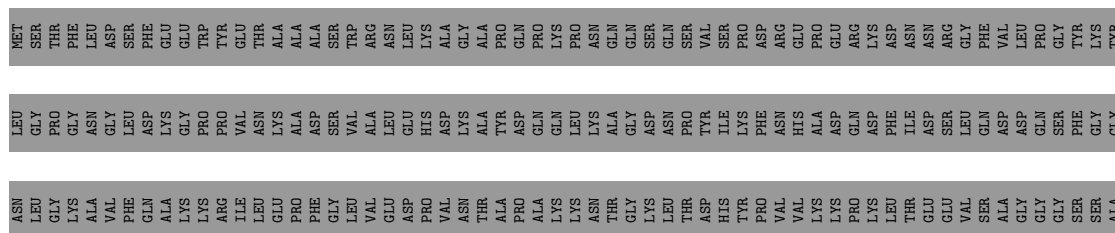
- Molecule 1: VP1

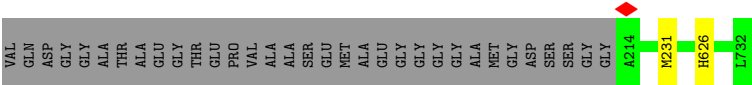
Chain m:  71% 29%



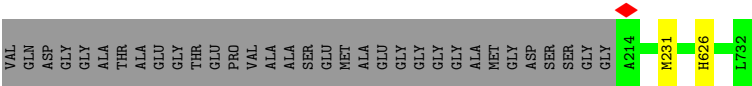
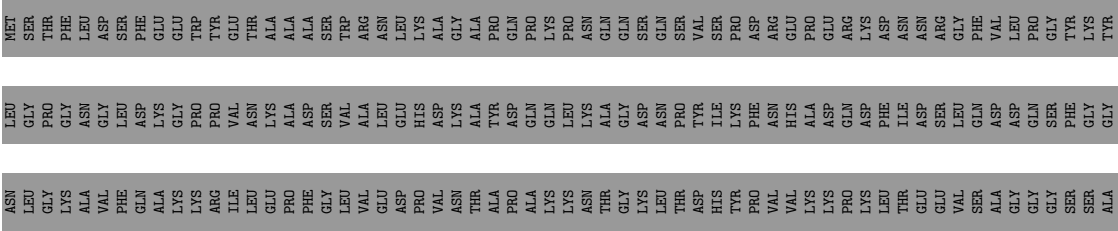
- Molecule 1: VP1

Chain n: 71% 29%

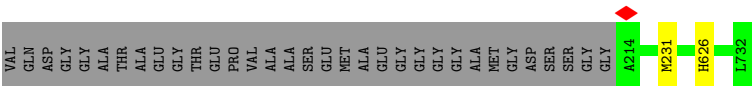
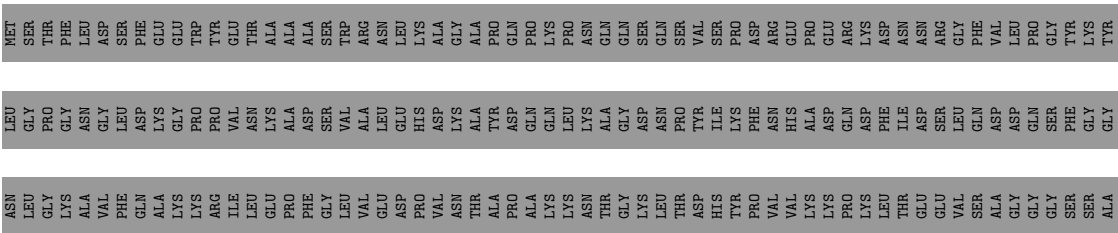




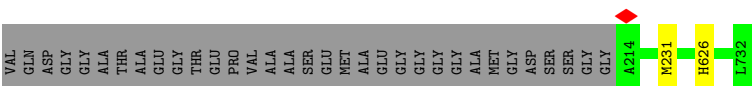
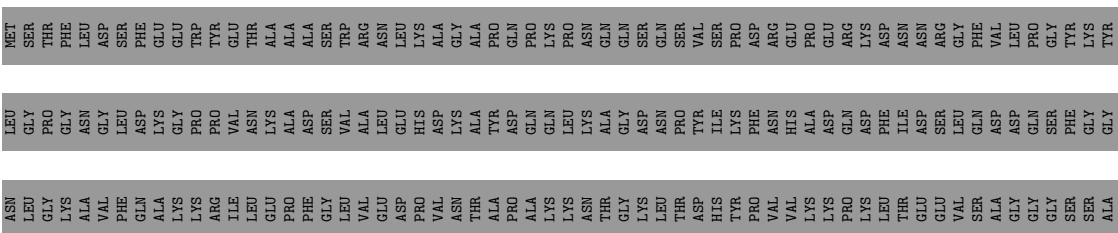
● Molecule 1: VP1



● Molecule 1: VP1



● Molecule 1: VP1



● Molecule 1: VP1

29%

VAL	GLN	ASP	GLY	GLY	ALA	THR	GLU	GLY	THR	GLU	PRO	VAL	ALA	ALA	SER	GLU	MET	ALA	GLU	GLY	GLY	GLY	ALA	MET	GLY	ASP	SER	SER	SER	GLY	GLY	GLY	A214	M231	H626	L732
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- Molecule 1: VP1

29%

VAL	GLN	ASP	GLY	GLY	ALA	THR	GLU	GLY	THR	PRO	GLU	MET	ALA	ALA	SER	GLU	MET	ALA	GLU	GLY	GLY	GLY	ALA	MET	GLY	ASP	SER	SER	GLY	GLY	GLY	A214	M231	H626	L732
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- Molecule 1: VP1

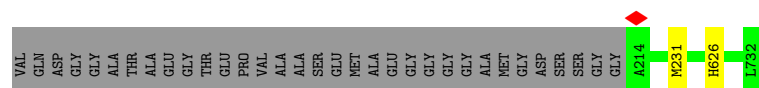
29%

[illegible]

- Molecule 1: VP1

29%

LEU	GLY	PRO	GLY	ASN	GLY	LEU	ASP	LYS	GLY	PRO	PRO	VAL	ASN	LYS	ALA	ASP	SER	VAL	ALA	ALA	LEU	HIS	ASP	LYS	TYR	ALA	ASP	GLN	GLN	LEU	LYS	ALA	ALA	ASP	ASN	ASN	HIS	ALA	ASP	GLN	ASP	PHE	LEU	ILE	THR	TYR	GLY	LYS	ASP	GLN	ASP	ASP	GLN	GLN	ASP	ASP	PHE	GLY	GLY
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15471	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	16.594	Depositor
Minimum map value	-8.236	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.51	1/4294 (0.0%)	0.55	0/5859
1	2	0.51	1/4294 (0.0%)	0.55	0/5859
1	3	0.51	1/4294 (0.0%)	0.55	0/5859
1	4	0.51	1/4294 (0.0%)	0.55	0/5859
1	5	0.51	1/4294 (0.0%)	0.55	0/5859
1	6	0.51	1/4294 (0.0%)	0.55	0/5859
1	7	0.51	1/4294 (0.0%)	0.55	0/5859
1	8	0.51	1/4294 (0.0%)	0.55	0/5859
1	A	0.51	1/4294 (0.0%)	0.55	0/5859
1	B	0.51	1/4294 (0.0%)	0.55	0/5859
1	C	0.51	1/4294 (0.0%)	0.55	0/5859
1	D	0.51	1/4294 (0.0%)	0.55	0/5859
1	E	0.51	1/4294 (0.0%)	0.55	0/5859
1	F	0.51	1/4294 (0.0%)	0.55	0/5859
1	G	0.51	1/4294 (0.0%)	0.55	0/5859
1	H	0.51	1/4294 (0.0%)	0.55	0/5859
1	I	0.51	1/4294 (0.0%)	0.55	0/5859
1	J	0.51	1/4294 (0.0%)	0.55	0/5859
1	K	0.51	1/4294 (0.0%)	0.55	0/5859
1	L	0.51	1/4294 (0.0%)	0.55	0/5859
1	M	0.51	1/4294 (0.0%)	0.55	0/5859
1	N	0.51	1/4294 (0.0%)	0.55	0/5859
1	O	0.51	1/4294 (0.0%)	0.55	0/5859
1	P	0.51	1/4294 (0.0%)	0.55	0/5859
1	Q	0.51	1/4294 (0.0%)	0.55	0/5859
1	R	0.51	1/4294 (0.0%)	0.55	0/5859
1	S	0.51	1/4294 (0.0%)	0.55	0/5859
1	T	0.51	1/4294 (0.0%)	0.55	0/5859
1	U	0.51	1/4294 (0.0%)	0.55	0/5859
1	V	0.51	1/4294 (0.0%)	0.55	0/5859
1	W	0.51	1/4294 (0.0%)	0.55	0/5859
1	X	0.51	1/4294 (0.0%)	0.55	0/5859
1	Y	0.51	1/4294 (0.0%)	0.55	0/5859
1	Z	0.51	1/4294 (0.0%)	0.55	0/5859

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.51	1/4294 (0.0%)	0.55	0/5859
1	b	0.51	1/4294 (0.0%)	0.55	0/5859
1	c	0.51	1/4294 (0.0%)	0.55	0/5859
1	d	0.51	1/4294 (0.0%)	0.55	0/5859
1	e	0.51	1/4294 (0.0%)	0.55	0/5859
1	f	0.51	1/4294 (0.0%)	0.55	0/5859
1	g	0.51	1/4294 (0.0%)	0.55	0/5859
1	h	0.51	1/4294 (0.0%)	0.55	0/5859
1	i	0.51	1/4294 (0.0%)	0.55	0/5859
1	j	0.51	1/4294 (0.0%)	0.55	0/5859
1	k	0.51	1/4294 (0.0%)	0.55	0/5859
1	l	0.51	1/4294 (0.0%)	0.55	0/5859
1	m	0.51	1/4294 (0.0%)	0.55	0/5859
1	n	0.51	1/4294 (0.0%)	0.55	0/5859
1	o	0.51	1/4294 (0.0%)	0.55	0/5859
1	p	0.51	1/4294 (0.0%)	0.55	0/5859
1	q	0.51	1/4294 (0.0%)	0.55	0/5859
1	r	0.51	1/4294 (0.0%)	0.55	0/5859
1	s	0.51	1/4294 (0.0%)	0.55	0/5859
1	t	0.51	1/4294 (0.0%)	0.55	0/5859
1	u	0.51	1/4294 (0.0%)	0.55	0/5859
1	v	0.51	1/4294 (0.0%)	0.55	0/5859
1	w	0.51	1/4294 (0.0%)	0.55	0/5859
1	x	0.51	1/4294 (0.0%)	0.55	0/5859
1	y	0.51	1/4294 (0.0%)	0.55	0/5859
1	z	0.51	1/4294 (0.0%)	0.55	0/5859
All	All	0.51	60/257640 (0.0%)	0.55	0/351540

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7	626	HIS	C-N	-5.75	1.23	1.34
1	m	626	HIS	C-N	-5.74	1.23	1.34
1	a	626	HIS	C-N	-5.73	1.23	1.34
1	v	626	HIS	C-N	-5.73	1.23	1.34
1	t	626	HIS	C-N	-5.73	1.23	1.34
1	s	626	HIS	C-N	-5.72	1.23	1.34
1	G	626	HIS	C-N	-5.72	1.23	1.34
1	O	626	HIS	C-N	-5.72	1.23	1.34
1	h	626	HIS	C-N	-5.72	1.23	1.34
1	8	626	HIS	C-N	-5.72	1.23	1.34
1	S	626	HIS	C-N	-5.72	1.23	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	626	HIS	C-N	-5.72	1.23	1.34
1	2	626	HIS	C-N	-5.72	1.23	1.34
1	i	626	HIS	C-N	-5.72	1.23	1.34
1	6	626	HIS	C-N	-5.72	1.23	1.34
1	K	626	HIS	C-N	-5.71	1.23	1.34
1	P	626	HIS	C-N	-5.71	1.23	1.34
1	j	626	HIS	C-N	-5.71	1.23	1.34
1	B	626	HIS	C-N	-5.70	1.23	1.34
1	Z	626	HIS	C-N	-5.70	1.23	1.34
1	o	626	HIS	C-N	-5.70	1.23	1.34
1	w	626	HIS	C-N	-5.70	1.23	1.34
1	z	626	HIS	C-N	-5.70	1.23	1.34
1	A	626	HIS	C-N	-5.69	1.23	1.34
1	b	626	HIS	C-N	-5.69	1.23	1.34
1	c	626	HIS	C-N	-5.69	1.23	1.34
1	d	626	HIS	C-N	-5.69	1.23	1.34
1	e	626	HIS	C-N	-5.69	1.23	1.34
1	y	626	HIS	C-N	-5.69	1.23	1.34
1	3	626	HIS	C-N	-5.69	1.23	1.34
1	C	626	HIS	C-N	-5.69	1.23	1.34
1	I	626	HIS	C-N	-5.69	1.23	1.34
1	Q	626	HIS	C-N	-5.69	1.23	1.34
1	V	626	HIS	C-N	-5.69	1.23	1.34
1	g	626	HIS	C-N	-5.69	1.23	1.34
1	p	626	HIS	C-N	-5.69	1.23	1.34
1	u	626	HIS	C-N	-5.69	1.23	1.34
1	T	626	HIS	C-N	-5.68	1.23	1.34
1	x	626	HIS	C-N	-5.68	1.23	1.34
1	4	626	HIS	C-N	-5.68	1.23	1.34
1	E	626	HIS	C-N	-5.68	1.23	1.34
1	H	626	HIS	C-N	-5.68	1.23	1.34
1	M	626	HIS	C-N	-5.68	1.23	1.34
1	N	626	HIS	C-N	-5.68	1.23	1.34
1	X	626	HIS	C-N	-5.68	1.23	1.34
1	Y	626	HIS	C-N	-5.68	1.23	1.34
1	l	626	HIS	C-N	-5.68	1.23	1.34
1	q	626	HIS	C-N	-5.68	1.23	1.34
1	5	626	HIS	C-N	-5.68	1.23	1.34
1	J	626	HIS	C-N	-5.67	1.23	1.34
1	L	626	HIS	C-N	-5.67	1.23	1.34
1	r	626	HIS	C-N	-5.67	1.23	1.34
1	D	626	HIS	C-N	-5.67	1.23	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	626	HIS	C-N	-5.67	1.23	1.34
1	U	626	HIS	C-N	-5.65	1.23	1.34
1	F	626	HIS	C-N	-5.65	1.23	1.34
1	f	626	HIS	C-N	-5.65	1.23	1.34
1	n	626	HIS	C-N	-5.65	1.23	1.34
1	R	626	HIS	C-N	-5.65	1.23	1.34
1	k	626	HIS	C-N	-5.65	1.23	1.34

There are no bond angle outliers.

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	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	2	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	3	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	4	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	5	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	6	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	7	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	8	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	A	517/732 (71%)	504 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	C	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	D	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	E	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	F	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	G	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	H	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	I	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	J	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	K	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	L	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	M	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	N	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	O	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	P	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	Q	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	R	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	S	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	T	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	U	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	V	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	W	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	X	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	Y	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	Z	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	a	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	b	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	c	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	d	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	e	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	f	517/732 (71%)	504 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	g	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	h	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	i	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	j	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	k	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	l	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	m	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	n	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	o	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	p	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	q	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	r	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	s	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	t	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	u	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	v	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	w	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	x	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	y	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
1	z	517/732 (71%)	504 (98%)	13 (2%)	0	100	100
All	All	31020/43920 (71%)	30240 (98%)	780 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	453/618 (73%)	452 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	3	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	4	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	5	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	6	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	7	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	8	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	A	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	B	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	C	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	D	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	E	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	F	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	G	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	H	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	I	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	J	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	K	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	L	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	M	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	N	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	O	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	P	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	Q	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	R	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	S	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	T	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	U	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	V	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	W	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	X	453/618 (73%)	452 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	Z	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	a	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	b	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	c	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	d	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	e	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	f	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	g	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	h	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	i	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	j	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	k	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	l	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	m	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	n	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	o	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	p	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	q	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	r	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	s	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	t	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	u	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	v	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	w	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	x	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	y	453/618 (73%)	452 (100%)	1 (0%)	92	96
1	z	453/618 (73%)	452 (100%)	1 (0%)	92	96
All	All	27180/37080 (73%)	27120 (100%)	60 (0%)	91	96

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	MET
1	B	231	MET
1	C	231	MET
1	D	231	MET
1	E	231	MET
1	F	231	MET
1	G	231	MET
1	H	231	MET
1	I	231	MET
1	J	231	MET
1	K	231	MET
1	L	231	MET
1	M	231	MET
1	N	231	MET
1	O	231	MET
1	P	231	MET
1	Q	231	MET
1	R	231	MET
1	S	231	MET
1	T	231	MET
1	U	231	MET
1	V	231	MET
1	W	231	MET
1	X	231	MET
1	Y	231	MET
1	Z	231	MET
1	a	231	MET
1	b	231	MET
1	c	231	MET
1	d	231	MET
1	e	231	MET
1	f	231	MET
1	g	231	MET
1	h	231	MET
1	i	231	MET
1	j	231	MET
1	k	231	MET
1	l	231	MET
1	m	231	MET
1	n	231	MET
1	o	231	MET
1	p	231	MET
1	q	231	MET

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Mol	Chain	Res	Type
1	r	231	MET
1	s	231	MET
1	t	231	MET
1	u	231	MET
1	v	231	MET
1	w	231	MET
1	x	231	MET
1	y	231	MET
1	z	231	MET
1	1	231	MET
1	2	231	MET
1	3	231	MET
1	4	231	MET
1	5	231	MET
1	6	231	MET
1	7	231	MET
1	8	231	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (705) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	HIS
1	A	322	GLN
1	A	337	GLN
1	A	400	GLN
1	A	425	HIS
1	A	427	GLN
1	A	479	GLN
1	A	581	GLN
1	A	637	HIS
1	A	642	GLN
1	A	669	GLN
1	A	731	ASN
1	B	284	HIS
1	B	322	GLN
1	B	337	GLN
1	B	425	HIS
1	B	427	GLN
1	B	479	GLN
1	B	581	GLN
1	B	637	HIS
1	B	642	GLN

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Mol	Chain	Res	Type
1	B	669	GLN
1	B	731	ASN
1	C	284	HIS
1	C	322	GLN
1	C	337	GLN
1	C	400	GLN
1	C	425	HIS
1	C	427	GLN
1	C	479	GLN
1	C	581	GLN
1	C	637	HIS
1	C	642	GLN
1	C	669	GLN
1	C	731	ASN
1	D	284	HIS
1	D	322	GLN
1	D	337	GLN
1	D	400	GLN
1	D	425	HIS
1	D	427	GLN
1	D	479	GLN
1	D	581	GLN
1	D	637	HIS
1	D	642	GLN
1	D	669	GLN
1	D	731	ASN
1	E	284	HIS
1	E	322	GLN
1	E	337	GLN
1	E	400	GLN
1	E	425	HIS
1	E	427	GLN
1	E	479	GLN
1	E	581	GLN
1	E	637	HIS
1	E	642	GLN
1	E	669	GLN
1	E	731	ASN
1	F	284	HIS
1	F	322	GLN
1	F	337	GLN
1	F	400	GLN

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Mol	Chain	Res	Type
1	F	425	HIS
1	F	427	GLN
1	F	479	GLN
1	F	581	GLN
1	F	637	HIS
1	F	642	GLN
1	F	669	GLN
1	F	731	ASN
1	G	284	HIS
1	G	322	GLN
1	G	337	GLN
1	G	400	GLN
1	G	425	HIS
1	G	427	GLN
1	G	479	GLN
1	G	581	GLN
1	G	637	HIS
1	G	642	GLN
1	G	669	GLN
1	G	731	ASN
1	H	284	HIS
1	H	322	GLN
1	H	337	GLN
1	H	400	GLN
1	H	425	HIS
1	H	427	GLN
1	H	479	GLN
1	H	581	GLN
1	H	637	HIS
1	H	642	GLN
1	H	669	GLN
1	H	731	ASN
1	I	284	HIS
1	I	322	GLN
1	I	337	GLN
1	I	400	GLN
1	I	425	HIS
1	I	427	GLN
1	I	479	GLN
1	I	581	GLN
1	I	637	HIS
1	I	642	GLN

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Mol	Chain	Res	Type
1	I	669	GLN
1	I	731	ASN
1	J	284	HIS
1	J	322	GLN
1	J	337	GLN
1	J	425	HIS
1	J	427	GLN
1	J	479	GLN
1	J	581	GLN
1	J	637	HIS
1	J	642	GLN
1	J	669	GLN
1	J	731	ASN
1	K	284	HIS
1	K	322	GLN
1	K	337	GLN
1	K	425	HIS
1	K	427	GLN
1	K	479	GLN
1	K	581	GLN
1	K	637	HIS
1	K	642	GLN
1	K	669	GLN
1	K	731	ASN
1	L	284	HIS
1	L	322	GLN
1	L	337	GLN
1	L	425	HIS
1	L	427	GLN
1	L	479	GLN
1	L	581	GLN
1	L	637	HIS
1	L	642	GLN
1	L	669	GLN
1	L	731	ASN
1	M	284	HIS
1	M	322	GLN
1	M	337	GLN
1	M	425	HIS
1	M	427	GLN
1	M	479	GLN
1	M	581	GLN

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Mol	Chain	Res	Type
1	M	637	HIS
1	M	642	GLN
1	M	669	GLN
1	M	731	ASN
1	N	284	HIS
1	N	322	GLN
1	N	337	GLN
1	N	400	GLN
1	N	425	HIS
1	N	427	GLN
1	N	479	GLN
1	N	581	GLN
1	N	637	HIS
1	N	642	GLN
1	N	669	GLN
1	N	731	ASN
1	O	284	HIS
1	O	322	GLN
1	O	337	GLN
1	O	400	GLN
1	O	425	HIS
1	O	427	GLN
1	O	479	GLN
1	O	581	GLN
1	O	637	HIS
1	O	642	GLN
1	O	669	GLN
1	O	731	ASN
1	P	284	HIS
1	P	322	GLN
1	P	337	GLN
1	P	425	HIS
1	P	427	GLN
1	P	479	GLN
1	P	581	GLN
1	P	637	HIS
1	P	642	GLN
1	P	669	GLN
1	P	731	ASN
1	Q	284	HIS
1	Q	322	GLN
1	Q	337	GLN

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Mol	Chain	Res	Type
1	Q	400	GLN
1	Q	425	HIS
1	Q	427	GLN
1	Q	479	GLN
1	Q	581	GLN
1	Q	637	HIS
1	Q	642	GLN
1	Q	669	GLN
1	Q	731	ASN
1	R	284	HIS
1	R	322	GLN
1	R	337	GLN
1	R	400	GLN
1	R	425	HIS
1	R	427	GLN
1	R	479	GLN
1	R	581	GLN
1	R	637	HIS
1	R	642	GLN
1	R	669	GLN
1	R	731	ASN
1	S	284	HIS
1	S	322	GLN
1	S	337	GLN
1	S	425	HIS
1	S	427	GLN
1	S	479	GLN
1	S	581	GLN
1	S	637	HIS
1	S	642	GLN
1	S	669	GLN
1	S	731	ASN
1	T	284	HIS
1	T	322	GLN
1	T	337	GLN
1	T	400	GLN
1	T	425	HIS
1	T	427	GLN
1	T	479	GLN
1	T	581	GLN
1	T	637	HIS
1	T	642	GLN

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Mol	Chain	Res	Type
1	T	669	GLN
1	T	731	ASN
1	U	284	HIS
1	U	322	GLN
1	U	337	GLN
1	U	400	GLN
1	U	425	HIS
1	U	427	GLN
1	U	479	GLN
1	U	581	GLN
1	U	637	HIS
1	U	642	GLN
1	U	669	GLN
1	U	731	ASN
1	V	284	HIS
1	V	322	GLN
1	V	337	GLN
1	V	400	GLN
1	V	425	HIS
1	V	427	GLN
1	V	479	GLN
1	V	581	GLN
1	V	637	HIS
1	V	642	GLN
1	V	669	GLN
1	V	731	ASN
1	W	284	HIS
1	W	322	GLN
1	W	337	GLN
1	W	400	GLN
1	W	425	HIS
1	W	427	GLN
1	W	479	GLN
1	W	581	GLN
1	W	637	HIS
1	W	642	GLN
1	W	669	GLN
1	W	731	ASN
1	X	284	HIS
1	X	322	GLN
1	X	337	GLN
1	X	400	GLN

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Mol	Chain	Res	Type
1	X	425	HIS
1	X	427	GLN
1	X	479	GLN
1	X	581	GLN
1	X	637	HIS
1	X	642	GLN
1	X	669	GLN
1	X	731	ASN
1	Y	284	HIS
1	Y	322	GLN
1	Y	337	GLN
1	Y	400	GLN
1	Y	425	HIS
1	Y	427	GLN
1	Y	479	GLN
1	Y	581	GLN
1	Y	637	HIS
1	Y	642	GLN
1	Y	669	GLN
1	Y	731	ASN
1	Z	284	HIS
1	Z	322	GLN
1	Z	337	GLN
1	Z	425	HIS
1	Z	427	GLN
1	Z	479	GLN
1	Z	581	GLN
1	Z	637	HIS
1	Z	642	GLN
1	Z	669	GLN
1	Z	731	ASN
1	a	284	HIS
1	a	322	GLN
1	a	337	GLN
1	a	400	GLN
1	a	425	HIS
1	a	427	GLN
1	a	479	GLN
1	a	581	GLN
1	a	637	HIS
1	a	642	GLN
1	a	669	GLN

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Mol	Chain	Res	Type
1	a	731	ASN
1	b	284	HIS
1	b	322	GLN
1	b	337	GLN
1	b	400	GLN
1	b	425	HIS
1	b	427	GLN
1	b	479	GLN
1	b	581	GLN
1	b	637	HIS
1	b	642	GLN
1	b	669	GLN
1	b	731	ASN
1	c	284	HIS
1	c	322	GLN
1	c	337	GLN
1	c	425	HIS
1	c	427	GLN
1	c	479	GLN
1	c	581	GLN
1	c	637	HIS
1	c	642	GLN
1	c	669	GLN
1	c	731	ASN
1	d	284	HIS
1	d	322	GLN
1	d	337	GLN
1	d	400	GLN
1	d	425	HIS
1	d	427	GLN
1	d	479	GLN
1	d	581	GLN
1	d	637	HIS
1	d	642	GLN
1	d	669	GLN
1	d	731	ASN
1	e	284	HIS
1	e	322	GLN
1	e	337	GLN
1	e	400	GLN
1	e	425	HIS
1	e	427	GLN

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Mol	Chain	Res	Type
1	e	479	GLN
1	e	581	GLN
1	e	637	HIS
1	e	642	GLN
1	e	669	GLN
1	e	731	ASN
1	f	284	HIS
1	f	322	GLN
1	f	337	GLN
1	f	400	GLN
1	f	425	HIS
1	f	427	GLN
1	f	479	GLN
1	f	581	GLN
1	f	637	HIS
1	f	642	GLN
1	f	669	GLN
1	f	731	ASN
1	g	284	HIS
1	g	322	GLN
1	g	337	GLN
1	g	400	GLN
1	g	425	HIS
1	g	427	GLN
1	g	479	GLN
1	g	581	GLN
1	g	637	HIS
1	g	642	GLN
1	g	669	GLN
1	g	731	ASN
1	h	284	HIS
1	h	322	GLN
1	h	337	GLN
1	h	425	HIS
1	h	427	GLN
1	h	479	GLN
1	h	581	GLN
1	h	637	HIS
1	h	642	GLN
1	h	669	GLN
1	h	731	ASN
1	i	284	HIS

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Mol	Chain	Res	Type
1	i	322	GLN
1	i	337	GLN
1	i	400	GLN
1	i	425	HIS
1	i	427	GLN
1	i	479	GLN
1	i	581	GLN
1	i	637	HIS
1	i	642	GLN
1	i	669	GLN
1	i	731	ASN
1	j	284	HIS
1	j	322	GLN
1	j	337	GLN
1	j	400	GLN
1	j	425	HIS
1	j	427	GLN
1	j	479	GLN
1	j	581	GLN
1	j	637	HIS
1	j	642	GLN
1	j	669	GLN
1	j	731	ASN
1	k	284	HIS
1	k	322	GLN
1	k	337	GLN
1	k	400	GLN
1	k	425	HIS
1	k	427	GLN
1	k	479	GLN
1	k	581	GLN
1	k	637	HIS
1	k	642	GLN
1	k	669	GLN
1	k	731	ASN
1	l	284	HIS
1	l	322	GLN
1	l	337	GLN
1	l	400	GLN
1	l	425	HIS
1	l	427	GLN
1	l	479	GLN

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Mol	Chain	Res	Type
1	l	581	GLN
1	l	637	HIS
1	l	642	GLN
1	l	669	GLN
1	l	731	ASN
1	m	284	HIS
1	m	322	GLN
1	m	337	GLN
1	m	400	GLN
1	m	425	HIS
1	m	427	GLN
1	m	479	GLN
1	m	581	GLN
1	m	637	HIS
1	m	642	GLN
1	m	669	GLN
1	m	731	ASN
1	n	284	HIS
1	n	322	GLN
1	n	337	GLN
1	n	400	GLN
1	n	425	HIS
1	n	427	GLN
1	n	479	GLN
1	n	581	GLN
1	n	637	HIS
1	n	642	GLN
1	n	669	GLN
1	n	731	ASN
1	o	284	HIS
1	o	322	GLN
1	o	337	GLN
1	o	400	GLN
1	o	425	HIS
1	o	427	GLN
1	o	479	GLN
1	o	581	GLN
1	o	637	HIS
1	o	642	GLN
1	o	669	GLN
1	o	731	ASN
1	p	284	HIS

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Mol	Chain	Res	Type
1	p	322	GLN
1	p	337	GLN
1	p	400	GLN
1	p	425	HIS
1	p	427	GLN
1	p	479	GLN
1	p	581	GLN
1	p	637	HIS
1	p	642	GLN
1	p	669	GLN
1	p	731	ASN
1	q	284	HIS
1	q	322	GLN
1	q	337	GLN
1	q	400	GLN
1	q	425	HIS
1	q	427	GLN
1	q	479	GLN
1	q	581	GLN
1	q	637	HIS
1	q	642	GLN
1	q	669	GLN
1	q	731	ASN
1	r	284	HIS
1	r	322	GLN
1	r	337	GLN
1	r	425	HIS
1	r	427	GLN
1	r	479	GLN
1	r	581	GLN
1	r	637	HIS
1	r	642	GLN
1	r	669	GLN
1	r	731	ASN
1	s	284	HIS
1	s	322	GLN
1	s	337	GLN
1	s	400	GLN
1	s	425	HIS
1	s	427	GLN
1	s	479	GLN
1	s	581	GLN

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Mol	Chain	Res	Type
1	s	637	HIS
1	s	642	GLN
1	s	669	GLN
1	s	731	ASN
1	t	284	HIS
1	t	322	GLN
1	t	337	GLN
1	t	400	GLN
1	t	425	HIS
1	t	427	GLN
1	t	479	GLN
1	t	581	GLN
1	t	637	HIS
1	t	642	GLN
1	t	669	GLN
1	t	731	ASN
1	u	284	HIS
1	u	322	GLN
1	u	337	GLN
1	u	400	GLN
1	u	425	HIS
1	u	427	GLN
1	u	479	GLN
1	u	581	GLN
1	u	637	HIS
1	u	642	GLN
1	u	669	GLN
1	u	731	ASN
1	v	284	HIS
1	v	322	GLN
1	v	337	GLN
1	v	400	GLN
1	v	425	HIS
1	v	427	GLN
1	v	479	GLN
1	v	581	GLN
1	v	637	HIS
1	v	642	GLN
1	v	669	GLN
1	v	731	ASN
1	w	284	HIS
1	w	322	GLN

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Mol	Chain	Res	Type
1	w	337	GLN
1	w	400	GLN
1	w	425	HIS
1	w	427	GLN
1	w	479	GLN
1	w	581	GLN
1	w	637	HIS
1	w	642	GLN
1	w	669	GLN
1	w	731	ASN
1	x	284	HIS
1	x	322	GLN
1	x	337	GLN
1	x	400	GLN
1	x	425	HIS
1	x	427	GLN
1	x	479	GLN
1	x	581	GLN
1	x	637	HIS
1	x	642	GLN
1	x	669	GLN
1	x	731	ASN
1	y	284	HIS
1	y	322	GLN
1	y	337	GLN
1	y	400	GLN
1	y	425	HIS
1	y	427	GLN
1	y	479	GLN
1	y	581	GLN
1	y	637	HIS
1	y	642	GLN
1	y	669	GLN
1	y	731	ASN
1	z	284	HIS
1	z	322	GLN
1	z	337	GLN
1	z	425	HIS
1	z	427	GLN
1	z	479	GLN
1	z	581	GLN
1	z	637	HIS

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Mol	Chain	Res	Type
1	z	642	GLN
1	z	669	GLN
1	z	731	ASN
1	1	284	HIS
1	1	322	GLN
1	1	337	GLN
1	1	425	HIS
1	1	427	GLN
1	1	479	GLN
1	1	581	GLN
1	1	637	HIS
1	1	642	GLN
1	1	669	GLN
1	1	731	ASN
1	2	284	HIS
1	2	322	GLN
1	2	337	GLN
1	2	425	HIS
1	2	427	GLN
1	2	479	GLN
1	2	581	GLN
1	2	637	HIS
1	2	642	GLN
1	2	669	GLN
1	2	731	ASN
1	3	284	HIS
1	3	322	GLN
1	3	337	GLN
1	3	400	GLN
1	3	425	HIS
1	3	427	GLN
1	3	479	GLN
1	3	581	GLN
1	3	637	HIS
1	3	642	GLN
1	3	669	GLN
1	3	731	ASN
1	4	284	HIS
1	4	322	GLN
1	4	337	GLN
1	4	400	GLN
1	4	425	HIS

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Mol	Chain	Res	Type
1	4	427	GLN
1	4	479	GLN
1	4	581	GLN
1	4	637	HIS
1	4	642	GLN
1	4	669	GLN
1	4	731	ASN
1	5	284	HIS
1	5	322	GLN
1	5	337	GLN
1	5	400	GLN
1	5	425	HIS
1	5	427	GLN
1	5	479	GLN
1	5	581	GLN
1	5	637	HIS
1	5	642	GLN
1	5	669	GLN
1	5	731	ASN
1	6	284	HIS
1	6	322	GLN
1	6	337	GLN
1	6	400	GLN
1	6	425	HIS
1	6	427	GLN
1	6	479	GLN
1	6	581	GLN
1	6	637	HIS
1	6	642	GLN
1	6	669	GLN
1	6	731	ASN
1	7	284	HIS
1	7	322	GLN
1	7	337	GLN
1	7	400	GLN
1	7	425	HIS
1	7	427	GLN
1	7	479	GLN
1	7	581	GLN
1	7	637	HIS
1	7	642	GLN
1	7	669	GLN

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Mol	Chain	Res	Type
1	7	731	ASN
1	8	284	HIS
1	8	322	GLN
1	8	337	GLN
1	8	425	HIS
1	8	427	GLN
1	8	479	GLN
1	8	581	GLN
1	8	637	HIS
1	8	642	GLN
1	8	669	GLN
1	8	731	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.

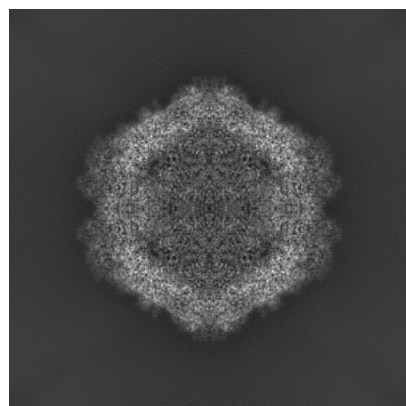
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48181. These allow visual inspection of the internal detail of the map and identification of artifacts.

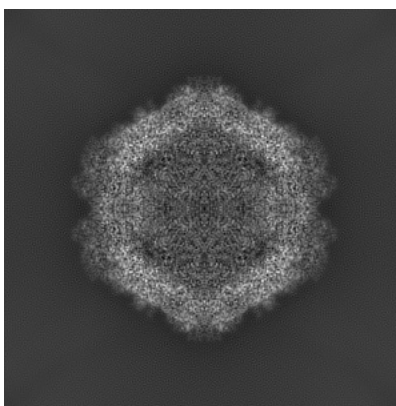
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

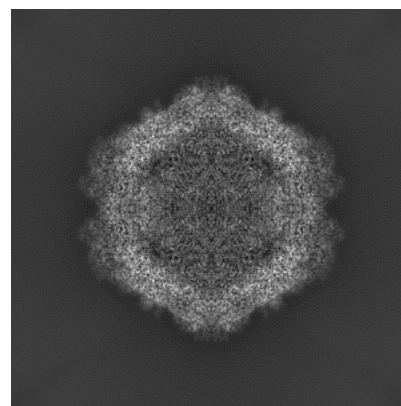
6.1.1 Primary map



X

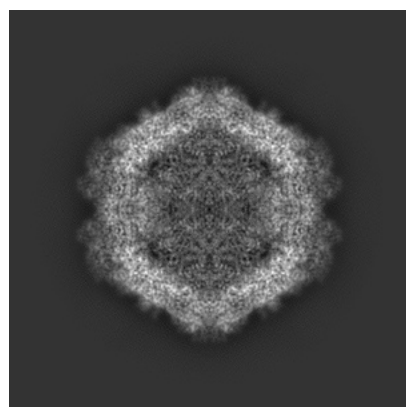


Y

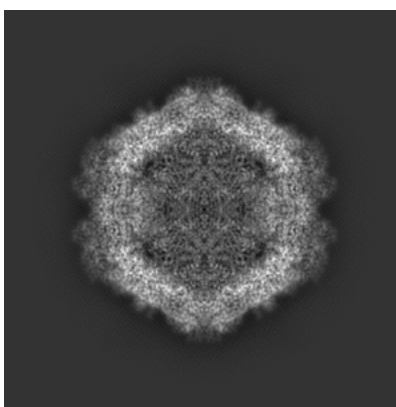


Z

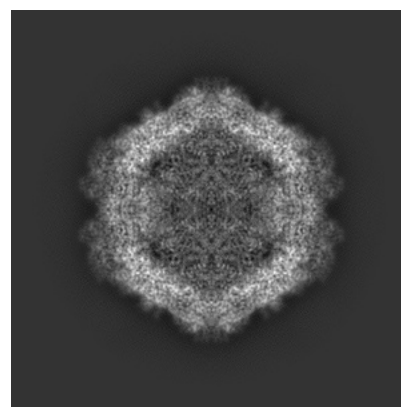
6.1.2 Raw map



X



Y

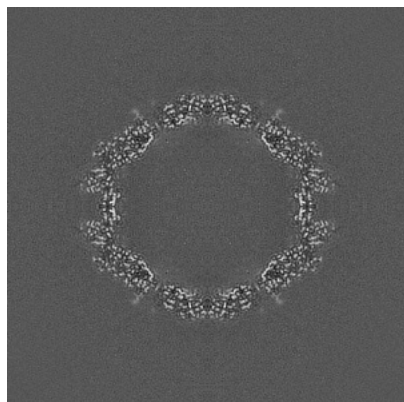


Z

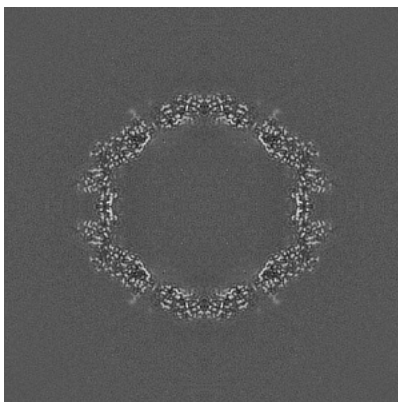
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

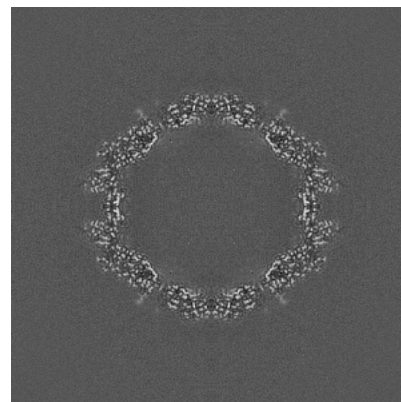
6.2.1 Primary map



X Index: 250

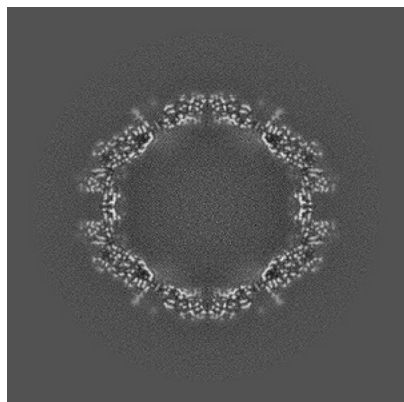


Y Index: 250

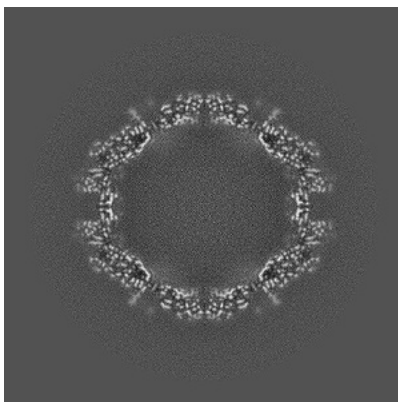


Z Index: 250

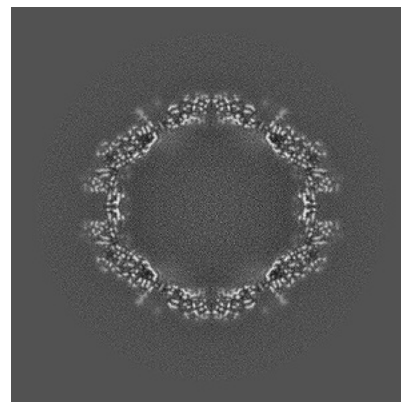
6.2.2 Raw map



X Index: 250



Y Index: 250

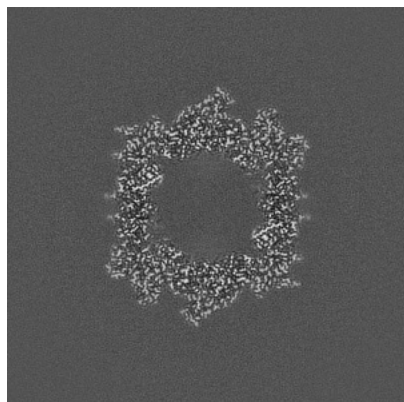


Z Index: 250

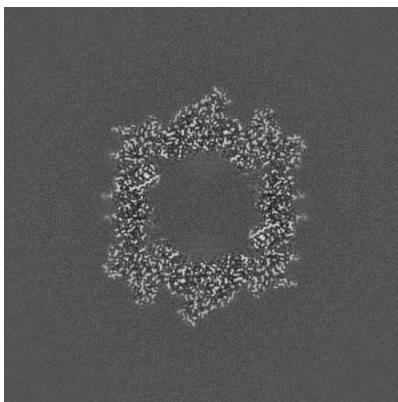
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

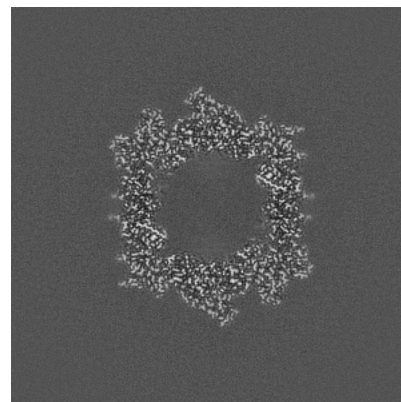
6.3.1 Primary map



X Index: 329

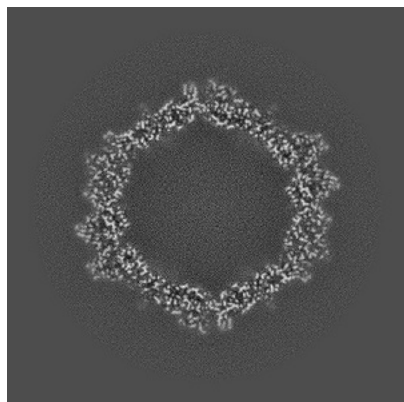


Y Index: 329

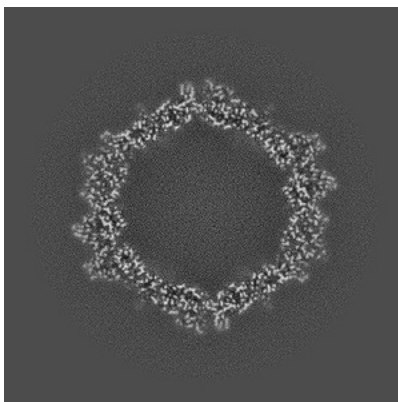


Z Index: 171

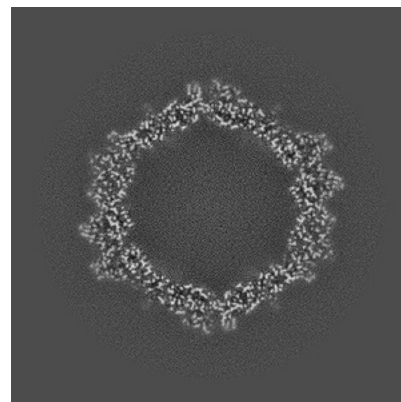
6.3.2 Raw map



X Index: 232



Y Index: 232

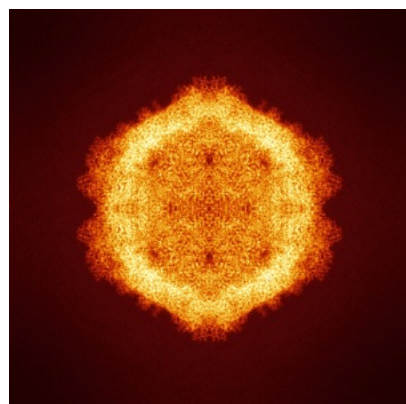


Z Index: 232

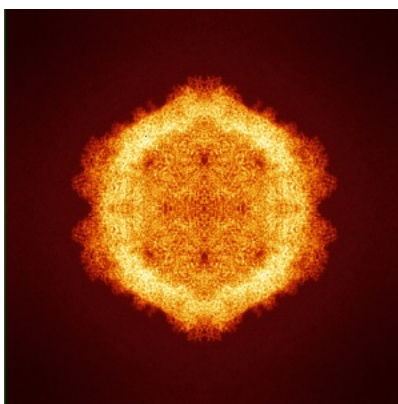
The images above show the largest variance slices of the map in three orthogonal directions.

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

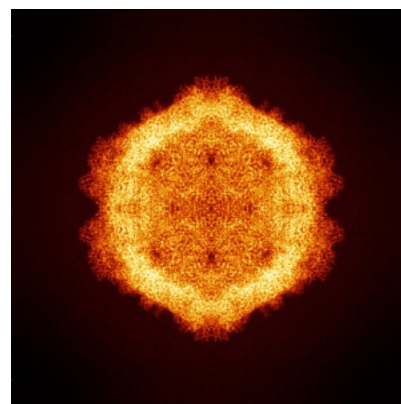
6.4.1 Primary map



X

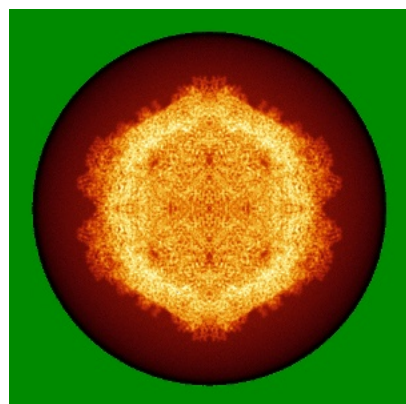


Y

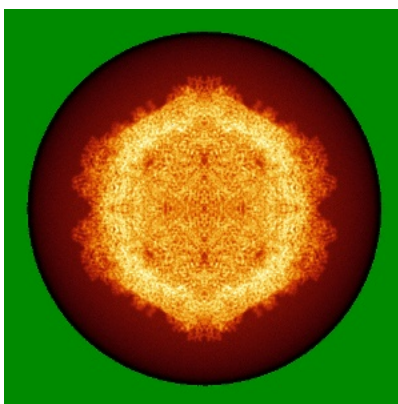


Z

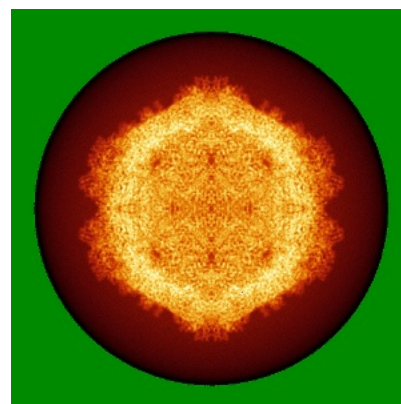
6.4.2 Raw map



X



Y

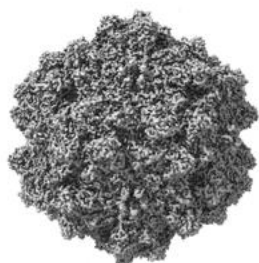


Z

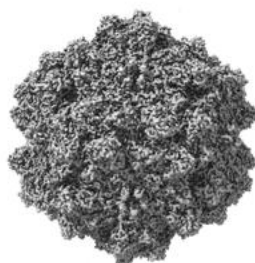
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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.

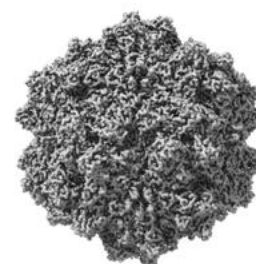
6.5.2 Raw map



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.

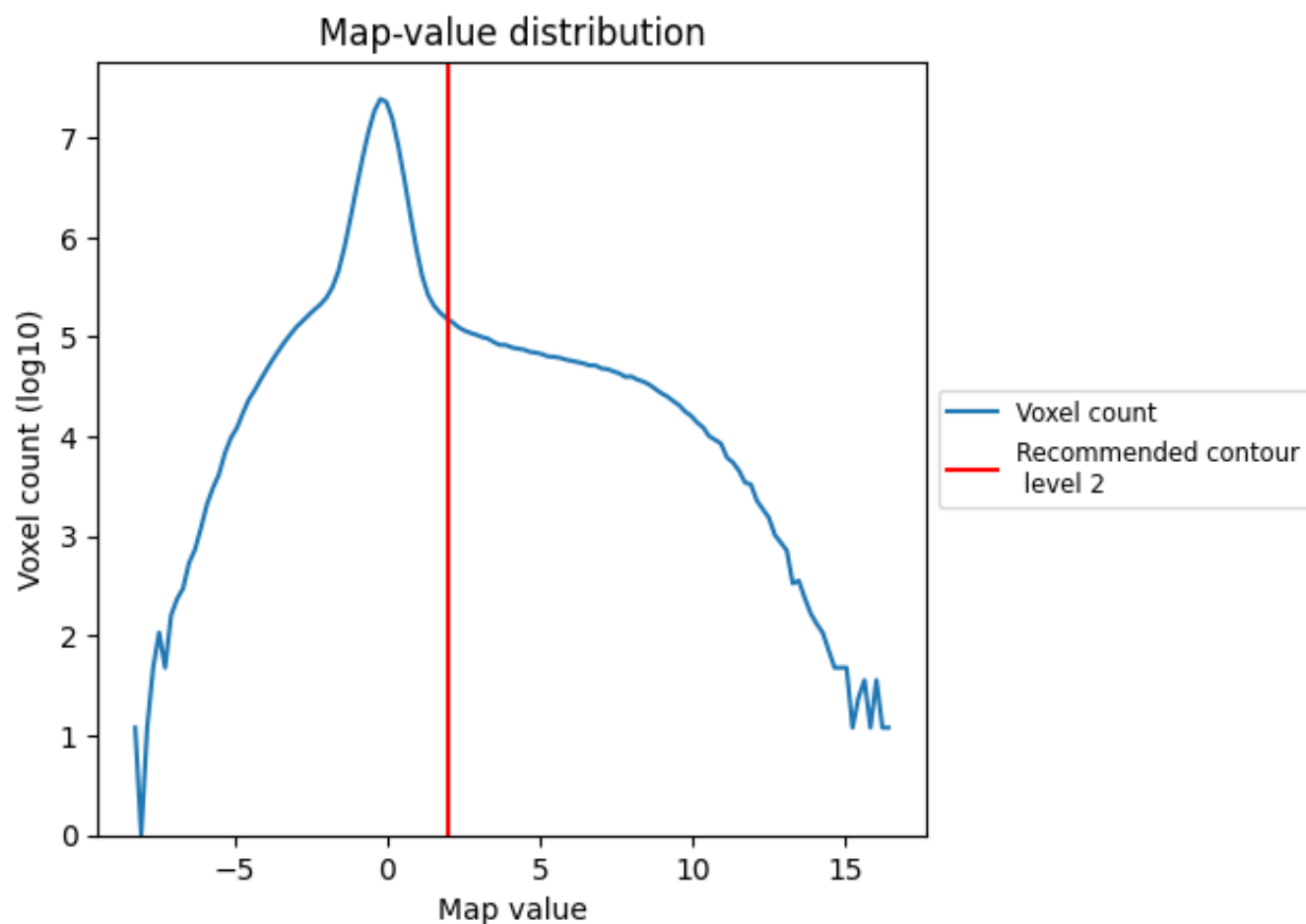
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

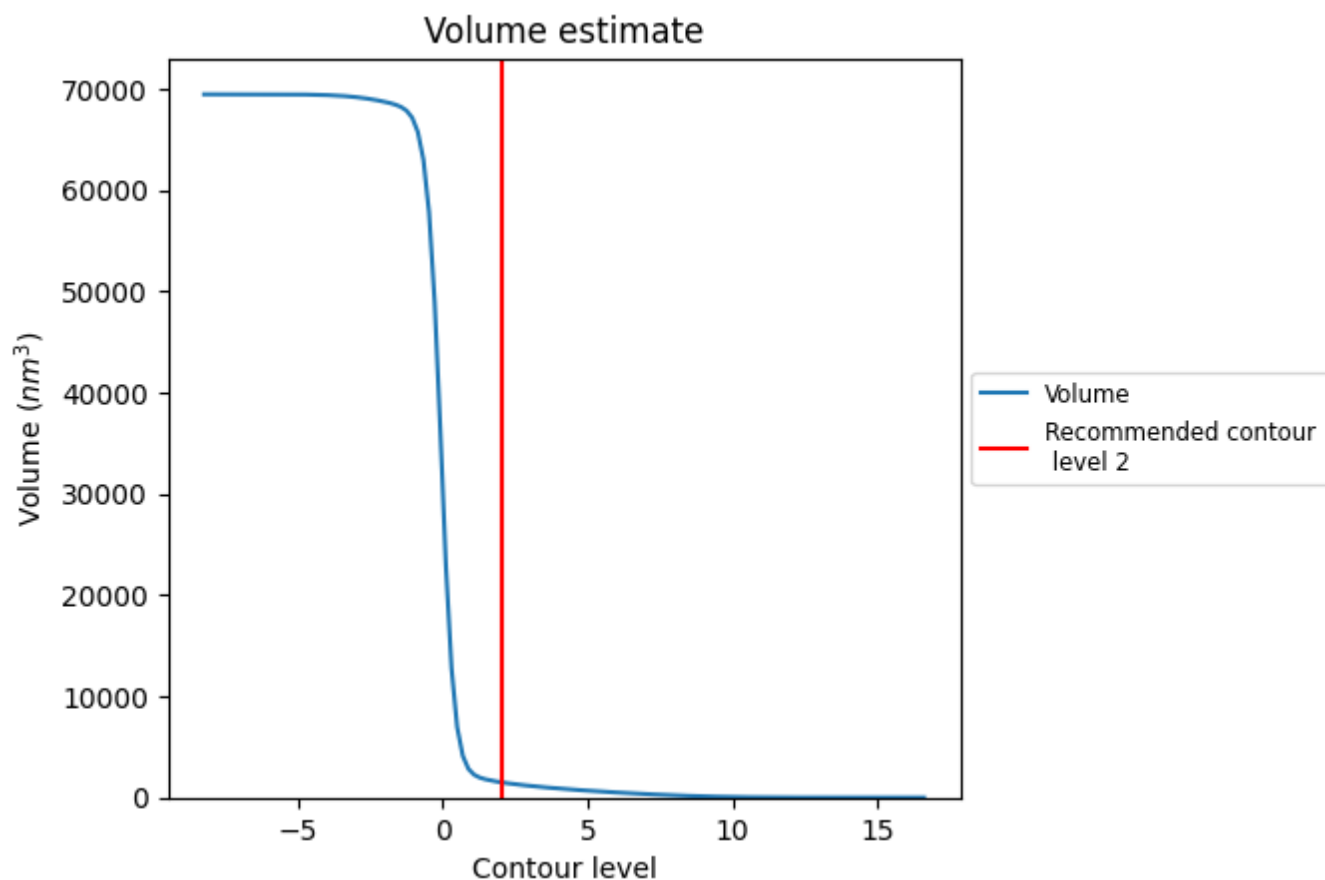
This section contains the results of statistical analysis of the map.

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.

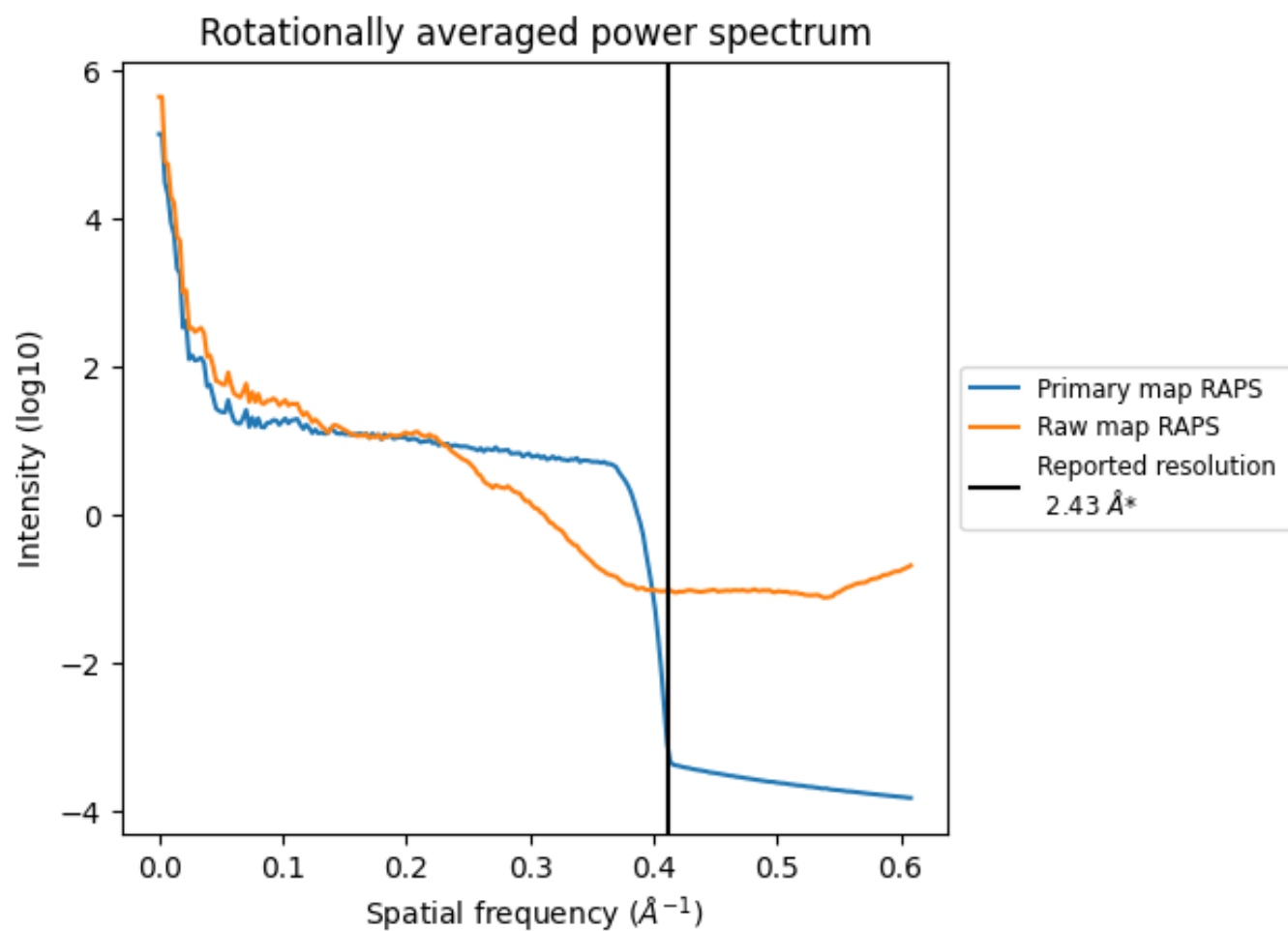
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1512 nm³; this corresponds to an approximate mass of 1366 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

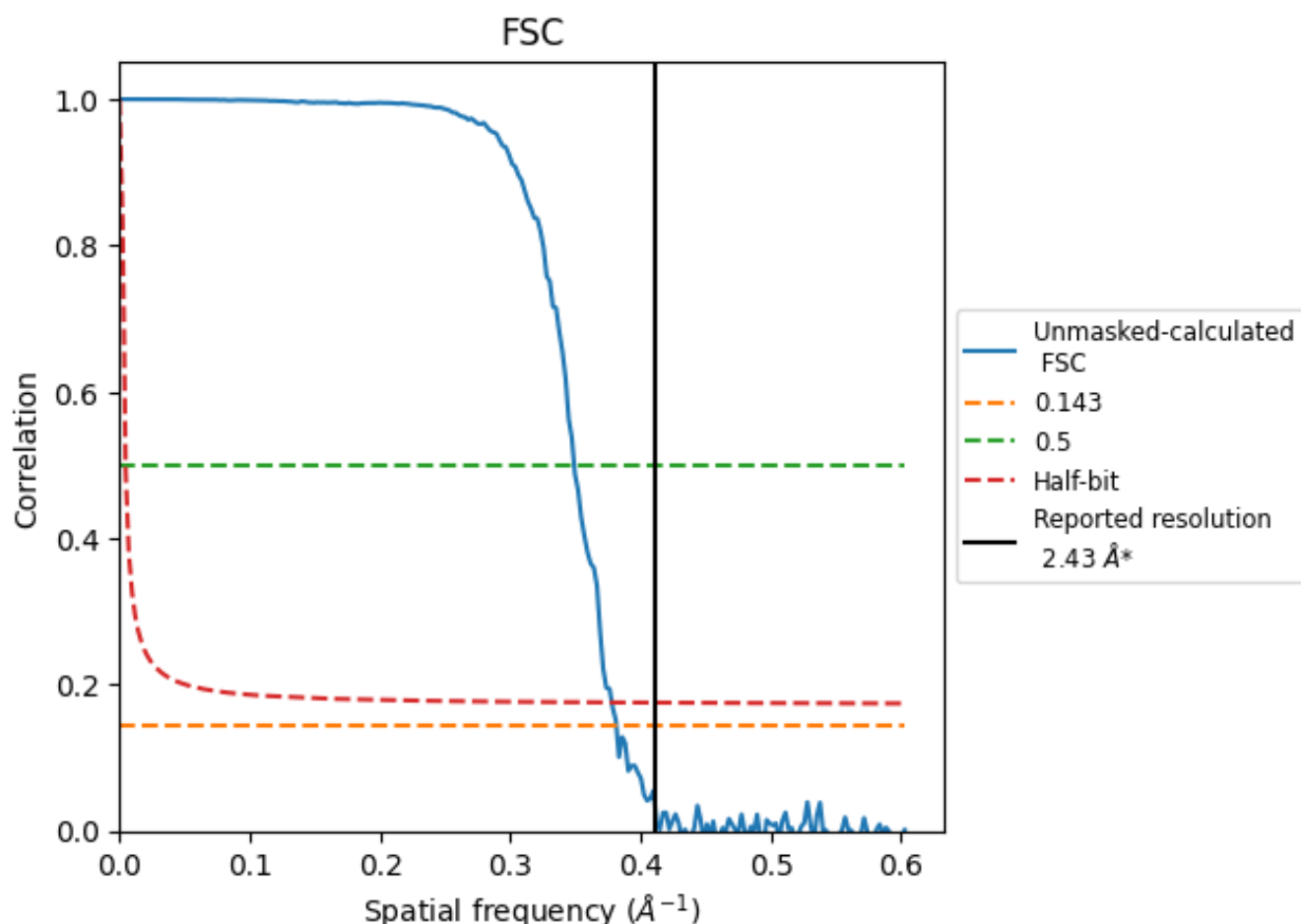


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

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 0.412 \AA^{-1}

8.2 Resolution estimates [i](#)

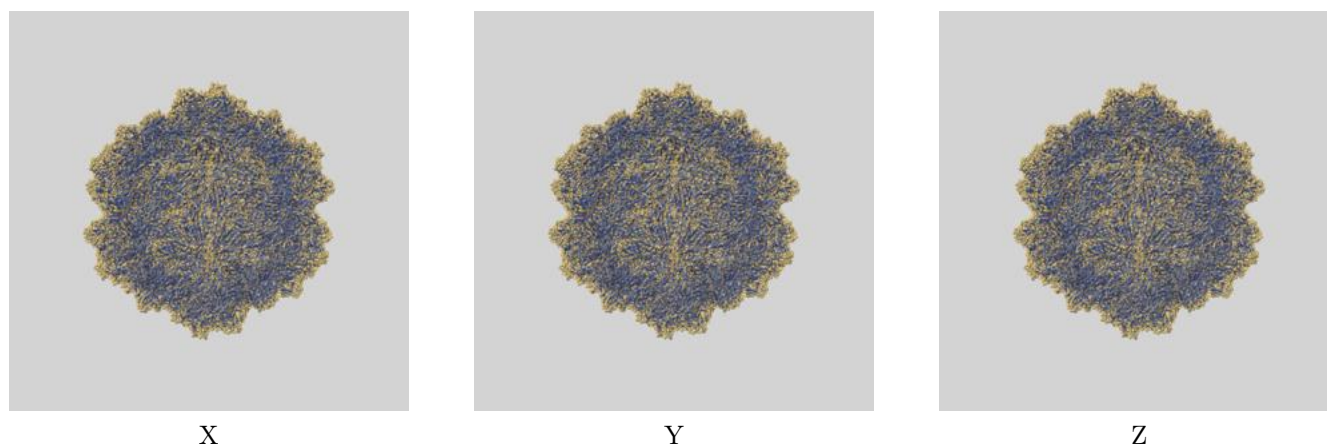
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.62	2.86	2.64

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

9 Map-model fit [i](#)

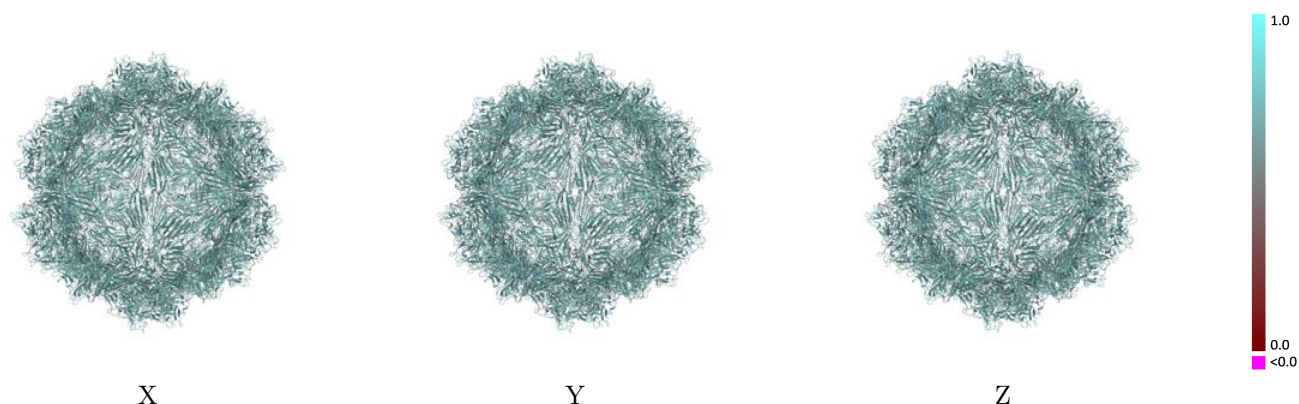
This section contains information regarding the fit between EMDB map EMD-48181 and PDB model 9ME0. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



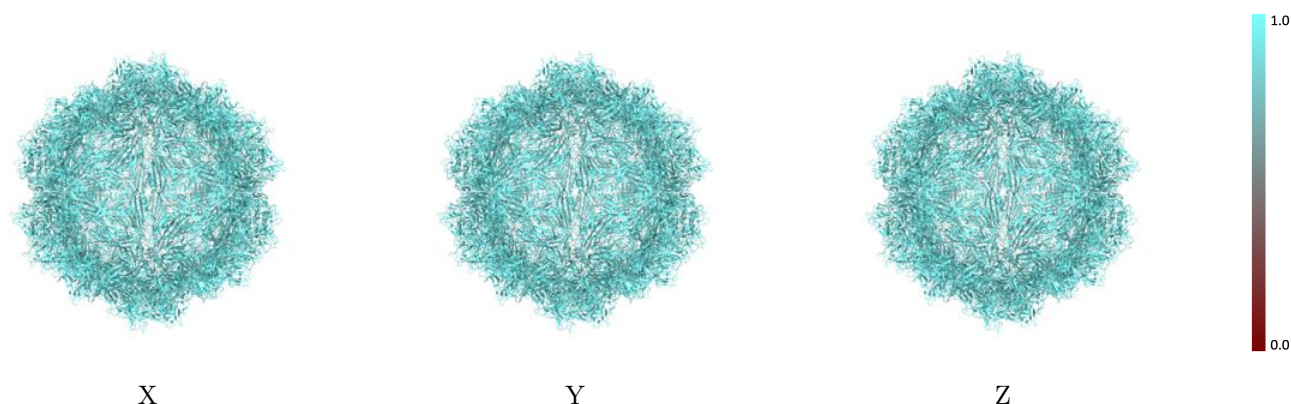
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



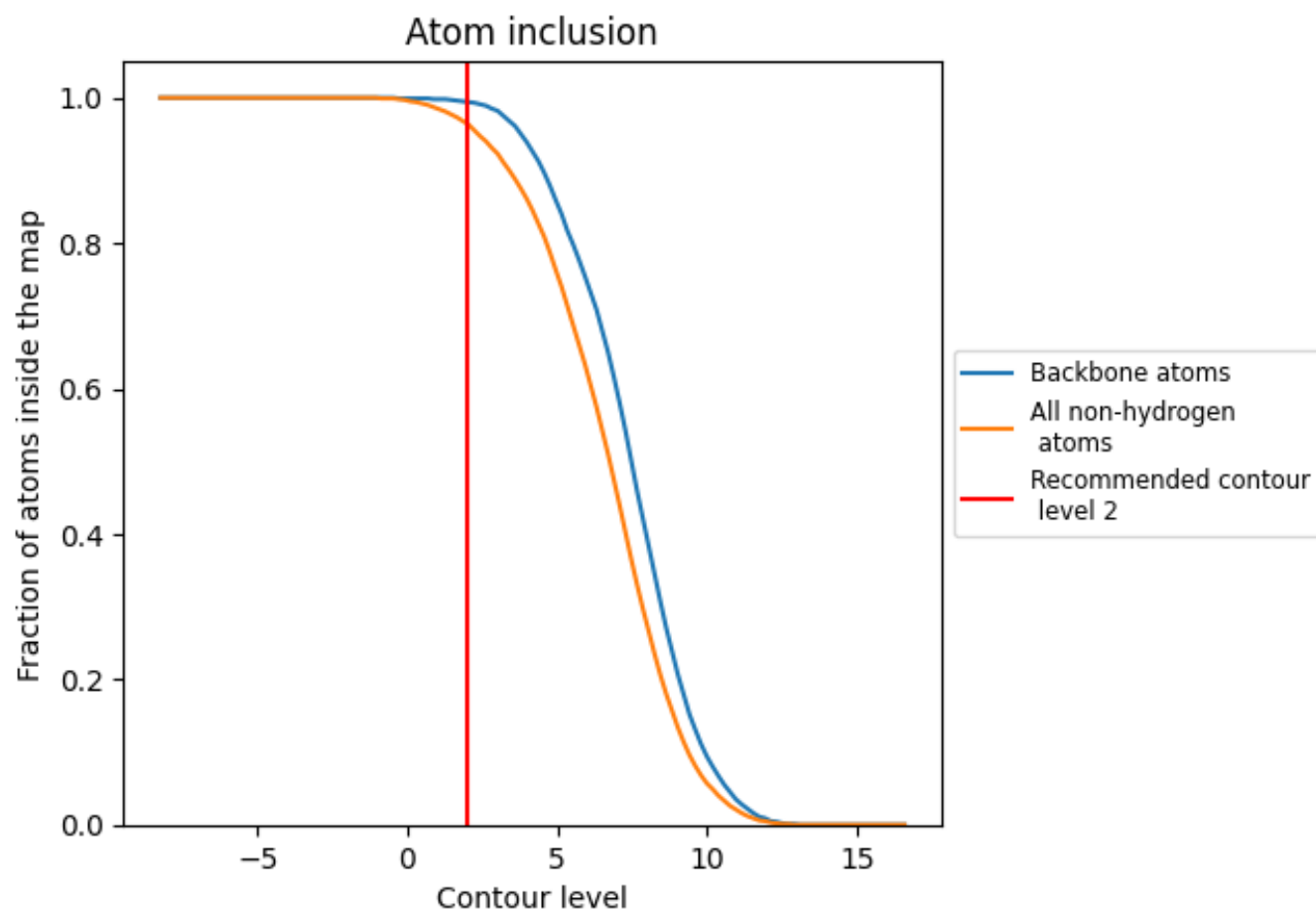
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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	 0.9640	 0.6730
1	 0.9630	 0.6730
2	 0.9630	 0.6730
3	 0.9640	 0.6730
4	 0.9650	 0.6730
5	 0.9650	 0.6740
6	 0.9650	 0.6740
7	 0.9650	 0.6730
8	 0.9640	 0.6730
A	 0.9640	 0.6740
B	 0.9630	 0.6730
C	 0.9650	 0.6730
D	 0.9650	 0.6730
E	 0.9640	 0.6730
F	 0.9640	 0.6730
G	 0.9640	 0.6730
H	 0.9650	 0.6740
I	 0.9650	 0.6730
J	 0.9630	 0.6730
K	 0.9650	 0.6730
L	 0.9630	 0.6730
M	 0.9640	 0.6730
N	 0.9650	 0.6730
O	 0.9640	 0.6730
P	 0.9650	 0.6730
Q	 0.9650	 0.6730
R	 0.9630	 0.6730
S	 0.9630	 0.6730
T	 0.9650	 0.6730
U	 0.9630	 0.6730
V	 0.9650	 0.6730
W	 0.9650	 0.6740
X	 0.9640	 0.6730
Y	 0.9650	 0.6730
Z	 0.9640	 0.6740



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Chain	Atom inclusion	Q-score
a	 0.9640	 0.6730
b	 0.9640	 0.6740
c	 0.9640	 0.6740
d	 0.9640	 0.6730
e	 0.9640	 0.6730
f	 0.9640	 0.6740
g	 0.9650	 0.6730
h	 0.9640	 0.6730
i	 0.9650	 0.6740
j	 0.9650	 0.6730
k	 0.9650	 0.6730
l	 0.9640	 0.6730
m	 0.9650	 0.6730
n	 0.9640	 0.6740
o	 0.9640	 0.6730
p	 0.9650	 0.6730
q	 0.9630	 0.6730
r	 0.9630	 0.6730
s	 0.9630	 0.6730
t	 0.9640	 0.6730
u	 0.9650	 0.6720
v	 0.9640	 0.6730
w	 0.9640	 0.6730
x	 0.9650	 0.6730
y	 0.9640	 0.6730
z	 0.9630	 0.6720