



Full wwPDB EM Validation Report ⓘ

Sep 7, 2024 – 01:38 PM EDT

PDB ID : 9CWS
EMDB ID : EMD-45973
Title : Bufavirus 1 at pH 2.6
Authors : Gulkis, M.C.; McKenna, R.; Bennett, A.D.
Deposited on : 2024-07-30
Resolution : 2.73 Å (reported)
Based on initial model : 6BWX

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.







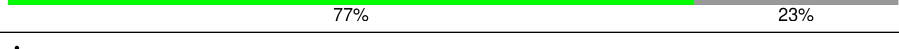
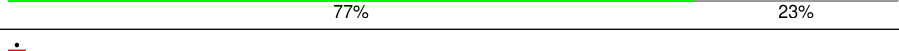
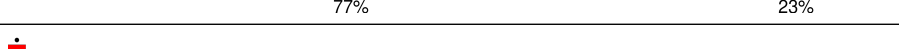
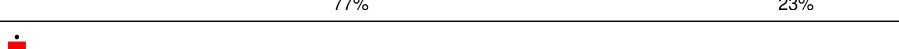
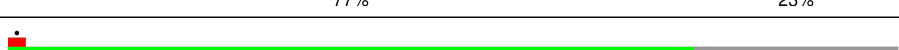

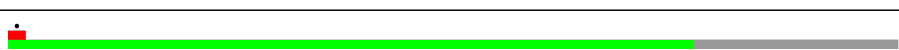

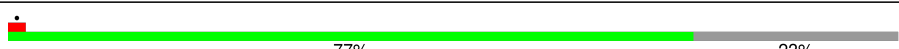





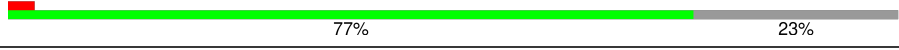
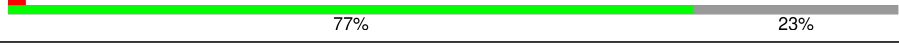



The types of validation reports are described at

<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:







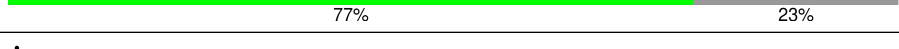
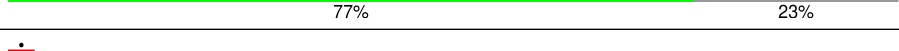
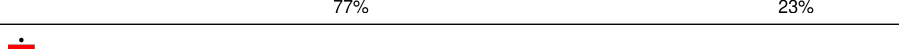
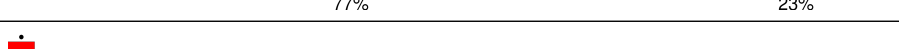
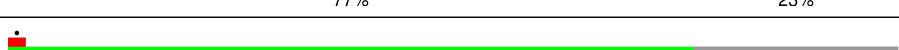

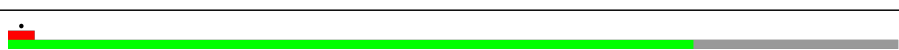

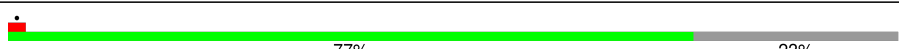





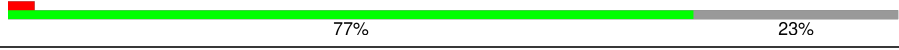
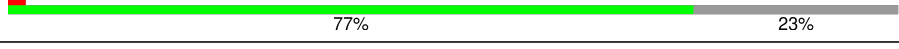



EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

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Mol	Chain	Length	Quality of chain	
1	B	707		
1	C	707		
1	D	707		
1	E	707		
1	F	707		
1	G	707		
1	H	707		
1	I	707		
1	J	707		
1	K	707		
1	L	707		
1	M	707		
1	N	707		
1	O	707		
1	P	707		
1	Q	707		
1	R	707		
1	S	707		
1	T	707		
1	U	707		
1	V	707		
1	W	707		
1	X	707		
1	Y	707		
1	Z	707		


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Mol	Chain	Length	Quality of chain	
1	a	707		77% 23%
1	b	707		77% 23%
1	c	707		77% 23%
1	d	707		77% 23%
1	e	707		77% 23%
1	f	707		77% 23%
1	g	707		77% 23%
1	h	707		77% 23%
1	i	707		77% 23%
1	j	707		77% 23%
1	k	707		77% 23%
1	l	707		77% 23%
1	m	707		77% 23%
1	n	707		77% 23%
1	o	707		77% 23%
1	p	707		77% 23%
1	q	707		77% 23%
1	r	707		77% 23%
1	s	707		77% 23%
1	t	707		77% 23%
1	u	707		77% 23%
1	v	707		77% 23%
1	w	707		77% 23%
1	x	707		77% 23%
1	y	707		77% 23%

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Mol	Chain	Length	Quality of chain
1	z	707	 77% 23%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 263940 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
			Total	C	N	O	S		
1	A	547	4399	2779	775	831	14	0	0
1	B	547	4399	2779	775	831	14	0	0
1	C	547	4399	2779	775	831	14	0	0
1	D	547	4399	2779	775	831	14	0	0
1	E	547	4399	2779	775	831	14	0	0
1	F	547	4399	2779	775	831	14	0	0
1	G	547	4399	2779	775	831	14	0	0
1	H	547	4399	2779	775	831	14	0	0
1	I	547	4399	2779	775	831	14	0	0
1	J	547	4399	2779	775	831	14	0	0
1	K	547	4399	2779	775	831	14	0	0
1	L	547	4399	2779	775	831	14	0	0
1	M	547	4399	2779	775	831	14	0	0
1	N	547	4399	2779	775	831	14	0	0
1	O	547	4399	2779	775	831	14	0	0
1	P	547	4399	2779	775	831	14	0	0
1	Q	547	4399	2779	775	831	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	S	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	T	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	U	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	V	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	W	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	X	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	Y	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	Z	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	a	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	b	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	c	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	d	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	e	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	f	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	g	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	h	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	i	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	j	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	k	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	l	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	n	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	o	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	p	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	q	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	r	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	s	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	t	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	u	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	v	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	w	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	x	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	y	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	z	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	1	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	2	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	3	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	4	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	5	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	6	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		
1	7	547	Total	C	N	O	S	0	0
			4399	2779	775	831	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	547	4399	2779	775	831	14	0	0

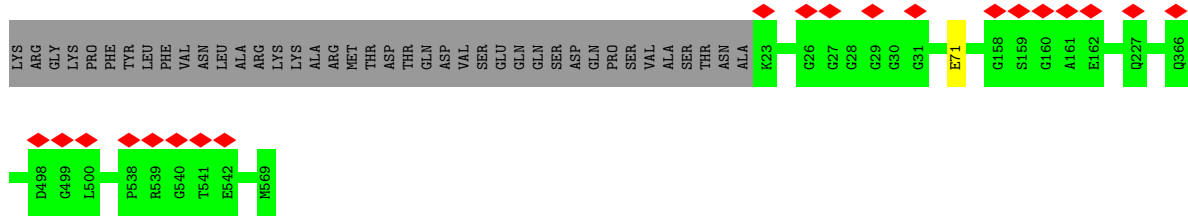
There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	VAL	ILE	conflict	UNP A0A097PIM0
B	35	VAL	ILE	conflict	UNP A0A097PIM0
C	35	VAL	ILE	conflict	UNP A0A097PIM0
D	35	VAL	ILE	conflict	UNP A0A097PIM0
E	35	VAL	ILE	conflict	UNP A0A097PIM0
F	35	VAL	ILE	conflict	UNP A0A097PIM0
G	35	VAL	ILE	conflict	UNP A0A097PIM0
H	35	VAL	ILE	conflict	UNP A0A097PIM0
I	35	VAL	ILE	conflict	UNP A0A097PIM0
J	35	VAL	ILE	conflict	UNP A0A097PIM0
K	35	VAL	ILE	conflict	UNP A0A097PIM0
L	35	VAL	ILE	conflict	UNP A0A097PIM0
M	35	VAL	ILE	conflict	UNP A0A097PIM0
N	35	VAL	ILE	conflict	UNP A0A097PIM0
O	35	VAL	ILE	conflict	UNP A0A097PIM0
P	35	VAL	ILE	conflict	UNP A0A097PIM0
Q	35	VAL	ILE	conflict	UNP A0A097PIM0
R	35	VAL	ILE	conflict	UNP A0A097PIM0
S	35	VAL	ILE	conflict	UNP A0A097PIM0
T	35	VAL	ILE	conflict	UNP A0A097PIM0
U	35	VAL	ILE	conflict	UNP A0A097PIM0
V	35	VAL	ILE	conflict	UNP A0A097PIM0
W	35	VAL	ILE	conflict	UNP A0A097PIM0
X	35	VAL	ILE	conflict	UNP A0A097PIM0
Y	35	VAL	ILE	conflict	UNP A0A097PIM0
Z	35	VAL	ILE	conflict	UNP A0A097PIM0
a	35	VAL	ILE	conflict	UNP A0A097PIM0
b	35	VAL	ILE	conflict	UNP A0A097PIM0
c	35	VAL	ILE	conflict	UNP A0A097PIM0
d	35	VAL	ILE	conflict	UNP A0A097PIM0
e	35	VAL	ILE	conflict	UNP A0A097PIM0
f	35	VAL	ILE	conflict	UNP A0A097PIM0
g	35	VAL	ILE	conflict	UNP A0A097PIM0
h	35	VAL	ILE	conflict	UNP A0A097PIM0
i	35	VAL	ILE	conflict	UNP A0A097PIM0
j	35	VAL	ILE	conflict	UNP A0A097PIM0

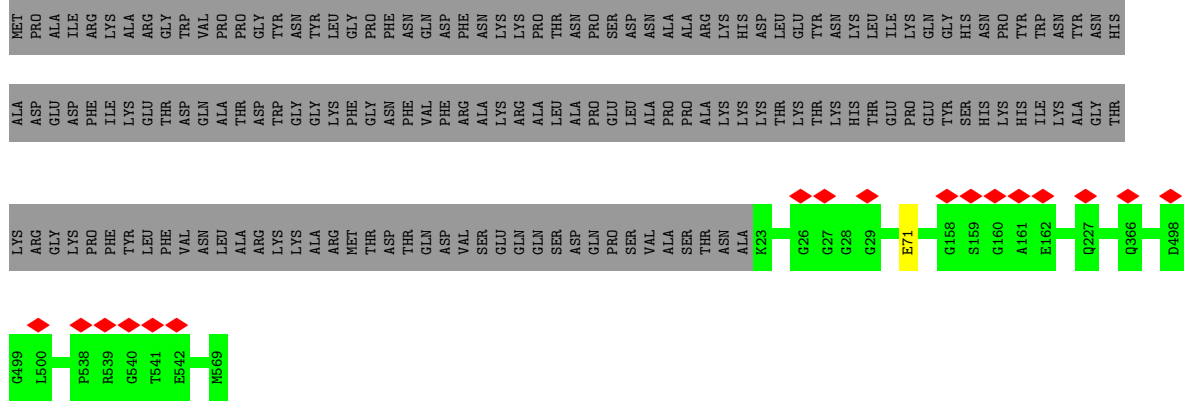
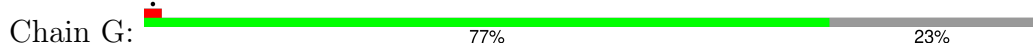
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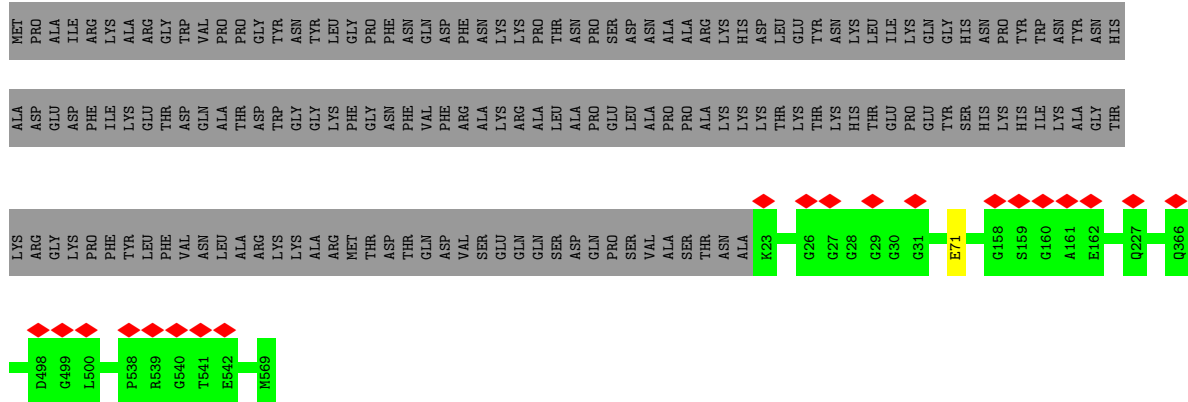
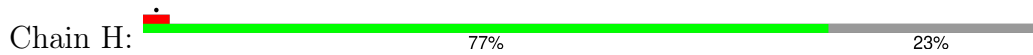
Chain	Residue	Modelled	Actual	Comment	Reference
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l	35	VAL	ILE	conflict	UNP A0A097PIM0
m	35	VAL	ILE	conflict	UNP A0A097PIM0
n	35	VAL	ILE	conflict	UNP A0A097PIM0
o	35	VAL	ILE	conflict	UNP A0A097PIM0
p	35	VAL	ILE	conflict	UNP A0A097PIM0
q	35	VAL	ILE	conflict	UNP A0A097PIM0
r	35	VAL	ILE	conflict	UNP A0A097PIM0
s	35	VAL	ILE	conflict	UNP A0A097PIM0
t	35	VAL	ILE	conflict	UNP A0A097PIM0
u	35	VAL	ILE	conflict	UNP A0A097PIM0
v	35	VAL	ILE	conflict	UNP A0A097PIM0
w	35	VAL	ILE	conflict	UNP A0A097PIM0
x	35	VAL	ILE	conflict	UNP A0A097PIM0
y	35	VAL	ILE	conflict	UNP A0A097PIM0
z	35	VAL	ILE	conflict	UNP A0A097PIM0
1	35	VAL	ILE	conflict	UNP A0A097PIM0
2	35	VAL	ILE	conflict	UNP A0A097PIM0
3	35	VAL	ILE	conflict	UNP A0A097PIM0
4	35	VAL	ILE	conflict	UNP A0A097PIM0
5	35	VAL	ILE	conflict	UNP A0A097PIM0
6	35	VAL	ILE	conflict	UNP A0A097PIM0
7	35	VAL	ILE	conflict	UNP A0A097PIM0
8	35	VAL	ILE	conflict	UNP A0A097PIM0



• Molecule 1: VP1

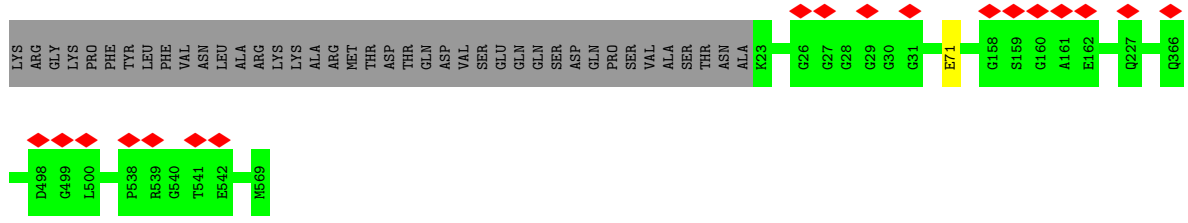


• Molecule 1: VP1

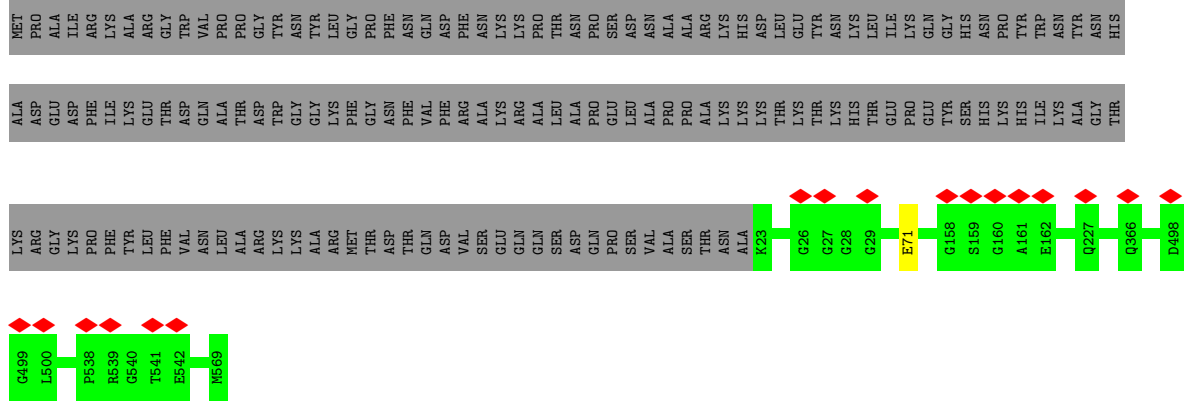
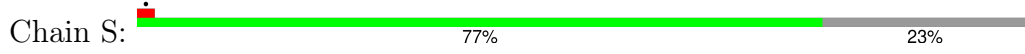


• Molecule 1: VP1

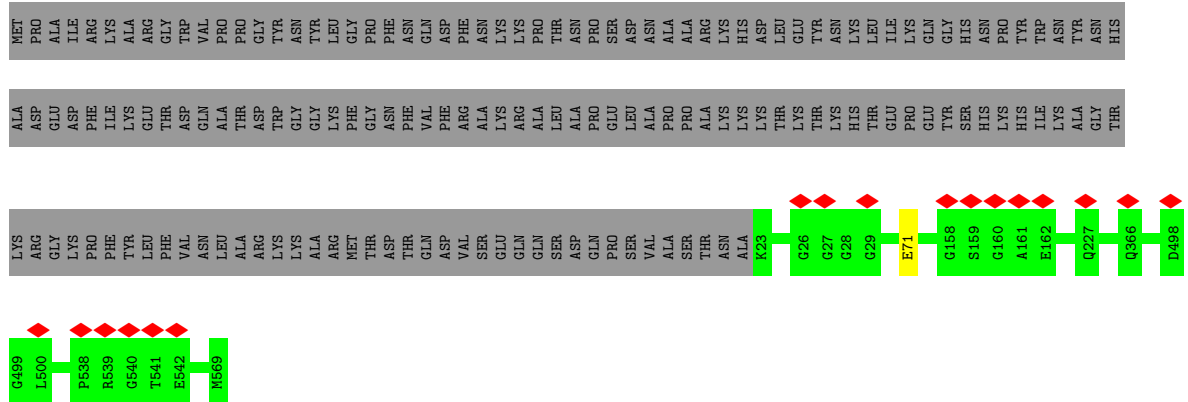
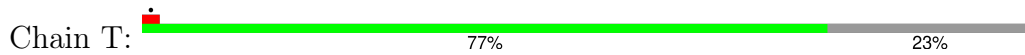




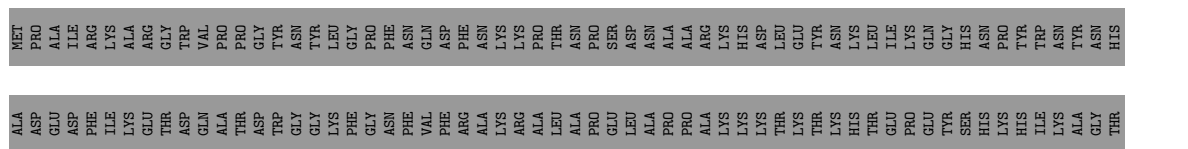
• Molecule 1: VP1

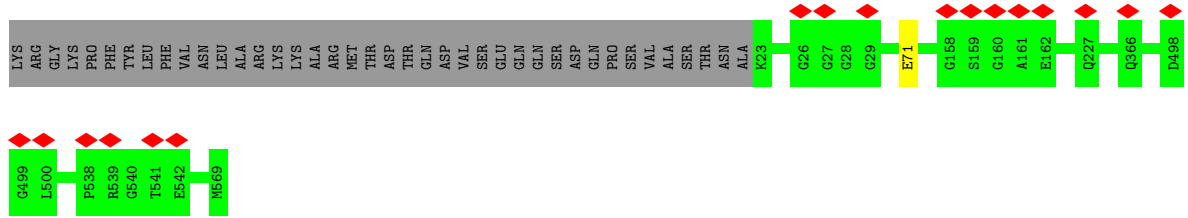


• Molecule 1: VP1

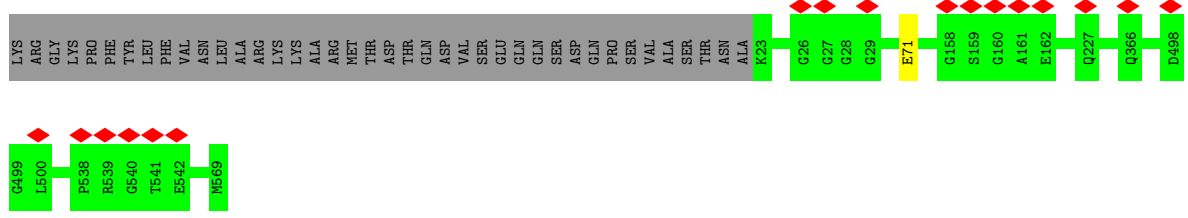
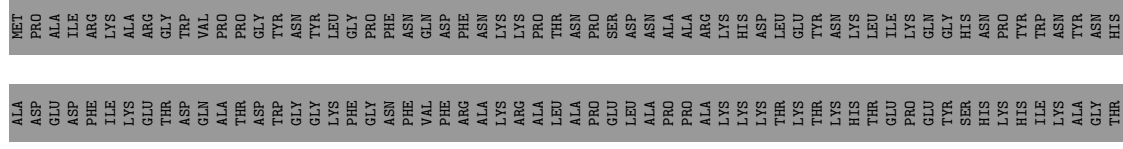
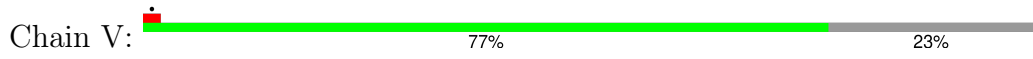


• Molecule 1: VP1

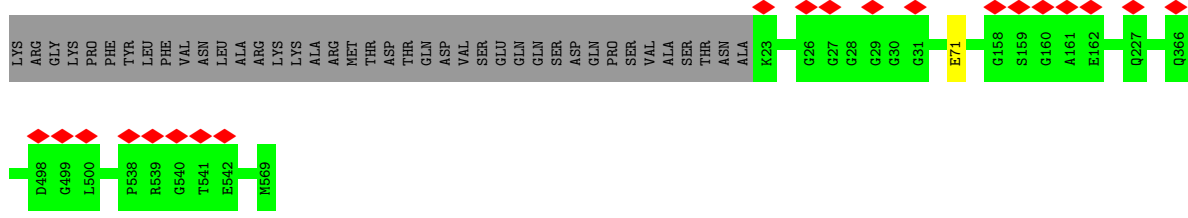
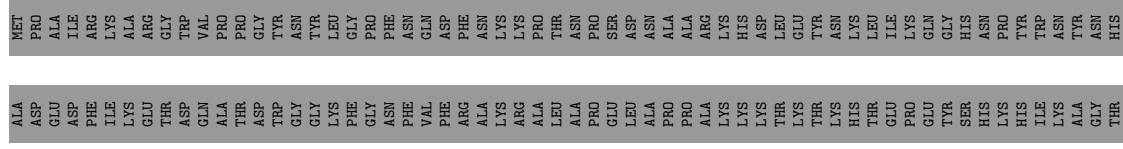
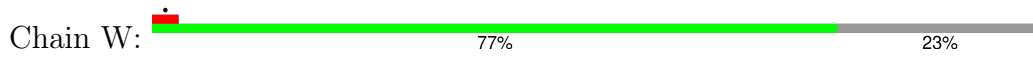




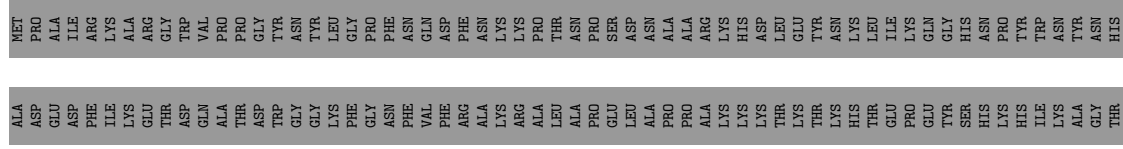
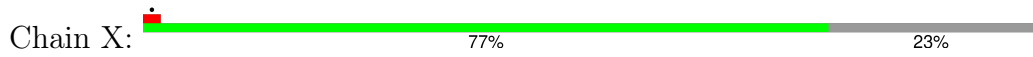
• Molecule 1: VP1

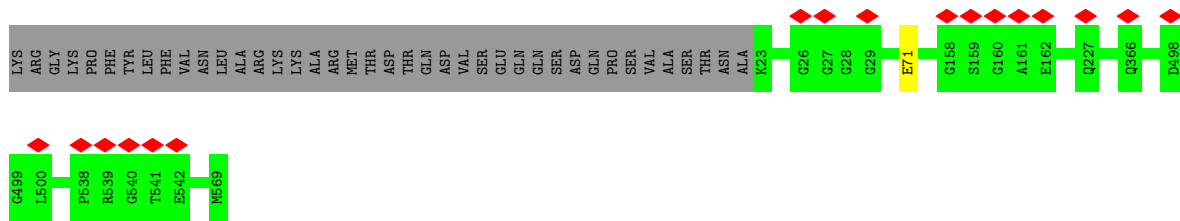


• Molecule 1: VP1

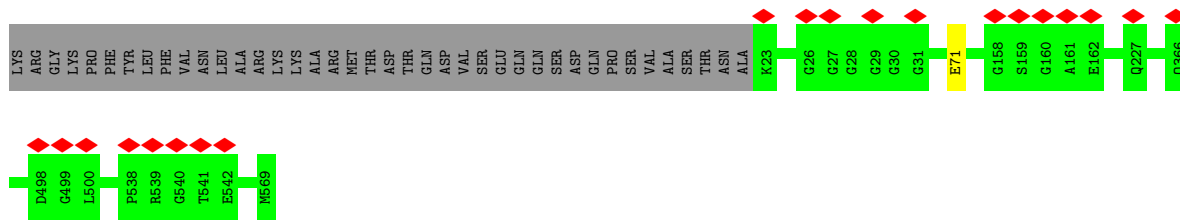
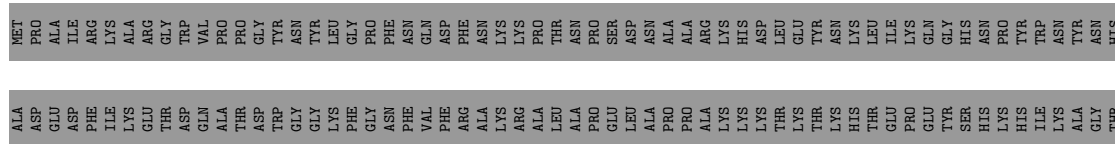
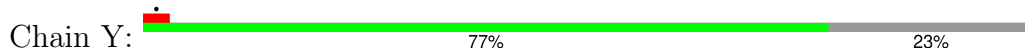


• Molecule 1: VP1

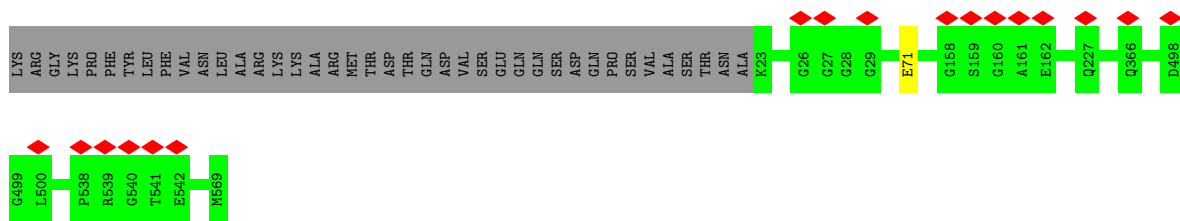
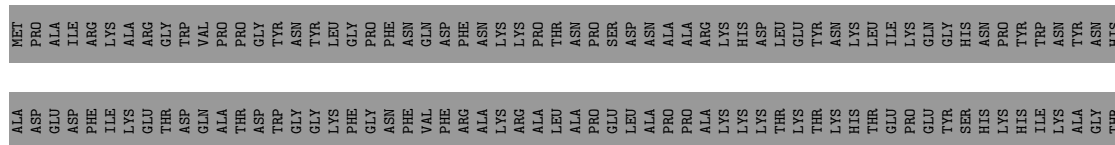
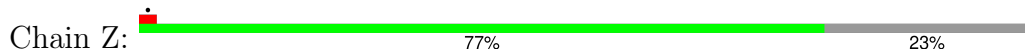




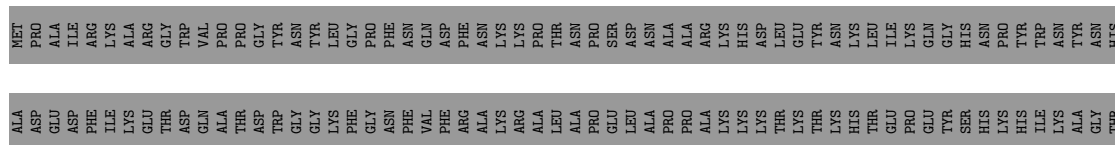
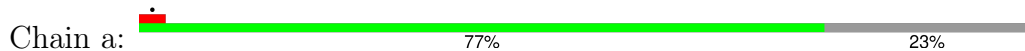
• Molecule 1: VP1

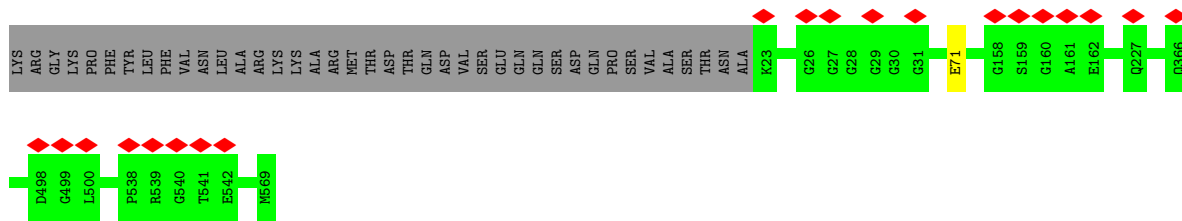


• Molecule 1: VP1



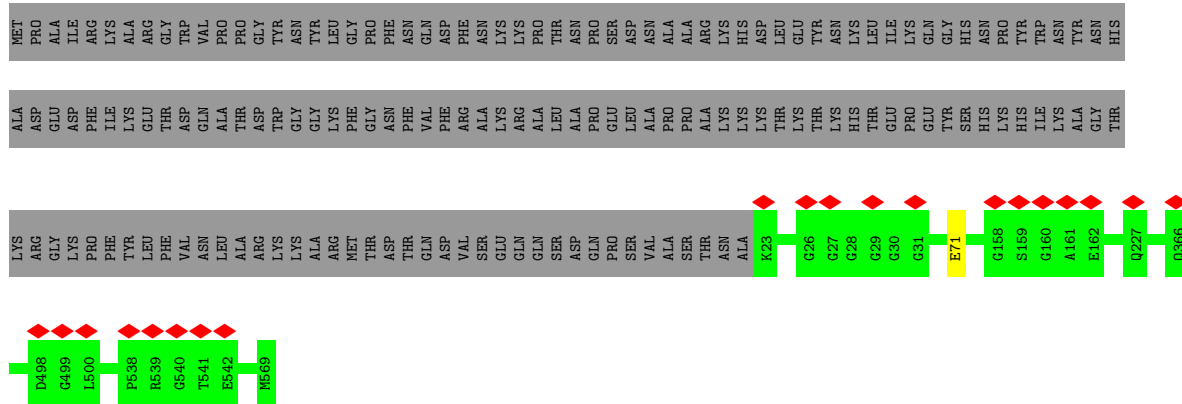
• Molecule 1: VP1





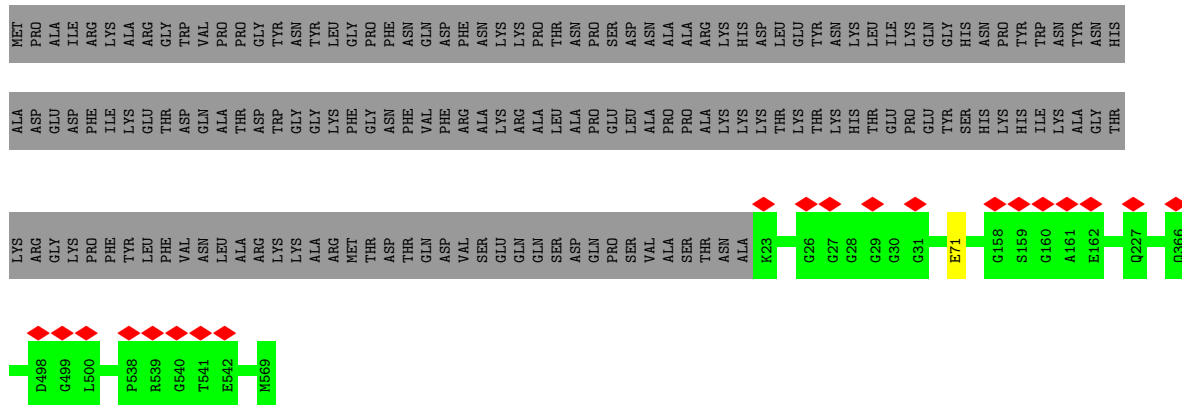
• Molecule 1: VP1

Chain b: 77% 23%



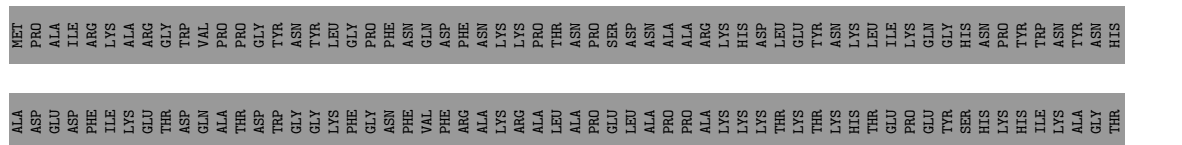
• Molecule 1: VP1

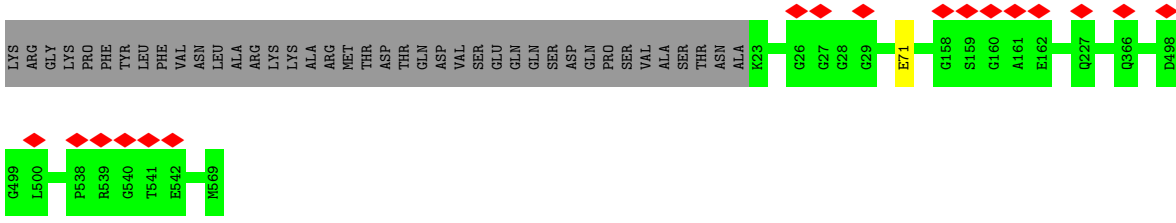
Chain c: 77% 23%



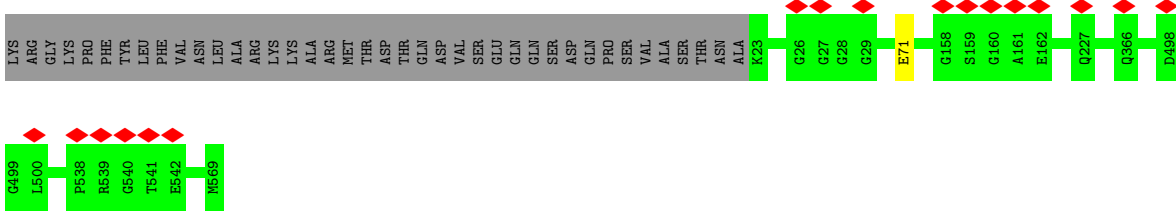
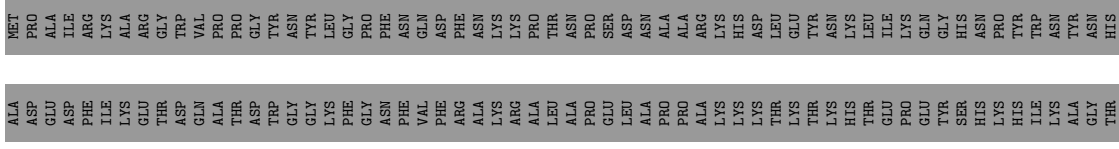
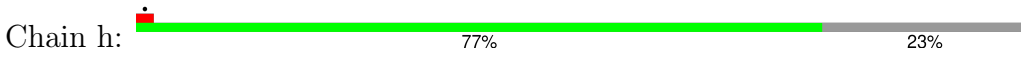
• Molecule 1: VP1

Chain d: 77% 23%

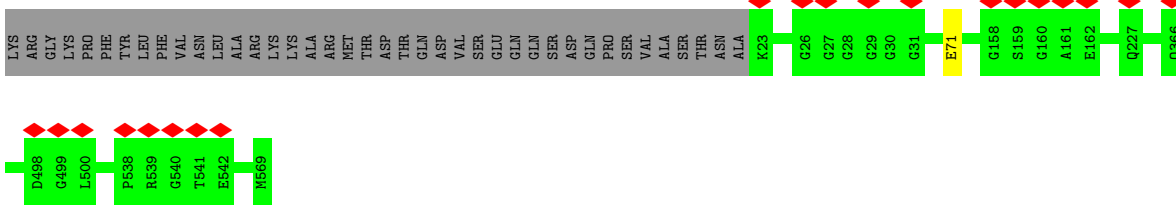
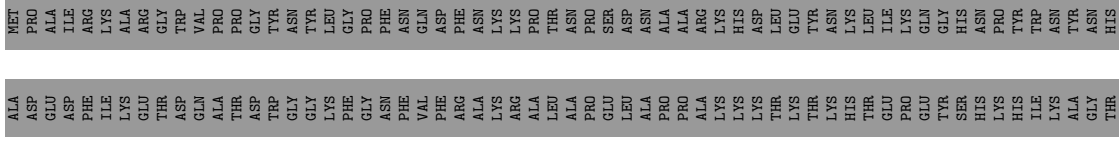
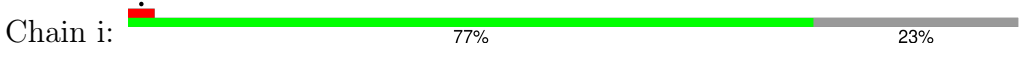




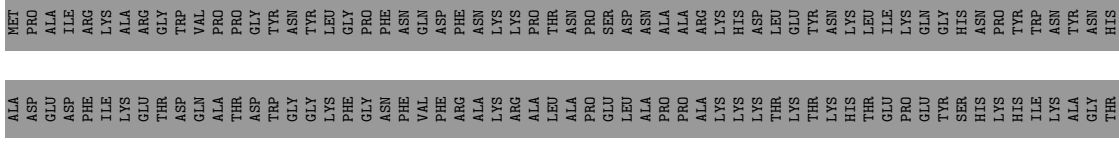
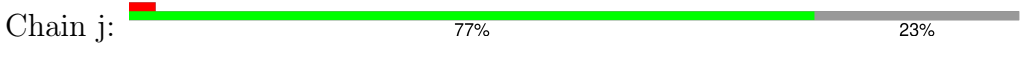
• Molecule 1: VP1

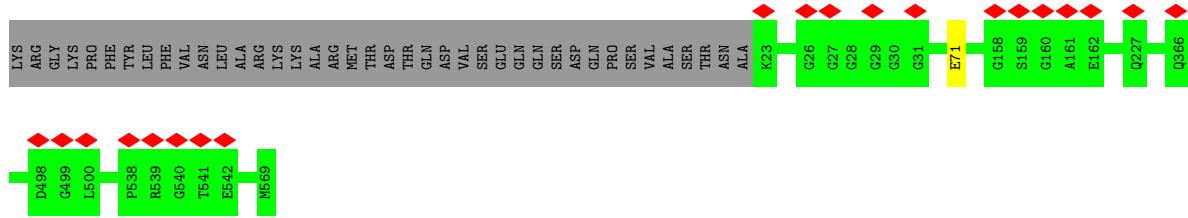


• Molecule 1: VP1

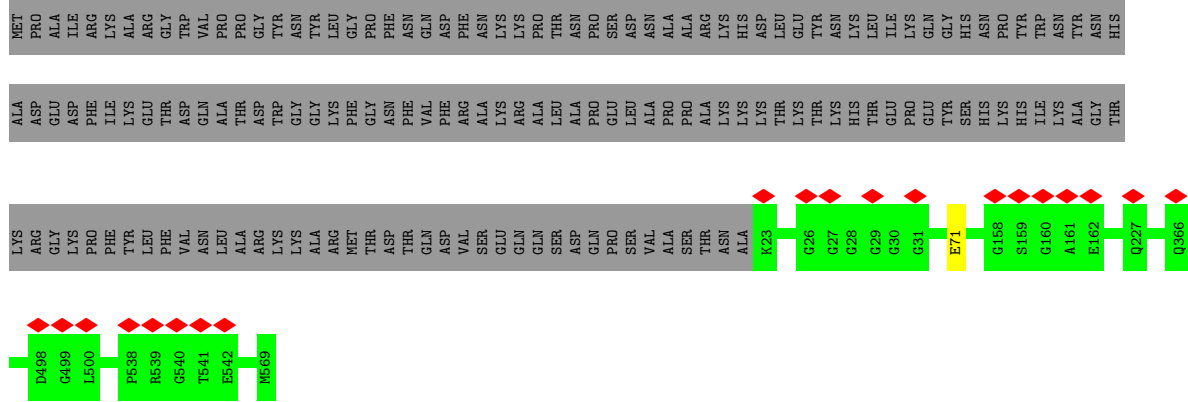
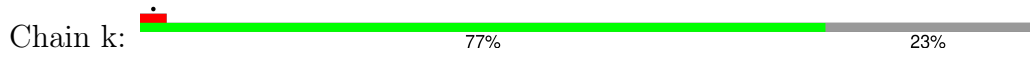


• Molecule 1: VP1

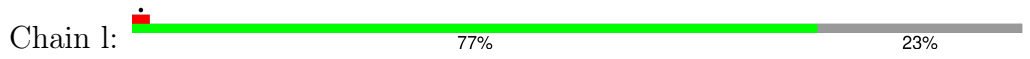




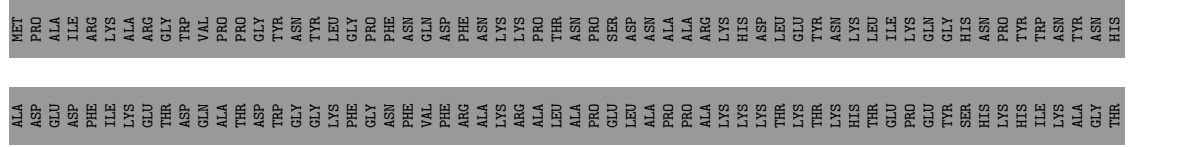
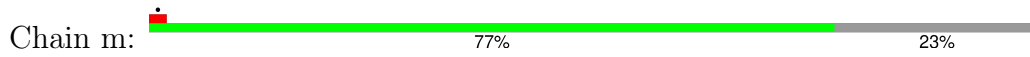
• Molecule 1: VP1

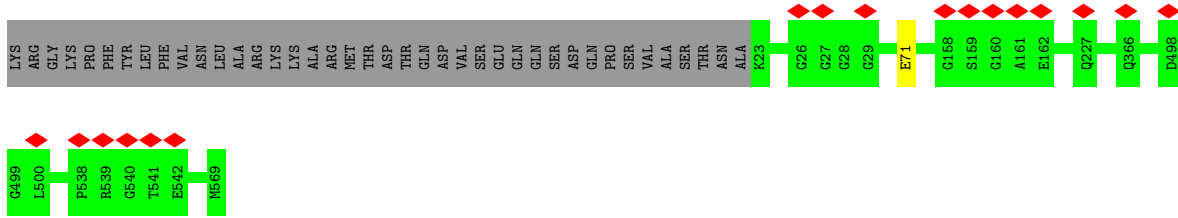


• Molecule 1: VP1

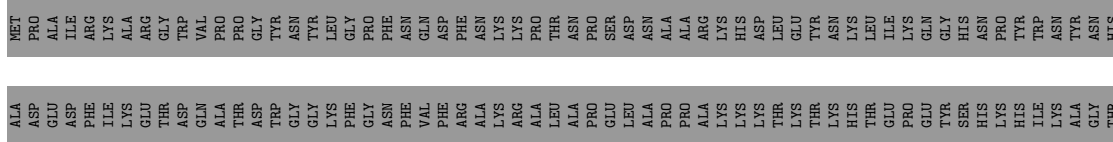
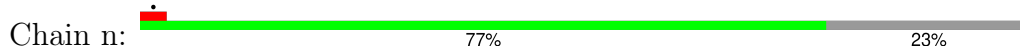


• Molecule 1: VP1

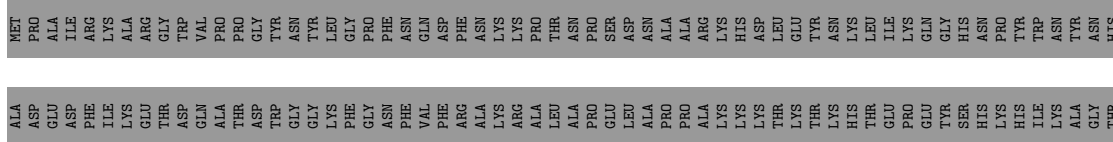
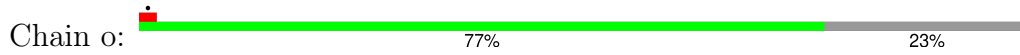




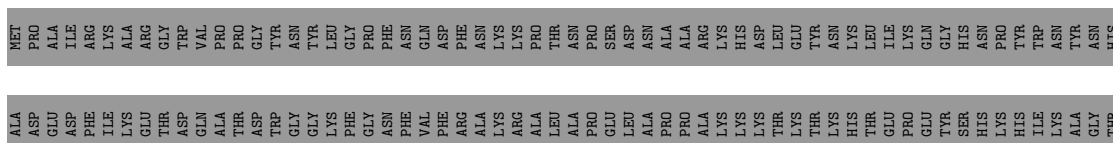
• Molecule 1: VP1

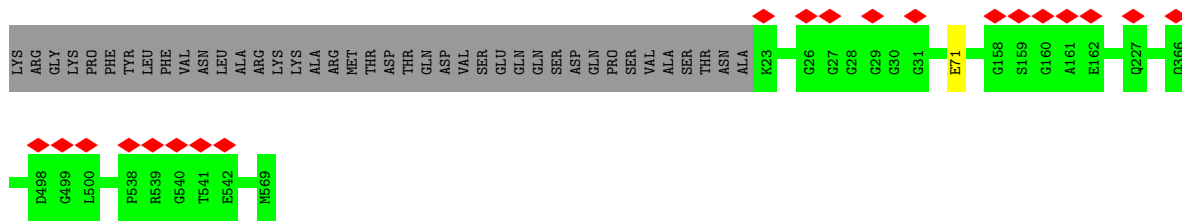


• Molecule 1: VP1

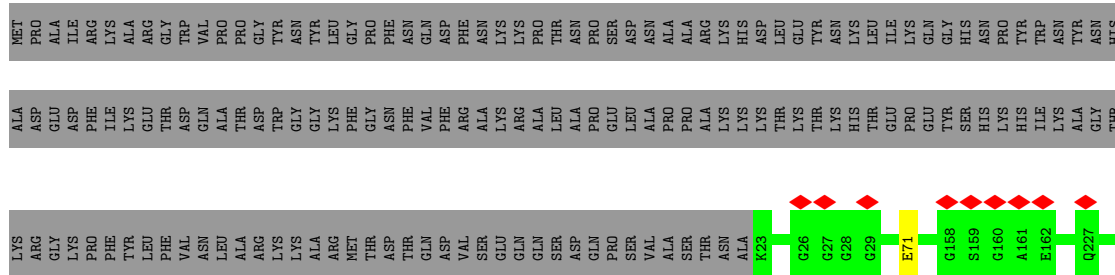
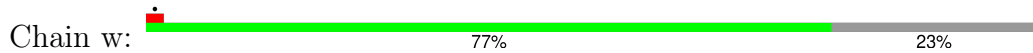


• Molecule 1: VP1

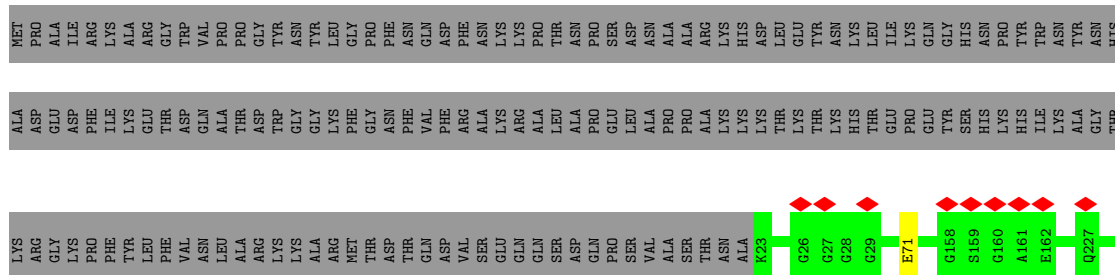
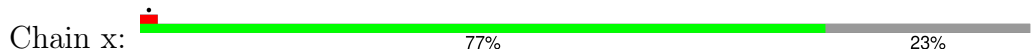




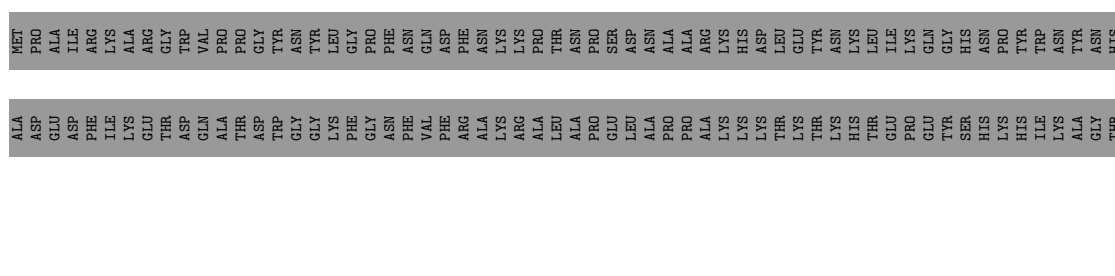
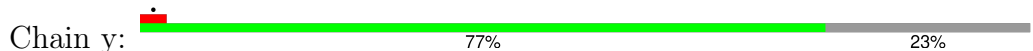
• Molecule 1: VP1

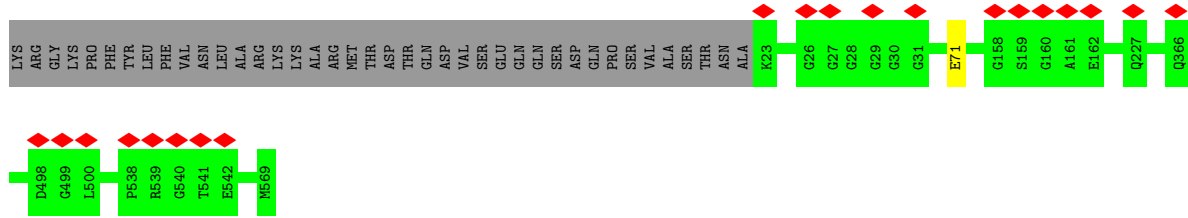


• Molecule 1: VP1

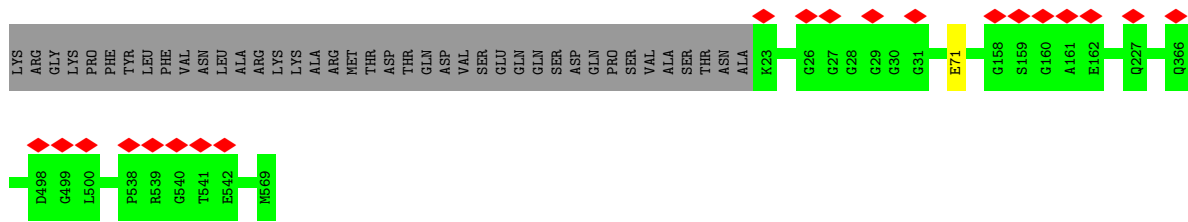
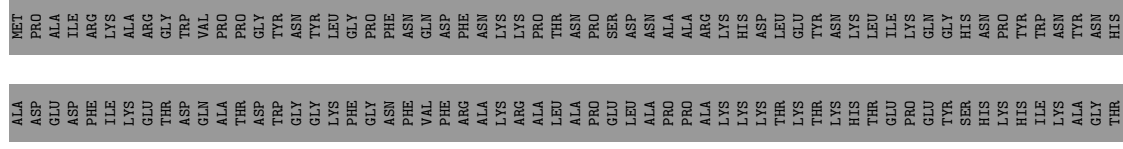
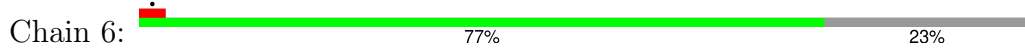


• Molecule 1: VP1

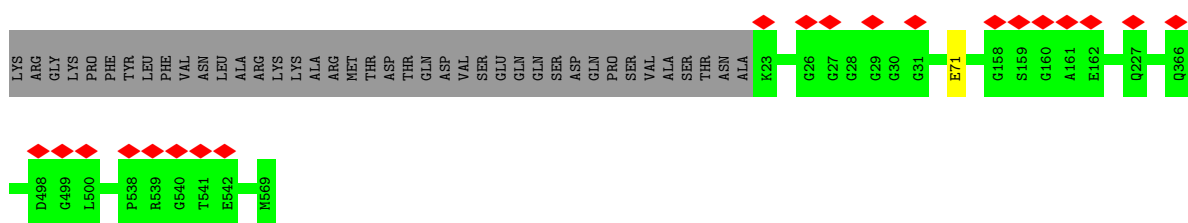
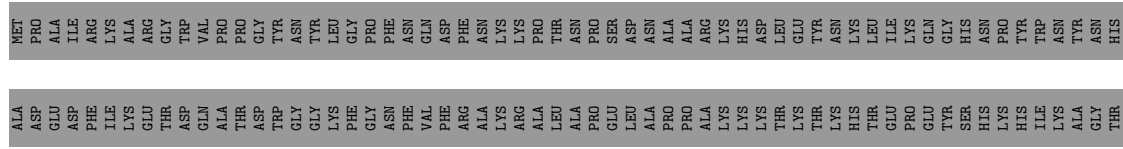
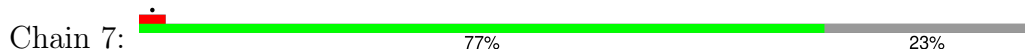




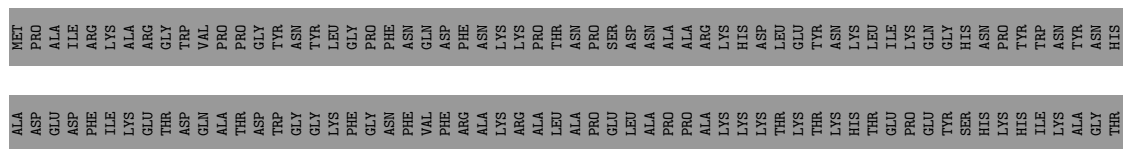
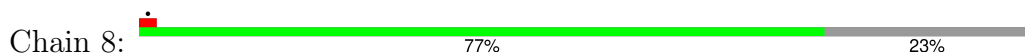
• Molecule 1: VP1

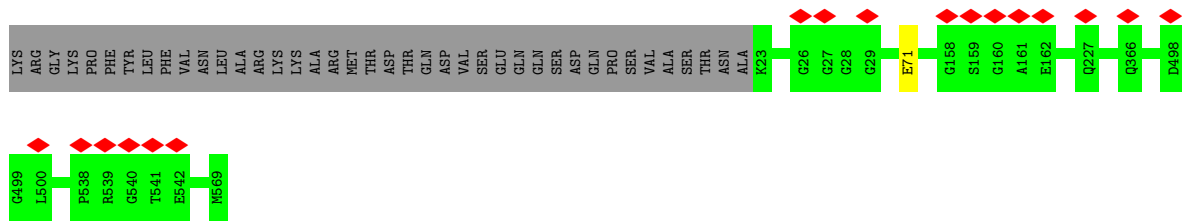


• Molecule 1: VP1



• Molecule 1: VP1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	121222	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 ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	100	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.380	Depositor
Minimum map value	-15.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size (\AA)	496.32, 496.32, 496.32	wwPDB
Map dimensions	470, 470, 470	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.056, 1.056, 1.056	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.47	0/4546	0.57	0/6214
1	2	0.47	0/4546	0.57	0/6214
1	3	0.47	0/4546	0.57	0/6214
1	4	0.47	0/4546	0.57	0/6214
1	5	0.47	0/4546	0.57	0/6214
1	6	0.47	0/4546	0.58	0/6214
1	7	0.47	0/4546	0.57	0/6214
1	8	0.47	0/4546	0.57	0/6214
1	A	0.47	0/4546	0.57	0/6214
1	B	0.47	0/4546	0.57	0/6214
1	C	0.47	0/4546	0.57	0/6214
1	D	0.47	0/4546	0.57	0/6214
1	E	0.47	0/4546	0.57	0/6214
1	F	0.47	0/4546	0.57	0/6214
1	G	0.47	0/4546	0.57	0/6214
1	H	0.47	0/4546	0.57	0/6214
1	I	0.47	0/4546	0.57	0/6214
1	J	0.47	0/4546	0.57	0/6214
1	K	0.47	0/4546	0.57	0/6214
1	L	0.47	0/4546	0.57	0/6214
1	M	0.47	0/4546	0.57	0/6214
1	N	0.47	0/4546	0.57	0/6214
1	O	0.47	0/4546	0.57	0/6214
1	P	0.47	0/4546	0.57	0/6214
1	Q	0.47	0/4546	0.57	0/6214
1	R	0.47	0/4546	0.57	0/6214
1	S	0.47	0/4546	0.57	0/6214
1	T	0.47	0/4546	0.58	0/6214
1	U	0.47	0/4546	0.57	0/6214
1	V	0.47	0/4546	0.57	0/6214
1	W	0.47	0/4546	0.57	0/6214
1	X	0.47	0/4546	0.57	0/6214
1	Y	0.47	0/4546	0.57	0/6214
1	Z	0.47	0/4546	0.57	0/6214

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.47	0/4546	0.57	0/6214
1	b	0.47	0/4546	0.57	0/6214
1	c	0.47	0/4546	0.57	0/6214
1	d	0.47	0/4546	0.57	0/6214
1	e	0.47	0/4546	0.57	0/6214
1	f	0.47	0/4546	0.57	0/6214
1	g	0.47	0/4546	0.57	0/6214
1	h	0.47	0/4546	0.57	0/6214
1	i	0.47	0/4546	0.57	0/6214
1	j	0.47	0/4546	0.57	0/6214
1	k	0.47	0/4546	0.58	0/6214
1	l	0.47	0/4546	0.57	0/6214
1	m	0.47	0/4546	0.57	0/6214
1	n	0.47	0/4546	0.57	0/6214
1	o	0.47	0/4546	0.57	0/6214
1	p	0.47	0/4546	0.57	0/6214
1	q	0.47	0/4546	0.57	0/6214
1	r	0.47	0/4546	0.57	0/6214
1	s	0.47	0/4546	0.57	0/6214
1	t	0.47	0/4546	0.57	0/6214
1	u	0.47	0/4546	0.57	0/6214
1	v	0.47	0/4546	0.57	0/6214
1	w	0.47	0/4546	0.57	0/6214
1	x	0.47	0/4546	0.57	0/6214
1	y	0.47	0/4546	0.57	0/6214
1	z	0.47	0/4546	0.57	0/6214
All	All	0.47	0/272760	0.57	0/372840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	2	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	3	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	4	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	5	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	6	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	7	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	8	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	A	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	B	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	C	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	D	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	E	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	F	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	G	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	H	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	I	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	J	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	K	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	L	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	M	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	N	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	O	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	P	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	Q	545/707 (77%)	510 (94%)	35 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	S	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	T	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	U	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	V	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	W	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	X	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	Y	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	Z	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	a	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	b	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	c	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	d	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	e	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	f	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	g	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	h	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	i	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	j	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	k	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	l	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	m	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	n	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	o	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	p	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	q	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	r	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	s	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	t	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	u	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	v	545/707 (77%)	510 (94%)	35 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	x	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	y	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
1	z	545/707 (77%)	510 (94%)	35 (6%)	0	100	100
All	All	32700/42420 (77%)	30600 (94%)	2100 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	2	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	3	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	4	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	5	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	6	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	7	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	8	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	A	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	B	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	C	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	D	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	E	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	F	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	G	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	H	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	I	474/609 (78%)	473 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	K	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	L	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	M	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	N	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	O	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	P	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	Q	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	R	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	S	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	T	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	U	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	V	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	W	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	X	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	Y	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	Z	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	a	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	b	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	c	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	d	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	e	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	f	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	g	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	h	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	i	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	j	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	k	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	l	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	m	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	n	474/609 (78%)	473 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	p	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	q	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	r	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	s	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	t	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	u	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	v	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	w	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	x	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	y	474/609 (78%)	473 (100%)	1 (0%)	92	96
1	z	474/609 (78%)	473 (100%)	1 (0%)	92	96
All	All	28440/36540 (78%)	28380 (100%)	60 (0%)	91	96

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

Mol	Chain	Res	Type
1	A	71	GLU
1	B	71	GLU
1	C	71	GLU
1	D	71	GLU
1	E	71	GLU
1	F	71	GLU
1	G	71	GLU
1	H	71	GLU
1	I	71	GLU
1	J	71	GLU
1	K	71	GLU
1	L	71	GLU
1	M	71	GLU
1	N	71	GLU
1	O	71	GLU
1	P	71	GLU
1	Q	71	GLU
1	R	71	GLU
1	S	71	GLU
1	T	71	GLU
1	U	71	GLU

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Mol	Chain	Res	Type
1	V	71	GLU
1	W	71	GLU
1	X	71	GLU
1	Y	71	GLU
1	Z	71	GLU
1	a	71	GLU
1	b	71	GLU
1	c	71	GLU
1	d	71	GLU
1	e	71	GLU
1	f	71	GLU
1	g	71	GLU
1	h	71	GLU
1	i	71	GLU
1	j	71	GLU
1	k	71	GLU
1	l	71	GLU
1	m	71	GLU
1	n	71	GLU
1	o	71	GLU
1	p	71	GLU
1	q	71	GLU
1	r	71	GLU
1	s	71	GLU
1	t	71	GLU
1	u	71	GLU
1	v	71	GLU
1	w	71	GLU
1	x	71	GLU
1	y	71	GLU
1	z	71	GLU
1	1	71	GLU
1	2	71	GLU
1	3	71	GLU
1	4	71	GLU
1	5	71	GLU
1	6	71	GLU
1	7	71	GLU
1	8	71	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1019) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	103	HIS
1	A	105	GLN
1	A	129	GLN
1	A	148	ASN
1	A	166	GLN
1	A	209	GLN
1	A	276	GLN
1	A	280	HIS
1	A	286	HIS
1	A	331	HIS
1	A	342	HIS
1	A	383	HIS
1	A	393	GLN
1	A	404	GLN
1	A	433	HIS
1	A	470	HIS
1	B	44	ASN
1	B	103	HIS
1	B	105	GLN
1	B	129	GLN
1	B	148	ASN
1	B	166	GLN
1	B	209	GLN
1	B	276	GLN
1	B	280	HIS
1	B	286	HIS
1	B	331	HIS
1	B	342	HIS
1	B	383	HIS
1	B	393	GLN
1	B	404	GLN
1	B	433	HIS
1	B	470	HIS
1	C	44	ASN
1	C	103	HIS
1	C	105	GLN
1	C	129	GLN
1	C	148	ASN
1	C	166	GLN
1	C	209	GLN
1	C	276	GLN
1	C	280	HIS

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Mol	Chain	Res	Type
1	C	286	HIS
1	C	331	HIS
1	C	342	HIS
1	C	383	HIS
1	C	393	GLN
1	C	404	GLN
1	C	433	HIS
1	C	470	HIS
1	D	44	ASN
1	D	103	HIS
1	D	105	GLN
1	D	129	GLN
1	D	148	ASN
1	D	166	GLN
1	D	209	GLN
1	D	276	GLN
1	D	280	HIS
1	D	286	HIS
1	D	331	HIS
1	D	342	HIS
1	D	383	HIS
1	D	393	GLN
1	D	404	GLN
1	D	433	HIS
1	D	470	HIS
1	E	44	ASN
1	E	103	HIS
1	E	105	GLN
1	E	129	GLN
1	E	148	ASN
1	E	166	GLN
1	E	209	GLN
1	E	276	GLN
1	E	280	HIS
1	E	286	HIS
1	E	331	HIS
1	E	342	HIS
1	E	383	HIS
1	E	393	GLN
1	E	404	GLN
1	E	433	HIS
1	E	470	HIS

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Mol	Chain	Res	Type
1	F	44	ASN
1	F	103	HIS
1	F	105	GLN
1	F	129	GLN
1	F	148	ASN
1	F	166	GLN
1	F	209	GLN
1	F	276	GLN
1	F	280	HIS
1	F	286	HIS
1	F	331	HIS
1	F	342	HIS
1	F	383	HIS
1	F	393	GLN
1	F	404	GLN
1	F	433	HIS
1	F	470	HIS
1	G	44	ASN
1	G	103	HIS
1	G	105	GLN
1	G	129	GLN
1	G	148	ASN
1	G	166	GLN
1	G	209	GLN
1	G	276	GLN
1	G	280	HIS
1	G	286	HIS
1	G	331	HIS
1	G	342	HIS
1	G	383	HIS
1	G	393	GLN
1	G	404	GLN
1	G	433	HIS
1	G	470	HIS
1	H	44	ASN
1	H	103	HIS
1	H	105	GLN
1	H	129	GLN
1	H	148	ASN
1	H	166	GLN
1	H	209	GLN
1	H	276	GLN

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Mol	Chain	Res	Type
1	H	280	HIS
1	H	286	HIS
1	H	331	HIS
1	H	342	HIS
1	H	383	HIS
1	H	393	GLN
1	H	404	GLN
1	H	433	HIS
1	H	470	HIS
1	I	44	ASN
1	I	103	HIS
1	I	105	GLN
1	I	129	GLN
1	I	148	ASN
1	I	166	GLN
1	I	209	GLN
1	I	276	GLN
1	I	280	HIS
1	I	286	HIS
1	I	331	HIS
1	I	342	HIS
1	I	383	HIS
1	I	393	GLN
1	I	404	GLN
1	I	433	HIS
1	I	470	HIS
1	J	44	ASN
1	J	103	HIS
1	J	105	GLN
1	J	129	GLN
1	J	148	ASN
1	J	166	GLN
1	J	209	GLN
1	J	276	GLN
1	J	280	HIS
1	J	286	HIS
1	J	331	HIS
1	J	342	HIS
1	J	383	HIS
1	J	393	GLN
1	J	404	GLN
1	J	433	HIS

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Mol	Chain	Res	Type
1	J	470	HIS
1	K	44	ASN
1	K	103	HIS
1	K	105	GLN
1	K	129	GLN
1	K	148	ASN
1	K	166	GLN
1	K	209	GLN
1	K	276	GLN
1	K	280	HIS
1	K	286	HIS
1	K	331	HIS
1	K	342	HIS
1	K	383	HIS
1	K	393	GLN
1	K	404	GLN
1	K	433	HIS
1	K	470	HIS
1	L	44	ASN
1	L	103	HIS
1	L	105	GLN
1	L	129	GLN
1	L	148	ASN
1	L	166	GLN
1	L	209	GLN
1	L	276	GLN
1	L	280	HIS
1	L	286	HIS
1	L	331	HIS
1	L	342	HIS
1	L	383	HIS
1	L	393	GLN
1	L	404	GLN
1	L	433	HIS
1	L	470	HIS
1	M	44	ASN
1	M	103	HIS
1	M	105	GLN
1	M	129	GLN
1	M	148	ASN
1	M	166	GLN
1	M	209	GLN

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Mol	Chain	Res	Type
1	M	276	GLN
1	M	280	HIS
1	M	286	HIS
1	M	331	HIS
1	M	342	HIS
1	M	383	HIS
1	M	393	GLN
1	M	404	GLN
1	M	433	HIS
1	M	470	HIS
1	N	44	ASN
1	N	103	HIS
1	N	105	GLN
1	N	129	GLN
1	N	148	ASN
1	N	166	GLN
1	N	209	GLN
1	N	276	GLN
1	N	280	HIS
1	N	286	HIS
1	N	331	HIS
1	N	342	HIS
1	N	383	HIS
1	N	393	GLN
1	N	404	GLN
1	N	433	HIS
1	N	470	HIS
1	O	44	ASN
1	O	103	HIS
1	O	105	GLN
1	O	129	GLN
1	O	148	ASN
1	O	166	GLN
1	O	209	GLN
1	O	276	GLN
1	O	280	HIS
1	O	286	HIS
1	O	331	HIS
1	O	342	HIS
1	O	383	HIS
1	O	393	GLN
1	O	404	GLN

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Mol	Chain	Res	Type
1	O	433	HIS
1	O	470	HIS
1	P	44	ASN
1	P	103	HIS
1	P	105	GLN
1	P	129	GLN
1	P	148	ASN
1	P	166	GLN
1	P	209	GLN
1	P	276	GLN
1	P	280	HIS
1	P	286	HIS
1	P	331	HIS
1	P	342	HIS
1	P	383	HIS
1	P	393	GLN
1	P	404	GLN
1	P	433	HIS
1	P	470	HIS
1	Q	44	ASN
1	Q	103	HIS
1	Q	105	GLN
1	Q	129	GLN
1	Q	148	ASN
1	Q	166	GLN
1	Q	209	GLN
1	Q	276	GLN
1	Q	280	HIS
1	Q	286	HIS
1	Q	331	HIS
1	Q	342	HIS
1	Q	383	HIS
1	Q	393	GLN
1	Q	404	GLN
1	Q	433	HIS
1	Q	470	HIS
1	R	44	ASN
1	R	103	HIS
1	R	105	GLN
1	R	129	GLN
1	R	148	ASN
1	R	166	GLN

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Mol	Chain	Res	Type
1	R	209	GLN
1	R	276	GLN
1	R	280	HIS
1	R	286	HIS
1	R	331	HIS
1	R	342	HIS
1	R	383	HIS
1	R	393	GLN
1	R	404	GLN
1	R	433	HIS
1	R	470	HIS
1	S	44	ASN
1	S	103	HIS
1	S	105	GLN
1	S	129	GLN
1	S	148	ASN
1	S	166	GLN
1	S	209	GLN
1	S	276	GLN
1	S	280	HIS
1	S	286	HIS
1	S	331	HIS
1	S	342	HIS
1	S	383	HIS
1	S	393	GLN
1	S	404	GLN
1	S	433	HIS
1	S	470	HIS
1	T	44	ASN
1	T	103	HIS
1	T	105	GLN
1	T	129	GLN
1	T	148	ASN
1	T	166	GLN
1	T	209	GLN
1	T	276	GLN
1	T	280	HIS
1	T	286	HIS
1	T	331	HIS
1	T	342	HIS
1	T	383	HIS
1	T	393	GLN

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Mol	Chain	Res	Type
1	T	404	GLN
1	T	433	HIS
1	T	470	HIS
1	U	44	ASN
1	U	103	HIS
1	U	105	GLN
1	U	129	GLN
1	U	148	ASN
1	U	166	GLN
1	U	209	GLN
1	U	276	GLN
1	U	280	HIS
1	U	286	HIS
1	U	331	HIS
1	U	342	HIS
1	U	383	HIS
1	U	393	GLN
1	U	404	GLN
1	U	433	HIS
1	U	470	HIS
1	V	44	ASN
1	V	103	HIS
1	V	105	GLN
1	V	129	GLN
1	V	148	ASN
1	V	166	GLN
1	V	209	GLN
1	V	276	GLN
1	V	280	HIS
1	V	286	HIS
1	V	331	HIS
1	V	342	HIS
1	V	383	HIS
1	V	393	GLN
1	V	404	GLN
1	V	433	HIS
1	V	470	HIS
1	W	44	ASN
1	W	103	HIS
1	W	105	GLN
1	W	129	GLN
1	W	148	ASN

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Mol	Chain	Res	Type
1	W	166	GLN
1	W	209	GLN
1	W	276	GLN
1	W	280	HIS
1	W	286	HIS
1	W	331	HIS
1	W	342	HIS
1	W	383	HIS
1	W	393	GLN
1	W	404	GLN
1	W	433	HIS
1	W	470	HIS
1	X	44	ASN
1	X	103	HIS
1	X	105	GLN
1	X	129	GLN
1	X	148	ASN
1	X	166	GLN
1	X	209	GLN
1	X	276	GLN
1	X	280	HIS
1	X	286	HIS
1	X	331	HIS
1	X	342	HIS
1	X	383	HIS
1	X	393	GLN
1	X	404	GLN
1	X	433	HIS
1	X	470	HIS
1	Y	44	ASN
1	Y	103	HIS
1	Y	105	GLN
1	Y	129	GLN
1	Y	148	ASN
1	Y	166	GLN
1	Y	209	GLN
1	Y	276	GLN
1	Y	280	HIS
1	Y	286	HIS
1	Y	331	HIS
1	Y	342	HIS
1	Y	383	HIS

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Mol	Chain	Res	Type
1	Y	393	GLN
1	Y	404	GLN
1	Y	433	HIS
1	Y	470	HIS
1	Z	44	ASN
1	Z	103	HIS
1	Z	105	GLN
1	Z	129	GLN
1	Z	148	ASN
1	Z	166	GLN
1	Z	209	GLN
1	Z	276	GLN
1	Z	280	HIS
1	Z	286	HIS
1	Z	331	HIS
1	Z	342	HIS
1	Z	383	HIS
1	Z	393	GLN
1	Z	404	GLN
1	Z	433	HIS
1	Z	470	HIS
1	a	44	ASN
1	a	103	HIS
1	a	105	GLN
1	a	129	GLN
1	a	148	ASN
1	a	166	GLN
1	a	209	GLN
1	a	276	GLN
1	a	280	HIS
1	a	286	HIS
1	a	331	HIS
1	a	342	HIS
1	a	383	HIS
1	a	393	GLN
1	a	404	GLN
1	a	433	HIS
1	a	470	HIS
1	b	44	ASN
1	b	103	HIS
1	b	105	GLN
1	b	129	GLN

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Mol	Chain	Res	Type
1	b	148	ASN
1	b	166	GLN
1	b	209	GLN
1	b	276	GLN
1	b	280	HIS
1	b	286	HIS
1	b	331	HIS
1	b	342	HIS
1	b	383	HIS
1	b	393	GLN
1	b	404	GLN
1	b	433	HIS
1	b	470	HIS
1	c	44	ASN
1	c	103	HIS
1	c	105	GLN
1	c	129	GLN
1	c	148	ASN
1	c	166	GLN
1	c	209	GLN
1	c	276	GLN
1	c	280	HIS
1	c	286	HIS
1	c	331	HIS
1	c	342	HIS
1	c	383	HIS
1	c	393	GLN
1	c	404	GLN
1	c	433	HIS
1	c	470	HIS
1	d	44	ASN
1	d	103	HIS
1	d	105	GLN
1	d	129	GLN
1	d	148	ASN
1	d	166	GLN
1	d	209	GLN
1	d	276	GLN
1	d	280	HIS
1	d	286	HIS
1	d	331	HIS
1	d	342	HIS

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Mol	Chain	Res	Type
1	d	383	HIS
1	d	393	GLN
1	d	404	GLN
1	d	433	HIS
1	d	470	HIS
1	e	44	ASN
1	e	103	HIS
1	e	105	GLN
1	e	129	GLN
1	e	148	ASN
1	e	166	GLN
1	e	209	GLN
1	e	276	GLN
1	e	280	HIS
1	e	286	HIS
1	e	331	HIS
1	e	342	HIS
1	e	383	HIS
1	e	393	GLN
1	e	404	GLN
1	e	433	HIS
1	e	470	HIS
1	f	44	ASN
1	f	103	HIS
1	f	105	GLN
1	f	129	GLN
1	f	148	ASN
1	f	166	GLN
1	f	209	GLN
1	f	276	GLN
1	f	280	HIS
1	f	286	HIS
1	f	331	HIS
1	f	342	HIS
1	f	383	HIS
1	f	393	GLN
1	f	404	GLN
1	f	433	HIS
1	f	470	HIS
1	g	44	ASN
1	g	103	HIS
1	g	105	GLN

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Mol	Chain	Res	Type
1	g	129	GLN
1	g	148	ASN
1	g	166	GLN
1	g	209	GLN
1	g	276	GLN
1	g	280	HIS
1	g	286	HIS
1	g	331	HIS
1	g	342	HIS
1	g	383	HIS
1	g	393	GLN
1	g	404	GLN
1	g	433	HIS
1	g	470	HIS
1	h	44	ASN
1	h	103	HIS
1	h	105	GLN
1	h	129	GLN
1	h	148	ASN
1	h	166	GLN
1	h	209	GLN
1	h	276	GLN
1	h	280	HIS
1	h	286	HIS
1	h	331	HIS
1	h	342	HIS
1	h	383	HIS
1	h	393	GLN
1	h	404	GLN
1	h	433	HIS
1	h	470	HIS
1	i	44	ASN
1	i	103	HIS
1	i	105	GLN
1	i	129	GLN
1	i	148	ASN
1	i	166	GLN
1	i	209	GLN
1	i	276	GLN
1	i	280	HIS
1	i	286	HIS
1	i	331	HIS

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Mol	Chain	Res	Type
1	i	342	HIS
1	i	383	HIS
1	i	393	GLN
1	i	404	GLN
1	i	433	HIS
1	i	470	HIS
1	j	44	ASN
1	j	103	HIS
1	j	105	GLN
1	j	129	GLN
1	j	148	ASN
1	j	166	GLN
1	j	209	GLN
1	j	276	GLN
1	j	280	HIS
1	j	286	HIS
1	j	331	HIS
1	j	342	HIS
1	j	383	HIS
1	j	393	GLN
1	j	404	GLN
1	j	433	HIS
1	j	470	HIS
1	k	44	ASN
1	k	103	HIS
1	k	105	GLN
1	k	129	GLN
1	k	148	ASN
1	k	166	GLN
1	k	209	GLN
1	k	276	GLN
1	k	280	HIS
1	k	286	HIS
1	k	331	HIS
1	k	342	HIS
1	k	383	HIS
1	k	393	GLN
1	k	404	GLN
1	k	433	HIS
1	k	470	HIS
1	l	44	ASN
1	l	103	HIS

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Mol	Chain	Res	Type
1	l	105	GLN
1	l	129	GLN
1	l	148	ASN
1	l	166	GLN
1	l	209	GLN
1	l	276	GLN
1	l	280	HIS
1	l	286	HIS
1	l	331	HIS
1	l	342	HIS
1	l	383	HIS
1	l	393	GLN
1	l	404	GLN
1	l	433	HIS
1	l	470	HIS
1	m	44	ASN
1	m	103	HIS
1	m	105	GLN
1	m	129	GLN
1	m	148	ASN
1	m	166	GLN
1	m	209	GLN
1	m	276	GLN
1	m	280	HIS
1	m	286	HIS
1	m	331	HIS
1	m	342	HIS
1	m	383	HIS
1	m	393	GLN
1	m	404	GLN
1	m	433	HIS
1	m	470	HIS
1	n	44	ASN
1	n	103	HIS
1	n	105	GLN
1	n	129	GLN
1	n	148	ASN
1	n	166	GLN
1	n	209	GLN
1	n	276	GLN
1	n	280	HIS
1	n	286	HIS

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Mol	Chain	Res	Type
1	n	331	HIS
1	n	342	HIS
1	n	383	HIS
1	n	393	GLN
1	n	404	GLN
1	n	433	HIS
1	n	470	HIS
1	o	44	ASN
1	o	103	HIS
1	o	105	GLN
1	o	129	GLN
1	o	148	ASN
1	o	166	GLN
1	o	209	GLN
1	o	276	GLN
1	o	280	HIS
1	o	286	HIS
1	o	331	HIS
1	o	342	HIS
1	o	383	HIS
1	o	393	GLN
1	o	404	GLN
1	o	433	HIS
1	o	470	HIS
1	p	44	ASN
1	p	103	HIS
1	p	105	GLN
1	p	129	GLN
1	p	148	ASN
1	p	166	GLN
1	p	209	GLN
1	p	276	GLN
1	p	280	HIS
1	p	286	HIS
1	p	331	HIS
1	p	342	HIS
1	p	383	HIS
1	p	393	GLN
1	p	404	GLN
1	p	433	HIS
1	p	470	HIS
1	q	44	ASN

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Mol	Chain	Res	Type
1	q	103	HIS
1	q	105	GLN
1	q	129	GLN
1	q	148	ASN
1	q	166	GLN
1	q	209	GLN
1	q	276	GLN
1	q	280	HIS
1	q	286	HIS
1	q	331	HIS
1	q	342	HIS
1	q	383	HIS
1	q	393	GLN
1	q	404	GLN
1	q	433	HIS
1	q	470	HIS
1	r	44	ASN
1	r	103	HIS
1	r	105	GLN
1	r	129	GLN
1	r	148	ASN
1	r	166	GLN
1	r	209	GLN
1	r	276	GLN
1	r	280	HIS
1	r	286	HIS
1	r	331	HIS
1	r	342	HIS
1	r	383	HIS
1	r	393	GLN
1	r	404	GLN
1	r	433	HIS
1	r	470	HIS
1	s	44	ASN
1	s	103	HIS
1	s	105	GLN
1	s	129	GLN
1	s	148	ASN
1	s	166	GLN
1	s	209	GLN
1	s	276	GLN
1	s	280	HIS

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Mol	Chain	Res	Type
1	s	286	HIS
1	s	331	HIS
1	s	342	HIS
1	s	383	HIS
1	s	393	GLN
1	s	404	GLN
1	s	433	HIS
1	s	470	HIS
1	t	44	ASN
1	t	103	HIS
1	t	105	GLN
1	t	129	GLN
1	t	148	ASN
1	t	166	GLN
1	t	209	GLN
1	t	276	GLN
1	t	280	HIS
1	t	286	HIS
1	t	331	HIS
1	t	342	HIS
1	t	383	HIS
1	t	393	GLN
1	t	404	GLN
1	t	433	HIS
1	t	470	HIS
1	u	44	ASN
1	u	103	HIS
1	u	105	GLN
1	u	129	GLN
1	u	148	ASN
1	u	166	GLN
1	u	209	GLN
1	u	276	GLN
1	u	280	HIS
1	u	286	HIS
1	u	331	HIS
1	u	342	HIS
1	u	383	HIS
1	u	393	GLN
1	u	404	GLN
1	u	433	HIS
1	u	470	HIS

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Mol	Chain	Res	Type
1	v	44	ASN
1	v	103	HIS
1	v	105	GLN
1	v	129	GLN
1	v	148	ASN
1	v	166	GLN
1	v	209	GLN
1	v	276	GLN
1	v	280	HIS
1	v	286	HIS
1	v	331	HIS
1	v	342	HIS
1	v	383	HIS
1	v	393	GLN
1	v	404	GLN
1	v	433	HIS
1	v	470	HIS
1	w	44	ASN
1	w	103	HIS
1	w	105	GLN
1	w	129	GLN
1	w	148	ASN
1	w	166	GLN
1	w	276	GLN
1	w	280	HIS
1	w	286	HIS
1	w	331	HIS
1	w	342	HIS
1	w	383	HIS
1	w	393	GLN
1	w	404	GLN
1	w	433	HIS
1	w	470	HIS
1	x	44	ASN
1	x	103	HIS
1	x	105	GLN
1	x	129	GLN
1	x	148	ASN
1	x	166	GLN
1	x	209	GLN
1	x	276	GLN
1	x	280	HIS

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Mol	Chain	Res	Type
1	x	286	HIS
1	x	331	HIS
1	x	342	HIS
1	x	383	HIS
1	x	393	GLN
1	x	404	GLN
1	x	433	HIS
1	x	470	HIS
1	y	44	ASN
1	y	103	HIS
1	y	105	GLN
1	y	129	GLN
1	y	148	ASN
1	y	166	GLN
1	y	209	GLN
1	y	276	GLN
1	y	280	HIS
1	y	286	HIS
1	y	331	HIS
1	y	342	HIS
1	y	383	HIS
1	y	393	GLN
1	y	404	GLN
1	y	433	HIS
1	y	470	HIS
1	z	44	ASN
1	z	103	HIS
1	z	105	GLN
1	z	129	GLN
1	z	148	ASN
1	z	166	GLN
1	z	209	GLN
1	z	276	GLN
1	z	280	HIS
1	z	286	HIS
1	z	331	HIS
1	z	342	HIS
1	z	383	HIS
1	z	393	GLN
1	z	404	GLN
1	z	433	HIS
1	z	470	HIS

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Mol	Chain	Res	Type
1	1	44	ASN
1	1	103	HIS
1	1	105	GLN
1	1	129	GLN
1	1	148	ASN
1	1	166	GLN
1	1	209	GLN
1	1	276	GLN
1	1	280	HIS
1	1	286	HIS
1	1	331	HIS
1	1	342	HIS
1	1	383	HIS
1	1	393	GLN
1	1	404	GLN
1	1	433	HIS
1	1	470	HIS
1	2	44	ASN
1	2	103	HIS
1	2	105	GLN
1	2	129	GLN
1	2	148	ASN
1	2	166	GLN
1	2	209	GLN
1	2	276	GLN
1	2	280	HIS
1	2	286	HIS
1	2	331	HIS
1	2	342	HIS
1	2	383	HIS
1	2	393	GLN
1	2	404	GLN
1	2	433	HIS
1	2	470	HIS
1	3	44	ASN
1	3	103	HIS
1	3	105	GLN
1	3	129	GLN
1	3	148	ASN
1	3	166	GLN
1	3	209	GLN
1	3	276	GLN

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Mol	Chain	Res	Type
1	3	280	HIS
1	3	286	HIS
1	3	331	HIS
1	3	342	HIS
1	3	383	HIS
1	3	393	GLN
1	3	404	GLN
1	3	433	HIS
1	3	470	HIS
1	4	44	ASN
1	4	103	HIS
1	4	105	GLN
1	4	129	GLN
1	4	148	ASN
1	4	166	GLN
1	4	209	GLN
1	4	276	GLN
1	4	280	HIS
1	4	286	HIS
1	4	331	HIS
1	4	342	HIS
1	4	383	HIS
1	4	393	GLN
1	4	404	GLN
1	4	433	HIS
1	4	470	HIS
1	5	44	ASN
1	5	103	HIS
1	5	105	GLN
1	5	129	GLN
1	5	148	ASN
1	5	166	GLN
1	5	209	GLN
1	5	276	GLN
1	5	280	HIS
1	5	286	HIS
1	5	331	HIS
1	5	342	HIS
1	5	383	HIS
1	5	393	GLN
1	5	404	GLN
1	5	433	HIS

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Mol	Chain	Res	Type
1	5	470	HIS
1	6	44	ASN
1	6	103	HIS
1	6	105	GLN
1	6	129	GLN
1	6	148	ASN
1	6	166	GLN
1	6	209	GLN
1	6	276	GLN
1	6	280	HIS
1	6	286	HIS
1	6	331	HIS
1	6	342	HIS
1	6	383	HIS
1	6	393	GLN
1	6	404	GLN
1	6	433	HIS
1	6	470	HIS
1	7	44	ASN
1	7	103	HIS
1	7	105	GLN
1	7	129	GLN
1	7	148	ASN
1	7	166	GLN
1	7	209	GLN
1	7	276	GLN
1	7	280	HIS
1	7	286	HIS
1	7	331	HIS
1	7	342	HIS
1	7	383	HIS
1	7	393	GLN
1	7	404	GLN
1	7	433	HIS
1	7	470	HIS
1	8	44	ASN
1	8	103	HIS
1	8	105	GLN
1	8	129	GLN
1	8	148	ASN
1	8	166	GLN
1	8	209	GLN

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Mol	Chain	Res	Type
1	8	276	GLN
1	8	280	HIS
1	8	286	HIS
1	8	331	HIS
1	8	342	HIS
1	8	383	HIS
1	8	393	GLN
1	8	404	GLN
1	8	433	HIS
1	8	470	HIS

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.

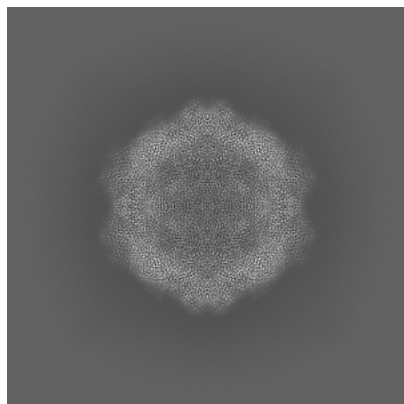
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45973. These allow visual inspection of the internal detail of the map and identification of artifacts.

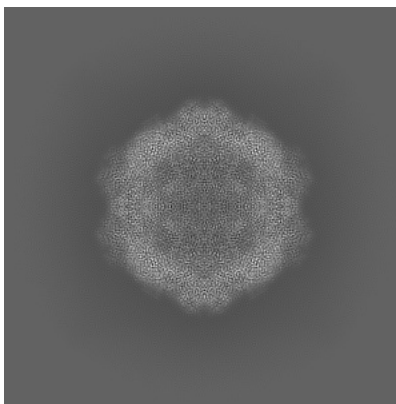
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

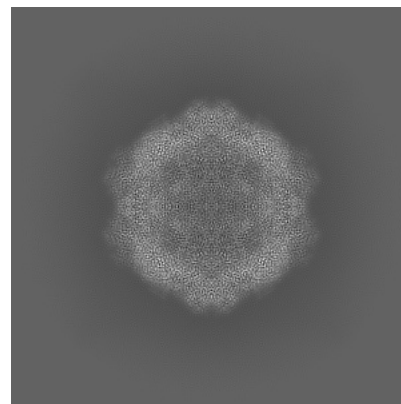
6.1.1 Primary map



X

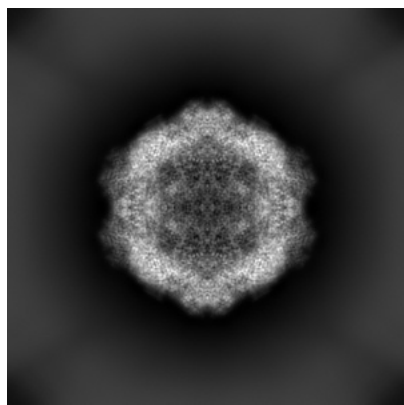


Y

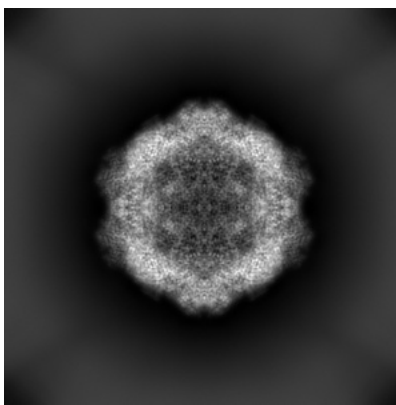


Z

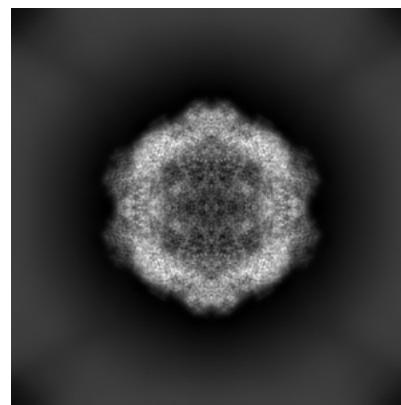
6.1.2 Raw map



X



Y

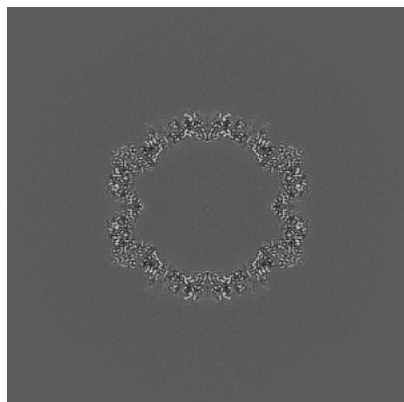


Z

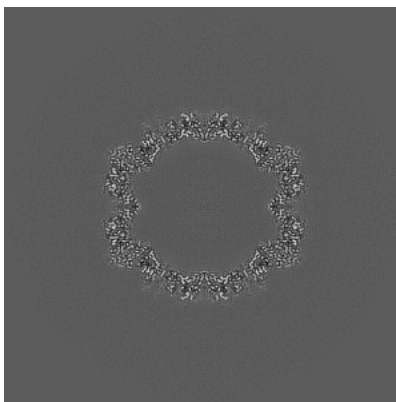
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

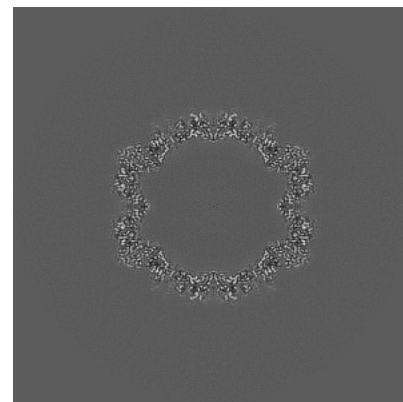
6.2.1 Primary map



X Index: 235

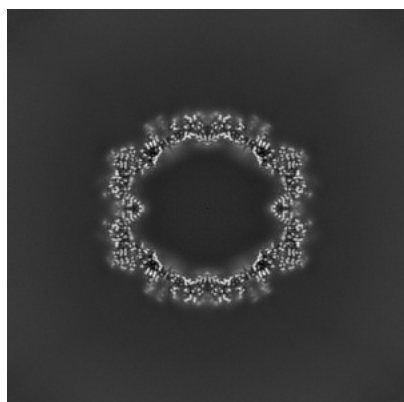


Y Index: 235

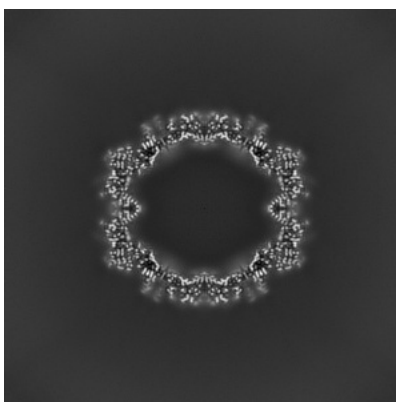


Z Index: 235

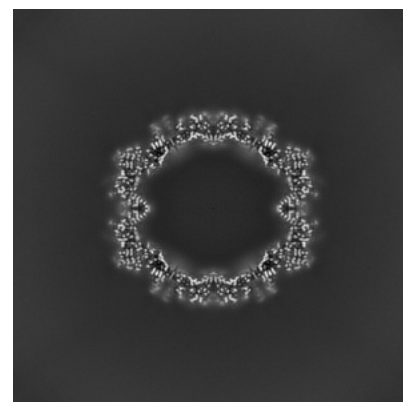
6.2.2 Raw map



X Index: 235



Y Index: 235

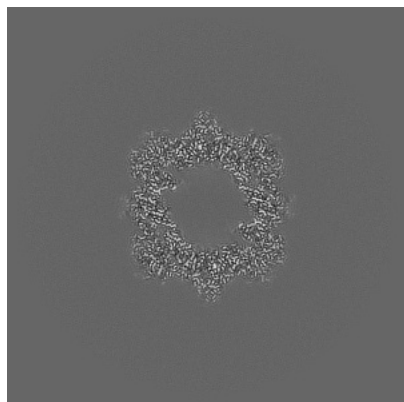


Z Index: 235

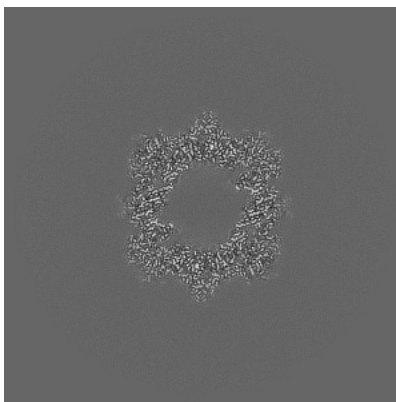
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

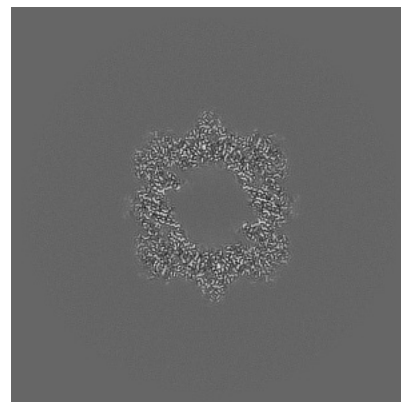
6.3.1 Primary map



X Index: 300

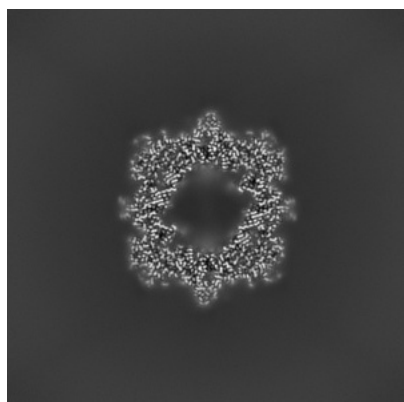


Y Index: 170

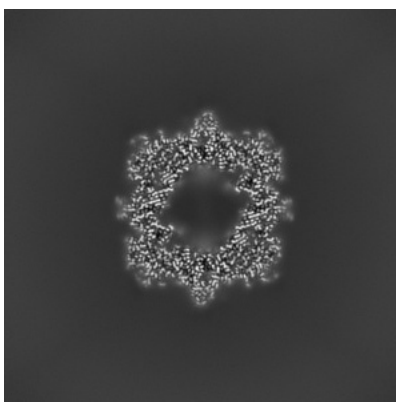


Z Index: 300

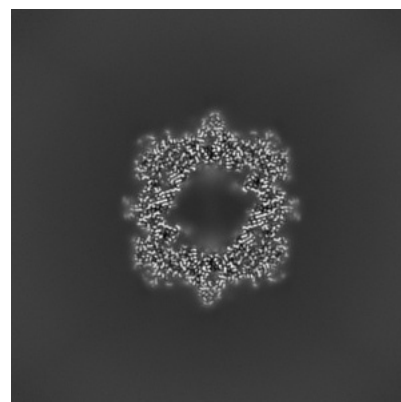
6.3.2 Raw map



X Index: 170



Y Index: 170

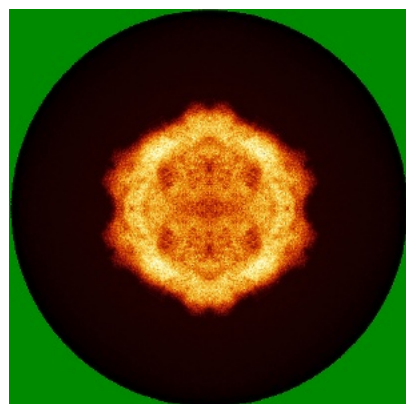


Z Index: 170

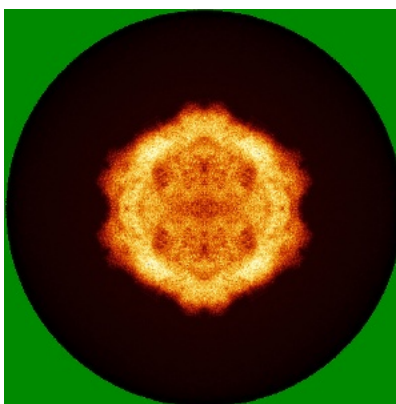
The images above show the largest variance slices of the map in three orthogonal directions.

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

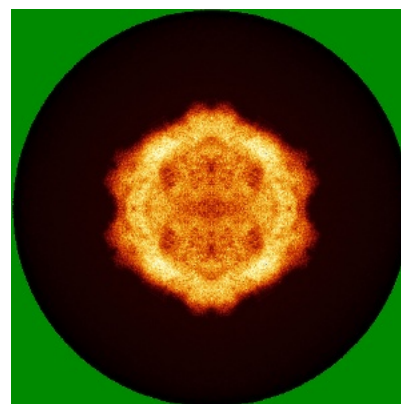
6.4.1 Primary map



X

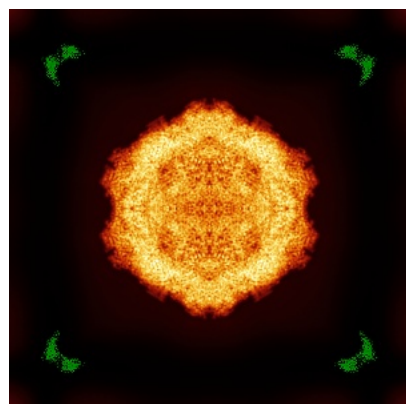


Y

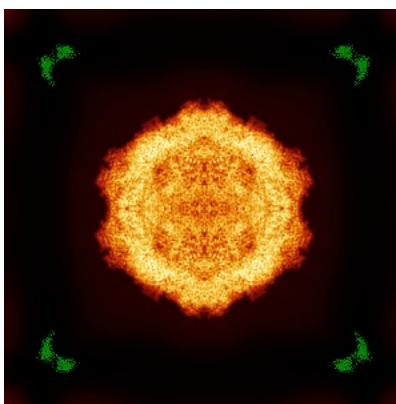


Z

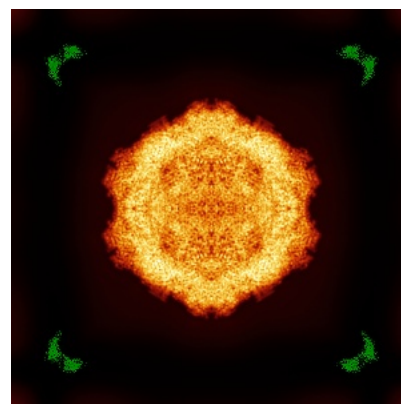
6.4.2 Raw map



X



Y

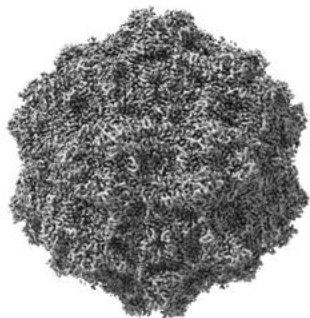


Z

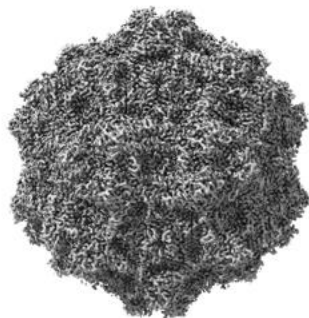
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

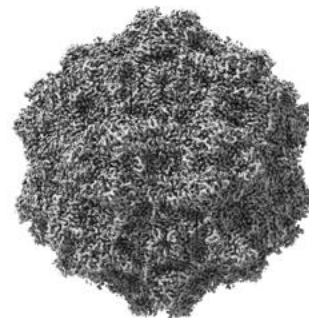
6.5.1 Primary map



X



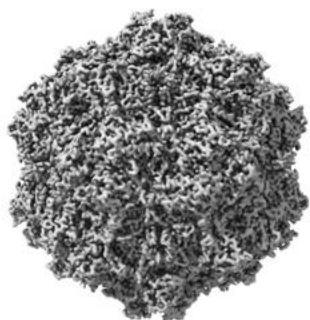
Y



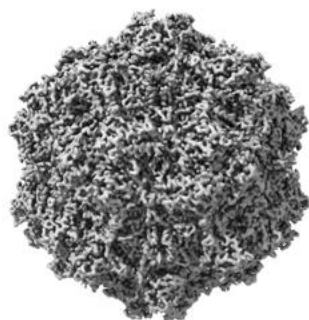
Z

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.

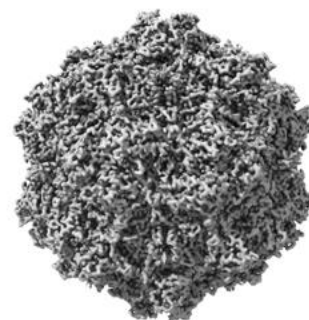
6.5.2 Raw map



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.

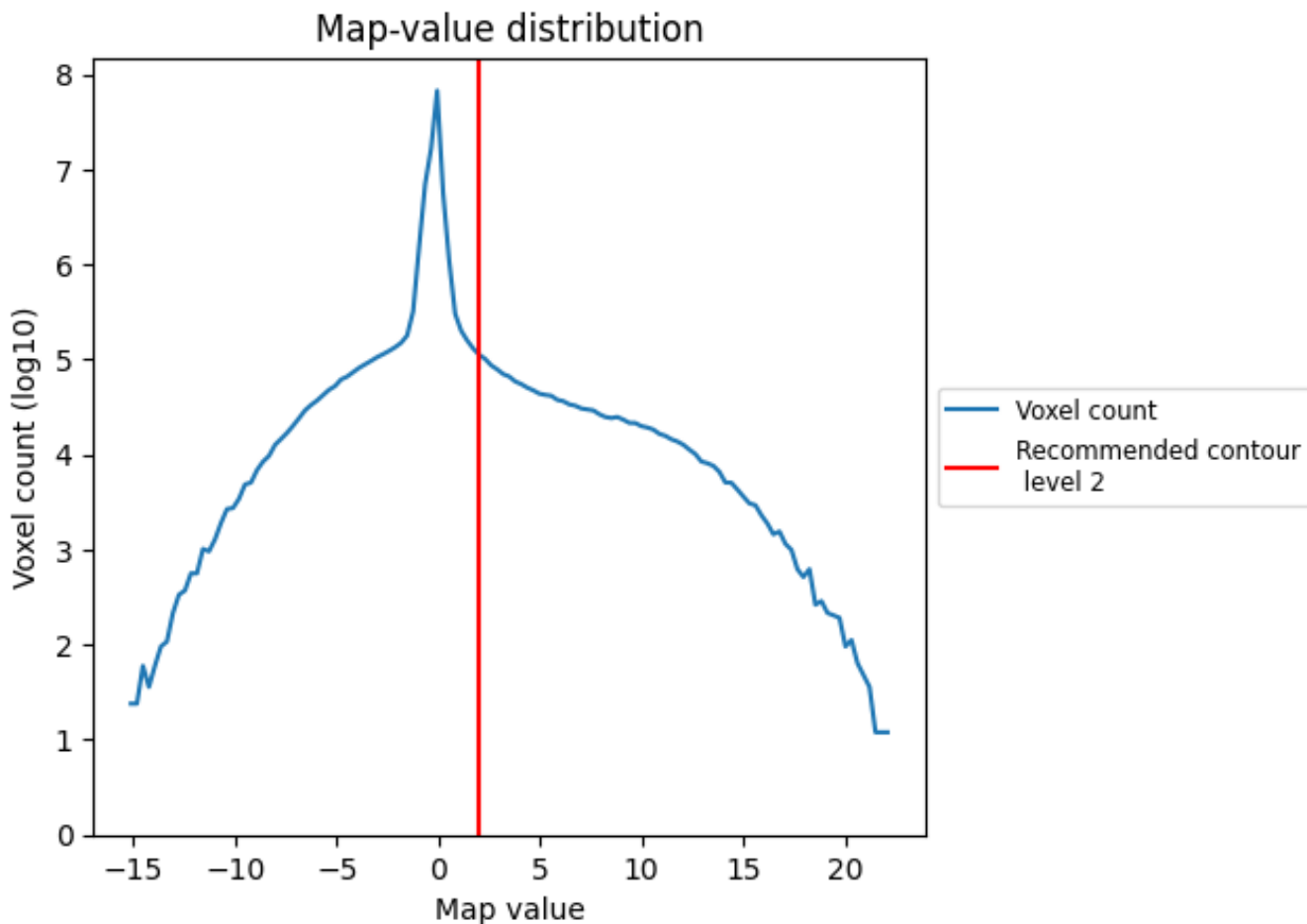
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

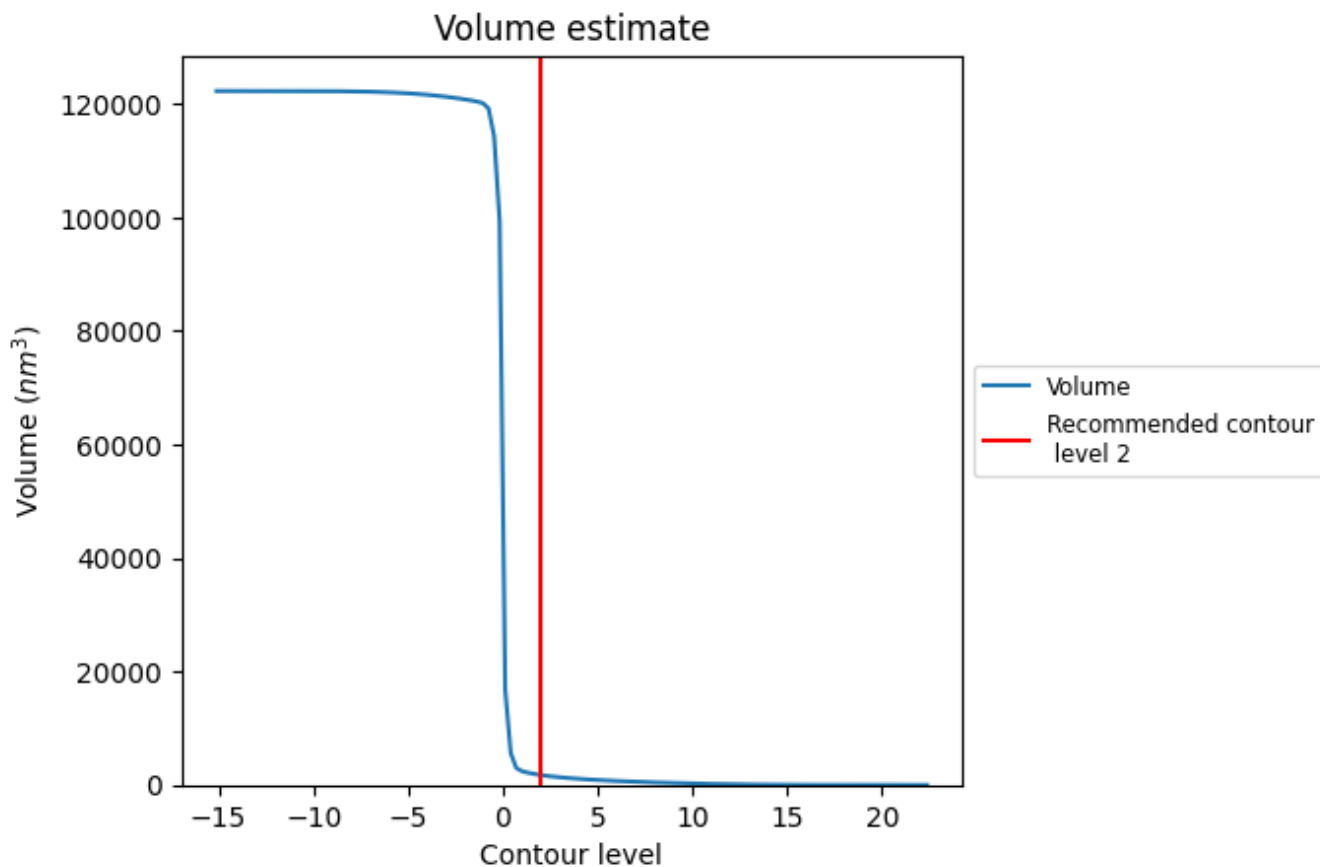
This section contains the results of statistical analysis of the map.

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.

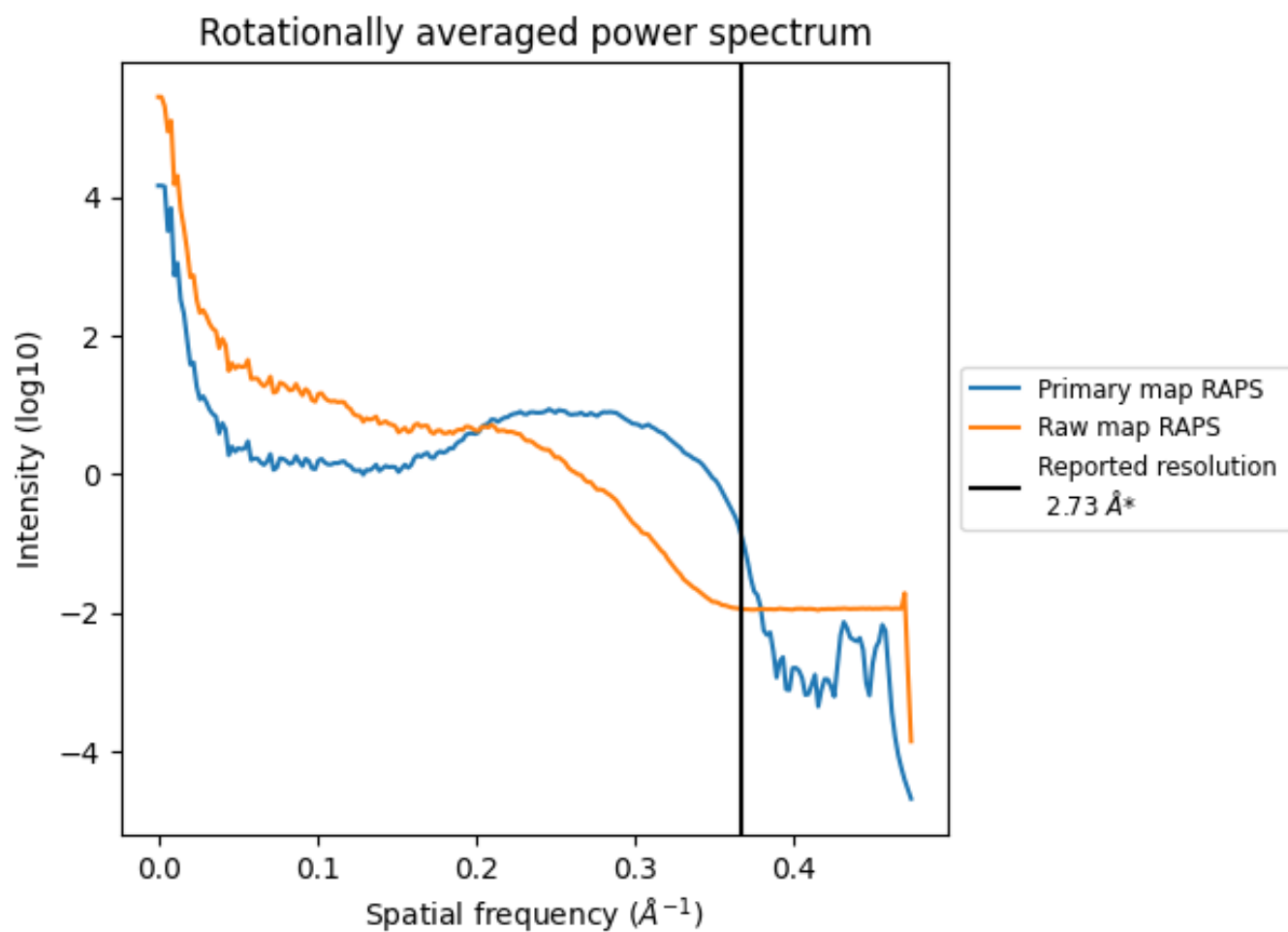
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1746 nm^3 ; this corresponds to an approximate mass of 1577 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

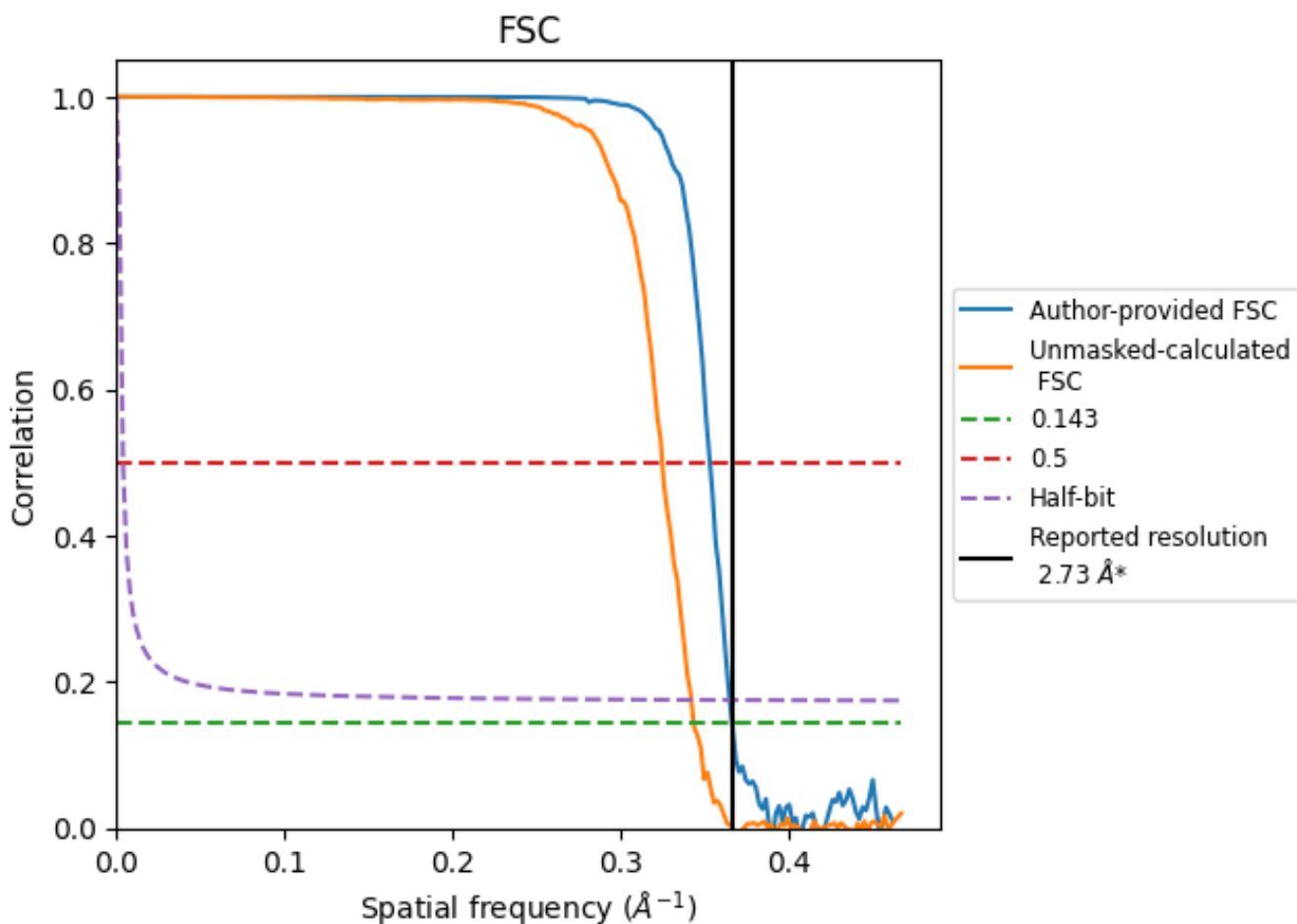


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 0.366 Å⁻¹

8.2 Resolution estimates [i](#)

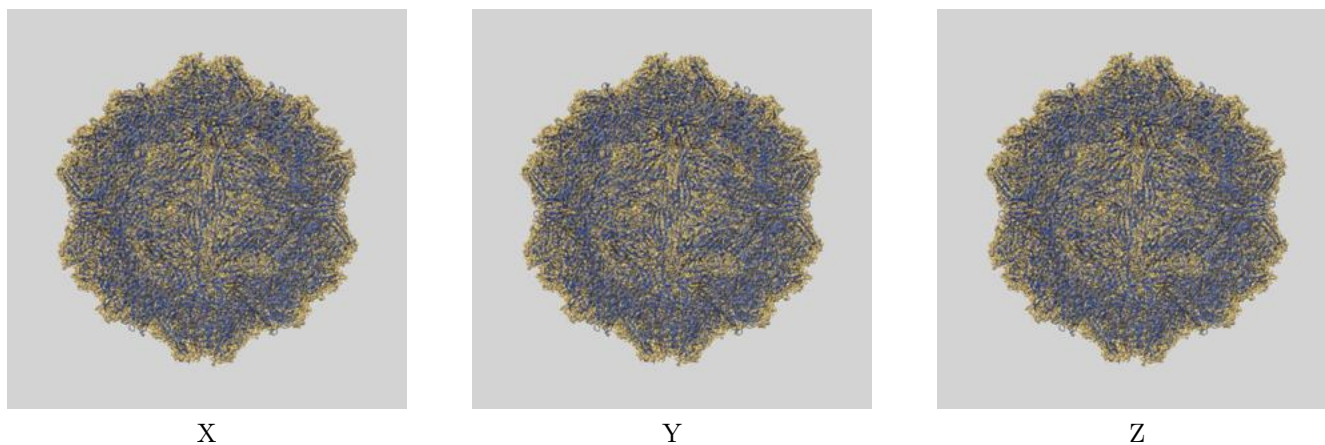
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	2.83	2.74
Unmasked-calculated*	2.91	3.08	2.92

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

9 Map-model fit [i](#)

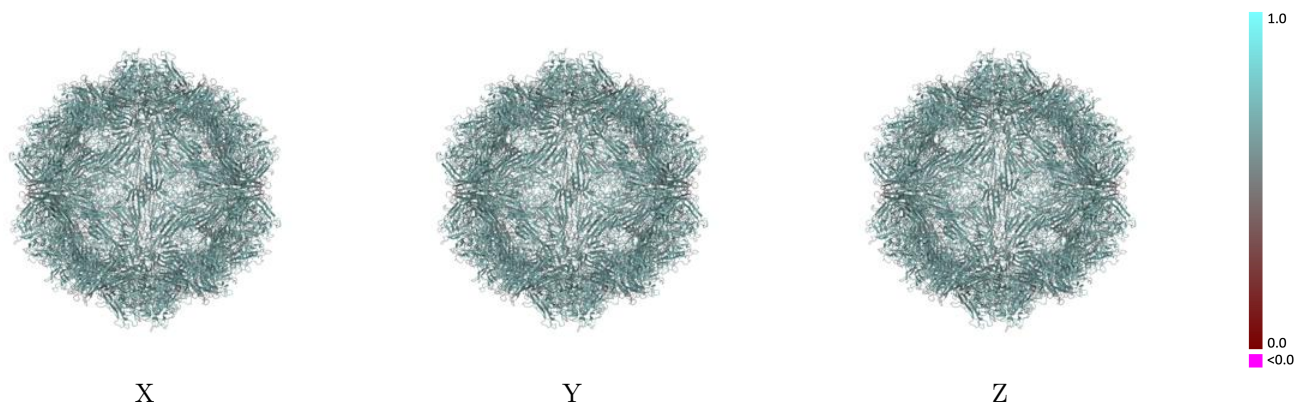
This section contains information regarding the fit between EMDB map EMD-45973 and PDB model 9CWS. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



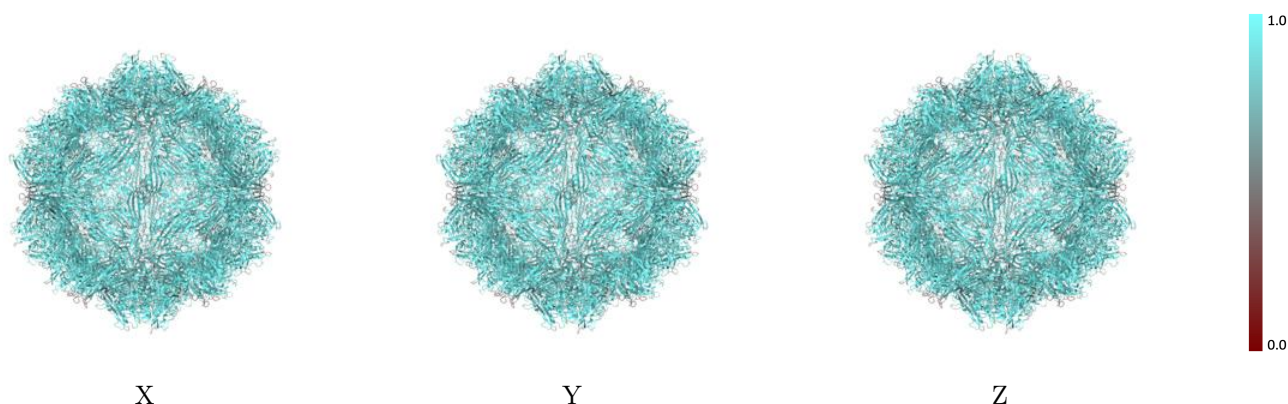
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



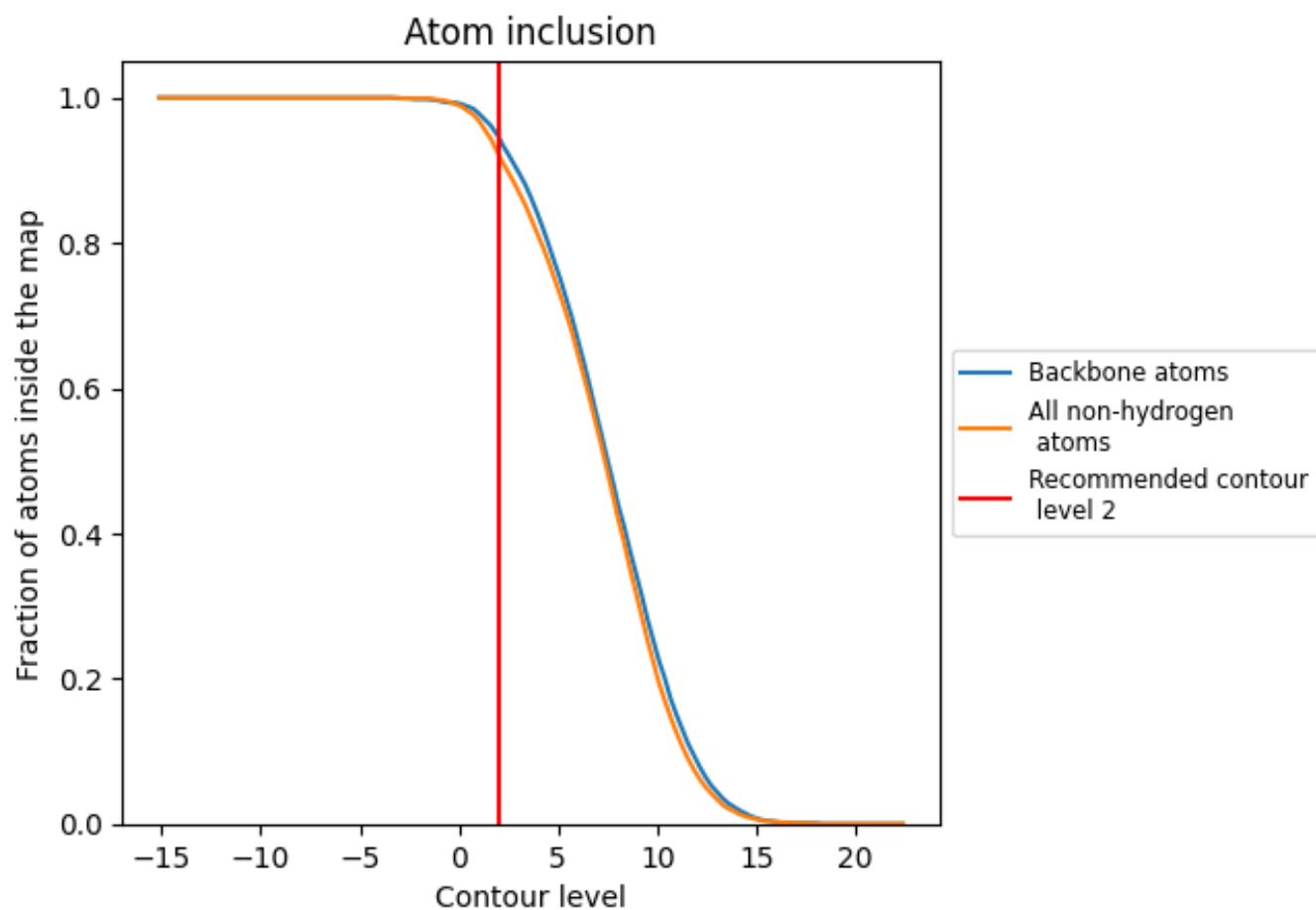
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9210	 0.6270
1	 0.9200	 0.6260
2	 0.9200	 0.6260
3	 0.9210	 0.6270
4	 0.9220	 0.6270
5	 0.9210	 0.6270
6	 0.9210	 0.6270
7	 0.9210	 0.6270
8	 0.9230	 0.6270
A	 0.9210	 0.6280
B	 0.9200	 0.6260
C	 0.9220	 0.6270
D	 0.9210	 0.6270
E	 0.9230	 0.6270
F	 0.9210	 0.6270
G	 0.9230	 0.6270
H	 0.9210	 0.6270
I	 0.9220	 0.6280
J	 0.9200	 0.6260
K	 0.9220	 0.6270
L	 0.9200	 0.6270
M	 0.9230	 0.6270
N	 0.9210	 0.6270
O	 0.9230	 0.6270
P	 0.9210	 0.6280
Q	 0.9220	 0.6270
R	 0.9200	 0.6260
S	 0.9200	 0.6260
T	 0.9220	 0.6280
U	 0.9200	 0.6270
V	 0.9220	 0.6280
W	 0.9210	 0.6280
X	 0.9230	 0.6270
Y	 0.9210	 0.6270
Z	 0.9230	 0.6270



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Chain	Atom inclusion	Q-score
a	 0.9210	 0.6270
b	 0.9210	 0.6270
c	 0.9210	 0.6270
d	 0.9210	 0.6270
e	 0.9210	 0.6270
f	 0.9210	 0.6270
g	 0.9220	 0.6280
h	 0.9230	 0.6270
i	 0.9210	 0.6270
j	 0.9210	 0.6270
k	 0.9210	 0.6280
l	 0.9230	 0.6270
m	 0.9220	 0.6280
n	 0.9210	 0.6270
o	 0.9230	 0.6260
p	 0.9220	 0.6270
q	 0.9200	 0.6260
r	 0.9200	 0.6270
s	 0.9200	 0.6260
t	 0.9230	 0.6270
u	 0.9220	 0.6270
v	 0.9210	 0.6260
w	 0.9230	 0.6260
x	 0.9220	 0.6270
y	 0.9210	 0.6270
z	 0.9190	 0.6270