



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2024 – 02:53 PM EDT

PDB ID : 6U3Q
EMDB ID : EMD-20630
Title : The atomic structure of a human adeno-associated virus capsid isolate (AAVhu69/AAVv66)
Authors : Hsu, H.-L.; Brown, A.; Loveland, A.; Tai, P.; Korostelev, A.; Gao, G.
Deposited on : 2019-08-22
Resolution : 2.46 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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:

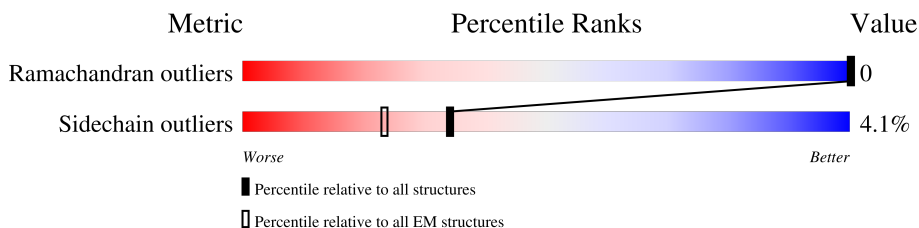
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













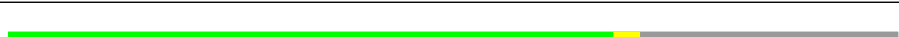


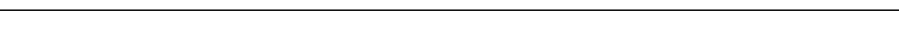
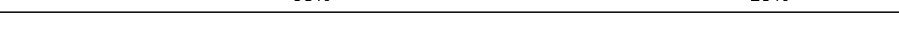
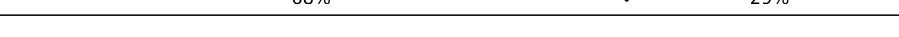



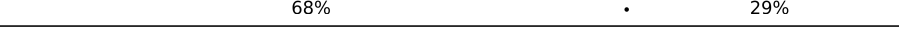





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain	
1	0	735	68%	29%
1	1	735	68%	29%
1	2	735	68%	29%
1	3	735	68%	29%
1	4	735	68%	29%
1	5	735	68%	29%
1	6	735	68%	29%
1	7	735	68%	29%
1	A	735	68%	29%


























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


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Mol	Chain	Length	Quality of chain
1	a	735	 68% 29%
1	b	735	 68% 29%
1	c	735	 68% 29%
1	d	735	 68% 29%
1	e	735	 68% 29%
1	f	735	 68% 29%
1	g	735	 68% 29%
1	h	735	 68% 29%
1	i	735	 68% 29%
1	j	735	 68% 29%
1	k	735	 68% 29%
1	l	735	 68% 29%
1	m	735	 68% 29%
1	n	735	 68% 29%
1	o	735	 68% 29%
1	p	735	 68% 29%
1	q	735	 68% 29%
1	r	735	 68% 29%
1	s	735	 68% 29%
1	t	735	 68% 29%
1	u	735	 68% 29%
1	v	735	 68% 29%
1	w	735	 68% 29%
1	x	735	 68% 29%
1	y	735	 68% 29%

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Mol	Chain	Length	Quality of chain
1	z	735	 68% 29%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 248280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	519	4138	2605	716	803	14	0	0
1	K	519	4138	2605	716	803	14	0	0
1	L	519	4138	2605	716	803	14	0	0
1	M	519	4138	2605	716	803	14	0	0
1	N	519	4138	2605	716	803	14	0	0
1	O	519	4138	2605	716	803	14	0	0
1	P	519	4138	2605	716	803	14	0	0
1	Q	519	4138	2605	716	803	14	0	0
1	R	519	4138	2605	716	803	14	0	0
1	S	519	4138	2605	716	803	14	0	0
1	T	519	4138	2605	716	803	14	0	0
1	B	519	4138	2605	716	803	14	0	0
1	U	519	4138	2605	716	803	14	0	0
1	V	519	4138	2605	716	803	14	0	0
1	W	519	4138	2605	716	803	14	0	0
1	X	519	4138	2605	716	803	14	0	0
1	Y	519	4138	2605	716	803	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	a	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	b	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	c	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	d	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	C	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	e	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	f	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	g	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	h	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	i	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	j	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	k	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	l	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	m	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	n	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	D	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	o	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	p	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	q	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	r	519	Total 4138	C 2605	N 716	O 803	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	s	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	t	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	u	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	v	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	w	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	x	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	E	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	y	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	z	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	0	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	1	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	2	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	3	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	4	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	5	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	6	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	7	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	F	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	G	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	H	519	Total 4138	C 2605	N 716	O 803	S 14	0	0
1	I	519	Total 4138	C 2605	N 716	O 803	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	519	4138	2605	716	803	14	0	0

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLN	LYS	conflict	UNP Q670R6
A	164	GLN	ASN	conflict	UNP Q670R6
A	312	ASN	SER	conflict	UNP Q670R6
A	447	LYS	ARG	conflict	UNP Q670R6
A	450	ALA	THR	conflict	UNP Q670R6
A	593	THR	SER	conflict	UNP Q670R6
K	39	GLN	LYS	conflict	UNP Q670R6
K	164	GLN	ASN	conflict	UNP Q670R6
K	312	ASN	SER	conflict	UNP Q670R6
K	447	LYS	ARG	conflict	UNP Q670R6
K	450	ALA	THR	conflict	UNP Q670R6
K	593	THR	SER	conflict	UNP Q670R6
L	39	GLN	LYS	conflict	UNP Q670R6
L	164	GLN	ASN	conflict	UNP Q670R6
L	312	ASN	SER	conflict	UNP Q670R6
L	447	LYS	ARG	conflict	UNP Q670R6
L	450	ALA	THR	conflict	UNP Q670R6
L	593	THR	SER	conflict	UNP Q670R6
M	39	GLN	LYS	conflict	UNP Q670R6
M	164	GLN	ASN	conflict	UNP Q670R6
M	312	ASN	SER	conflict	UNP Q670R6
M	447	LYS	ARG	conflict	UNP Q670R6
M	450	ALA	THR	conflict	UNP Q670R6
M	593	THR	SER	conflict	UNP Q670R6
N	39	GLN	LYS	conflict	UNP Q670R6
N	164	GLN	ASN	conflict	UNP Q670R6
N	312	ASN	SER	conflict	UNP Q670R6
N	447	LYS	ARG	conflict	UNP Q670R6
N	450	ALA	THR	conflict	UNP Q670R6
N	593	THR	SER	conflict	UNP Q670R6
O	39	GLN	LYS	conflict	UNP Q670R6
O	164	GLN	ASN	conflict	UNP Q670R6
O	312	ASN	SER	conflict	UNP Q670R6
O	447	LYS	ARG	conflict	UNP Q670R6
O	450	ALA	THR	conflict	UNP Q670R6
O	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
P	39	GLN	LYS	conflict	UNP Q670R6
P	164	GLN	ASN	conflict	UNP Q670R6
P	312	ASN	SER	conflict	UNP Q670R6
P	447	LYS	ARG	conflict	UNP Q670R6
P	450	ALA	THR	conflict	UNP Q670R6
P	593	THR	SER	conflict	UNP Q670R6
Q	39	GLN	LYS	conflict	UNP Q670R6
Q	164	GLN	ASN	conflict	UNP Q670R6
Q	312	ASN	SER	conflict	UNP Q670R6
Q	447	LYS	ARG	conflict	UNP Q670R6
Q	450	ALA	THR	conflict	UNP Q670R6
Q	593	THR	SER	conflict	UNP Q670R6
R	39	GLN	LYS	conflict	UNP Q670R6
R	164	GLN	ASN	conflict	UNP Q670R6
R	312	ASN	SER	conflict	UNP Q670R6
R	447	LYS	ARG	conflict	UNP Q670R6
R	450	ALA	THR	conflict	UNP Q670R6
R	593	THR	SER	conflict	UNP Q670R6
S	39	GLN	LYS	conflict	UNP Q670R6
S	164	GLN	ASN	conflict	UNP Q670R6
S	312	ASN	SER	conflict	UNP Q670R6
S	447	LYS	ARG	conflict	UNP Q670R6
S	450	ALA	THR	conflict	UNP Q670R6
S	593	THR	SER	conflict	UNP Q670R6
T	39	GLN	LYS	conflict	UNP Q670R6
T	164	GLN	ASN	conflict	UNP Q670R6
T	312	ASN	SER	conflict	UNP Q670R6
T	447	LYS	ARG	conflict	UNP Q670R6
T	450	ALA	THR	conflict	UNP Q670R6
T	593	THR	SER	conflict	UNP Q670R6
B	39	GLN	LYS	conflict	UNP Q670R6
B	164	GLN	ASN	conflict	UNP Q670R6
B	312	ASN	SER	conflict	UNP Q670R6
B	447	LYS	ARG	conflict	UNP Q670R6
B	450	ALA	THR	conflict	UNP Q670R6
B	593	THR	SER	conflict	UNP Q670R6
U	39	GLN	LYS	conflict	UNP Q670R6
U	164	GLN	ASN	conflict	UNP Q670R6
U	312	ASN	SER	conflict	UNP Q670R6
U	447	LYS	ARG	conflict	UNP Q670R6
U	450	ALA	THR	conflict	UNP Q670R6
U	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
V	39	GLN	LYS	conflict	UNP Q670R6
V	164	GLN	ASN	conflict	UNP Q670R6
V	312	ASN	SER	conflict	UNP Q670R6
V	447	LYS	ARG	conflict	UNP Q670R6
V	450	ALA	THR	conflict	UNP Q670R6
V	593	THR	SER	conflict	UNP Q670R6
W	39	GLN	LYS	conflict	UNP Q670R6
W	164	GLN	ASN	conflict	UNP Q670R6
W	312	ASN	SER	conflict	UNP Q670R6
W	447	LYS	ARG	conflict	UNP Q670R6
W	450	ALA	THR	conflict	UNP Q670R6
W	593	THR	SER	conflict	UNP Q670R6
X	39	GLN	LYS	conflict	UNP Q670R6
X	164	GLN	ASN	conflict	UNP Q670R6
X	312	ASN	SER	conflict	UNP Q670R6
X	447	LYS	ARG	conflict	UNP Q670R6
X	450	ALA	THR	conflict	UNP Q670R6
X	593	THR	SER	conflict	UNP Q670R6
Y	39	GLN	LYS	conflict	UNP Q670R6
Y	164	GLN	ASN	conflict	UNP Q670R6
Y	312	ASN	SER	conflict	UNP Q670R6
Y	447	LYS	ARG	conflict	UNP Q670R6
Y	450	ALA	THR	conflict	UNP Q670R6
Y	593	THR	SER	conflict	UNP Q670R6
Z	39	GLN	LYS	conflict	UNP Q670R6
Z	164	GLN	ASN	conflict	UNP Q670R6
Z	312	ASN	SER	conflict	UNP Q670R6
Z	447	LYS	ARG	conflict	UNP Q670R6
Z	450	ALA	THR	conflict	UNP Q670R6
Z	593	THR	SER	conflict	UNP Q670R6
a	39	GLN	LYS	conflict	UNP Q670R6
a	164	GLN	ASN	conflict	UNP Q670R6
a	312	ASN	SER	conflict	UNP Q670R6
a	447	LYS	ARG	conflict	UNP Q670R6
a	450	ALA	THR	conflict	UNP Q670R6
a	593	THR	SER	conflict	UNP Q670R6
b	39	GLN	LYS	conflict	UNP Q670R6
b	164	GLN	ASN	conflict	UNP Q670R6
b	312	ASN	SER	conflict	UNP Q670R6
b	447	LYS	ARG	conflict	UNP Q670R6
b	450	ALA	THR	conflict	UNP Q670R6
b	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
c	39	GLN	LYS	conflict	UNP Q670R6
c	164	GLN	ASN	conflict	UNP Q670R6
c	312	ASN	SER	conflict	UNP Q670R6
c	447	LYS	ARG	conflict	UNP Q670R6
c	450	ALA	THR	conflict	UNP Q670R6
c	593	THR	SER	conflict	UNP Q670R6
d	39	GLN	LYS	conflict	UNP Q670R6
d	164	GLN	ASN	conflict	UNP Q670R6
d	312	ASN	SER	conflict	UNP Q670R6
d	447	LYS	ARG	conflict	UNP Q670R6
d	450	ALA	THR	conflict	UNP Q670R6
d	593	THR	SER	conflict	UNP Q670R6
C	39	GLN	LYS	conflict	UNP Q670R6
C	164	GLN	ASN	conflict	UNP Q670R6
C	312	ASN	SER	conflict	UNP Q670R6
C	447	LYS	ARG	conflict	UNP Q670R6
C	450	ALA	THR	conflict	UNP Q670R6
C	593	THR	SER	conflict	UNP Q670R6
e	39	GLN	LYS	conflict	UNP Q670R6
e	164	GLN	ASN	conflict	UNP Q670R6
e	312	ASN	SER	conflict	UNP Q670R6
e	447	LYS	ARG	conflict	UNP Q670R6
e	450	ALA	THR	conflict	UNP Q670R6
e	593	THR	SER	conflict	UNP Q670R6
f	39	GLN	LYS	conflict	UNP Q670R6
f	164	GLN	ASN	conflict	UNP Q670R6
f	312	ASN	SER	conflict	UNP Q670R6
f	447	LYS	ARG	conflict	UNP Q670R6
f	450	ALA	THR	conflict	UNP Q670R6
f	593	THR	SER	conflict	UNP Q670R6
g	39	GLN	LYS	conflict	UNP Q670R6
g	164	GLN	ASN	conflict	UNP Q670R6
g	312	ASN	SER	conflict	UNP Q670R6
g	447	LYS	ARG	conflict	UNP Q670R6
g	450	ALA	THR	conflict	UNP Q670R6
g	593	THR	SER	conflict	UNP Q670R6
h	39	GLN	LYS	conflict	UNP Q670R6
h	164	GLN	ASN	conflict	UNP Q670R6
h	312	ASN	SER	conflict	UNP Q670R6
h	447	LYS	ARG	conflict	UNP Q670R6
h	450	ALA	THR	conflict	UNP Q670R6
h	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
i	39	GLN	LYS	conflict	UNP Q670R6
i	164	GLN	ASN	conflict	UNP Q670R6
i	312	ASN	SER	conflict	UNP Q670R6
i	447	LYS	ARG	conflict	UNP Q670R6
i	450	ALA	THR	conflict	UNP Q670R6
i	593	THR	SER	conflict	UNP Q670R6
j	39	GLN	LYS	conflict	UNP Q670R6
j	164	GLN	ASN	conflict	UNP Q670R6
j	312	ASN	SER	conflict	UNP Q670R6
j	447	LYS	ARG	conflict	UNP Q670R6
j	450	ALA	THR	conflict	UNP Q670R6
j	593	THR	SER	conflict	UNP Q670R6
k	39	GLN	LYS	conflict	UNP Q670R6
k	164	GLN	ASN	conflict	UNP Q670R6
k	312	ASN	SER	conflict	UNP Q670R6
k	447	LYS	ARG	conflict	UNP Q670R6
k	450	ALA	THR	conflict	UNP Q670R6
k	593	THR	SER	conflict	UNP Q670R6
l	39	GLN	LYS	conflict	UNP Q670R6
l	164	GLN	ASN	conflict	UNP Q670R6
l	312	ASN	SER	conflict	UNP Q670R6
l	447	LYS	ARG	conflict	UNP Q670R6
l	450	ALA	THR	conflict	UNP Q670R6
l	593	THR	SER	conflict	UNP Q670R6
m	39	GLN	LYS	conflict	UNP Q670R6
m	164	GLN	ASN	conflict	UNP Q670R6
m	312	ASN	SER	conflict	UNP Q670R6
m	447	LYS	ARG	conflict	UNP Q670R6
m	450	ALA	THR	conflict	UNP Q670R6
m	593	THR	SER	conflict	UNP Q670R6
n	39	GLN	LYS	conflict	UNP Q670R6
n	164	GLN	ASN	conflict	UNP Q670R6
n	312	ASN	SER	conflict	UNP Q670R6
n	447	LYS	ARG	conflict	UNP Q670R6
n	450	ALA	THR	conflict	UNP Q670R6
n	593	THR	SER	conflict	UNP Q670R6
D	39	GLN	LYS	conflict	UNP Q670R6
D	164	GLN	ASN	conflict	UNP Q670R6
D	312	ASN	SER	conflict	UNP Q670R6
D	447	LYS	ARG	conflict	UNP Q670R6
D	450	ALA	THR	conflict	UNP Q670R6
D	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
o	39	GLN	LYS	conflict	UNP Q670R6
o	164	GLN	ASN	conflict	UNP Q670R6
o	312	ASN	SER	conflict	UNP Q670R6
o	447	LYS	ARG	conflict	UNP Q670R6
o	450	ALA	THR	conflict	UNP Q670R6
o	593	THR	SER	conflict	UNP Q670R6
p	39	GLN	LYS	conflict	UNP Q670R6
p	164	GLN	ASN	conflict	UNP Q670R6
p	312	ASN	SER	conflict	UNP Q670R6
p	447	LYS	ARG	conflict	UNP Q670R6
p	450	ALA	THR	conflict	UNP Q670R6
p	593	THR	SER	conflict	UNP Q670R6
q	39	GLN	LYS	conflict	UNP Q670R6
q	164	GLN	ASN	conflict	UNP Q670R6
q	312	ASN	SER	conflict	UNP Q670R6
q	447	LYS	ARG	conflict	UNP Q670R6
q	450	ALA	THR	conflict	UNP Q670R6
q	593	THR	SER	conflict	UNP Q670R6
r	39	GLN	LYS	conflict	UNP Q670R6
r	164	GLN	ASN	conflict	UNP Q670R6
r	312	ASN	SER	conflict	UNP Q670R6
r	447	LYS	ARG	conflict	UNP Q670R6
r	450	ALA	THR	conflict	UNP Q670R6
r	593	THR	SER	conflict	UNP Q670R6
s	39	GLN	LYS	conflict	UNP Q670R6
s	164	GLN	ASN	conflict	UNP Q670R6
s	312	ASN	SER	conflict	UNP Q670R6
s	447	LYS	ARG	conflict	UNP Q670R6
s	450	ALA	THR	conflict	UNP Q670R6
s	593	THR	SER	conflict	UNP Q670R6
t	39	GLN	LYS	conflict	UNP Q670R6
t	164	GLN	ASN	conflict	UNP Q670R6
t	312	ASN	SER	conflict	UNP Q670R6
t	447	LYS	ARG	conflict	UNP Q670R6
t	450	ALA	THR	conflict	UNP Q670R6
t	593	THR	SER	conflict	UNP Q670R6
u	39	GLN	LYS	conflict	UNP Q670R6
u	164	GLN	ASN	conflict	UNP Q670R6
u	312	ASN	SER	conflict	UNP Q670R6
u	447	LYS	ARG	conflict	UNP Q670R6
u	450	ALA	THR	conflict	UNP Q670R6
u	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
v	39	GLN	LYS	conflict	UNP Q670R6
v	164	GLN	ASN	conflict	UNP Q670R6
v	312	ASN	SER	conflict	UNP Q670R6
v	447	LYS	ARG	conflict	UNP Q670R6
v	450	ALA	THR	conflict	UNP Q670R6
v	593	THR	SER	conflict	UNP Q670R6
w	39	GLN	LYS	conflict	UNP Q670R6
w	164	GLN	ASN	conflict	UNP Q670R6
w	312	ASN	SER	conflict	UNP Q670R6
w	447	LYS	ARG	conflict	UNP Q670R6
w	450	ALA	THR	conflict	UNP Q670R6
w	593	THR	SER	conflict	UNP Q670R6
x	39	GLN	LYS	conflict	UNP Q670R6
x	164	GLN	ASN	conflict	UNP Q670R6
x	312	ASN	SER	conflict	UNP Q670R6
x	447	LYS	ARG	conflict	UNP Q670R6
x	450	ALA	THR	conflict	UNP Q670R6
x	593	THR	SER	conflict	UNP Q670R6
E	39	GLN	LYS	conflict	UNP Q670R6
E	164	GLN	ASN	conflict	UNP Q670R6
E	312	ASN	SER	conflict	UNP Q670R6
E	447	LYS	ARG	conflict	UNP Q670R6
E	450	ALA	THR	conflict	UNP Q670R6
E	593	THR	SER	conflict	UNP Q670R6
y	39	GLN	LYS	conflict	UNP Q670R6
y	164	GLN	ASN	conflict	UNP Q670R6
y	312	ASN	SER	conflict	UNP Q670R6
y	447	LYS	ARG	conflict	UNP Q670R6
y	450	ALA	THR	conflict	UNP Q670R6
y	593	THR	SER	conflict	UNP Q670R6
z	39	GLN	LYS	conflict	UNP Q670R6
z	164	GLN	ASN	conflict	UNP Q670R6
z	312	ASN	SER	conflict	UNP Q670R6
z	447	LYS	ARG	conflict	UNP Q670R6
z	450	ALA	THR	conflict	UNP Q670R6
z	593	THR	SER	conflict	UNP Q670R6
0	39	GLN	LYS	conflict	UNP Q670R6
0	164	GLN	ASN	conflict	UNP Q670R6
0	312	ASN	SER	conflict	UNP Q670R6
0	447	LYS	ARG	conflict	UNP Q670R6
0	450	ALA	THR	conflict	UNP Q670R6
0	593	THR	SER	conflict	UNP Q670R6

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Chain	Residue	Modelled	Actual	Comment	Reference
1	39	GLN	LYS	conflict	UNP Q670R6
1	164	GLN	ASN	conflict	UNP Q670R6
1	312	ASN	SER	conflict	UNP Q670R6
1	447	LYS	ARG	conflict	UNP Q670R6
1	450	ALA	THR	conflict	UNP Q670R6
1	593	THR	SER	conflict	UNP Q670R6
2	39	GLN	LYS	conflict	UNP Q670R6
2	164	GLN	ASN	conflict	UNP Q670R6
2	312	ASN	SER	conflict	UNP Q670R6
2	447	LYS	ARG	conflict	UNP Q670R6
2	450	ALA	THR	conflict	UNP Q670R6
2	593	THR	SER	conflict	UNP Q670R6
3	39	GLN	LYS	conflict	UNP Q670R6
3	164	GLN	ASN	conflict	UNP Q670R6
3	312	ASN	SER	conflict	UNP Q670R6
3	447	LYS	ARG	conflict	UNP Q670R6
3	450	ALA	THR	conflict	UNP Q670R6
3	593	THR	SER	conflict	UNP Q670R6
4	39	GLN	LYS	conflict	UNP Q670R6
4	164	GLN	ASN	conflict	UNP Q670R6
4	312	ASN	SER	conflict	UNP Q670R6
4	447	LYS	ARG	conflict	UNP Q670R6
4	450	ALA	THR	conflict	UNP Q670R6
4	593	THR	SER	conflict	UNP Q670R6
5	39	GLN	LYS	conflict	UNP Q670R6
5	164	GLN	ASN	conflict	UNP Q670R6
5	312	ASN	SER	conflict	UNP Q670R6
5	447	LYS	ARG	conflict	UNP Q670R6
5	450	ALA	THR	conflict	UNP Q670R6
5	593	THR	SER	conflict	UNP Q670R6
6	39	GLN	LYS	conflict	UNP Q670R6
6	164	GLN	ASN	conflict	UNP Q670R6
6	312	ASN	SER	conflict	UNP Q670R6
6	447	LYS	ARG	conflict	UNP Q670R6
6	450	ALA	THR	conflict	UNP Q670R6
6	593	THR	SER	conflict	UNP Q670R6
7	39	GLN	LYS	conflict	UNP Q670R6
7	164	GLN	ASN	conflict	UNP Q670R6
7	312	ASN	SER	conflict	UNP Q670R6
7	447	LYS	ARG	conflict	UNP Q670R6
7	450	ALA	THR	conflict	UNP Q670R6
7	593	THR	SER	conflict	UNP Q670R6

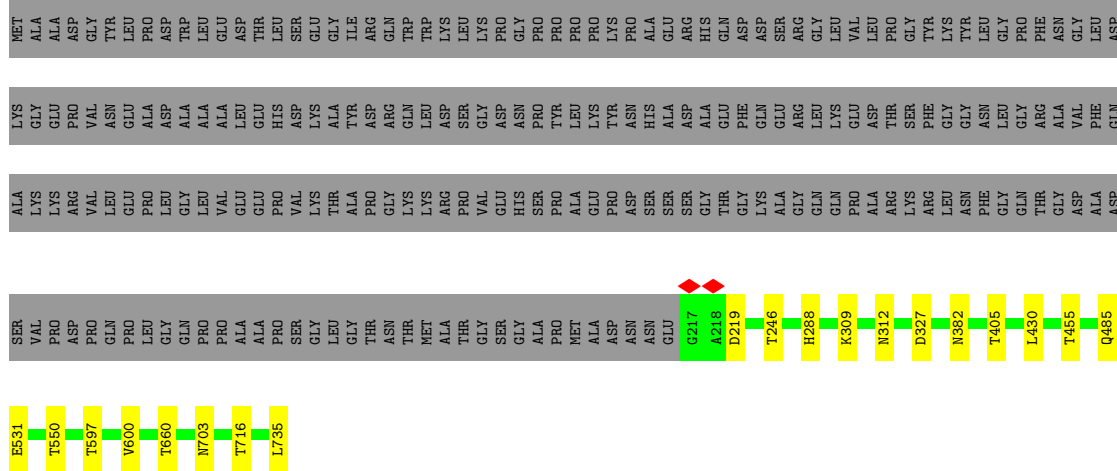
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Chain	Residue	Modelled	Actual	Comment	Reference
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F	164	GLN	ASN	conflict	UNP Q670R6
F	312	ASN	SER	conflict	UNP Q670R6
F	447	LYS	ARG	conflict	UNP Q670R6
F	450	ALA	THR	conflict	UNP Q670R6
F	593	THR	SER	conflict	UNP Q670R6
G	39	GLN	LYS	conflict	UNP Q670R6
G	164	GLN	ASN	conflict	UNP Q670R6
G	312	ASN	SER	conflict	UNP Q670R6
G	447	LYS	ARG	conflict	UNP Q670R6
G	450	ALA	THR	conflict	UNP Q670R6
G	593	THR	SER	conflict	UNP Q670R6
H	39	GLN	LYS	conflict	UNP Q670R6
H	164	GLN	ASN	conflict	UNP Q670R6
H	312	ASN	SER	conflict	UNP Q670R6
H	447	LYS	ARG	conflict	UNP Q670R6
H	450	ALA	THR	conflict	UNP Q670R6
H	593	THR	SER	conflict	UNP Q670R6
I	39	GLN	LYS	conflict	UNP Q670R6
I	164	GLN	ASN	conflict	UNP Q670R6
I	312	ASN	SER	conflict	UNP Q670R6
I	447	LYS	ARG	conflict	UNP Q670R6
I	450	ALA	THR	conflict	UNP Q670R6
I	593	THR	SER	conflict	UNP Q670R6
J	39	GLN	LYS	conflict	UNP Q670R6
J	164	GLN	ASN	conflict	UNP Q670R6
J	312	ASN	SER	conflict	UNP Q670R6
J	447	LYS	ARG	conflict	UNP Q670R6
J	450	ALA	THR	conflict	UNP Q670R6
J	593	THR	SER	conflict	UNP Q670R6



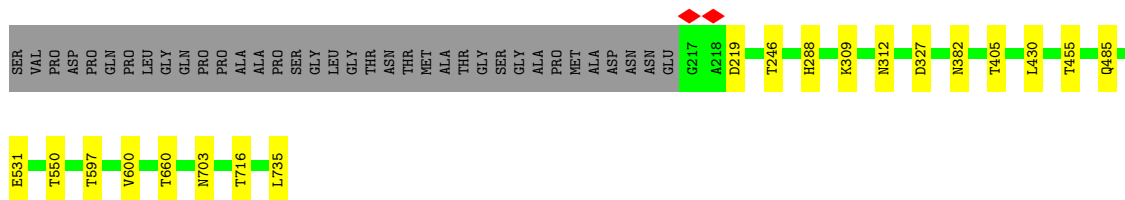
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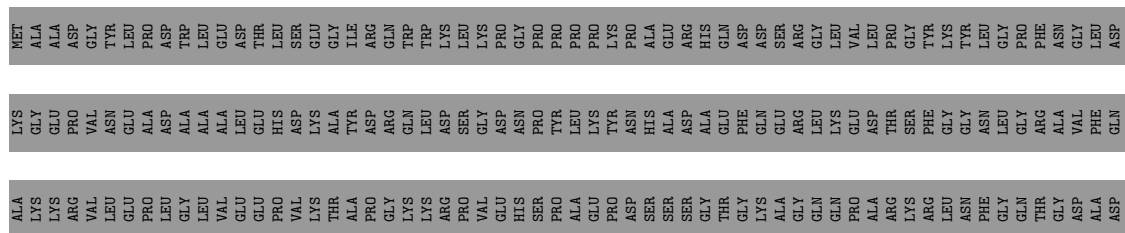
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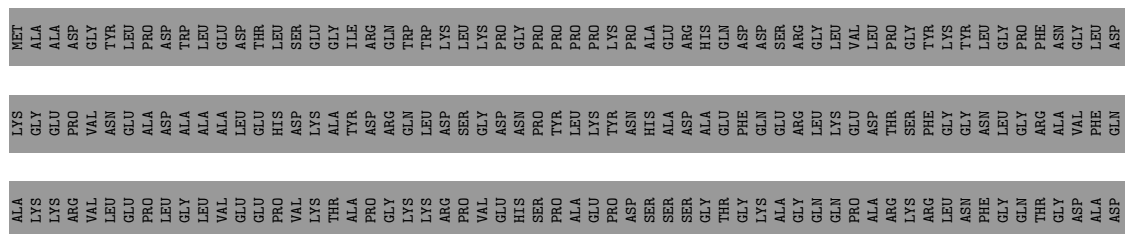
● Molecule 1: Capsid protein VP1



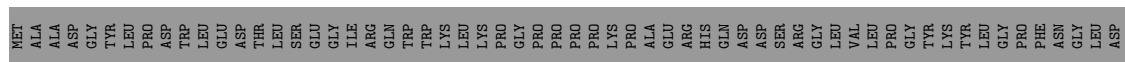
• Molecule 1: Capsid protein VP1

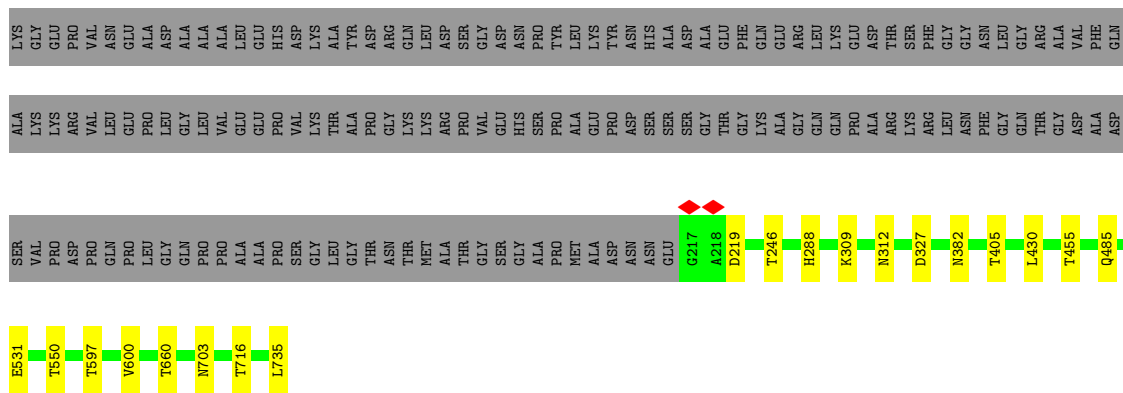


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

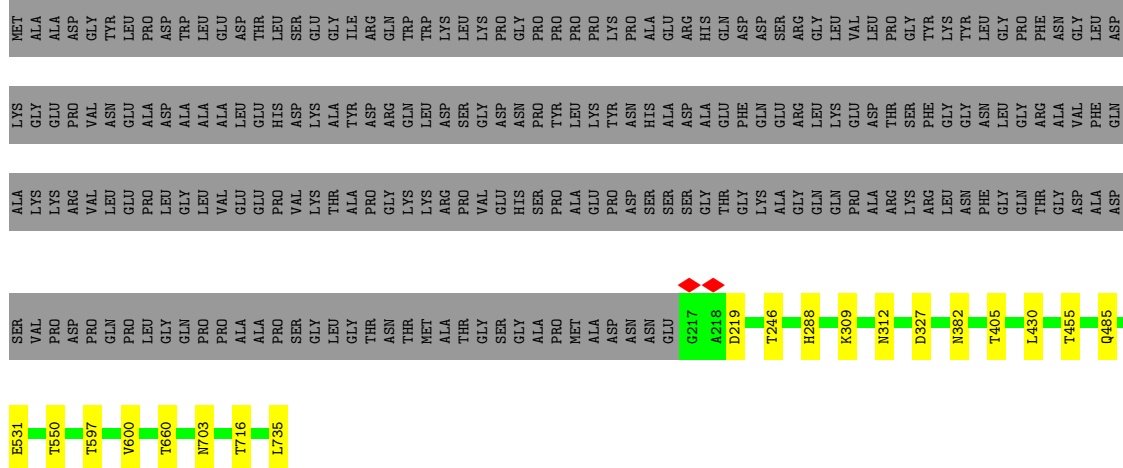




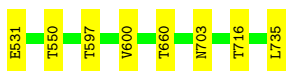
● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1

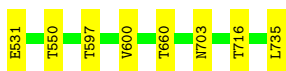
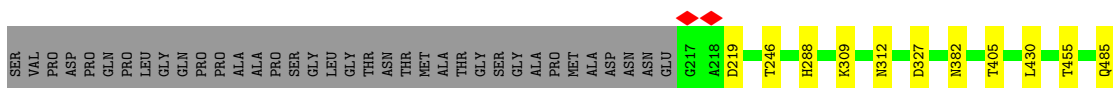
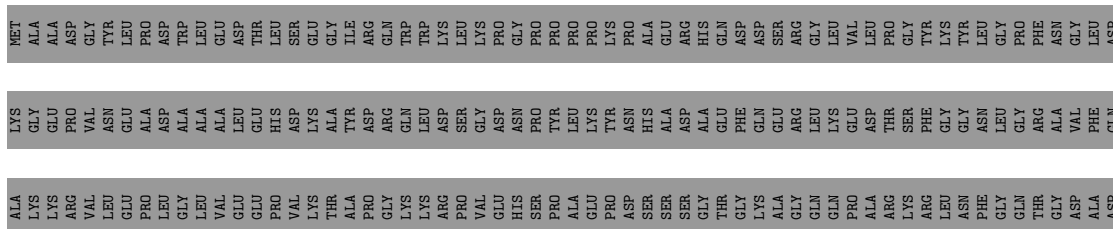


● Molecule 1: Capsid protein VP1



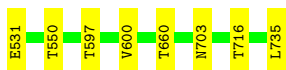
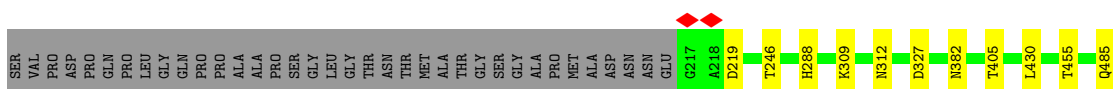
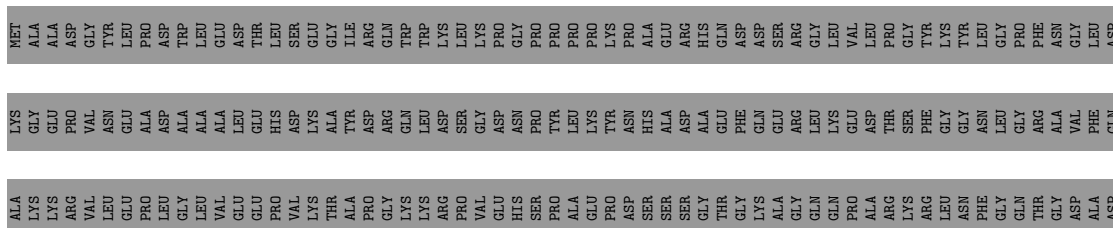
- Molecule 1: Capsid protein VP1

Chain i: 68% 29%



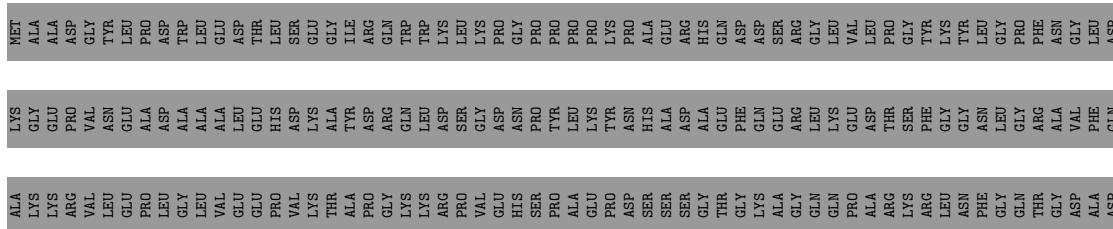
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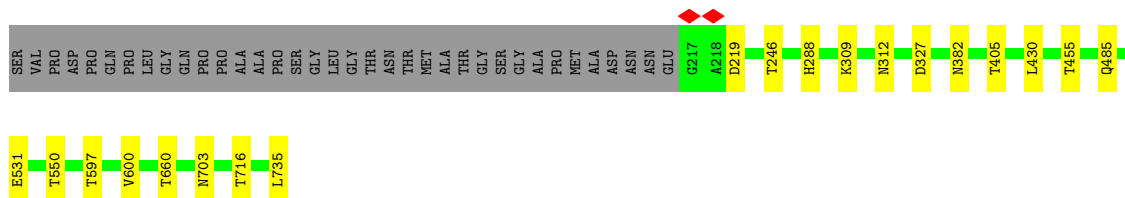
Chain j: 68% 29%



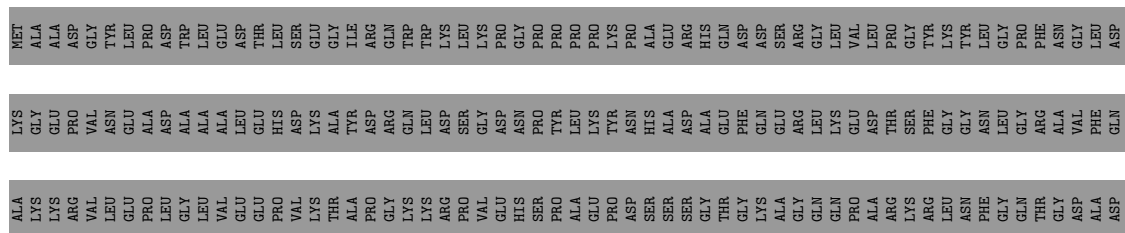
- Molecule 1: Capsid protein VP1

Chain k: 68% 29%

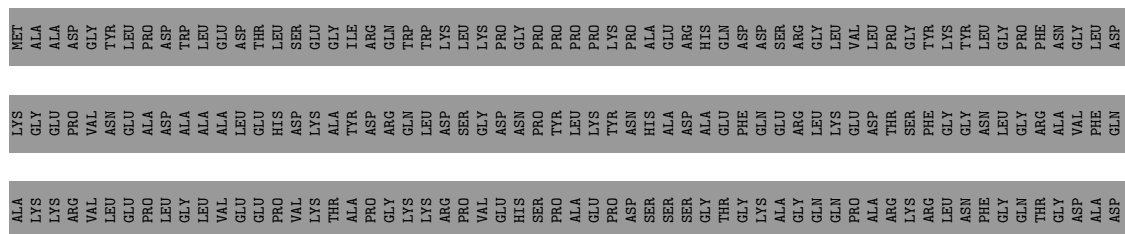




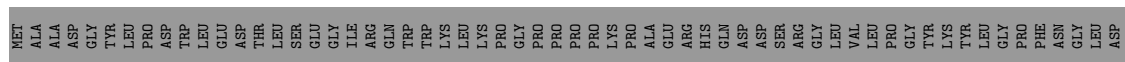
• Molecule 1: Capsid protein VP1

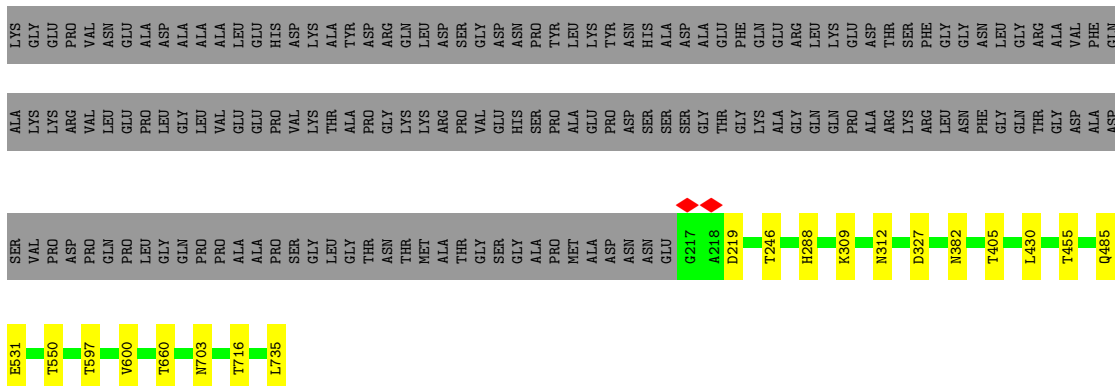


• Molecule 1: Capsid protein VP1



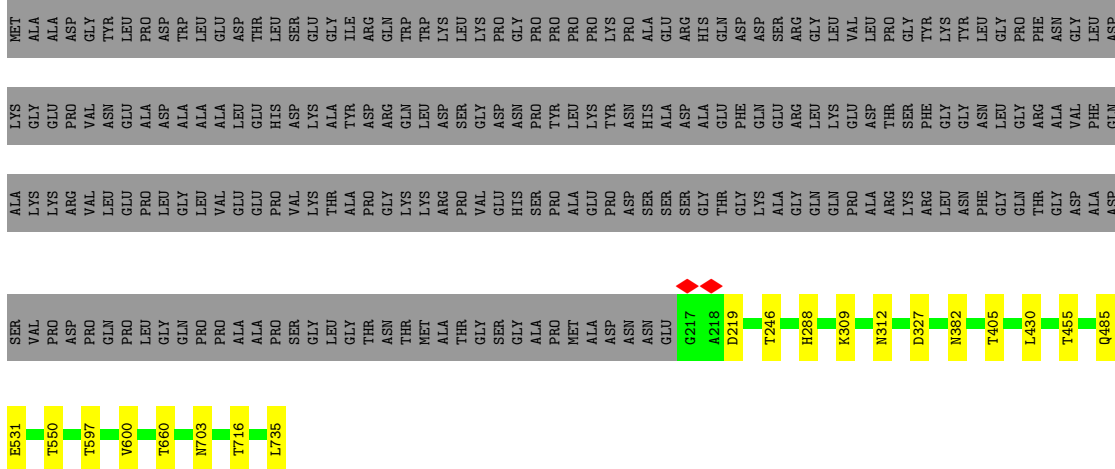
• Molecule 1: Capsid protein VP1





Molecule 1: Capsid protein VP1

Chain D: 68% 29%



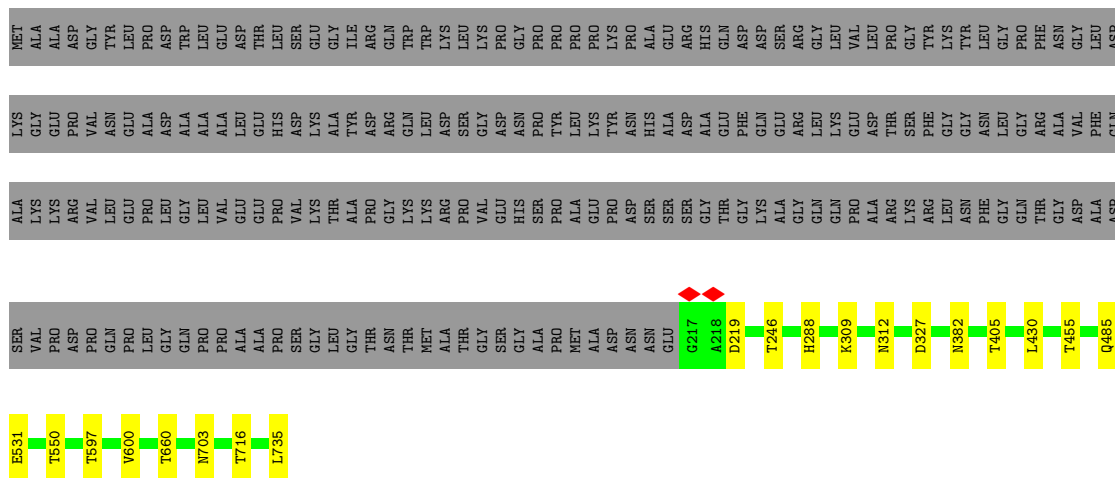
Molecule 1: Capsid protein VP1

Chain o: 68% 29%



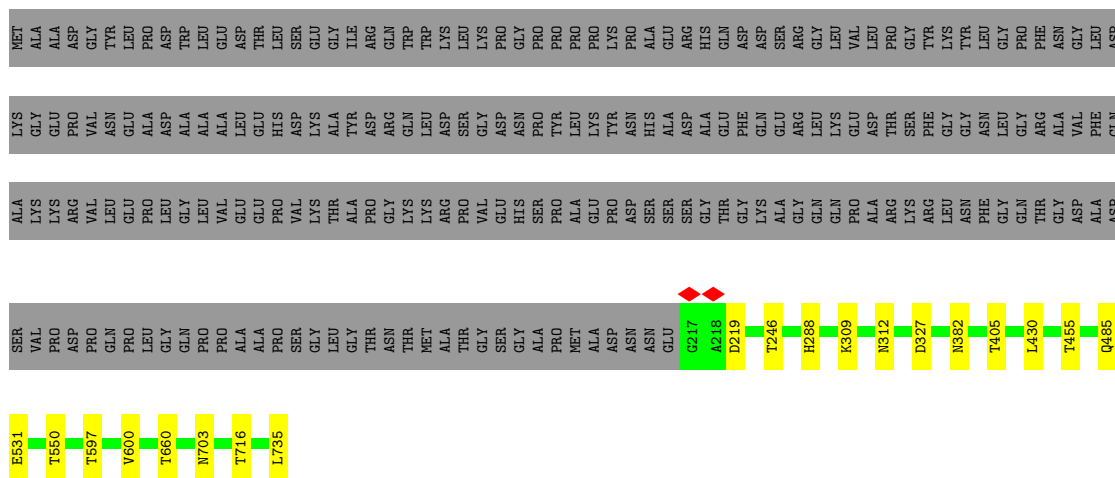
Molecule 1: Capsid protein VP1

Chain p:  68% 29%



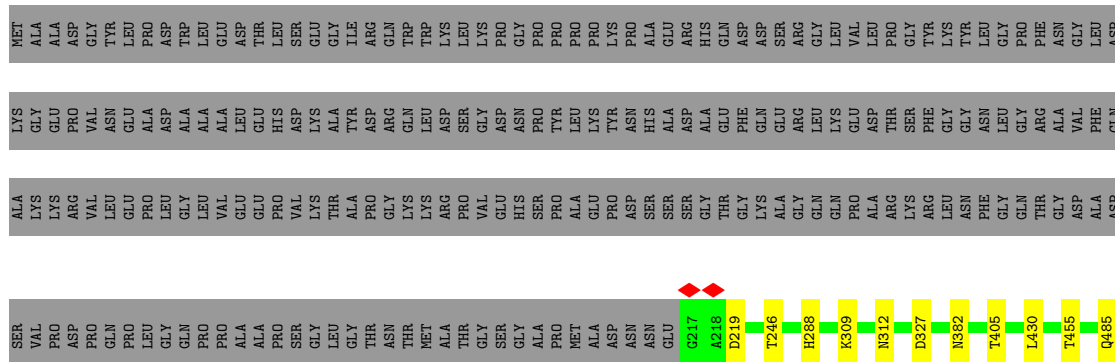
• Molecule 1: Capsid protein VP1

Chain q:  68% 29%



• Molecule 1: Capsid protein VP1

Chain r:  68% 29%





- Molecule 1: Capsid protein VP1

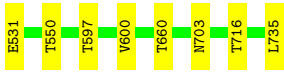
Chain s: 68% 29%

MET ALA
ALA ALA
GLY VAL
ASP ASP
TRP TYR
LEU LEU
PRO PRO
ASP ASP
TRP TRP
GLY ALA
LEU LEU
GLU VAL
ASP ASP
THR THR

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

ALA LYS
LYS LYS
ARG ARG
VAL VAL
LEU LEU
GLU GLU
PRO PRO
GLY GLY
TRP TRP
VAL VAL
GLU GLU
PRO PRO
VAL VAL
SER SER
THR THR
ALA ALA
PRO PRO
GLY GLY
LEU LEU
SER SER
ASP ASP
VAL VAL
THR THR
LEU LEU
GLY GLY
TYR TYR
ASN ASN
MET MET
LEU LEU
SER SER
THR THR
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SER VAL
PRO PRO
ASP ASP
PRO PRO
GLN GLN
LEU LEU
PRO PRO
GLY GLY
TRP TRP
GLN GLN
PRO PRO
ALA ALA
LEU LEU
GLU VAL
ALA ALA
ALA ALA
SER SER
SER SER
LEU LEU
GLY GLY
SER SER
GLY GLY
THR THR
LYS LYS
ASP ASP
GLY GLY
PRO PRO
ALA ALA
MET MET
ALA ALA
PRO PRO
ASP ASP
ASN ASN
SER SER
ALA ALA
SER SER
SER SER
GLU GLU
G217
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- Molecule 1: Capsid protein VP1

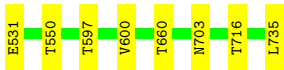
Chain t: 68% 29%

MET ALA
ALA ALA
GLY VAL
ASP ASP
TRP TYR
LEU LEU
PRO PRO
ASP ASP
TRP TRP
GLY ALA
LEU LEU
GLU VAL
ASP ASP
THR THR

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

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

SER VAL
PRO PRO
ASP ASP
PRO PRO
GLN GLN
LEU LEU
PRO PRO
GLY GLY
TRP TRP
GLN GLN
PRO PRO
ALA ALA
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GLU VAL
ALA ALA
ALA ALA
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SER SER
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THR THR
LYS LYS
ASP ASP
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PRO PRO
ALA ALA
MET MET
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PRO PRO
ASP ASP
ASN ASN
SER SER
ALA ALA
SER SER
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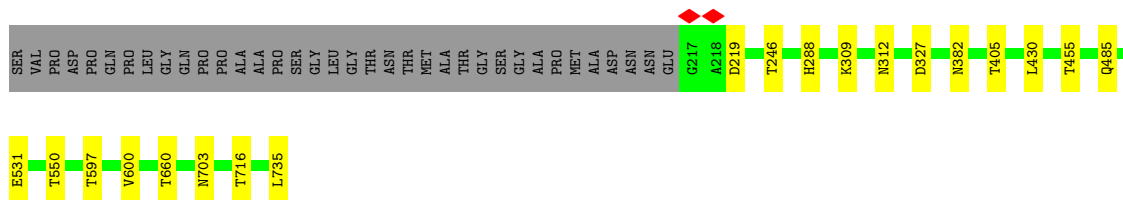
- Molecule 1: Capsid protein VP1

Chain u: 68% 29%

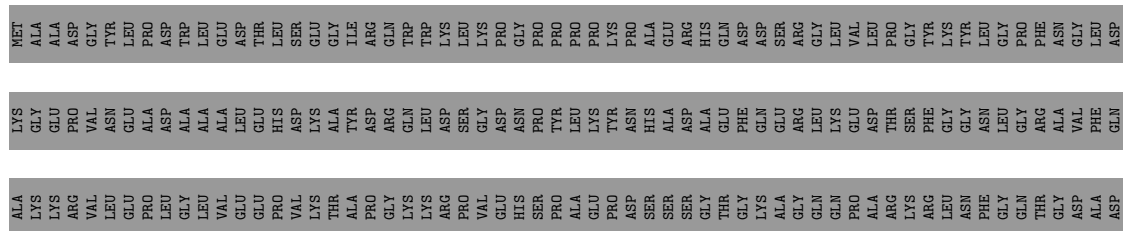
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GLY VAL
ASP ASP
TRP TYR
LEU LEU
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ASP ASP
TRP TRP
GLY ALA
LEU LEU
GLU VAL
ASP ASP
THR THR

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

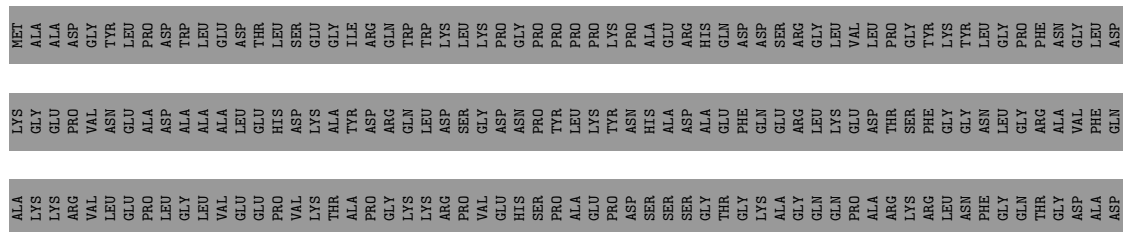
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LYS LYS
ARG ARG
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LEU LEU
GLU GLU
PRO PRO
GLY GLY
TRP TRP
VAL VAL
GLU GLU
PRO PRO
VAL VAL
SER SER
THR THR
ALA ALA
PRO PRO
GLY GLY
LEU LEU
SER SER
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ASN ASN
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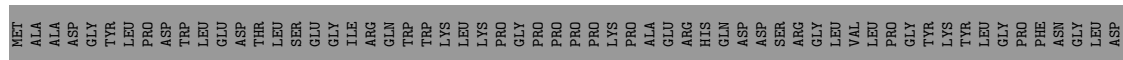
• Molecule 1: Capsid protein VP1

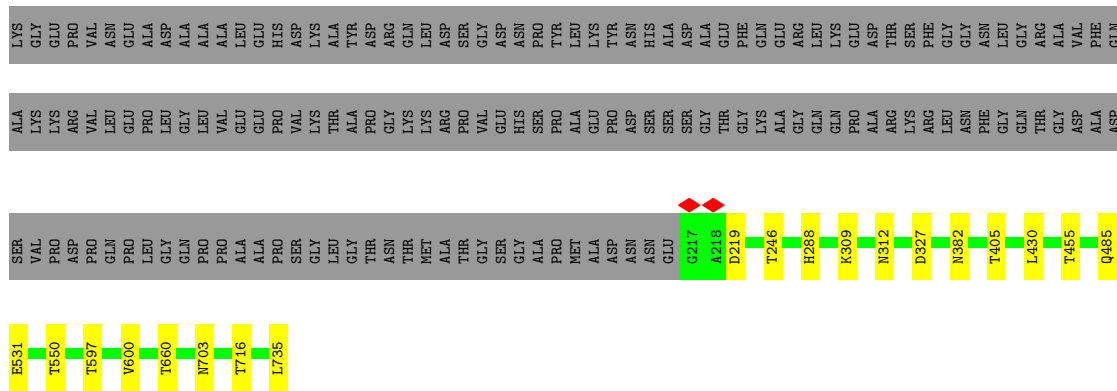


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

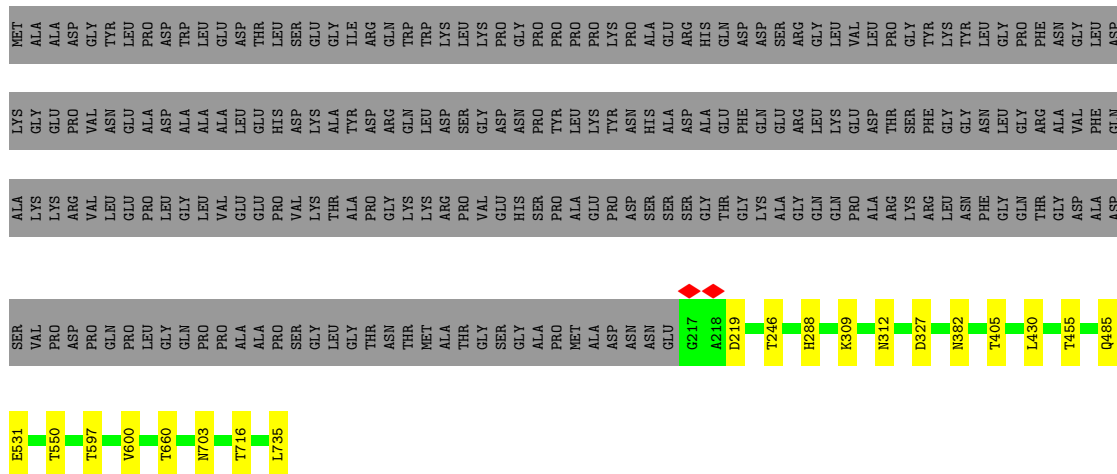




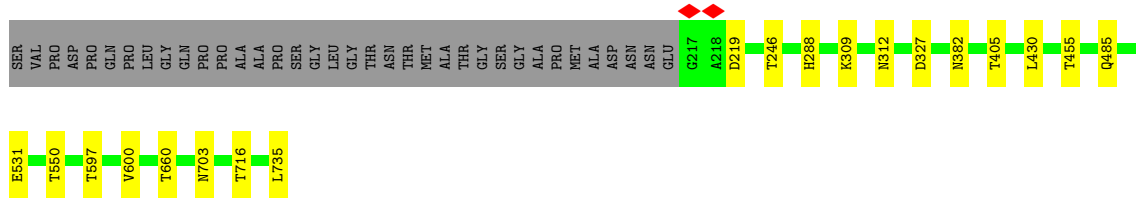
• Molecule 1: Capsid protein VP1



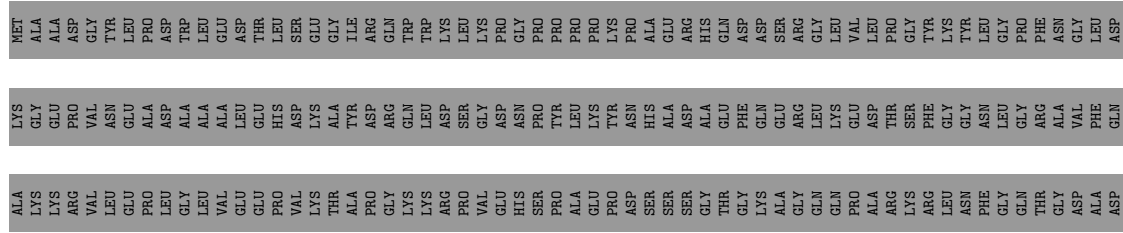
• Molecule 1: Capsid protein VP1



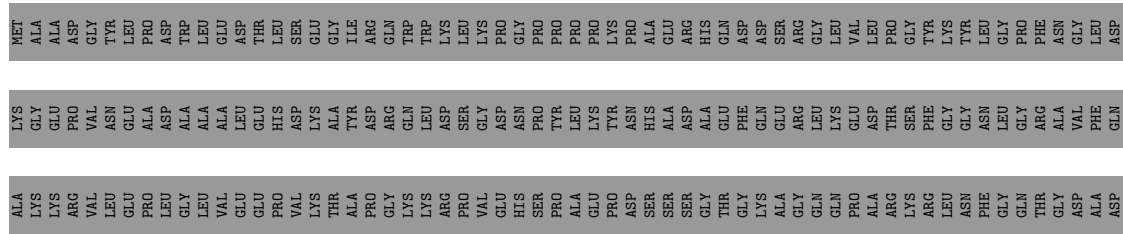
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

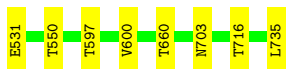


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52874	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.946	Depositor
Minimum map value	-7.268	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.6	Depositor
Map size (\AA)	609.984, 609.984, 609.984	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.059, 1.059, 1.059	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	0	0.46	0/4261	0.46	0/5811
1	1	0.46	0/4261	0.46	0/5811
1	2	0.46	0/4261	0.46	0/5811
1	3	0.46	0/4261	0.46	0/5811
1	4	0.46	0/4261	0.46	0/5811
1	5	0.46	0/4261	0.46	0/5811
1	6	0.46	0/4261	0.46	0/5811
1	7	0.46	0/4261	0.46	0/5811
1	A	0.46	0/4261	0.46	0/5811
1	B	0.46	0/4261	0.46	0/5811
1	C	0.46	0/4261	0.46	0/5811
1	D	0.46	0/4261	0.46	0/5811
1	E	0.46	0/4261	0.46	0/5811
1	F	0.46	0/4261	0.46	0/5811
1	G	0.46	0/4261	0.46	0/5811
1	H	0.46	0/4261	0.46	0/5811
1	I	0.46	0/4261	0.46	0/5811
1	J	0.46	0/4261	0.46	0/5811
1	K	0.46	0/4261	0.46	0/5811
1	L	0.46	0/4261	0.46	0/5811
1	M	0.46	0/4261	0.46	0/5811
1	N	0.46	0/4261	0.46	0/5811
1	O	0.46	0/4261	0.46	0/5811
1	P	0.46	0/4261	0.46	0/5811
1	Q	0.46	0/4261	0.46	0/5811
1	R	0.46	0/4261	0.46	0/5811
1	S	0.46	0/4261	0.46	0/5811
1	T	0.46	0/4261	0.46	0/5811
1	U	0.46	0/4261	0.46	0/5811
1	V	0.46	0/4261	0.46	0/5811
1	W	0.46	0/4261	0.46	0/5811
1	X	0.46	0/4261	0.46	0/5811
1	Y	0.46	0/4261	0.46	0/5811
1	Z	0.46	0/4261	0.46	0/5811

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.46	0/4261	0.46	0/5811
1	b	0.46	0/4261	0.46	0/5811
1	c	0.46	0/4261	0.46	0/5811
1	d	0.46	0/4261	0.46	0/5811
1	e	0.46	0/4261	0.46	0/5811
1	f	0.46	0/4261	0.46	0/5811
1	g	0.46	0/4261	0.46	0/5811
1	h	0.46	0/4261	0.46	0/5811
1	i	0.46	0/4261	0.46	0/5811
1	j	0.46	0/4261	0.46	0/5811
1	k	0.46	0/4261	0.46	0/5811
1	l	0.46	0/4261	0.46	0/5811
1	m	0.46	0/4261	0.46	0/5811
1	n	0.46	0/4261	0.46	0/5811
1	o	0.46	0/4261	0.46	0/5811
1	p	0.46	0/4261	0.46	0/5811
1	q	0.46	0/4261	0.46	0/5811
1	r	0.46	0/4261	0.46	0/5811
1	s	0.46	0/4261	0.46	0/5811
1	t	0.46	0/4261	0.46	0/5811
1	u	0.46	0/4261	0.46	0/5811
1	v	0.46	0/4261	0.46	0/5811
1	w	0.46	0/4261	0.46	0/5811
1	x	0.46	0/4261	0.46	0/5811
1	y	0.46	0/4261	0.46	0/5811
1	z	0.46	0/4261	0.46	0/5811
All	All	0.46	0/255660	0.46	0/348660

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	0	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	1	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	2	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	3	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	4	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	5	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	6	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	7	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	A	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	B	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	C	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	D	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	E	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	F	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	G	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	H	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	I	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	J	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	K	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	L	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	M	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	N	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	O	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	P	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Q	517/735 (70%)	501 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	S	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	T	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	U	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	V	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	W	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	X	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Y	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	Z	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	a	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	b	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	c	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	d	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	e	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	f	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	g	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	h	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	i	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	j	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	k	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	l	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	m	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	n	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	o	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	p	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	q	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	r	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	s	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	t	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	u	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	v	517/735 (70%)	501 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	x	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	y	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
1	z	517/735 (70%)	501 (97%)	16 (3%)	0	100	100
All	All	31020/44100 (70%)	30060 (97%)	960 (3%)	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	0	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	1	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	2	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	3	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	4	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	5	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	6	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	7	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	A	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	B	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	C	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	D	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	E	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	F	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	G	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	H	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	I	458/628 (73%)	439 (96%)	19 (4%)	30	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	K	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	L	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	M	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	N	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	O	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	P	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	Q	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	R	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	S	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	T	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	U	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	V	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	W	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	X	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	Y	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	Z	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	a	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	b	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	c	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	d	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	e	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	f	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	g	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	h	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	i	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	j	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	k	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	l	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	m	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	n	458/628 (73%)	439 (96%)	19 (4%)	30	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	p	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	q	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	r	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	s	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	t	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	u	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	v	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	w	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	x	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	y	458/628 (73%)	439 (96%)	19 (4%)	30	40
1	z	458/628 (73%)	439 (96%)	19 (4%)	30	40
All	All	27480/37680 (73%)	26340 (96%)	1140 (4%)	34	40

5 of 1140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	600	VAL
1	3	309	LYS
1	1	597	THR
1	7	600	VAL
1	c	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 858 such sidechains are listed below:

Mol	Chain	Res	Type
1	n	485	GLN
1	u	325	GLN
1	F	709	ASN
1	D	385	GLN
1	n	385	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

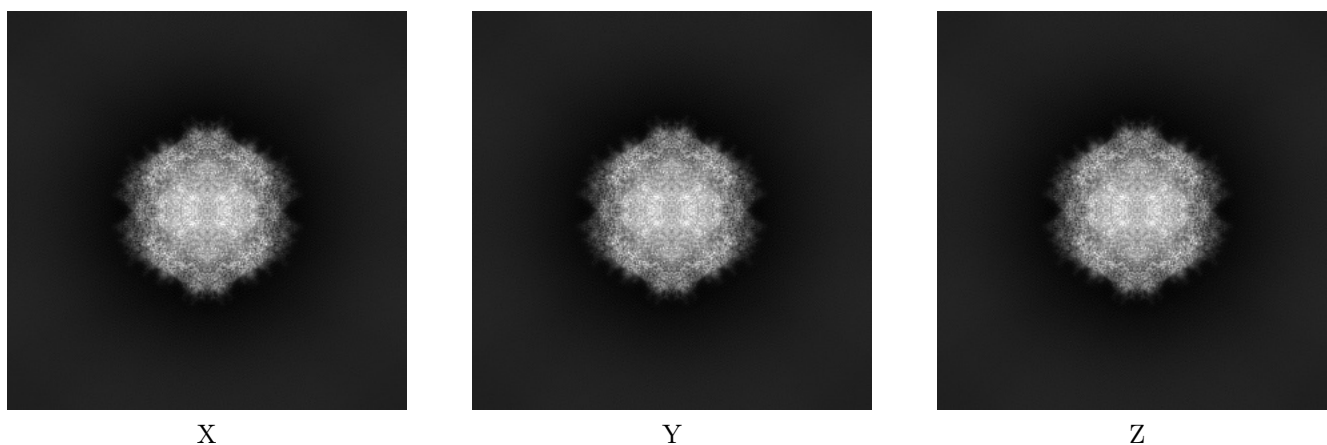
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20630. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

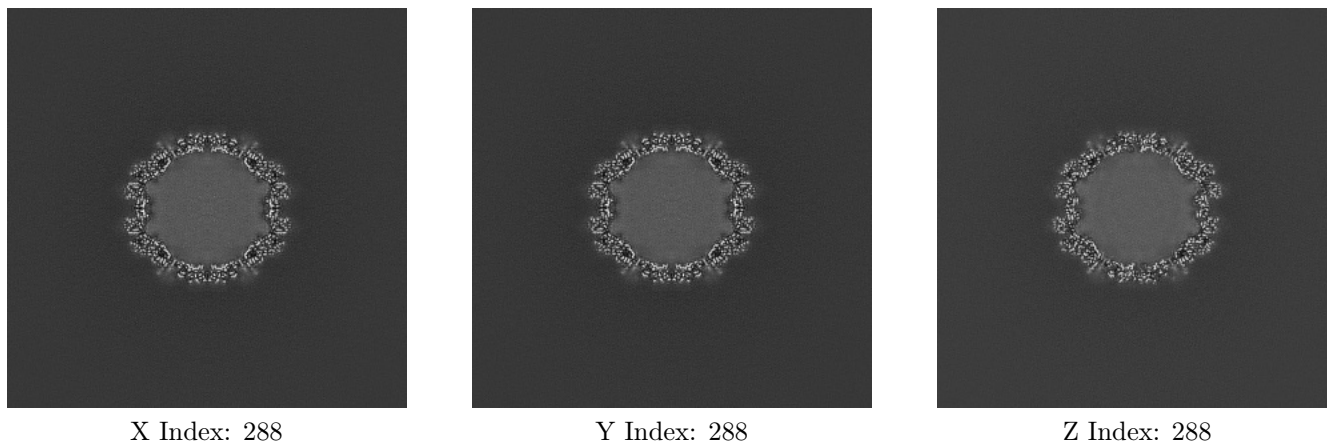
6.1.1 Primary map



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

6.2 Central slices [i](#)

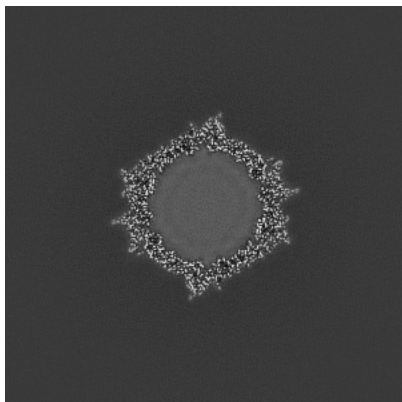
6.2.1 Primary map



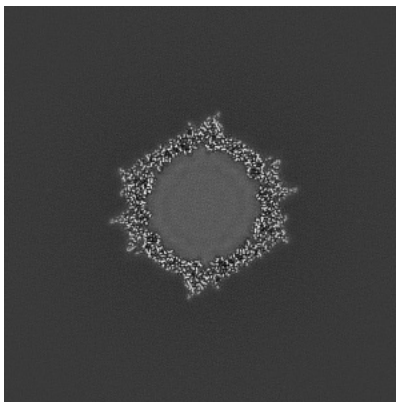
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

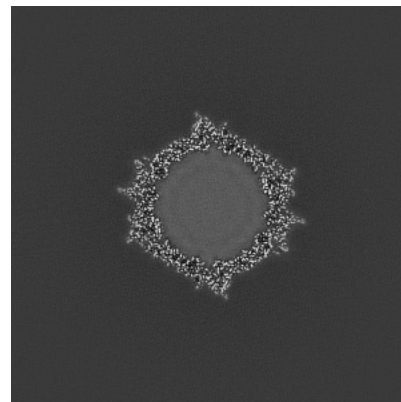
6.3.1 Primary map



X Index: 308



Y Index: 308

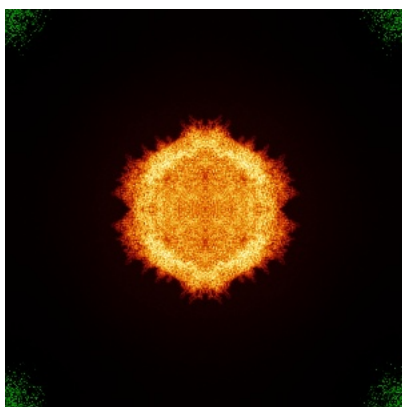


Z Index: 267

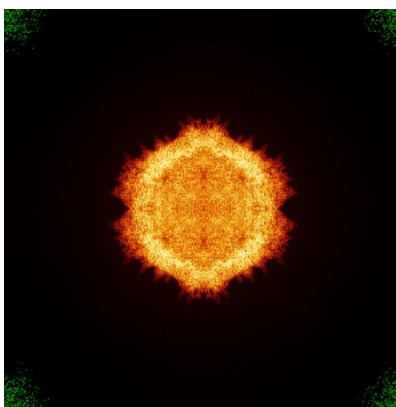
The images above show the largest variance slices of the map in three orthogonal directions.

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

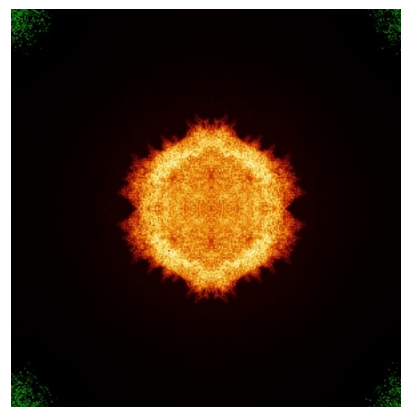
6.4.1 Primary map



X



Y

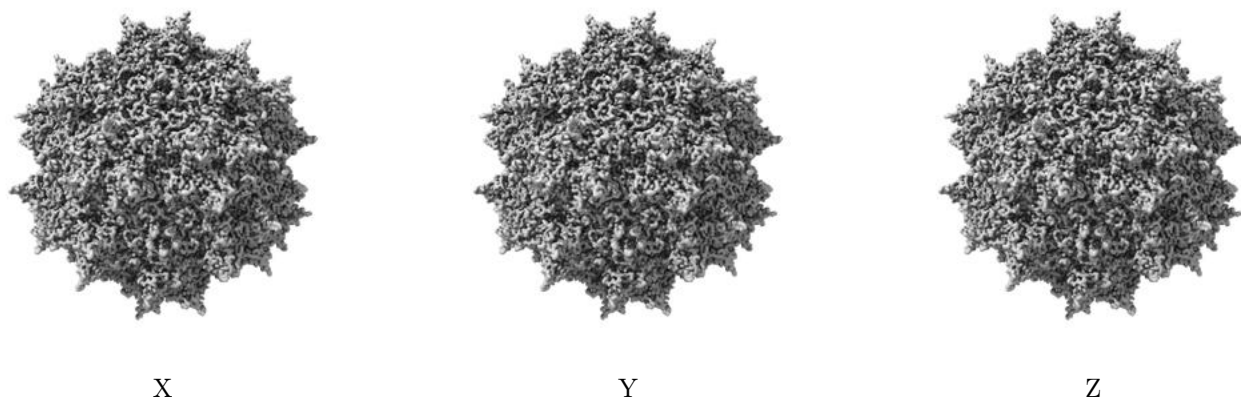


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

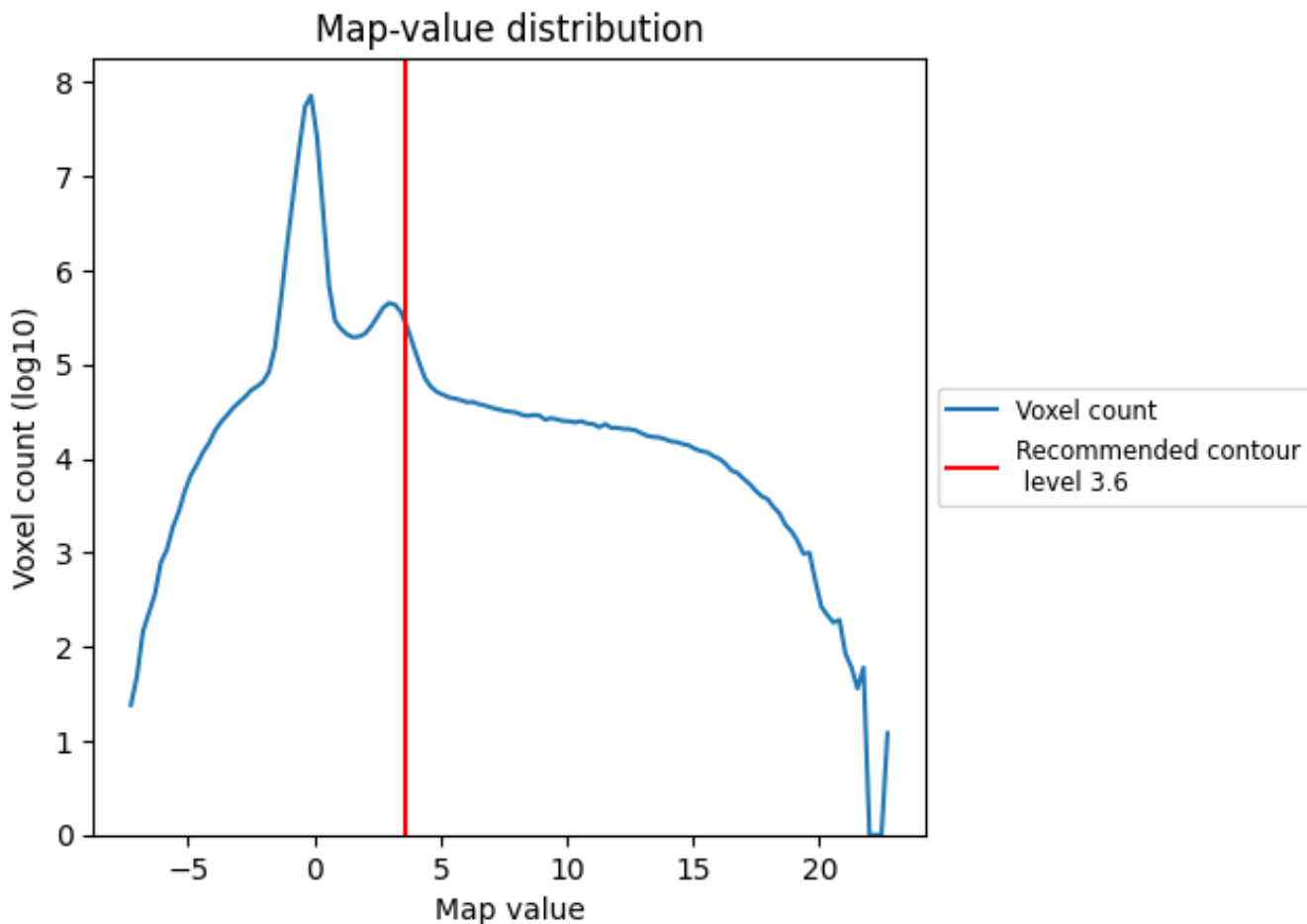
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

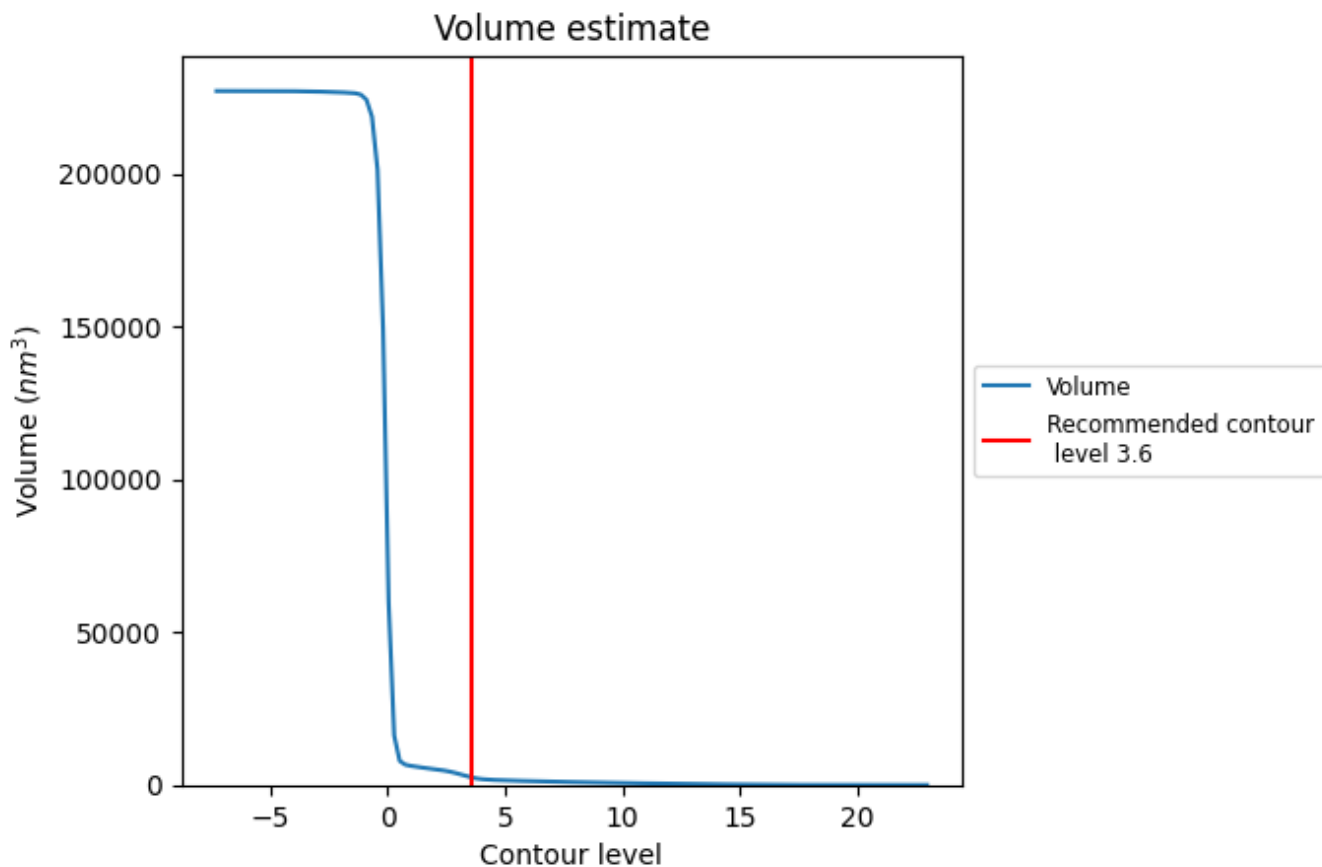
This section contains the results of statistical analysis of the map.

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.

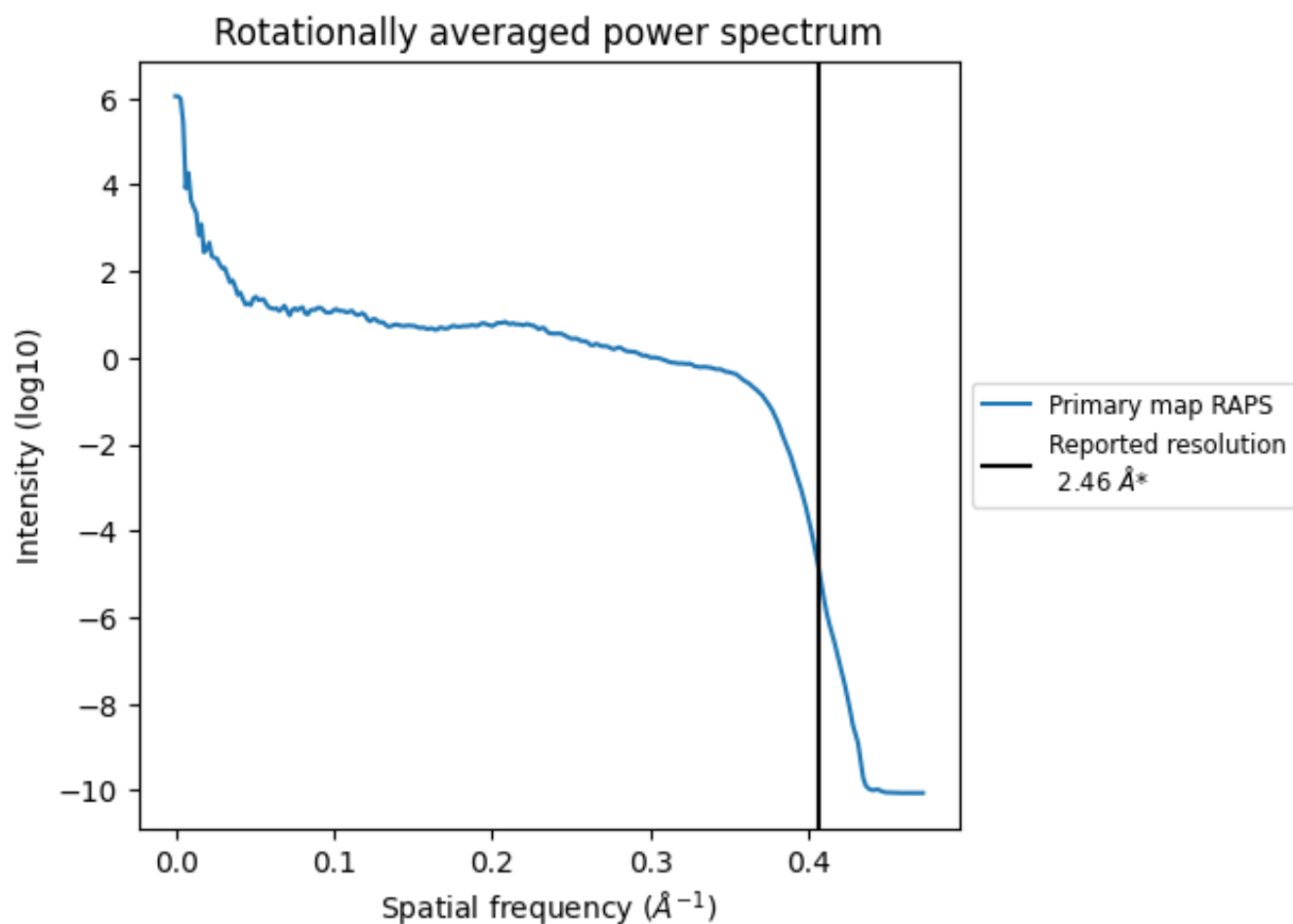
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2421 nm^3 ; this corresponds to an approximate mass of 2187 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 0.407 Å⁻¹

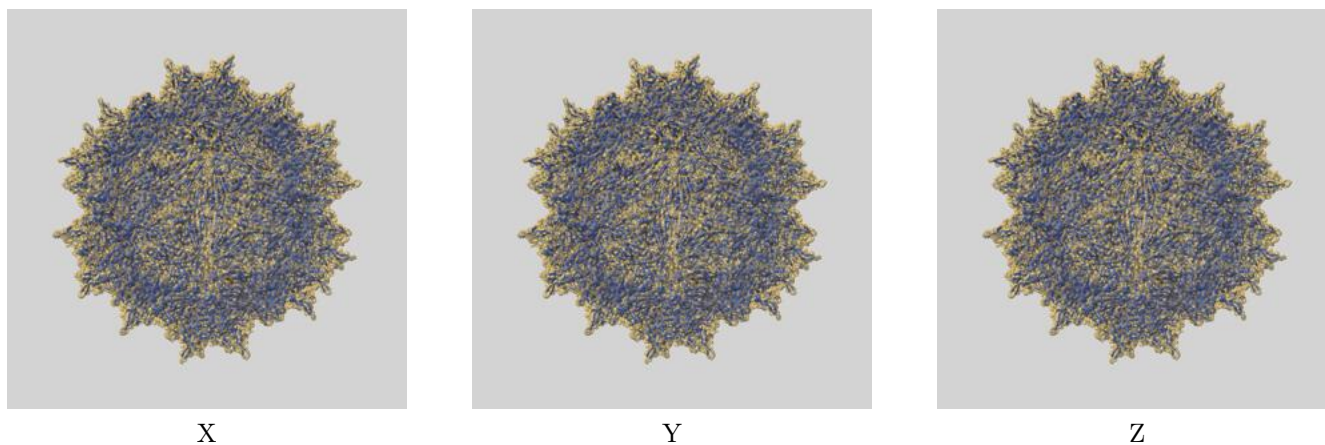
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

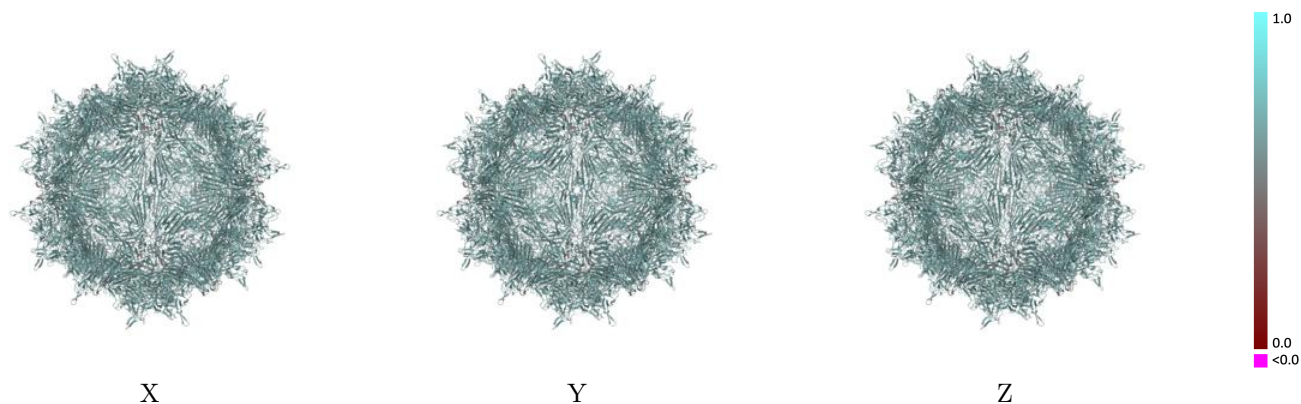
This section contains information regarding the fit between EMDB map EMD-20630 and PDB model 6U3Q. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



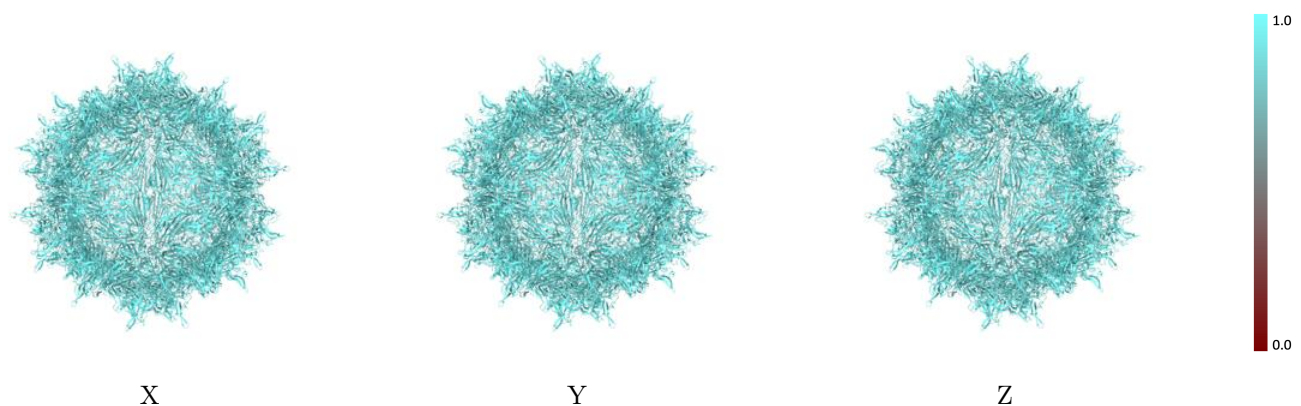
The images above show the 3D surface view of the map at the recommended contour level 3.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



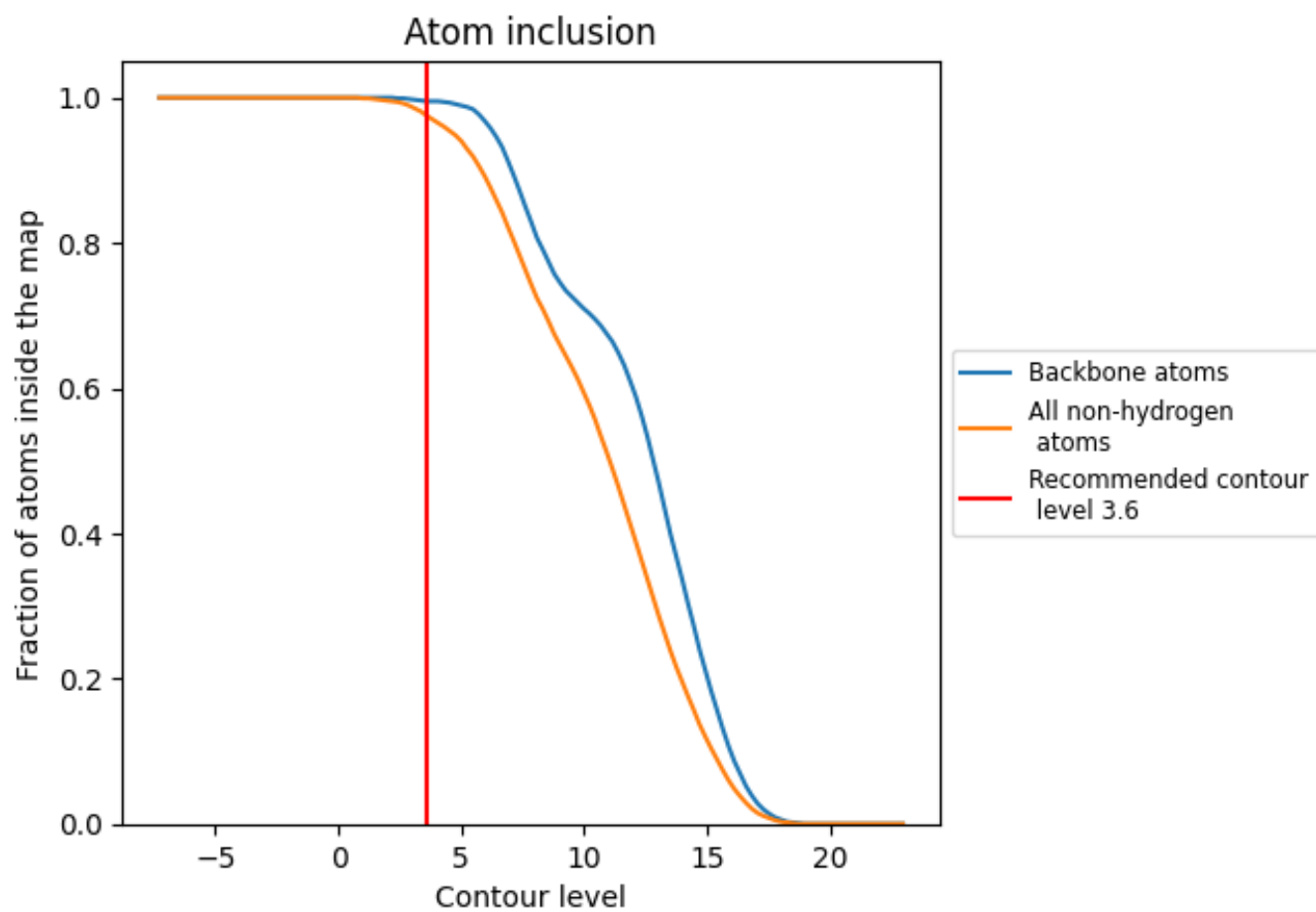
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.6300
0	 0.9760	 0.6290
1	 0.9760	 0.6290
2	 0.9760	 0.6300
3	 0.9760	 0.6290
4	 0.9750	 0.6290
5	 0.9760	 0.6300
6	 0.9760	 0.6300
7	 0.9760	 0.6300
A	 0.9760	 0.6290
B	 0.9760	 0.6290
C	 0.9760	 0.6310
D	 0.9750	 0.6300
E	 0.9760	 0.6300
F	 0.9750	 0.6280
G	 0.9750	 0.6280
H	 0.9750	 0.6290
I	 0.9760	 0.6300
J	 0.9760	 0.6300
K	 0.9750	 0.6300
L	 0.9760	 0.6300
M	 0.9760	 0.6300
N	 0.9740	 0.6300
O	 0.9760	 0.6300
P	 0.9760	 0.6290
Q	 0.9770	 0.6300
R	 0.9750	 0.6290
S	 0.9750	 0.6300
T	 0.9760	 0.6290
U	 0.9760	 0.6300
V	 0.9750	 0.6290
W	 0.9760	 0.6290
X	 0.9750	 0.6300
Y	 0.9760	 0.6300
Z	 0.9760	 0.6290



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Chain	Atom inclusion	Q-score
a	 0.9760	 0.6300
b	 0.9750	 0.6300
c	 0.9750	 0.6290
d	 0.9750	 0.6290
e	 0.9740	 0.6290
f	 0.9760	 0.6290
g	 0.9760	 0.6310
h	 0.9770	 0.6290
i	 0.9750	 0.6290
j	 0.9760	 0.6300
k	 0.9750	 0.6300
l	 0.9770	 0.6300
m	 0.9740	 0.6300
n	 0.9740	 0.6290
o	 0.9740	 0.6290
p	 0.9760	 0.6290
q	 0.9760	 0.6290
r	 0.9740	 0.6310
s	 0.9760	 0.6310
t	 0.9750	 0.6290
u	 0.9740	 0.6300
v	 0.9760	 0.6290
w	 0.9760	 0.6290
x	 0.9760	 0.6300
y	 0.9760	 0.6300
z	 0.9750	 0.6300