



wwPDB EM Model Validation Summary Report ⓘ

May 18, 2020 – 12:00 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 Model Validation Summary Report for a publicly released PDB/EMDB 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

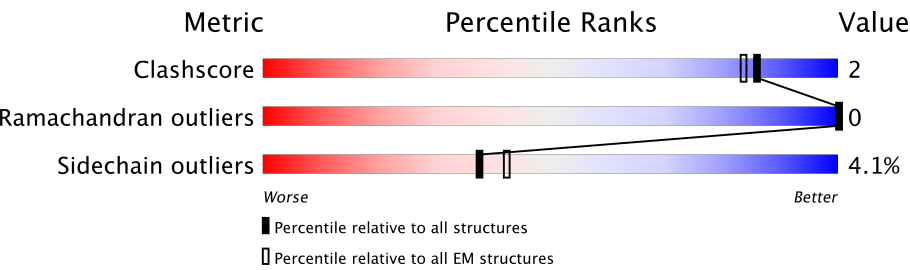
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.46 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)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	735	63% 7% • 29%
1	1	735	63% 7% • 29%
1	2	735	63% 7% • 29%
1	3	735	63% 7% • 29%
1	4	735	62% 8% • 29%
1	5	735	62% 8% • 29%
1	6	735	63% 7% • 29%
1	7	735	63% 7% • 29%
1	A	735	62% 8% • 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	
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	

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Mol	Chain	Length	Quality of chain
1	z	735	<div><div></div><div>68%</div><div></div><div>•</div><div>29%</div></div>

2 Entry composition

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
1	A	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	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
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	B	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	Y	519	Total 4138	C 2605	N 716	O 803	S 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
1	J	519	Total	C	N	O	S	0	0
			4138	2605	716	803	14		

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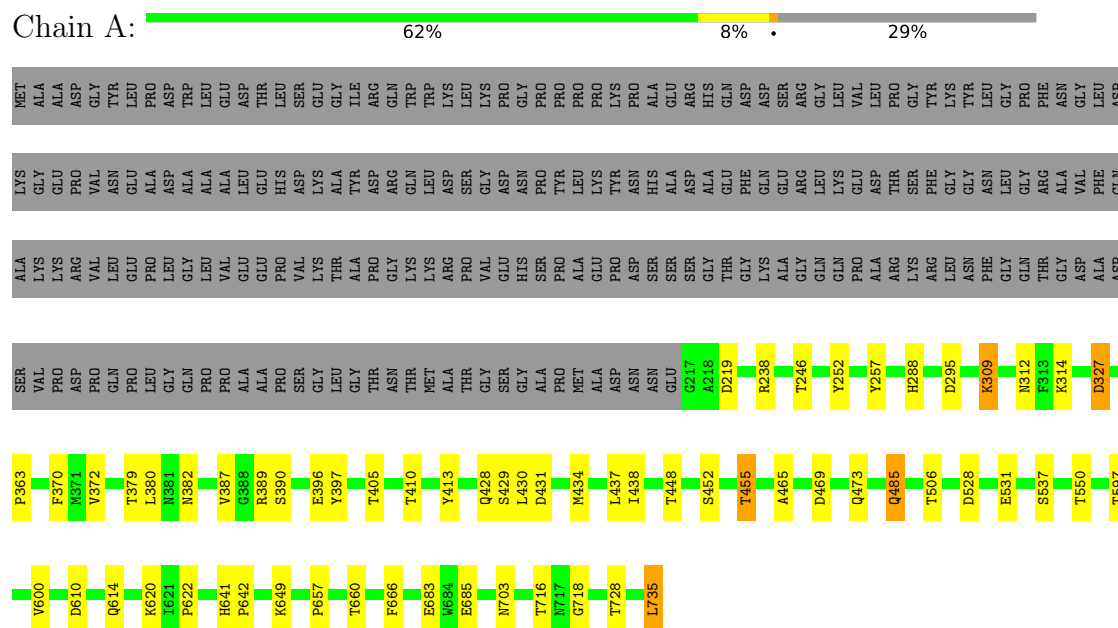
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Chain	Residue	Modelled	Actual	Comment	Reference
F	39	GLN	LYS	conflict	UNP Q670R6
F	164	GLN	ASN	conflict	UNP Q670R6
F	312	ASN	SER	conflict	UNP Q670R6
F	447	LYS	ARG	conflict	UNP Q670R6
F	450	ALA	THR	conflict	UNP Q670R6
F	593	THR	SER	conflict	UNP Q670R6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

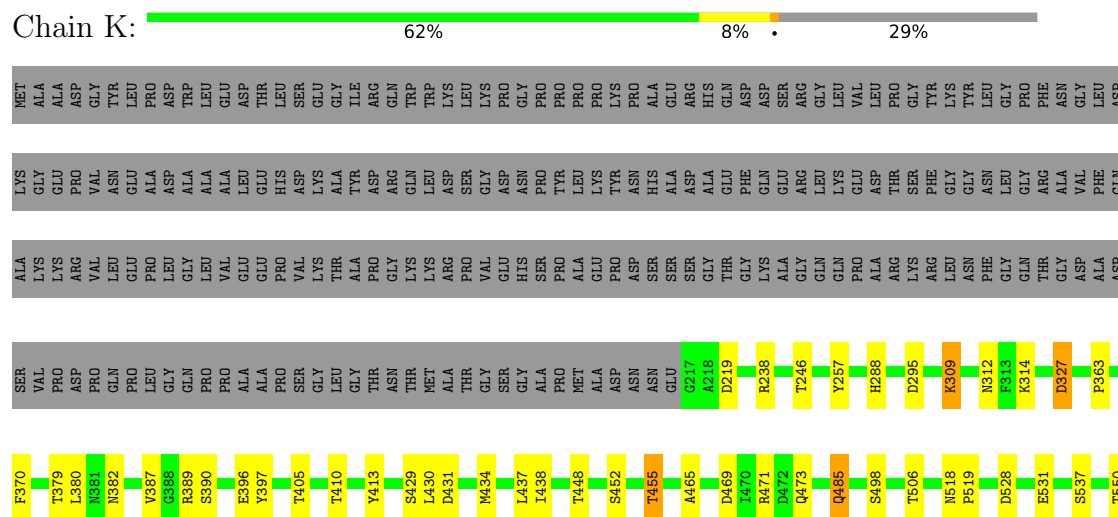
3 Residue-property plots [i](#)

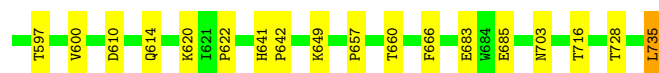
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: Capsid protein VP1



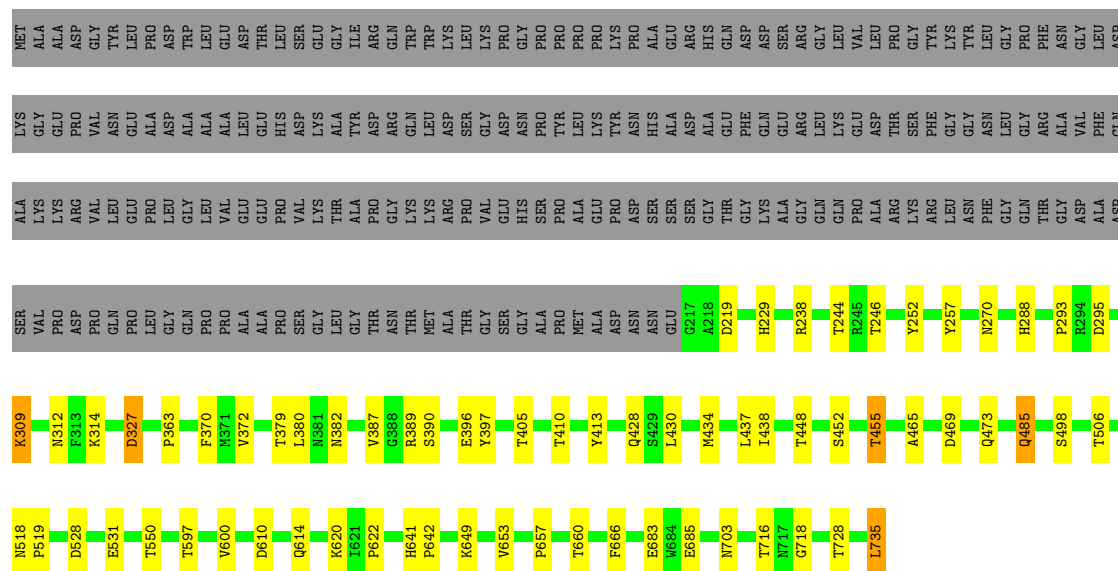
• Molecule 1: Capsid protein VP1





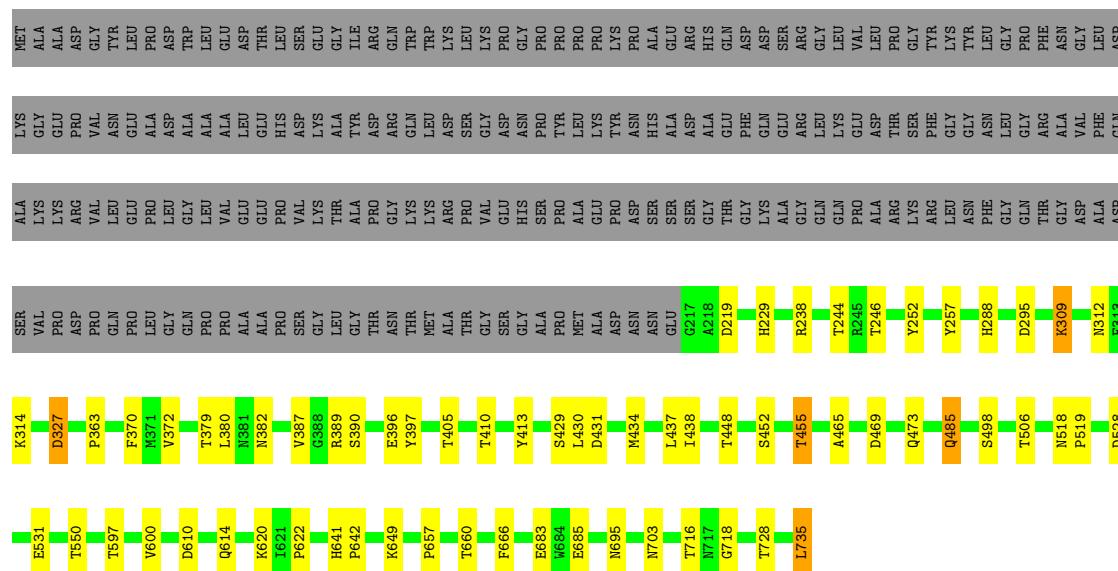
• Molecule 1: Capsid protein VP1

Chain L: 61% 9% 29%



• Molecule 1: Capsid protein VP1

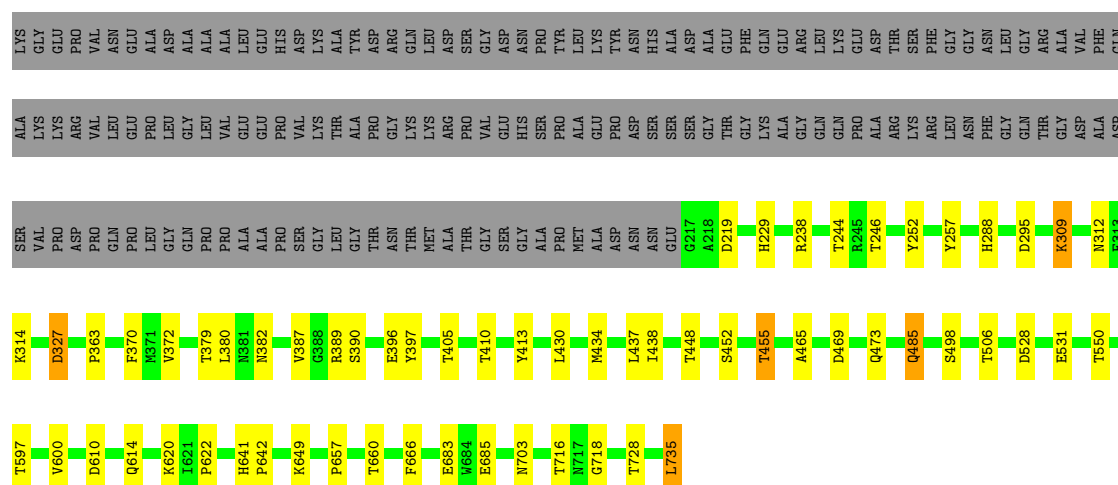
Chain M: 61% 8% 29%



• Molecule 1: Capsid protein VP1

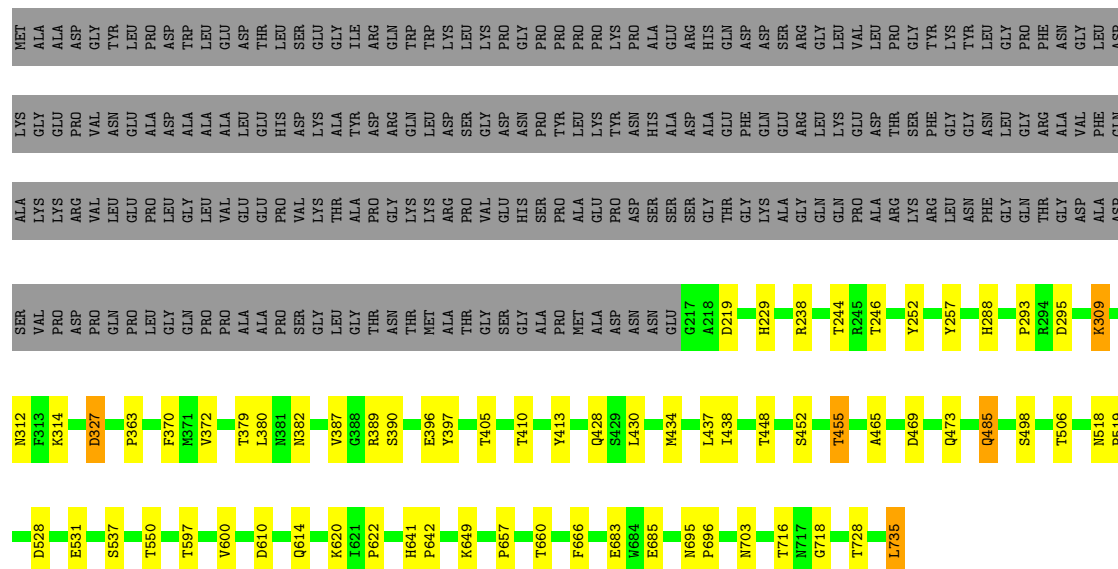
Chain N: 62% 8% 29%





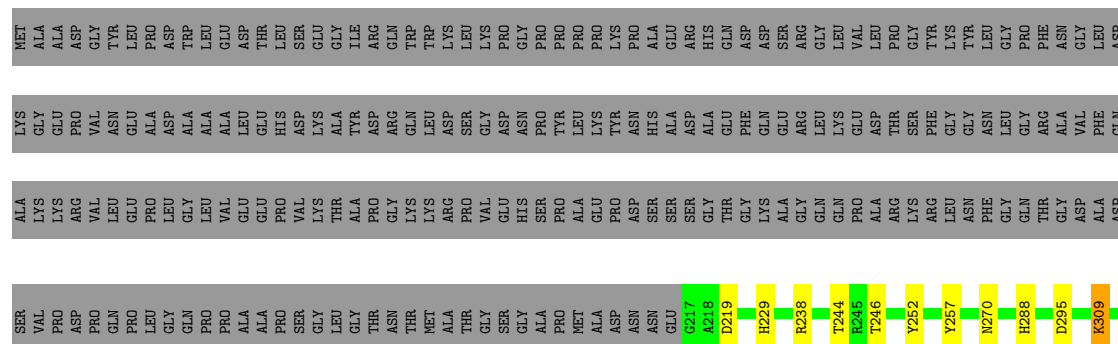
- Molecule 1: Capsid protein VP1

Chain O:  61% 9% 29%



- Molecule 1: Capsid protein VP1

Chain P:  62% 8% 29%





Category	Percentage
Very good	62%
Good	8%
Not good	29%
Very bad	1%

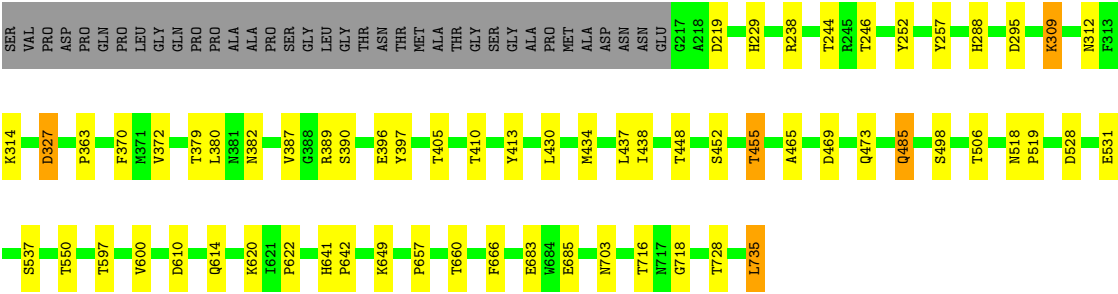


Response	Percentage
Yes	63%
No	7%
Don't know	29%

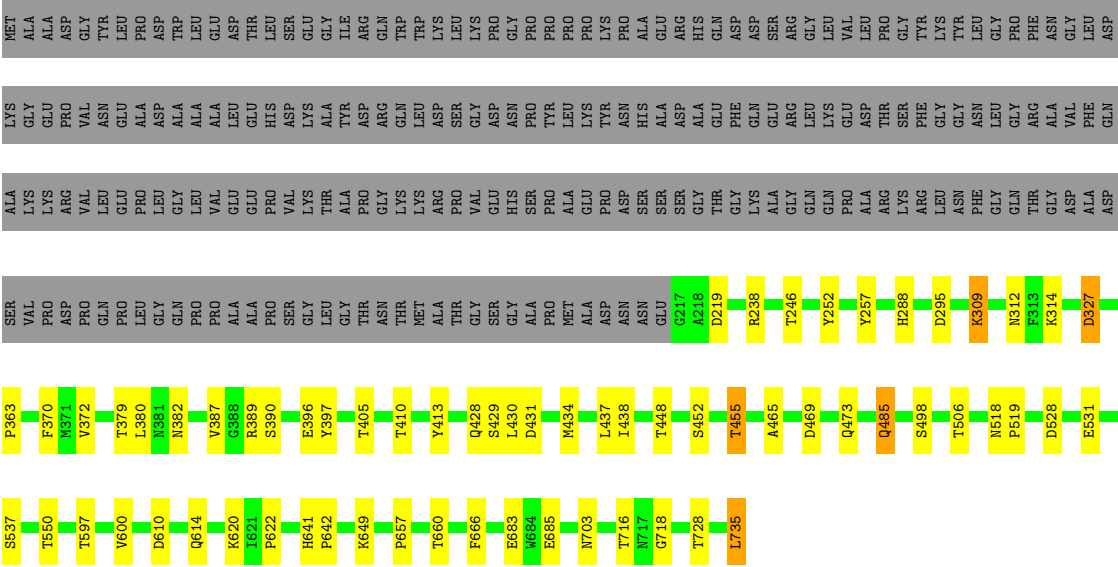


Response	Percentage
Yes, the U.S. is a democracy	62%
No, the U.S. is not a democracy	8%
Don't know	29%

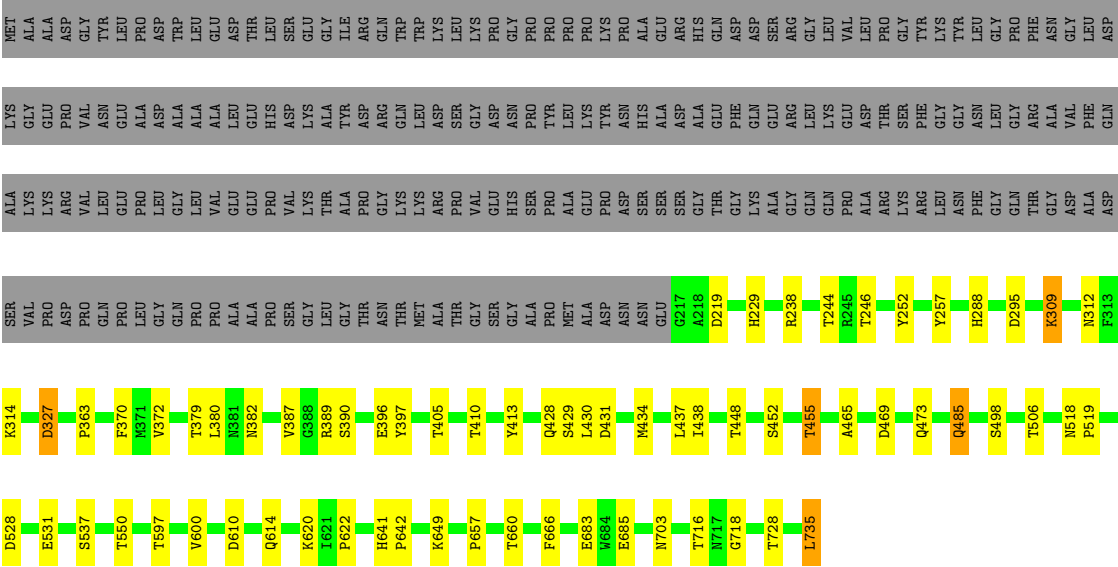


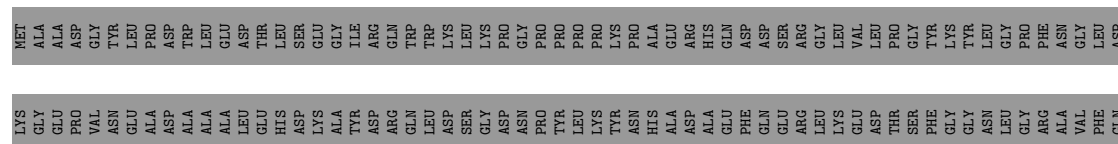


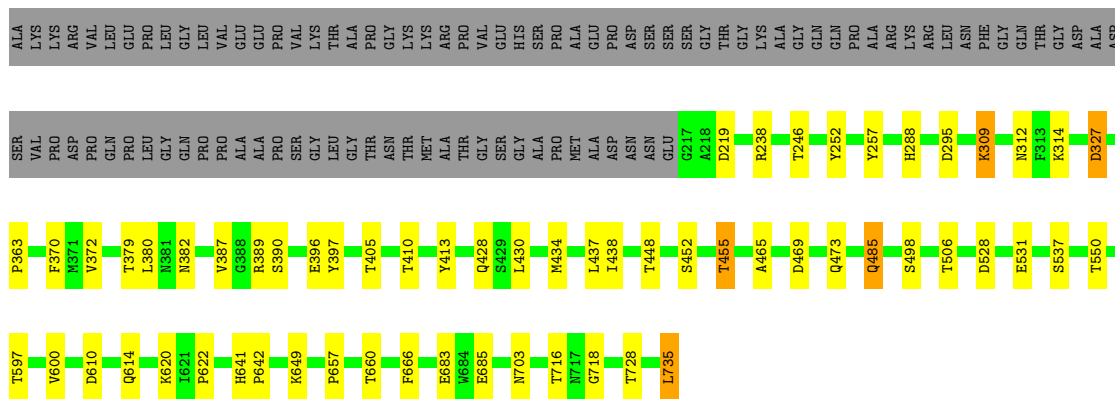
• Molecule 1: Capsid protein VP1



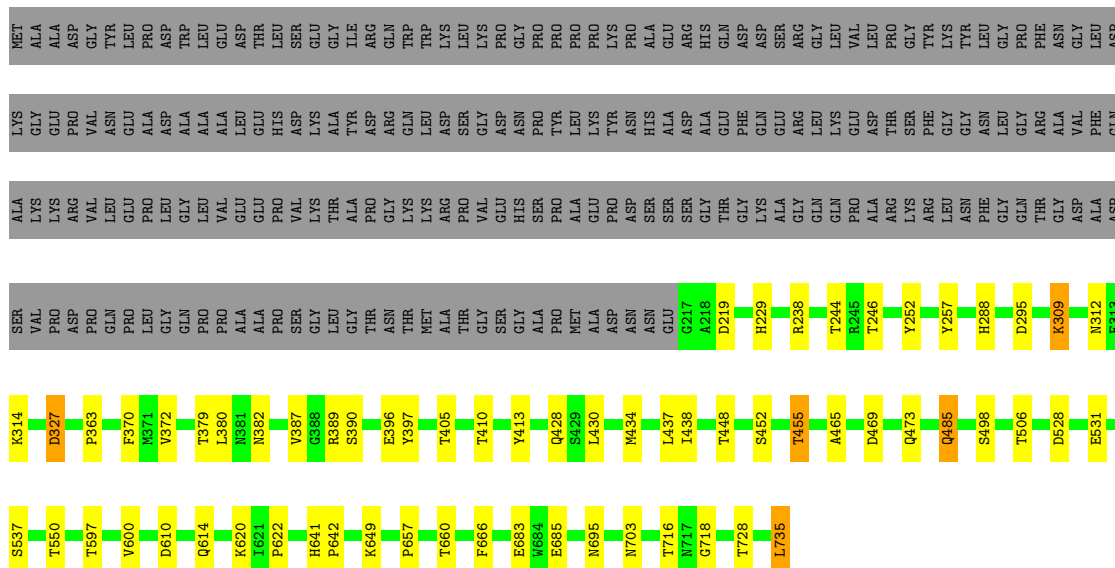
• Molecule 1: Capsid protein VP1



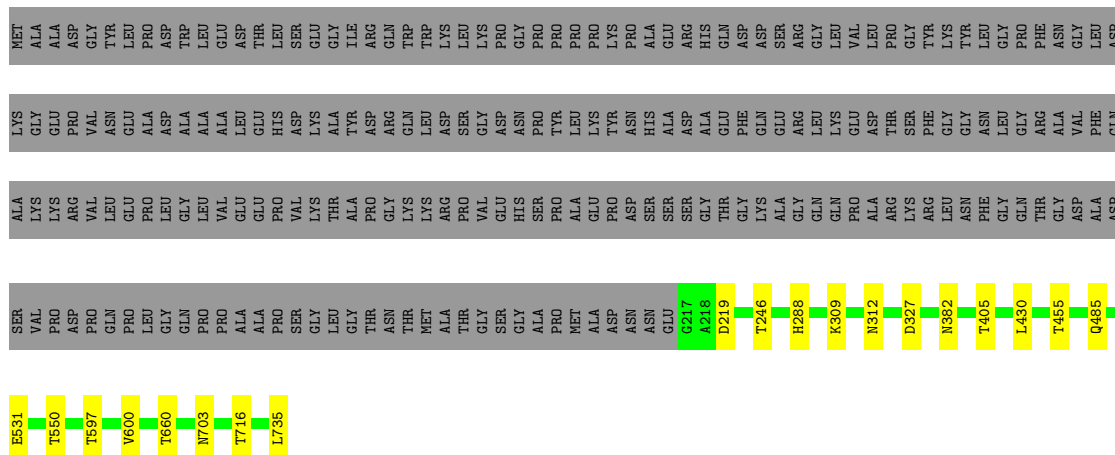




- Molecule 1: Capsid protein VP1

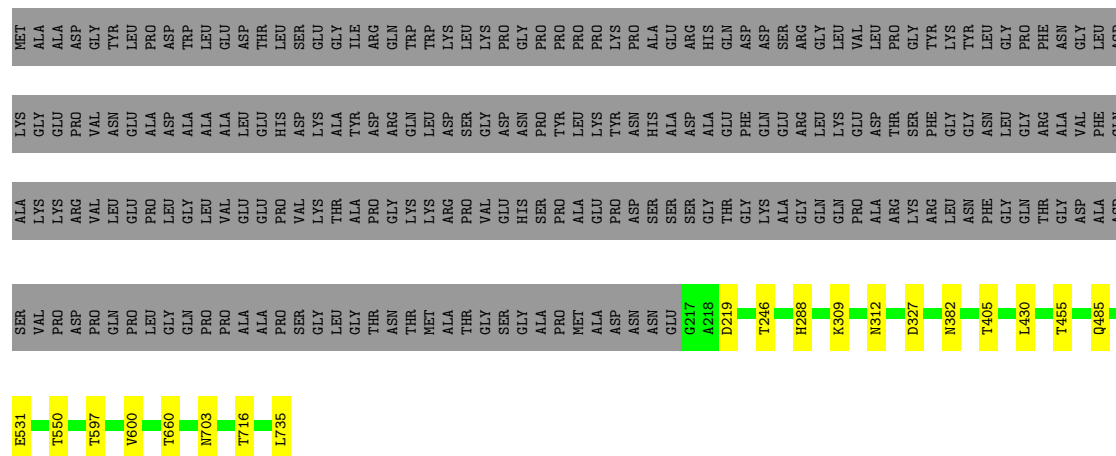


- Molecule 1: Capsid protein VP1



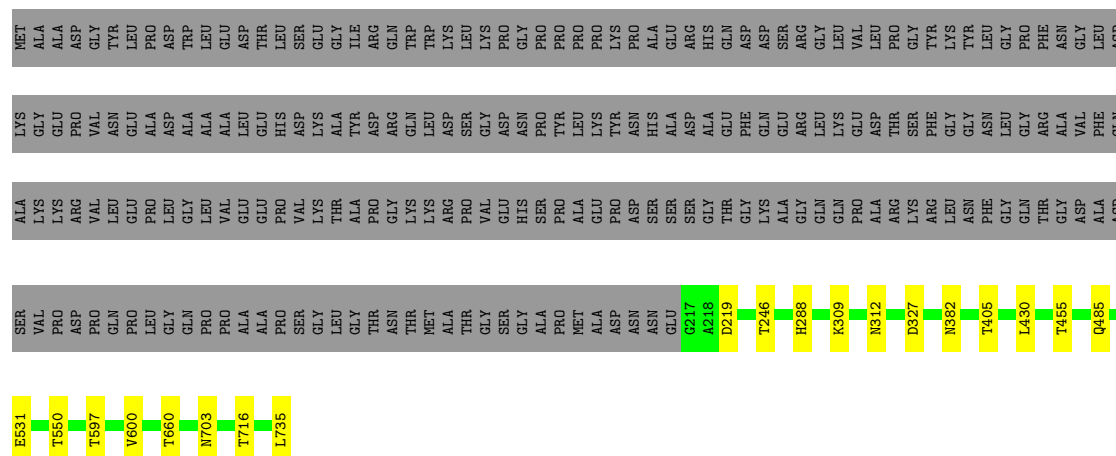
- Molecule 1: Capsid protein VP1

Chain b:  68% 29%



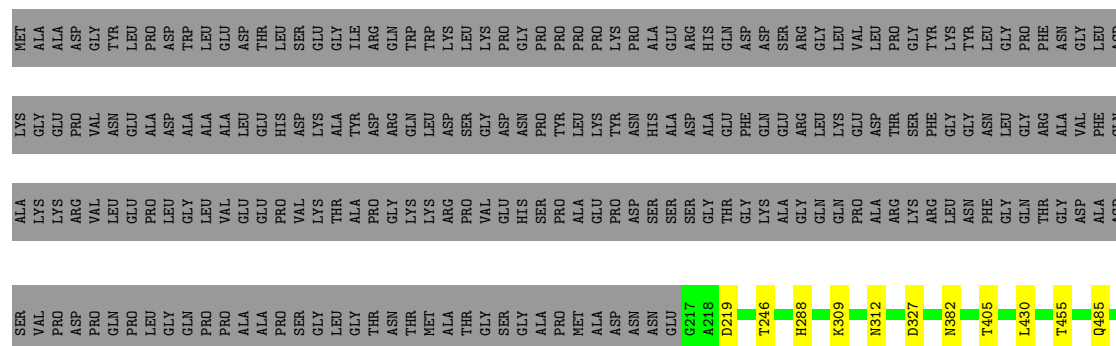
- Molecule 1: Capsid protein VP1

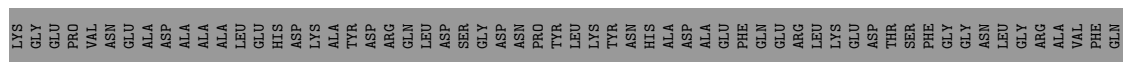
Chain c: 68% . 29%



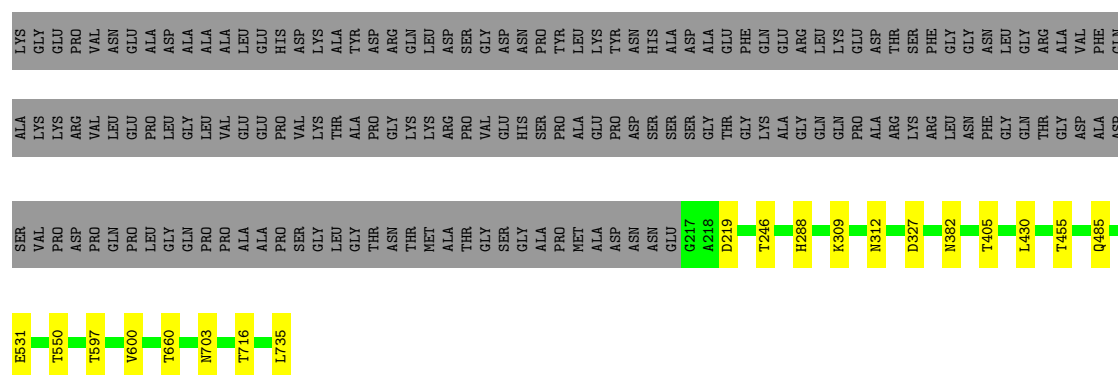
- Molecule 1: Capsid protein VP1

Chain d:  68% 29%

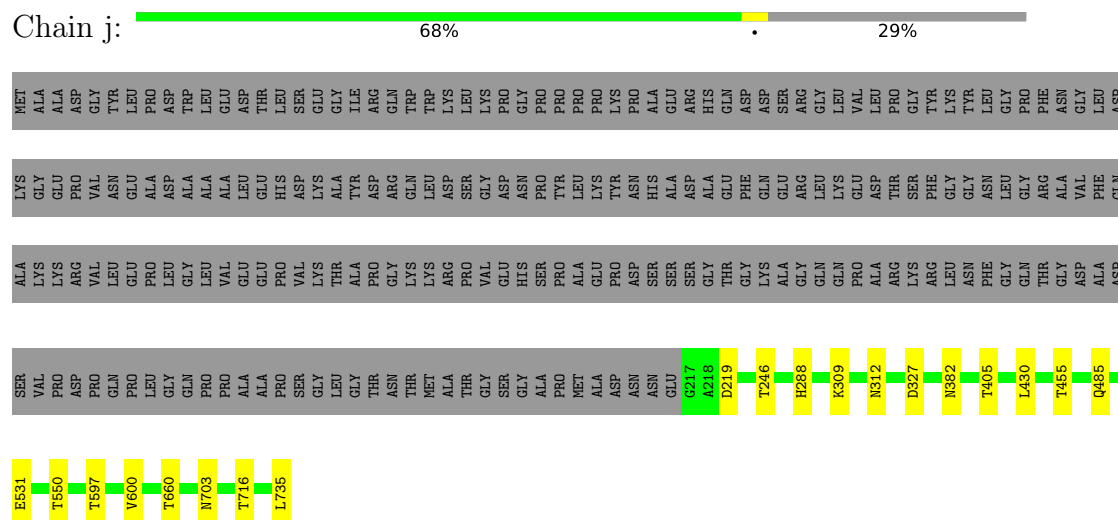




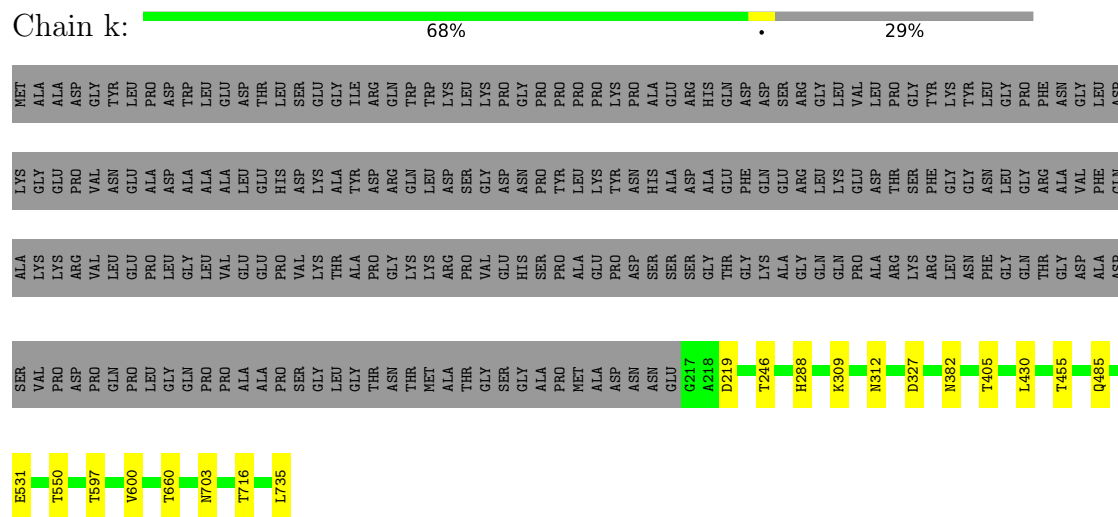




- Molecule 1: Capsid protein VP1

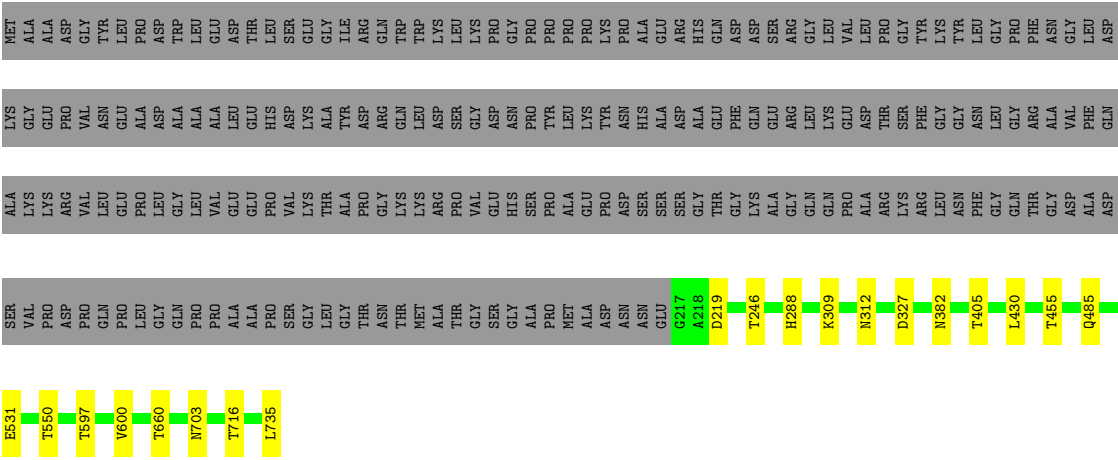


- Molecule 1: Capsid protein VP1



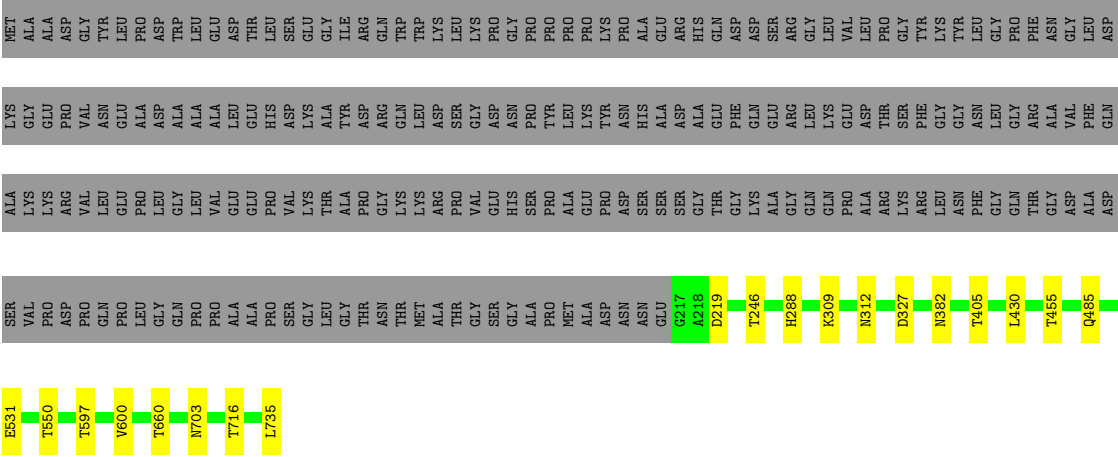
- Molecule 1: Capsid protein VP1





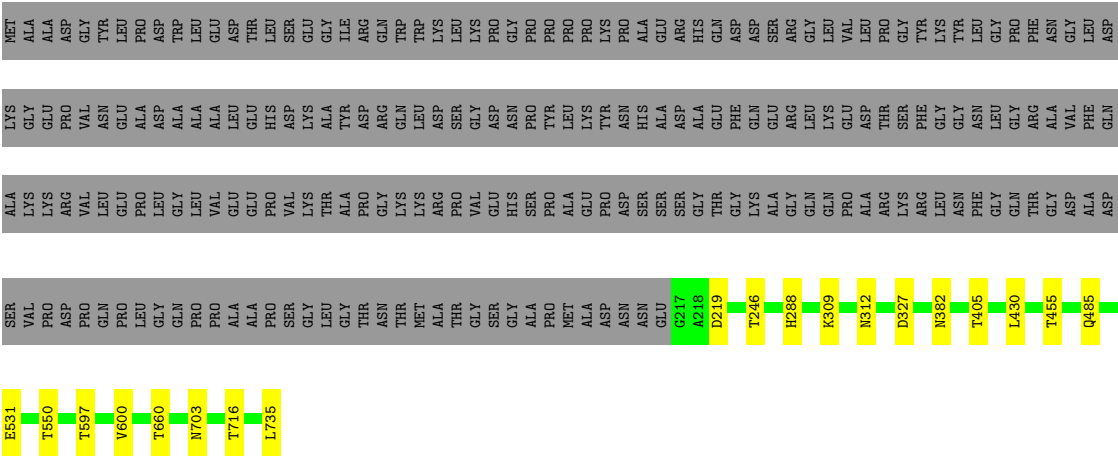
• Molecule 1: Capsid protein VP1

Chain m: 68% 29%



• Molecule 1: Capsid protein VP1

Chain n: 68% 29%



• Molecule 1: Capsid protein VP1

Response	Percentage
Yes	62%
No	8%
Don't know	29%

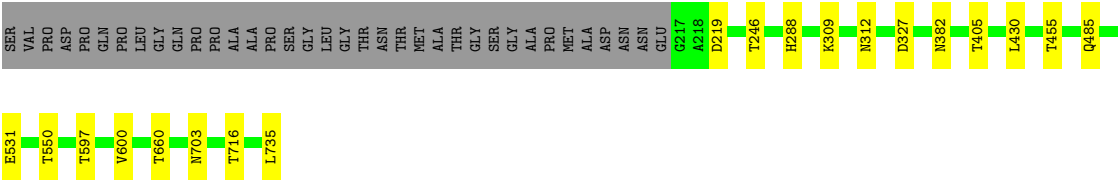


68% . 29%

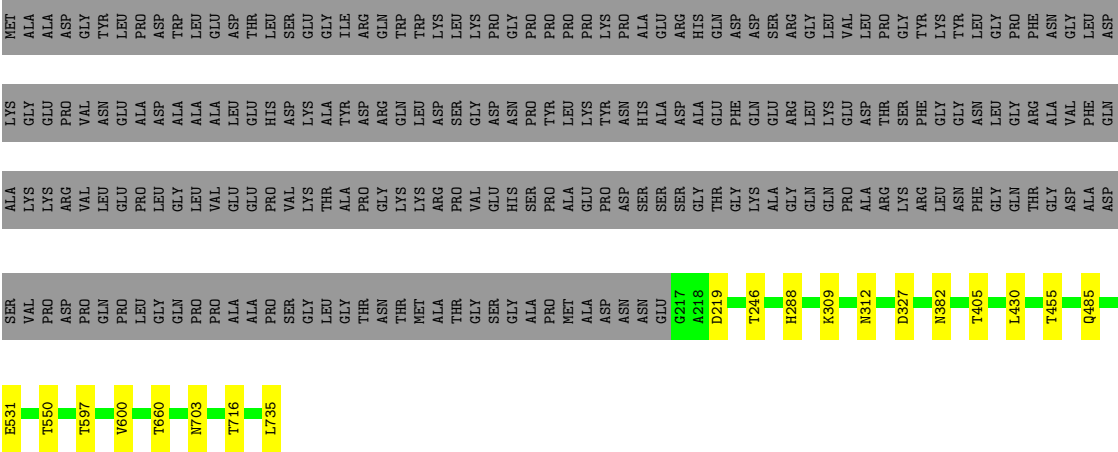


Response	Percentage
Yes, the U.S. is a democracy	68%
No, the U.S. is not a democracy	29%

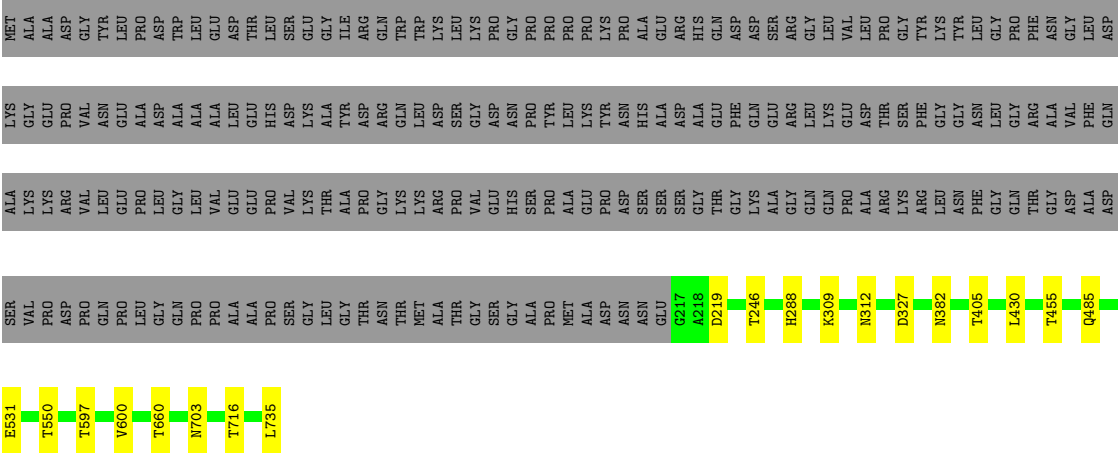




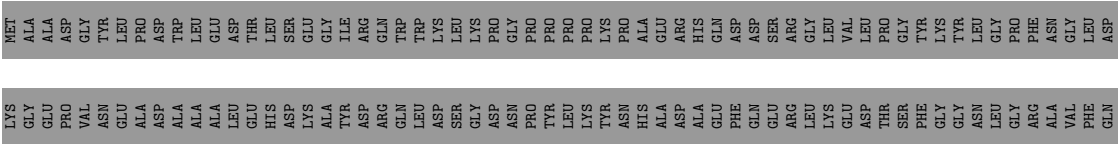
• Molecule 1: Capsid protein VP1

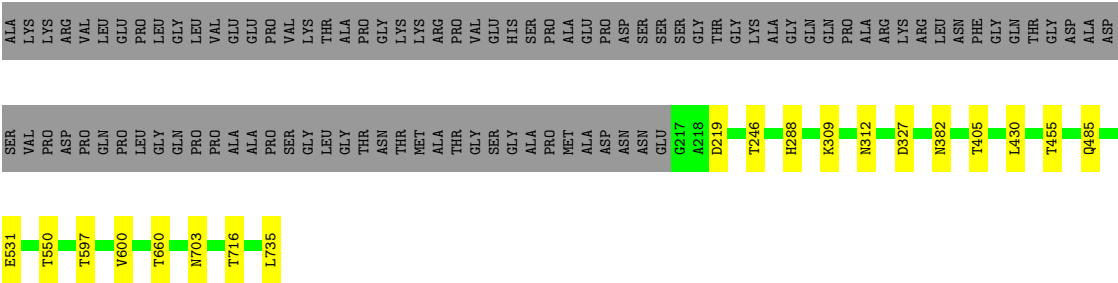


• Molecule 1: Capsid protein VP1

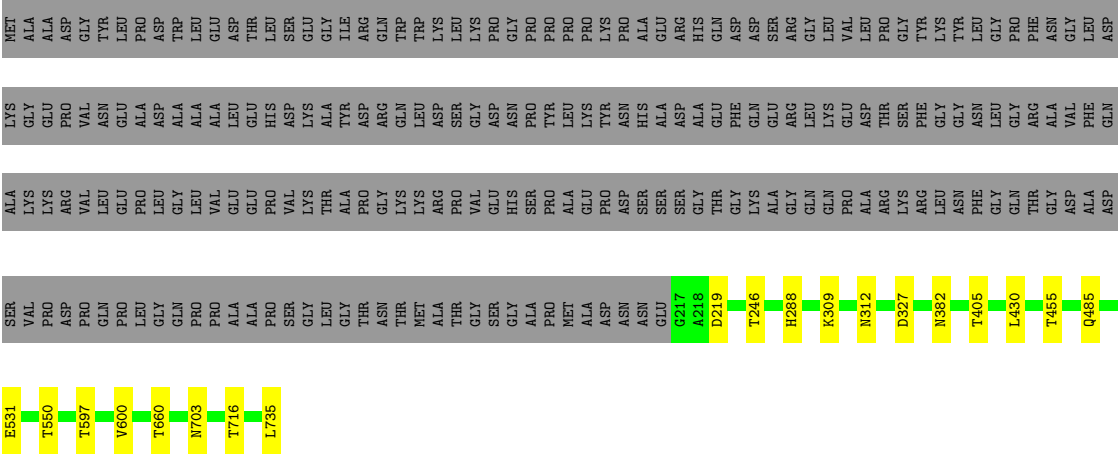


• Molecule 1: Capsid protein VP1

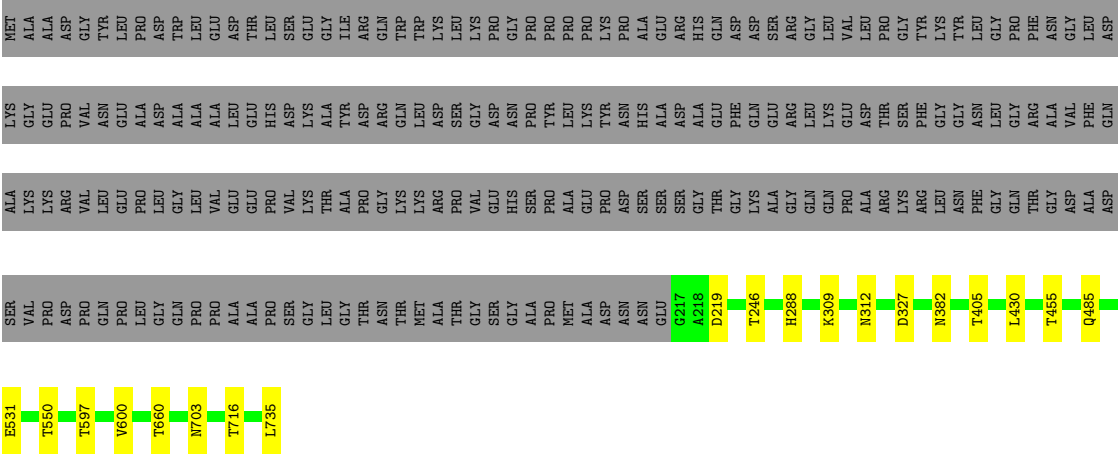




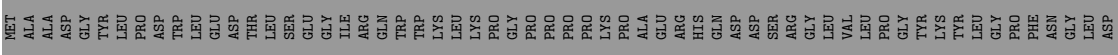
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1





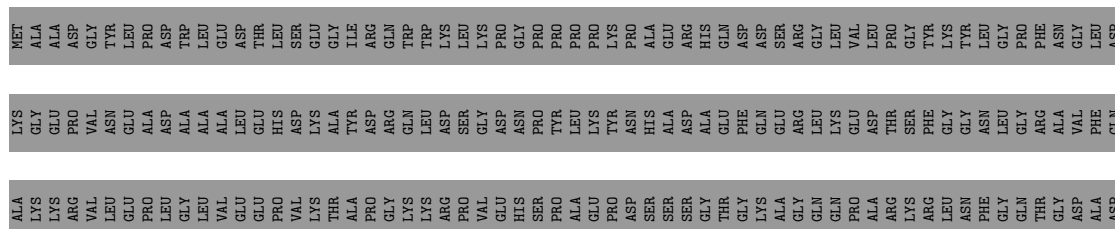
Response	Percentage
Yes, the U.S. is a democracy	63%
No, the U.S. is not a democracy	7%
Don't know	29%



Response	Percentage
Yes, the U.S. is a democracy	63%
No, the U.S. is not a democracy	7%
Don't know	29%



Response	Percentage
Yes	63%
No	7%
Don't know	29%

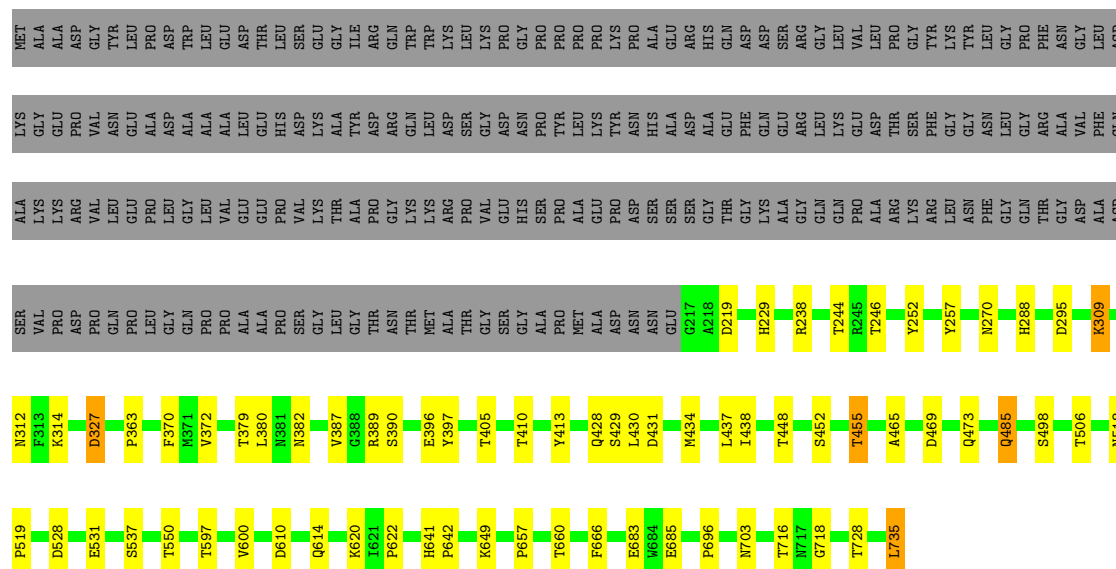






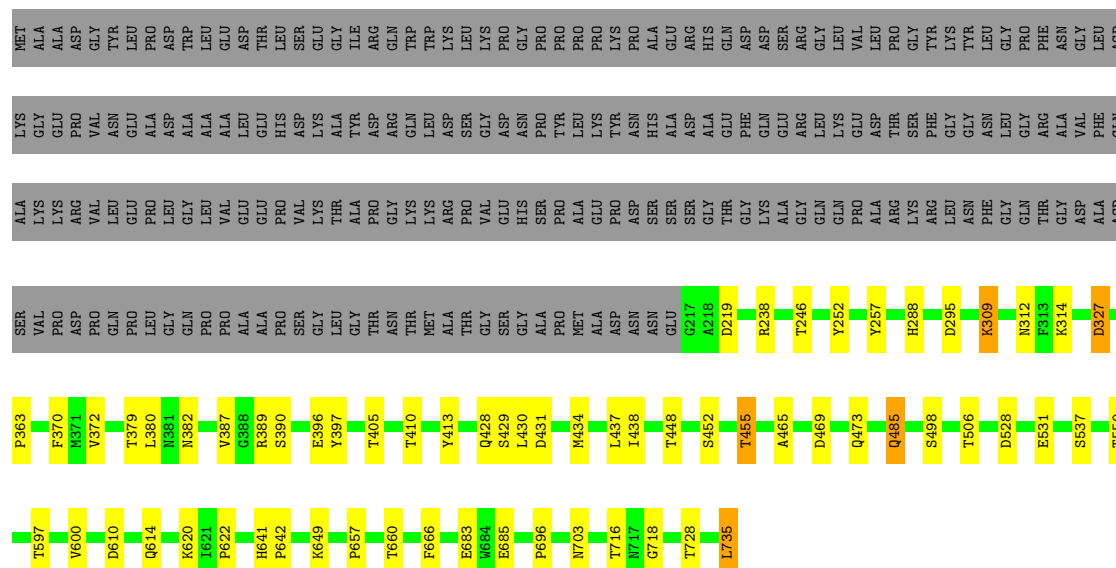
- Molecule 1: Capsid protein VP1

Chain H: 61% 9% 29%



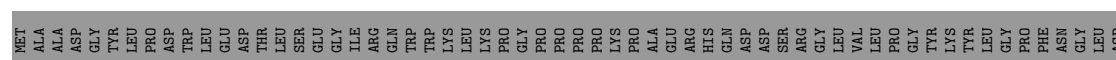
- Molecule 1: Capsid protein VP1

Chain I: 62% 8% 29%



- Molecule 1: Capsid protein VP1

Chain J: 62% 8% 29%



LYS	LYS	ALA	SER
GLY	LYS	LYS	VAL
GLU	LYS	ARG	ASP
PRO	ARG	VAL	PRO
ASN	VAL	GLN	GLN
GLU	LEU	PRO	PRO
ALA	GLU	LEU	LEU
ASP	LEU	GLY	GLY
ALA	GLY	GLN	GLN
ALA	LEU	PRO	PRO
LEU	VAL	ALA	ALA
GLU	GLU	ALA	ALA
HIS	GLU	PRO	PRO
ASP	HIS	VAL	SER
LYS	LYS	LYS	E396
ALA	THR	LEU	Y397
TYR	ALA	GLY	T405
ASP	PRO	THR	T410
ARG	GLY	ASN	T413
GLN	LYS	THR	Y413
LEU	LYS	ALA	L430
ASP	ARG	THR	M434
SER	PRO	GLY	L437
GLY	VAL	SER	I438
ASP	GLU	GLY	T448
ASN	GLU	GLY	S452
PRO	HIS	ALA	T455
TYR	TYR	ASP	A465
LYS	ALA	ASN	Q473
LEU	LEU	GLU	Q485
GLY	ARG	GLN	S498
LEU	LEU	GLN	T506
LYS	LYS	PRO	N518
ASP	THR	ALA	P519
THR	ARG	ARG	D528
PHE	LYS	LEU	E531
GLY	PHE	ASN	S537
GLY	GLY	PHE	T550
ASN	ASN	GLN	T597
LEU	GLY	THR	
LEU	GLY	GLY	
ARG	ARG	ASP	
ALA	ALA	ALA	
PHE	PHE	GLN	
GLN	ASP		

P363	F370	N371	V372	T379	L380	N381	N382	V387	G388	R389	S390	E396	Y397	T405	T410	Y413	L430	M434	L437	I438	T448	S452	T455	A465	Q473	Q485	S498	T506	N518	P519	D528	E531	S537	T550	T597
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

V600	D610	Q614	K620	F621	P622	H641	P642	K649	P657	T660	F666	E683	V684	E685	N695	N703	T716	H717	G718	T728	L736
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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 ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4138	0	3887	30	0
1	1	4138	0	3887	30	0
1	2	4138	0	3887	28	0
1	3	4138	0	3887	29	0
1	4	4138	0	3887	34	0
1	5	4138	0	3887	32	0
1	6	4138	0	3887	29	0
1	7	4138	0	3887	26	0
1	A	4138	0	3887	40	0
1	B	4138	0	3887	42	0
1	C	4138	0	3887	38	0
1	D	4138	0	3887	40	0
1	E	4138	0	3887	39	0
1	F	4138	0	3887	36	0
1	G	4138	0	3887	40	0
1	H	4138	0	3887	42	0
1	I	4138	0	3887	42	0
1	J	4138	0	3887	38	0
1	K	4138	0	3887	38	0
1	L	4138	0	3887	44	0
1	M	4138	0	3887	41	0
1	N	4138	0	3887	35	0
1	O	4138	0	3887	41	0
1	P	4138	0	3887	36	0
1	Q	4138	0	3887	39	0
1	R	4138	0	3887	43	0
1	S	4138	0	3887	37	0
1	T	4138	0	3887	37	0
1	U	4138	0	3887	43	0
1	V	4138	0	3887	43	0
1	W	4138	0	3887	39	0
1	X	4138	0	3887	41	0
1	Y	4138	0	3887	37	0
1	Z	4138	0	3887	43	0
1	a	4138	0	3887	0	0
1	b	4138	0	3887	0	0
1	c	4138	0	3887	0	0
1	d	4138	0	3887	0	0
1	e	4138	0	3887	0	0
1	f	4138	0	3887	0	0
1	g	4138	0	3887	0	0
1	h	4138	0	3887	0	0
1	i	4138	0	3887	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4138	0	3887	0	0
1	k	4138	0	3887	0	0
1	l	4138	0	3887	0	0
1	m	4138	0	3887	0	0
1	n	4138	0	3887	0	0
1	o	4138	0	3887	0	0
1	p	4138	0	3887	0	0
1	q	4138	0	3887	0	0
1	r	4138	0	3887	0	0
1	s	4138	0	3887	0	0
1	t	4138	0	3887	0	0
1	u	4138	0	3887	0	0
1	v	4138	0	3887	0	0
1	w	4138	0	3887	0	0
1	x	4138	0	3887	0	0
1	y	4138	0	3887	0	0
1	z	4138	0	3887	0	0
All	All	248280	0	233220	1086	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 1086 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:657:PRO:HB3	1:N:666:PHE:HZ	1.59	0.68
1:E:657:PRO:HB3	1:E:666:PHE:HZ	1.59	0.68
1:L:657:PRO:HB3	1:L:666:PHE:HZ	1.59	0.68
1:O:657:PRO:HB3	1:O:666:PHE:HZ	1.59	0.68
1:4:657:PRO:HB3	1:4:666:PHE:HZ	1.59	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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
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
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 ⓘ

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%)	33	44
1	1	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	2	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	3	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	4	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	5	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	6	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	7	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	A	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	B	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	C	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	D	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	E	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	F	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	G	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	H	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	I	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	J	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	K	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	L	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	M	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	N	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	O	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	P	458/628 (73%)	439 (96%)	19 (4%)	33	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	R	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	S	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	T	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	U	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	V	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	W	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	X	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	Y	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	Z	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	a	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	b	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	c	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	d	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	e	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	f	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	g	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	h	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	i	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	j	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	k	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	l	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	m	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	n	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	o	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	p	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	q	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	r	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	s	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	t	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	u	458/628 (73%)	439 (96%)	19 (4%)	33	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	w	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	x	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	y	458/628 (73%)	439 (96%)	19 (4%)	33	44
1	z	458/628 (73%)	439 (96%)	19 (4%)	33	44
All	All	27480/37680 (73%)	26340 (96%)	1140 (4%)	38	44

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

Mol	Chain	Res	Type
1	i	288	HIS
1	D	531	GLU
1	F	430	LEU
1	i	716	THR
1	l	430	LEU

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

Mol	Chain	Res	Type
1	i	359	GLN
1	D	589	GLN
1	F	359	GLN
1	j	270	ASN
1	l	536	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates 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.