



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:39 PM UTC

PDB ID : 6V1Z / pdb_00006v1z
EMDB ID : EMD-21020
Title : genome-containing AAVrh.39 particles
Authors : Mietzsch, M.; Agbandje-McKenna, M.
Deposited on : 2019-11-21
Resolution : 3.58 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

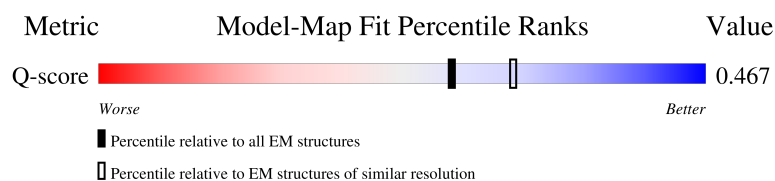
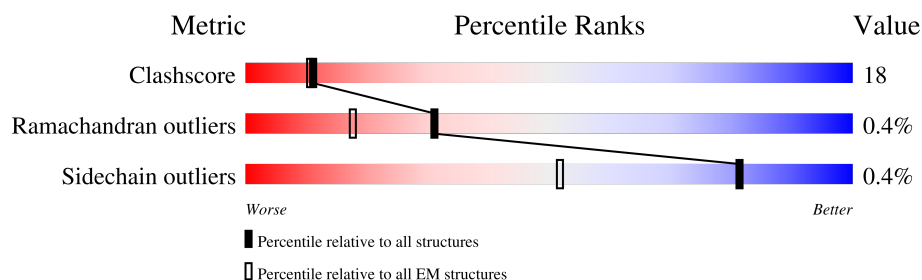
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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.



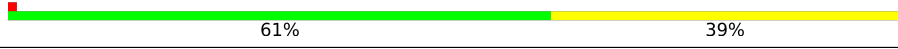
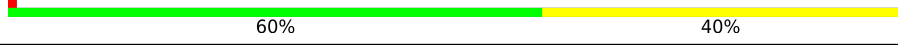
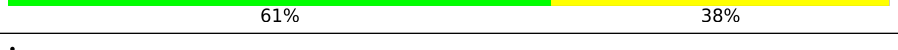
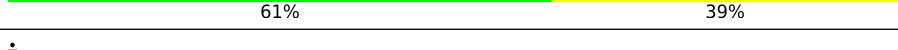
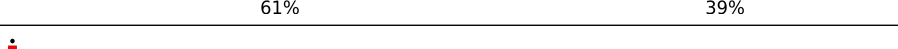
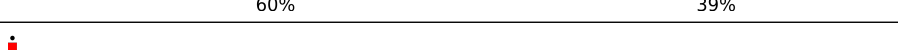
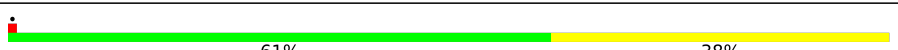
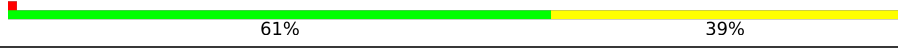
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12629 (3.08 - 4.08)

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

Mol	Chain	Length	Quality of chain
1	1	521	
1	2	521	
1	3	521	
1	4	521	

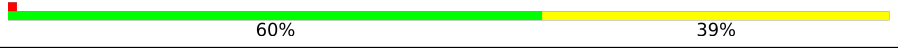
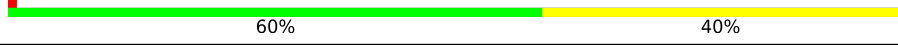
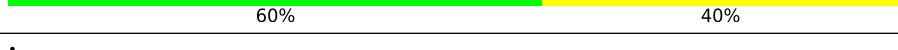
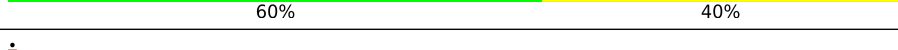
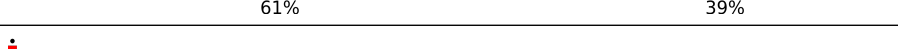
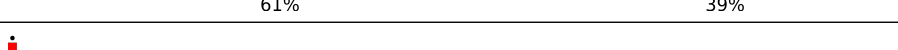
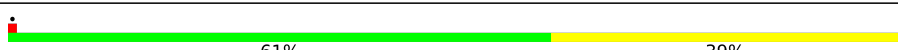
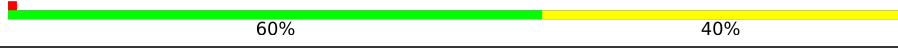
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Mol	Chain	Length	Quality of chain
1	5	521	
1	6	521	
1	7	521	
1	8	521	
1	A	521	
1	B	521	
1	C	521	
1	D	521	
1	E	521	
1	F	521	
1	G	521	
1	H	521	
1	I	521	
1	J	521	
1	K	521	
1	L	521	
1	M	521	
1	N	521	
1	O	521	
1	P	521	
1	Q	521	
1	R	521	
1	S	521	
1	T	521	
1	U	521	

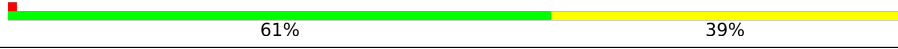
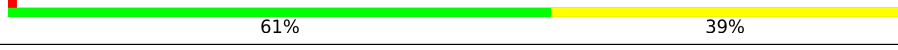
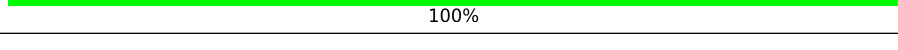
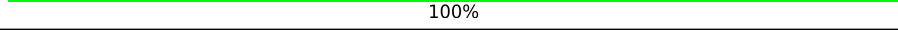
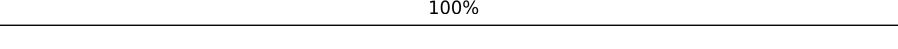
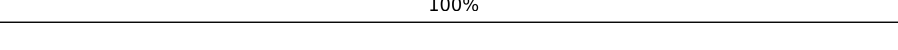
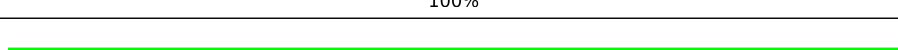
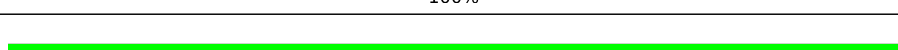
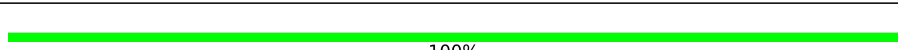
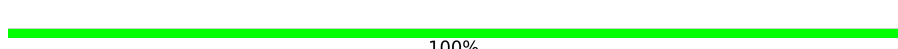
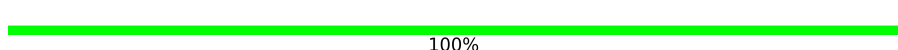
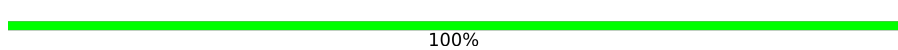
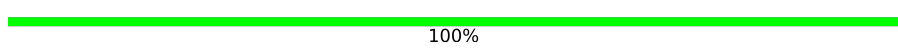
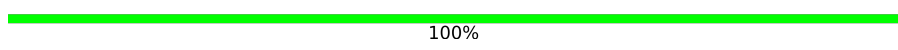
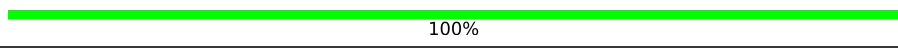
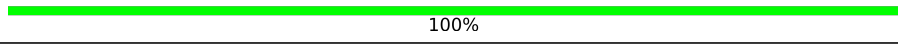
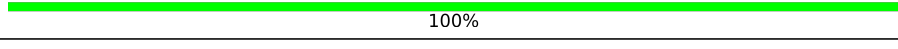
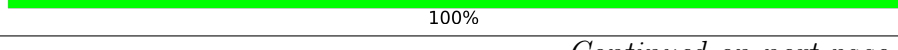
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Mol	Chain	Length	Quality of chain	
1	V	521		
1	W	521		
1	X	521		
1	Y	521		
1	Z	521		
1	a	521		
1	b	521		
1	c	521		
1	d	521		
1	e	521		
1	f	521		
1	g	521		
1	h	521		
1	i	521		
1	j	521		
1	k	521		
1	l	521		
1	m	521		
1	n	521		
1	o	521		
1	p	521		
1	q	521		
1	r	521		
1	s	521		
1	t	521		

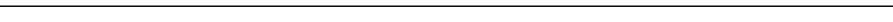
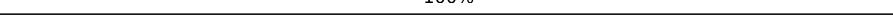
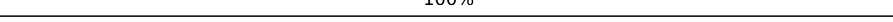
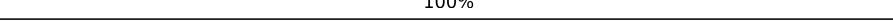
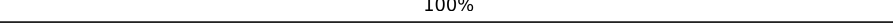
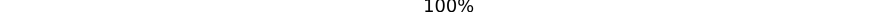
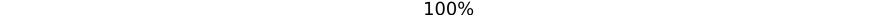
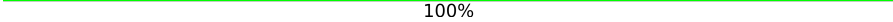
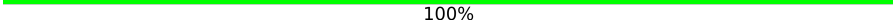
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Mol	Chain	Length	Quality of chain
1	u	521	 61%39%
1	v	521	 60%40%
1	w	521	 61%39%
1	x	521	 61%39%
1	y	521	 60%39%
1	z	521	 61%39%
2	0	2	 100%
2	0A	2	 100%
2	1A	2	 100%
2	2A	2	 100%
2	3A	2	 100%
2	4A	2	 100%
2	5A	2	 100%
2	9	2	 100%
2	AA	2	 100%
2	BA	2	 100%
2	CA	2	 100%
2	DA	2	 100%
2	EA	2	 100%
2	FA	2	 100%
2	GA	2	 100%
2	HA	2	 100%
2	IA	2	 100%
2	JA	2	 100%
2	KA	2	 100%

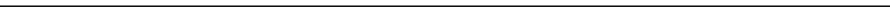
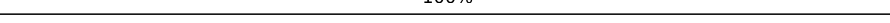
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Mol	Chain	Length	Quality of chain
2	LA	2	 100%
2	MA	2	 100%
2	NA	2	 100%
2	OA	2	 100%
2	PA	2	 100%
2	QA	2	 100%
2	RA	2	 100%
2	SA	2	 100%
2	TA	2	 100%
2	UA	2	 100%
2	VA	2	 100%
2	WA	2	 100%
2	XA	2	 100%
2	YA	2	 100%
2	ZA	2	 100%
2	aA	2	 100%
2	bA	2	 100%
2	cA	2	 100%
2	dA	2	 100%
2	eA	2	 100%
2	fA	2	 100%
2	gA	2	 100%
2	hA	2	 100%
2	iA	2	 100%
2	jA	2	 100%

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Mol	Chain	Length	Quality of chain
2	kA	2	 100%
2	lA	2	 100%
2	mA	2	 100%
2	nA	2	 100%
2	oA	2	 100%
2	pA	2	 100%
2	qA	2	 100%
2	rA	2	 100%
2	sA	2	 100%
2	tA	2	 100%
2	uA	2	 100%
2	vA	2	 100%
2	wA	2	 100%
2	xA	2	 100%
2	yA	2	 100%
2	zA	2	 100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 250920 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	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	B	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	C	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	D	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	E	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	F	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	G	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	H	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	I	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	J	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	K	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	L	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	M	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	N	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	O	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	P	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	Q	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	S	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	T	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	U	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	V	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	W	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	X	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	Y	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	Z	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	a	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	b	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	c	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	d	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	e	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	f	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	g	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	h	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	i	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	j	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	k	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	l	521	Total 4145	C 2617	N 717	O 797	S 14	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	n	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	o	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	p	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	q	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	r	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	s	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	t	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	u	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	v	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	w	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	x	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	y	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	z	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	1	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	2	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	3	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	4	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	5	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	6	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	7	521	Total 4145	C 2617	N 717	O 797	S 14	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ASN	SER	conflict	UNP B4Y886
A	417	GLN	THR	conflict	UNP B4Y886
B	315	ASN	SER	conflict	UNP B4Y886
B	417	GLN	THR	conflict	UNP B4Y886
C	315	ASN	SER	conflict	UNP B4Y886
C	417	GLN	THR	conflict	UNP B4Y886
D	315	ASN	SER	conflict	UNP B4Y886
D	417	GLN	THR	conflict	UNP B4Y886
E	315	ASN	SER	conflict	UNP B4Y886
E	417	GLN	THR	conflict	UNP B4Y886
F	315	ASN	SER	conflict	UNP B4Y886
F	417	GLN	THR	conflict	UNP B4Y886
G	315	ASN	SER	conflict	UNP B4Y886
G	417	GLN	THR	conflict	UNP B4Y886
H	315	ASN	SER	conflict	UNP B4Y886
H	417	GLN	THR	conflict	UNP B4Y886
I	315	ASN	SER	conflict	UNP B4Y886
I	417	GLN	THR	conflict	UNP B4Y886
J	315	ASN	SER	conflict	UNP B4Y886
J	417	GLN	THR	conflict	UNP B4Y886
K	315	ASN	SER	conflict	UNP B4Y886
K	417	GLN	THR	conflict	UNP B4Y886
L	315	ASN	SER	conflict	UNP B4Y886
L	417	GLN	THR	conflict	UNP B4Y886
M	315	ASN	SER	conflict	UNP B4Y886
M	417	GLN	THR	conflict	UNP B4Y886
N	315	ASN	SER	conflict	UNP B4Y886
N	417	GLN	THR	conflict	UNP B4Y886
O	315	ASN	SER	conflict	UNP B4Y886
O	417	GLN	THR	conflict	UNP B4Y886
P	315	ASN	SER	conflict	UNP B4Y886
P	417	GLN	THR	conflict	UNP B4Y886
Q	315	ASN	SER	conflict	UNP B4Y886
Q	417	GLN	THR	conflict	UNP B4Y886
R	315	ASN	SER	conflict	UNP B4Y886
R	417	GLN	THR	conflict	UNP B4Y886

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Chain	Residue	Modelled	Actual	Comment	Reference
S	315	ASN	SER	conflict	UNP B4Y886
S	417	GLN	THR	conflict	UNP B4Y886
T	315	ASN	SER	conflict	UNP B4Y886
T	417	GLN	THR	conflict	UNP B4Y886
U	315	ASN	SER	conflict	UNP B4Y886
U	417	GLN	THR	conflict	UNP B4Y886
V	315	ASN	SER	conflict	UNP B4Y886
V	417	GLN	THR	conflict	UNP B4Y886
W	315	ASN	SER	conflict	UNP B4Y886
W	417	GLN	THR	conflict	UNP B4Y886
X	315	ASN	SER	conflict	UNP B4Y886
X	417	GLN	THR	conflict	UNP B4Y886
Y	315	ASN	SER	conflict	UNP B4Y886
Y	417	GLN	THR	conflict	UNP B4Y886
Z	315	ASN	SER	conflict	UNP B4Y886
Z	417	GLN	THR	conflict	UNP B4Y886
a	315	ASN	SER	conflict	UNP B4Y886
a	417	GLN	THR	conflict	UNP B4Y886
b	315	ASN	SER	conflict	UNP B4Y886
b	417	GLN	THR	conflict	UNP B4Y886
c	315	ASN	SER	conflict	UNP B4Y886
c	417	GLN	THR	conflict	UNP B4Y886
d	315	ASN	SER	conflict	UNP B4Y886
d	417	GLN	THR	conflict	UNP B4Y886
e	315	ASN	SER	conflict	UNP B4Y886
e	417	GLN	THR	conflict	UNP B4Y886
f	315	ASN	SER	conflict	UNP B4Y886
f	417	GLN	THR	conflict	UNP B4Y886
g	315	ASN	SER	conflict	UNP B4Y886
g	417	GLN	THR	conflict	UNP B4Y886
h	315	ASN	SER	conflict	UNP B4Y886
h	417	GLN	THR	conflict	UNP B4Y886
i	315	ASN	SER	conflict	UNP B4Y886
i	417	GLN	THR	conflict	UNP B4Y886
j	315	ASN	SER	conflict	UNP B4Y886
j	417	GLN	THR	conflict	UNP B4Y886
k	315	ASN	SER	conflict	UNP B4Y886
k	417	GLN	THR	conflict	UNP B4Y886
l	315	ASN	SER	conflict	UNP B4Y886
l	417	GLN	THR	conflict	UNP B4Y886
m	315	ASN	SER	conflict	UNP B4Y886
m	417	GLN	THR	conflict	UNP B4Y886

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Chain	Residue	Modelled	Actual	Comment	Reference
n	315	ASN	SER	conflict	UNP B4Y886
n	417	GLN	THR	conflict	UNP B4Y886
o	315	ASN	SER	conflict	UNP B4Y886
o	417	GLN	THR	conflict	UNP B4Y886
p	315	ASN	SER	conflict	UNP B4Y886
p	417	GLN	THR	conflict	UNP B4Y886
q	315	ASN	SER	conflict	UNP B4Y886
q	417	GLN	THR	conflict	UNP B4Y886
r	315	ASN	SER	conflict	UNP B4Y886
r	417	GLN	THR	conflict	UNP B4Y886
s	315	ASN	SER	conflict	UNP B4Y886
s	417	GLN	THR	conflict	UNP B4Y886
t	315	ASN	SER	conflict	UNP B4Y886
t	417	GLN	THR	conflict	UNP B4Y886
u	315	ASN	SER	conflict	UNP B4Y886
u	417	GLN	THR	conflict	UNP B4Y886
v	315	ASN	SER	conflict	UNP B4Y886
v	417	GLN	THR	conflict	UNP B4Y886
w	315	ASN	SER	conflict	UNP B4Y886
w	417	GLN	THR	conflict	UNP B4Y886
x	315	ASN	SER	conflict	UNP B4Y886
x	417	GLN	THR	conflict	UNP B4Y886
y	315	ASN	SER	conflict	UNP B4Y886
y	417	GLN	THR	conflict	UNP B4Y886
z	315	ASN	SER	conflict	UNP B4Y886
z	417	GLN	THR	conflict	UNP B4Y886
1	315	ASN	SER	conflict	UNP B4Y886
1	417	GLN	THR	conflict	UNP B4Y886
2	315	ASN	SER	conflict	UNP B4Y886
2	417	GLN	THR	conflict	UNP B4Y886
3	315	ASN	SER	conflict	UNP B4Y886
3	417	GLN	THR	conflict	UNP B4Y886
4	315	ASN	SER	conflict	UNP B4Y886
4	417	GLN	THR	conflict	UNP B4Y886
5	315	ASN	SER	conflict	UNP B4Y886
5	417	GLN	THR	conflict	UNP B4Y886
6	315	ASN	SER	conflict	UNP B4Y886
6	417	GLN	THR	conflict	UNP B4Y886
7	315	ASN	SER	conflict	UNP B4Y886
7	417	GLN	THR	conflict	UNP B4Y886
8	315	ASN	SER	conflict	UNP B4Y886
8	417	GLN	THR	conflict	UNP B4Y886

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	9	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	AA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	BA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	CA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	DA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	EA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	FA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	GA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	HA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	IA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	JA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	KA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	LA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	MA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	NA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	OA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	PA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	QA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	RA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	SA	2	Total 37	C 19	N 8	O 9	P 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	TA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	UA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	VA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	WA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	XA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	YA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	ZA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	aA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	bA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	cA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	dA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	eA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	fA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	gA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	hA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	iA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	jA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	kA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	lA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	mA	2	Total 37	C 19	N 8	O 9	P 1	0	0
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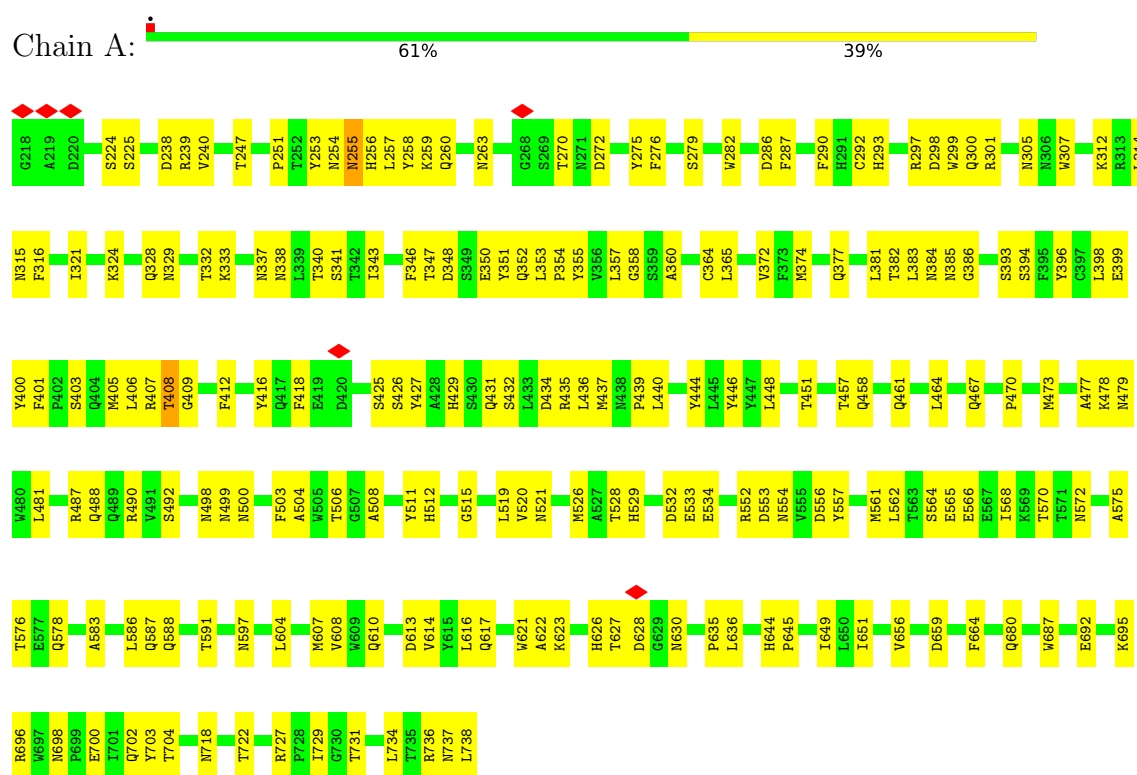
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Mol	Chain	Residues	Atoms					AltConf	Trace
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2	pA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	qA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	rA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	sA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	tA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	uA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	vA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	wA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	xA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	yA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	zA	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	0A	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	1A	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	2A	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	3A	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	4A	2	Total 37	C 19	N 8	O 9	P 1	0	0
2	5A	2	Total 37	C 19	N 8	O 9	P 1	0	0

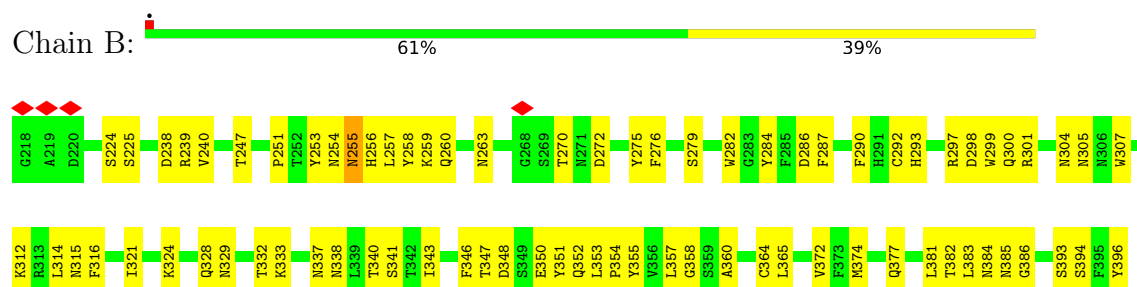
3 Residue-property plots

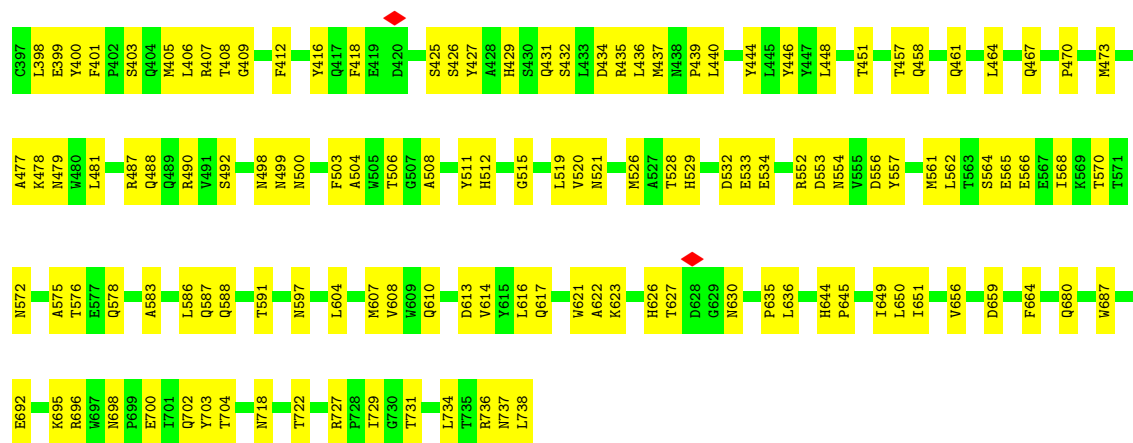
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Capsid protein VP1

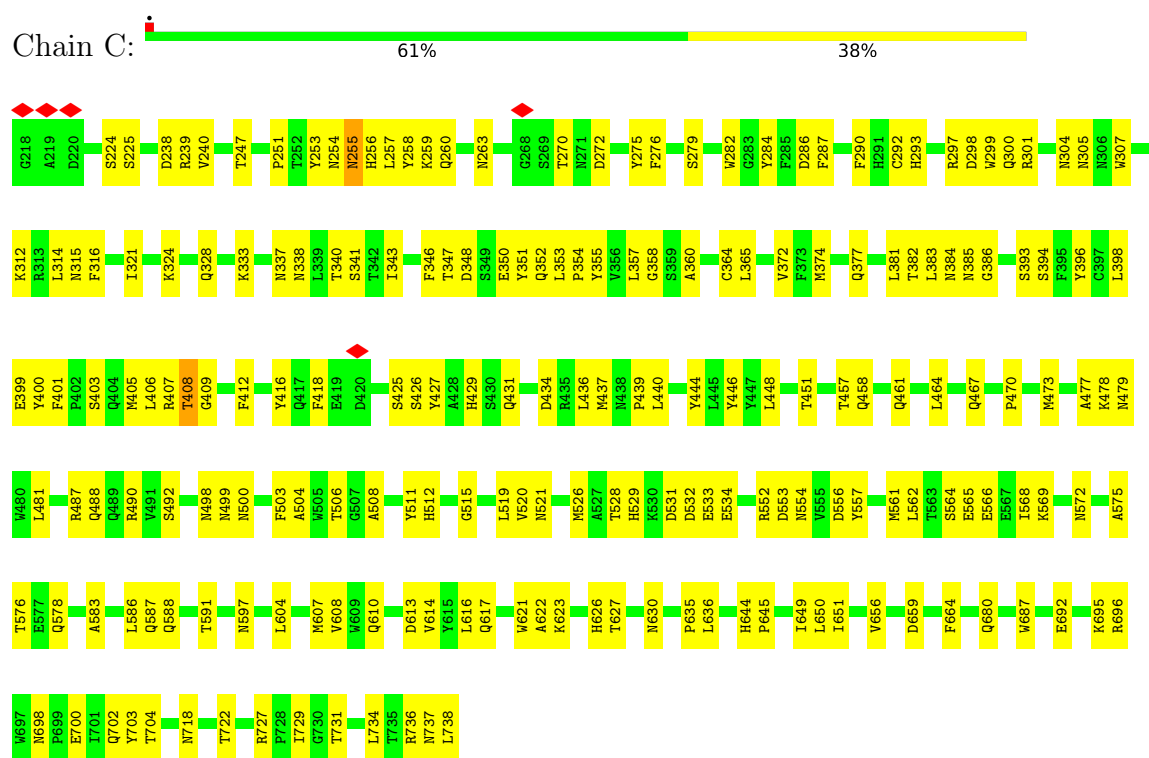


• Molecule 1: Capsid protein VP1

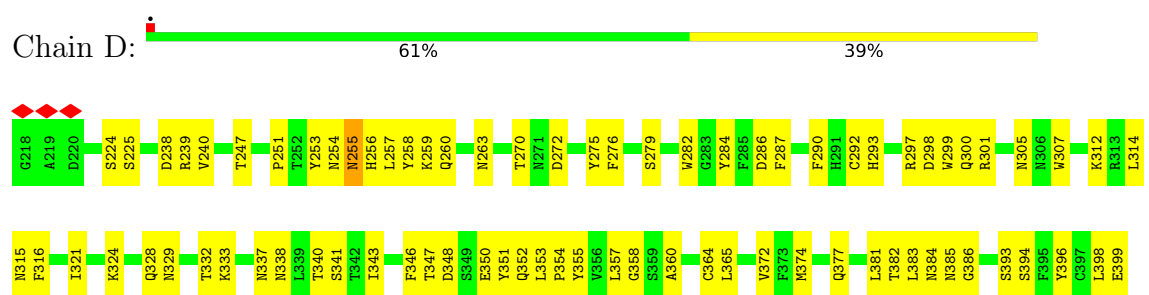


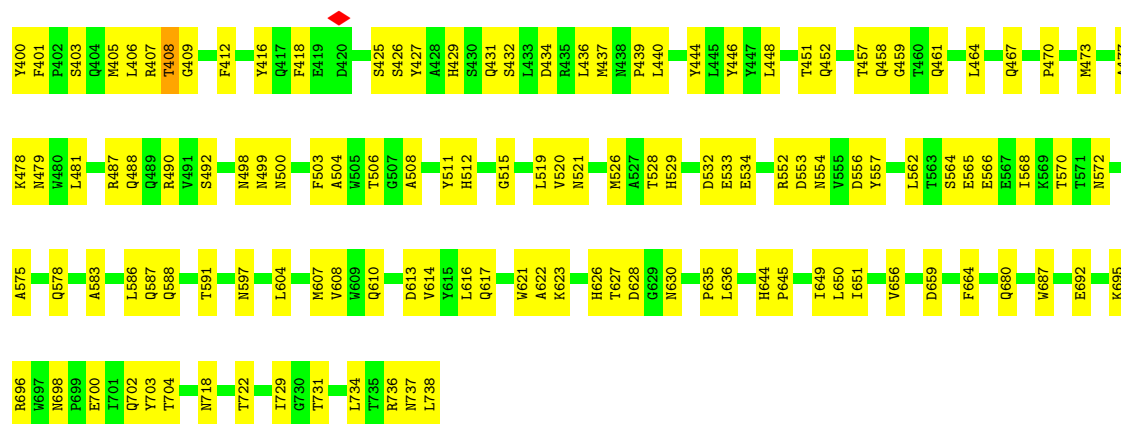


• Molecule 1: Capsid protein VP1

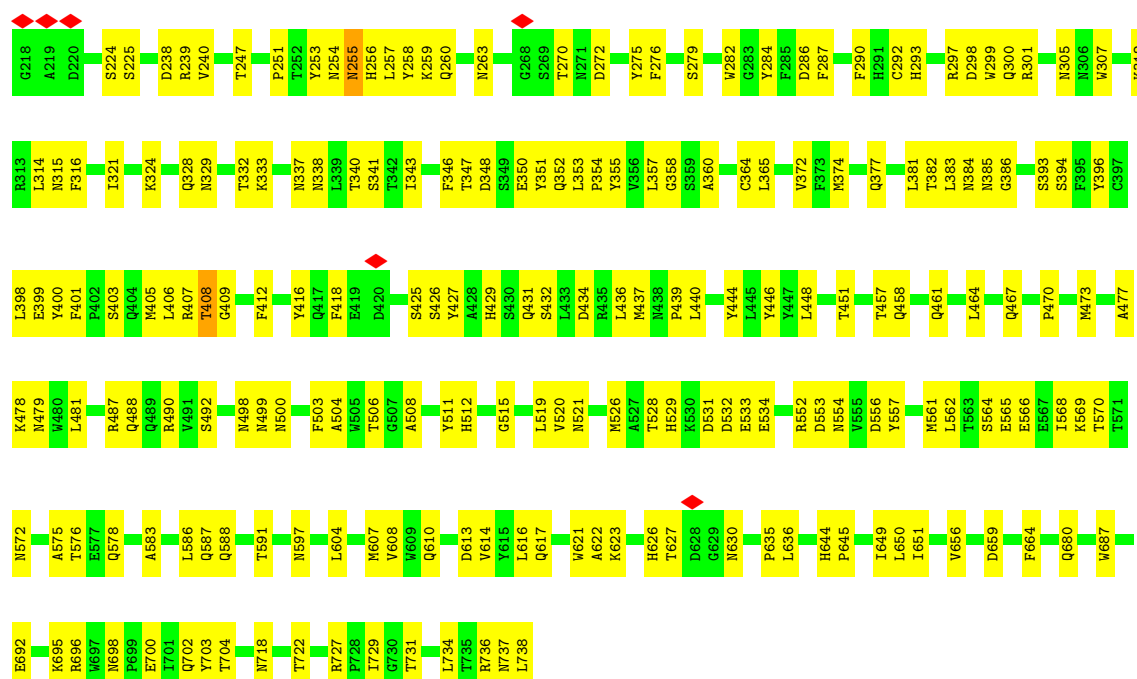


• Molecule 1: Capsid protein VP1

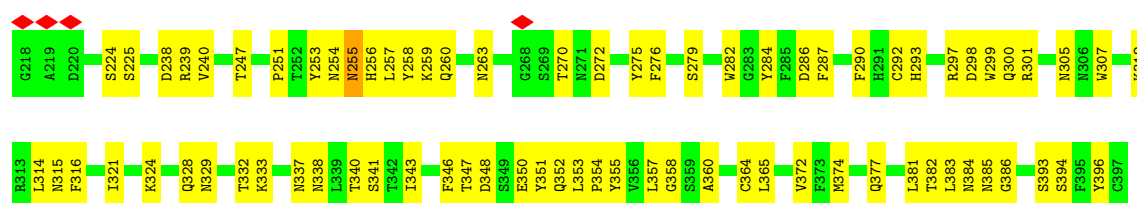


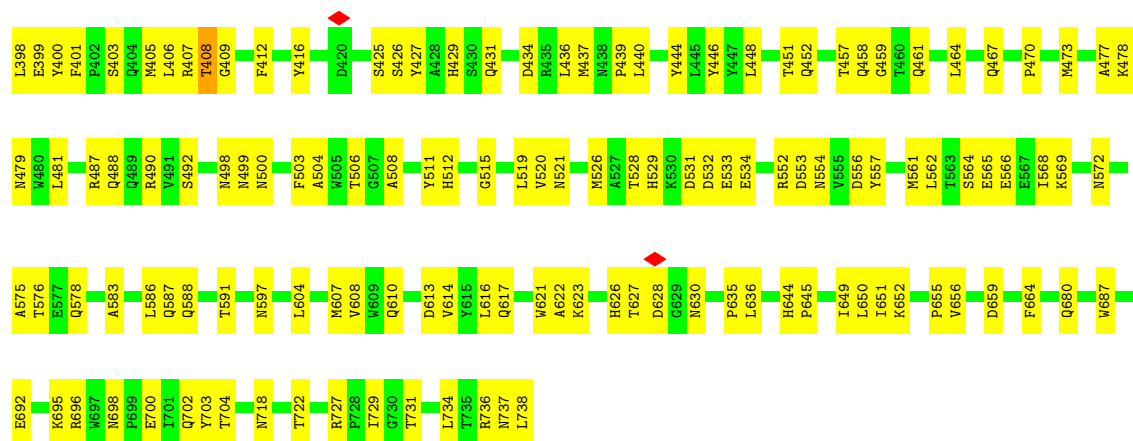


• Molecule 1: Capsid protein VP1

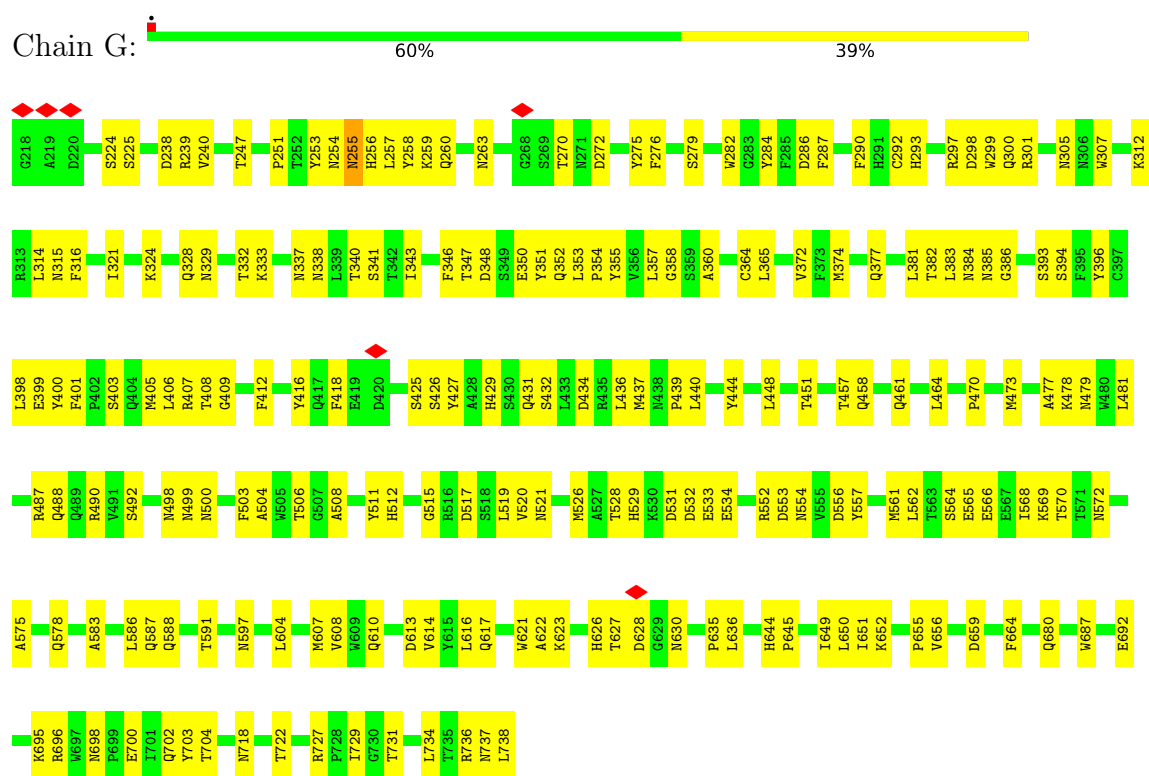


• Molecule 1: Capsid protein VP1

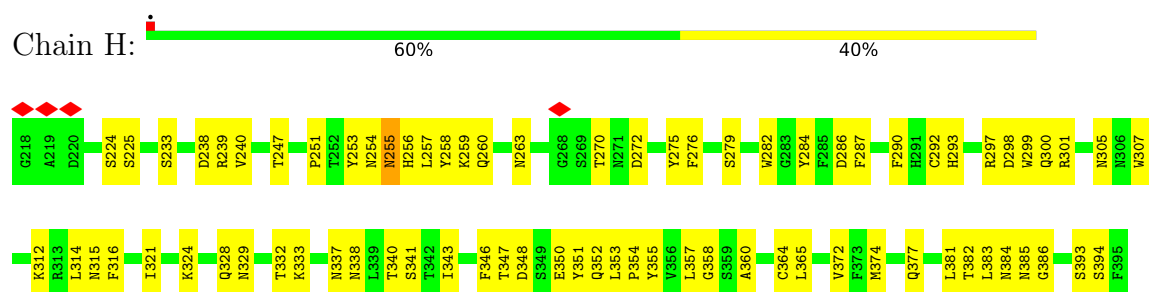


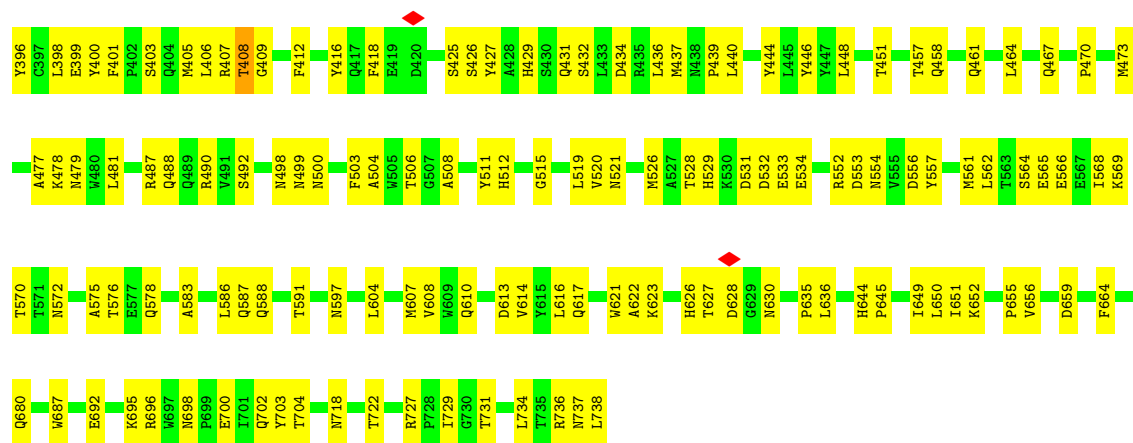


• Molecule 1: Capsid protein VP1

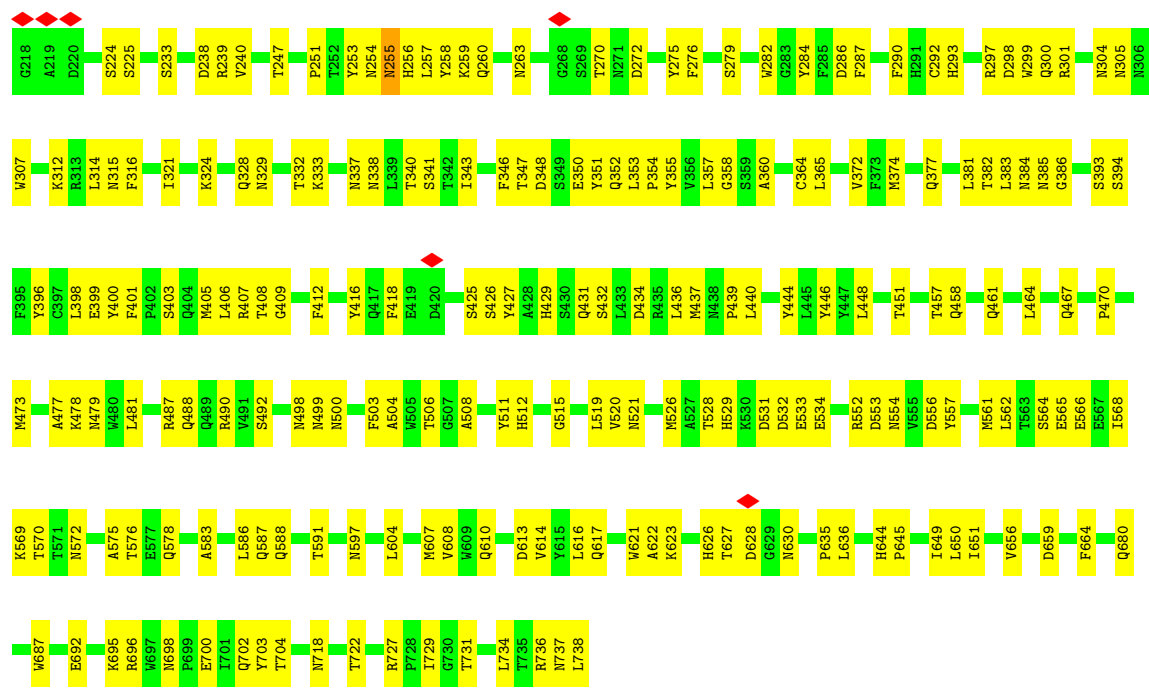


• Molecule 1: Capsid protein VP1

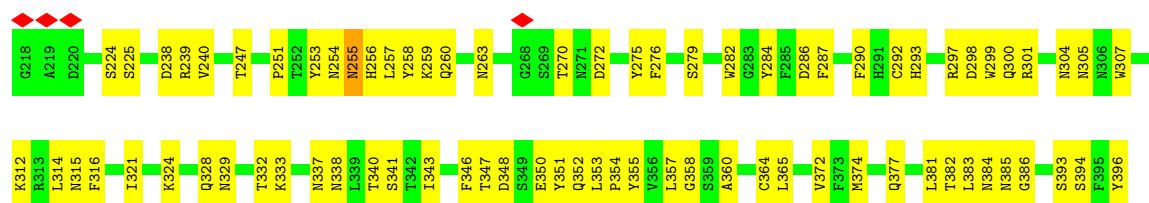


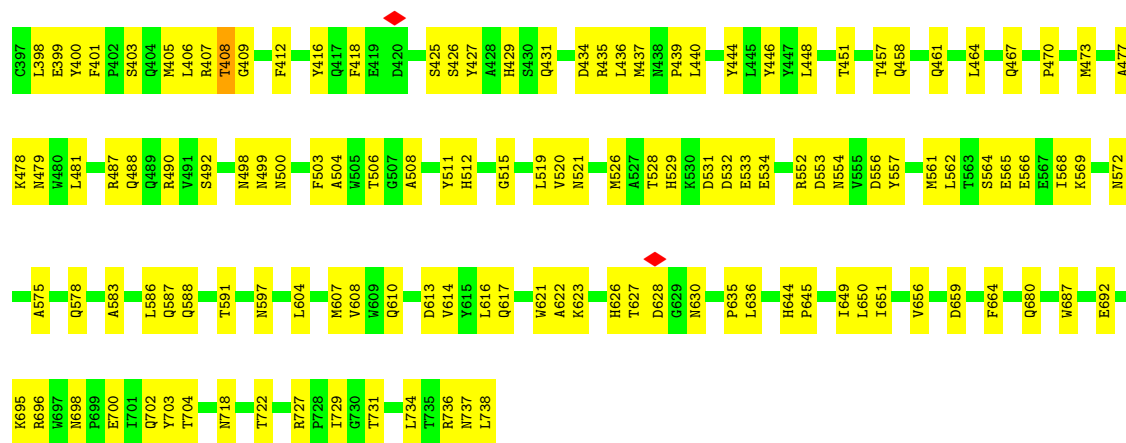


• Molecule 1: Capsid protein VP1

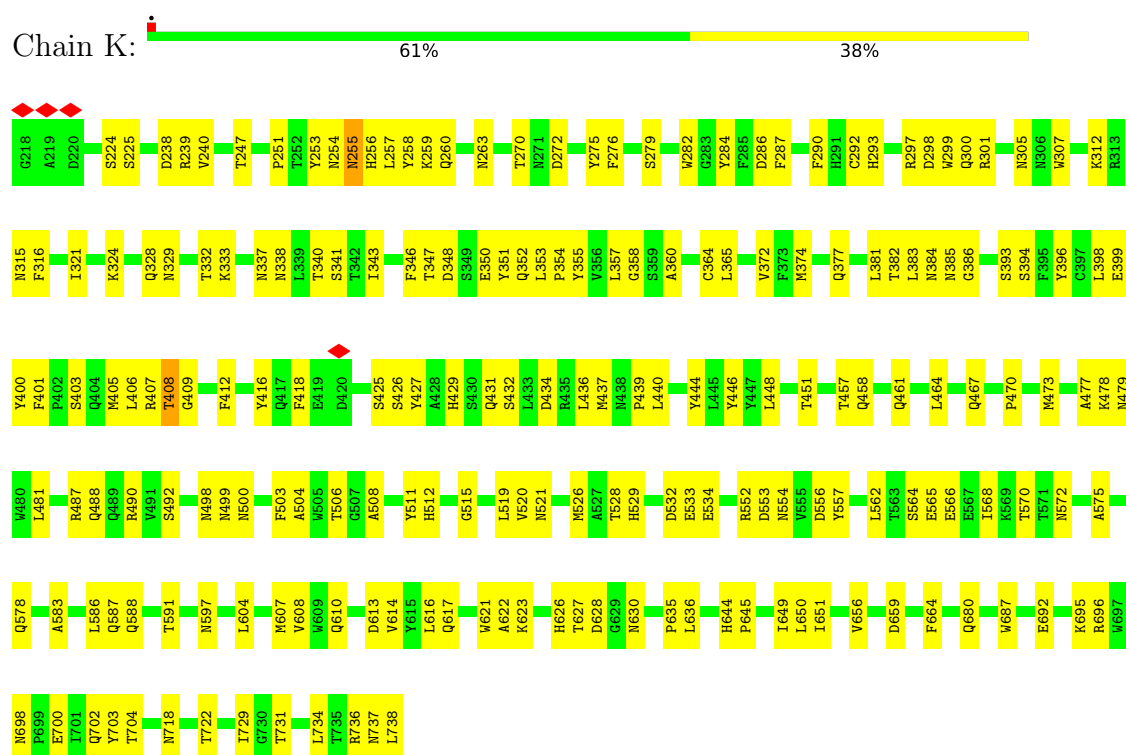


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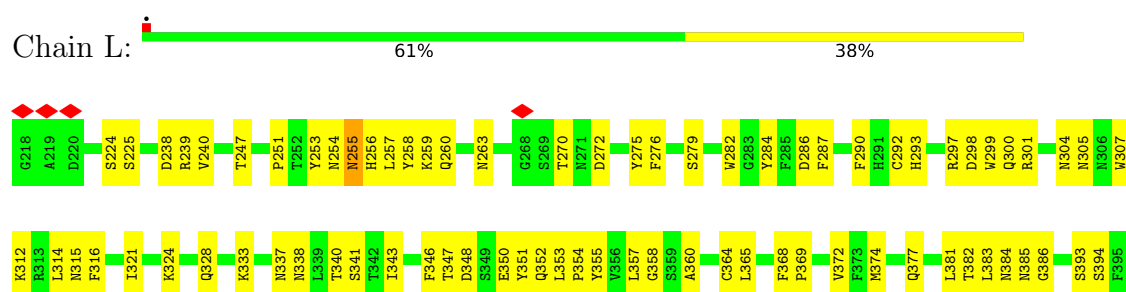


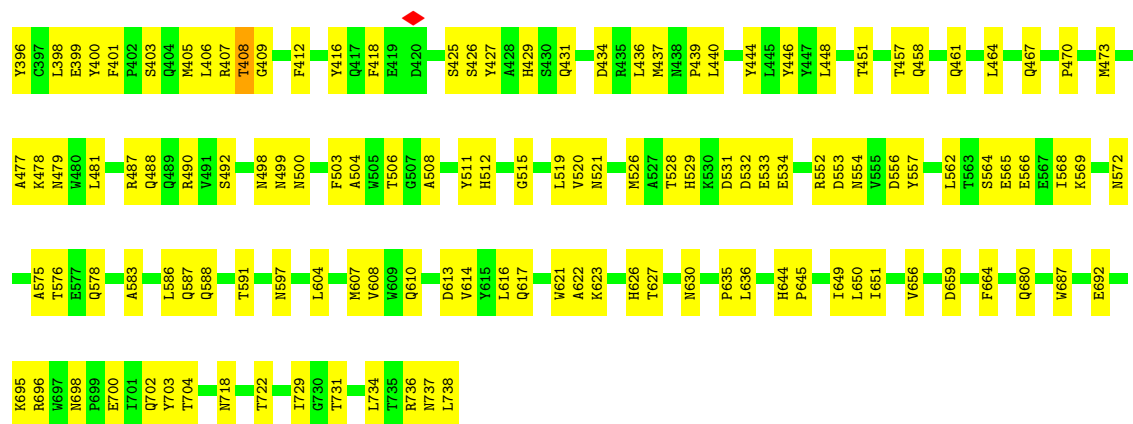


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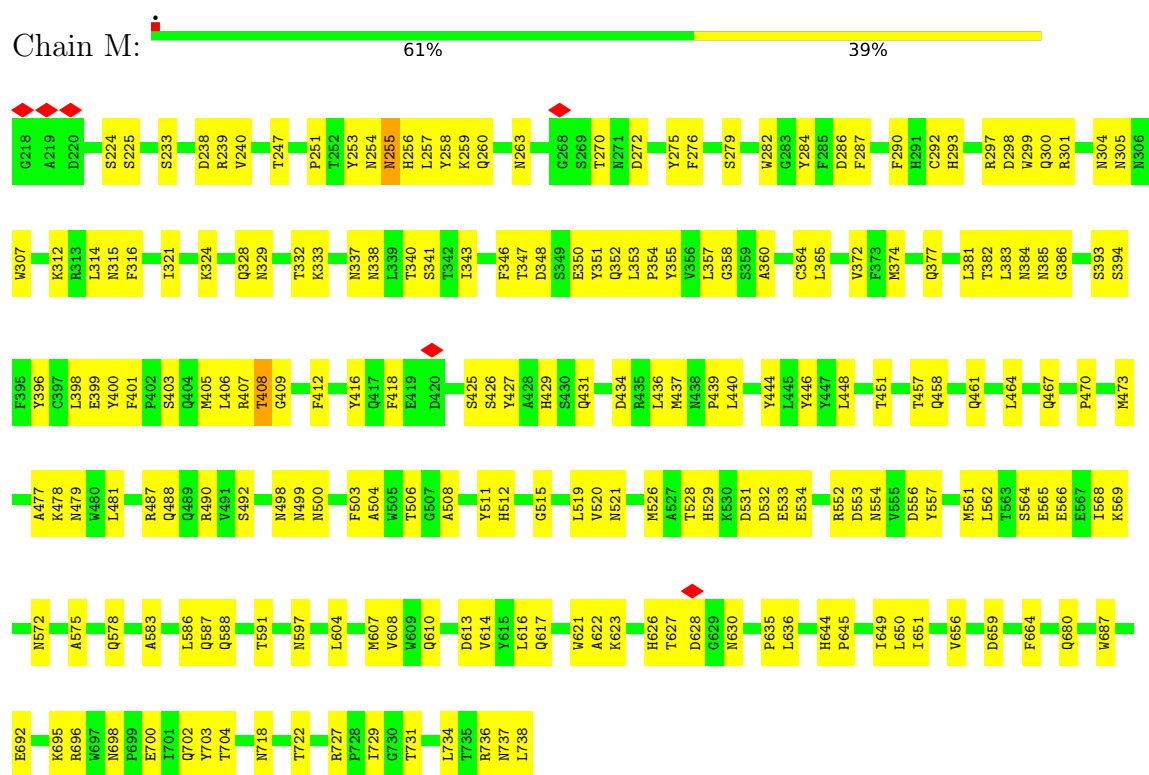


• Molecule 1: Capsid protein VP1

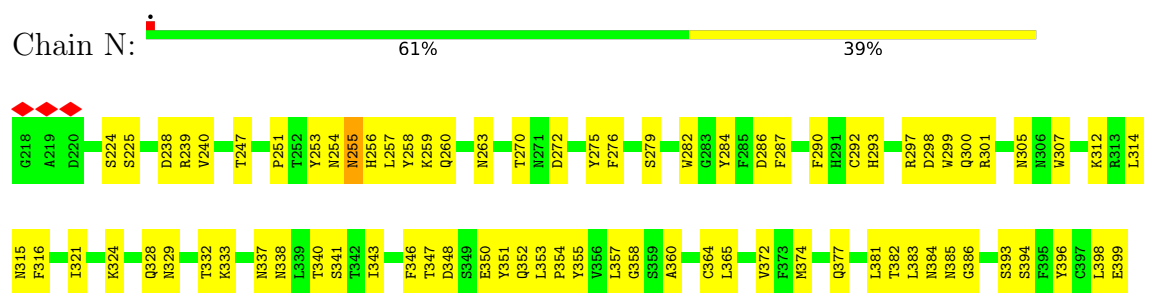




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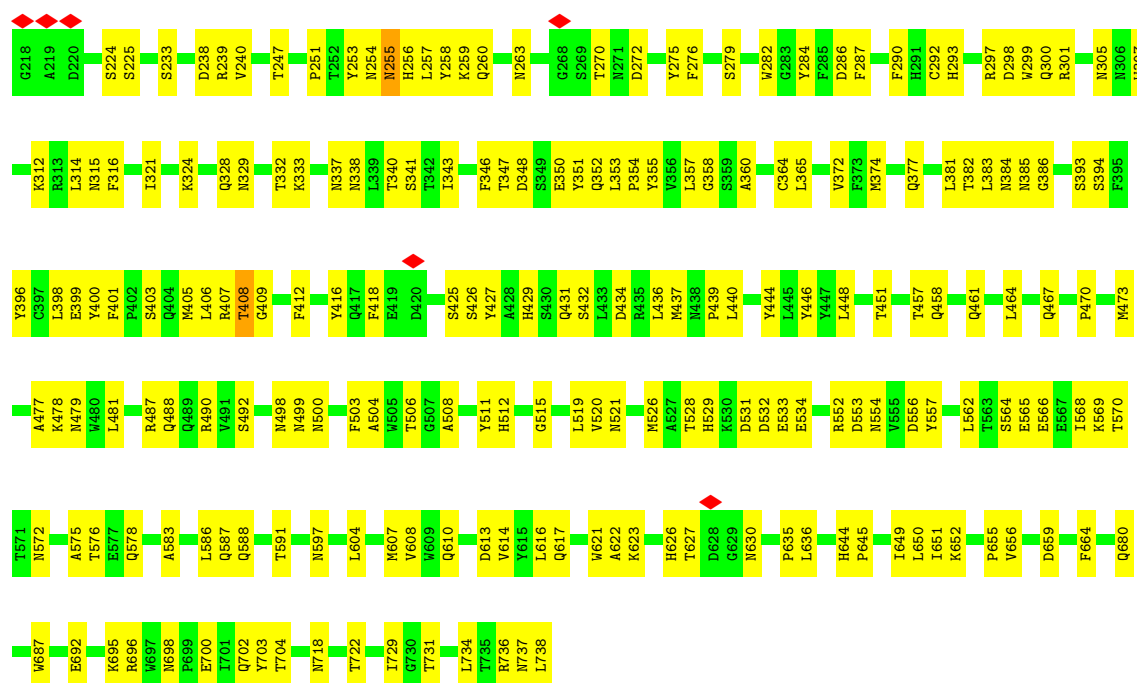


• Molecule 1: Capsid protein VP1

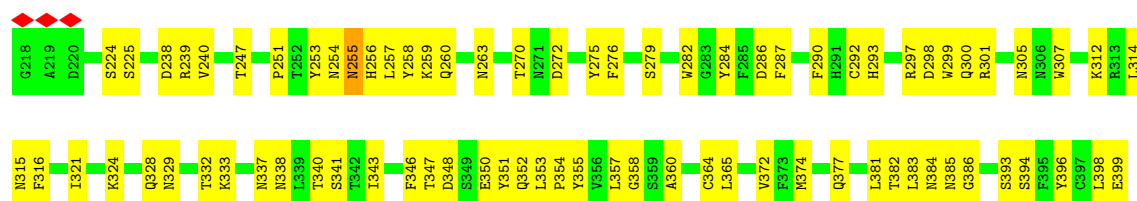


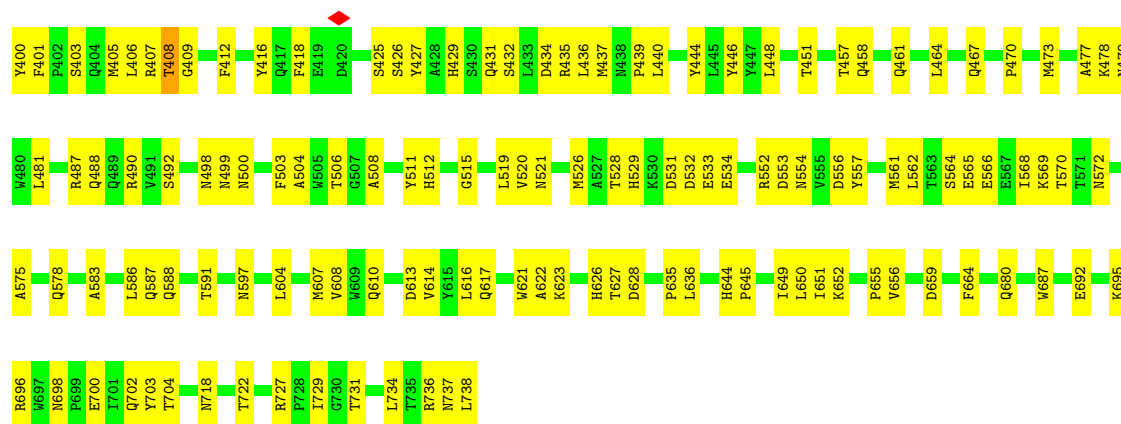


• Molecule 1: Capsid protein VP1

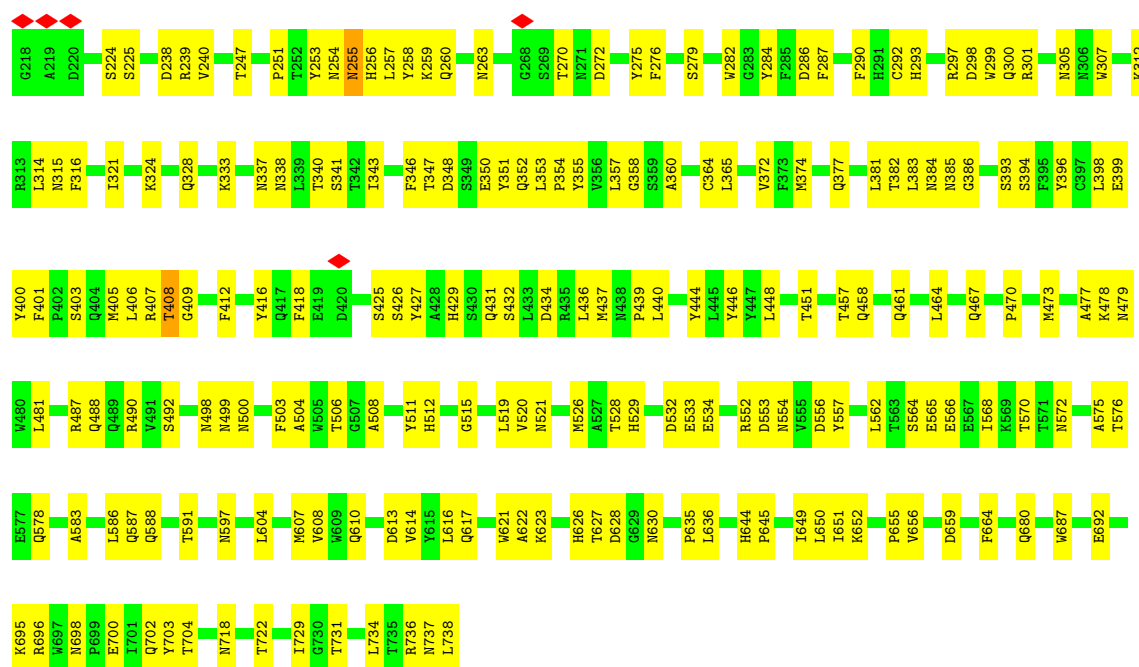


• Molecule 1: Capsid protein VP1

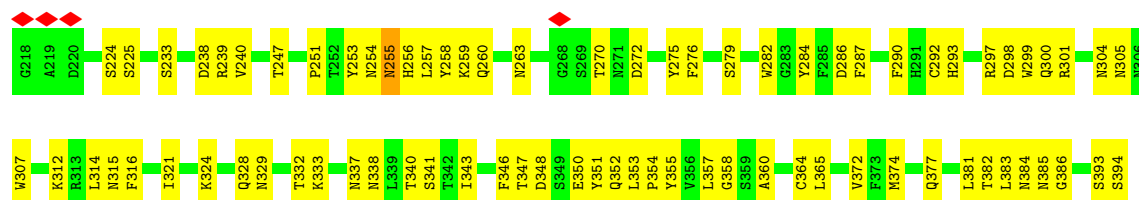


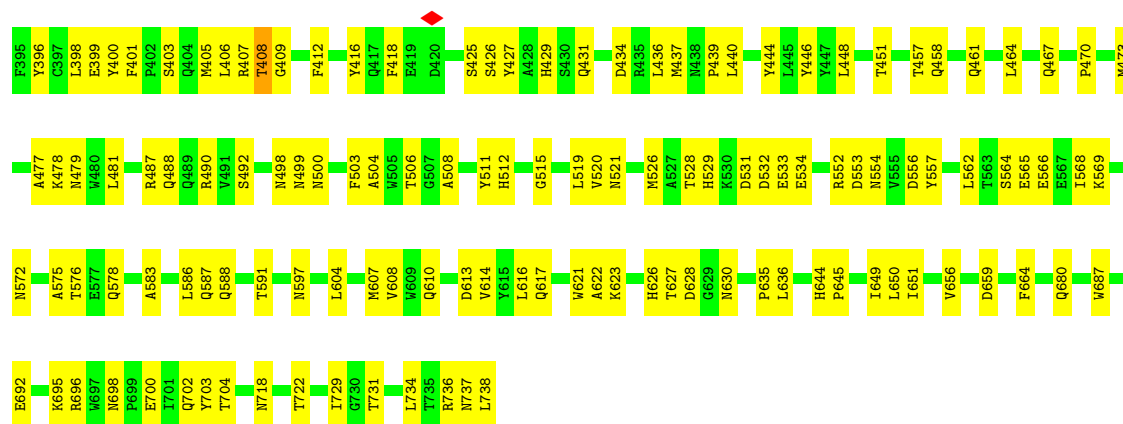


• Molecule 1: Capsid protein VP1

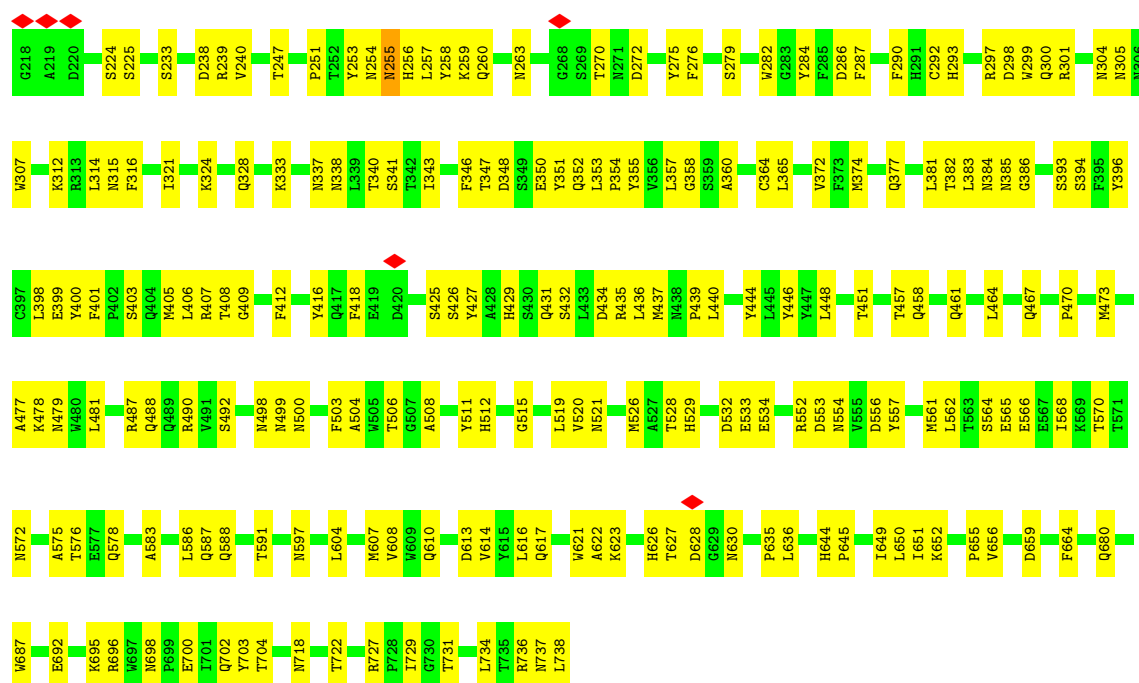


• Molecule 1: Capsid protein VP1

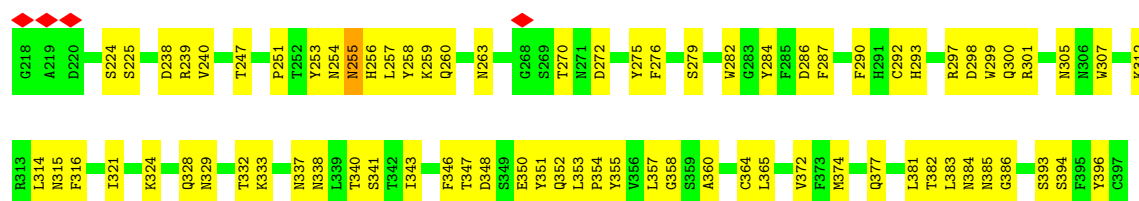


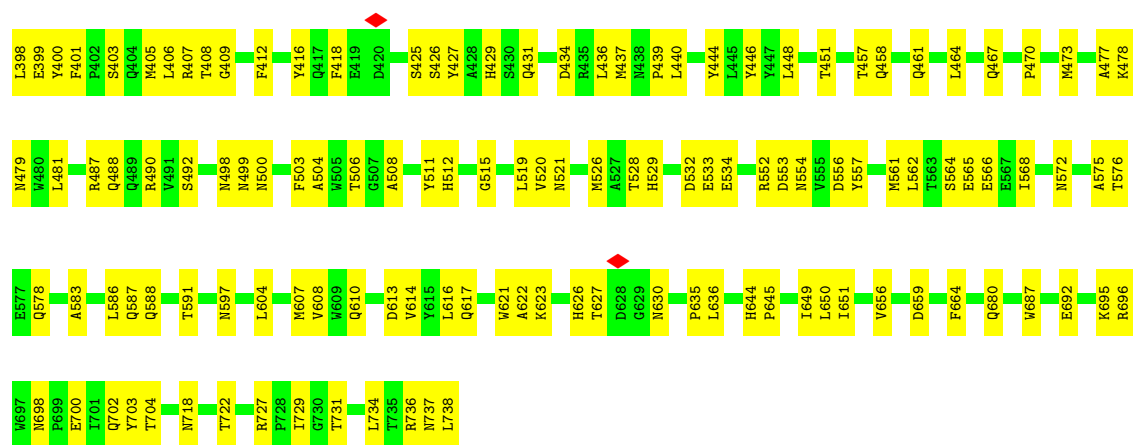


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

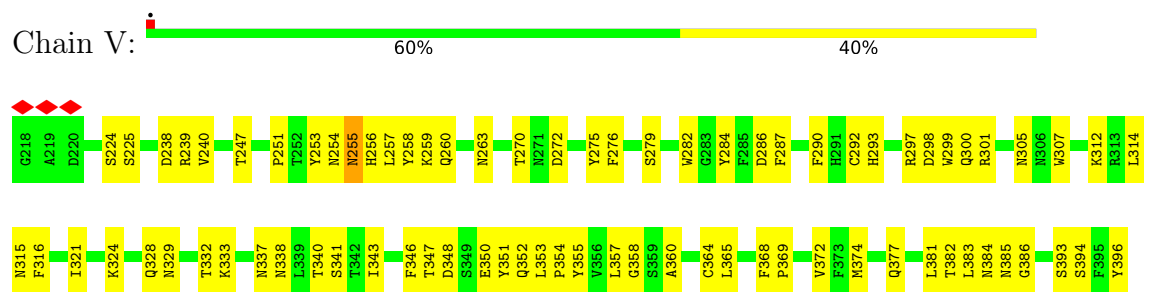




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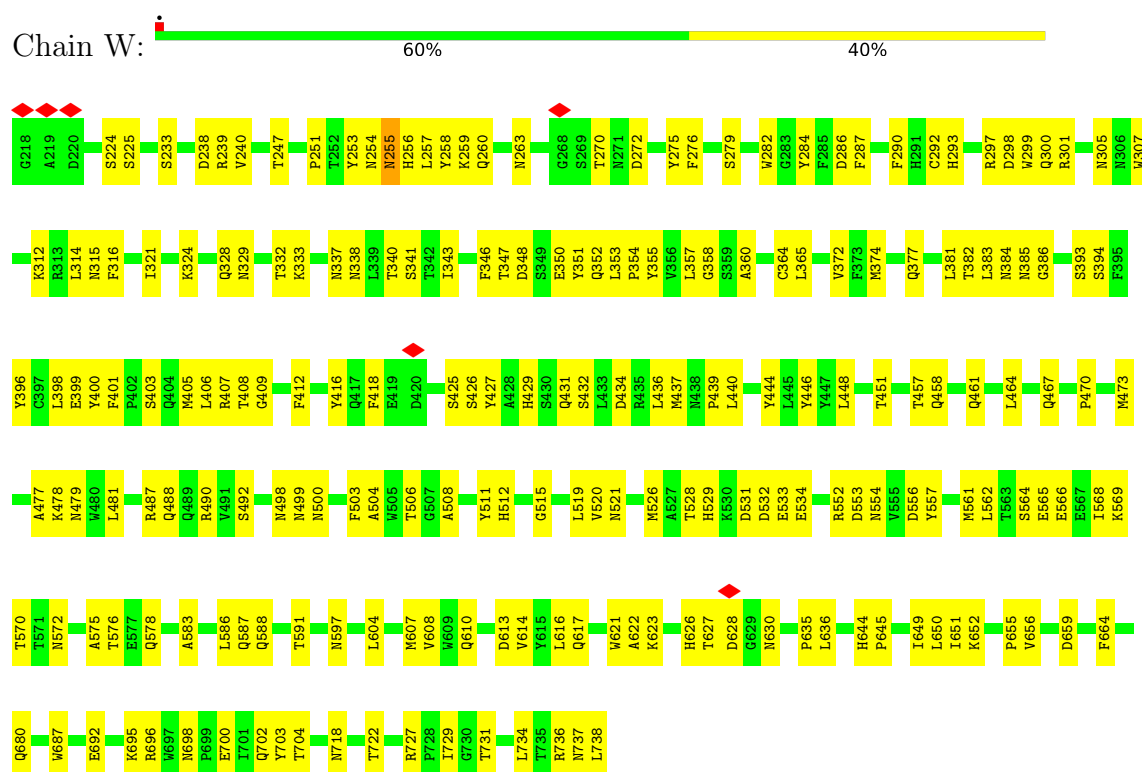


• Molecule 1: Capsid protein VP1

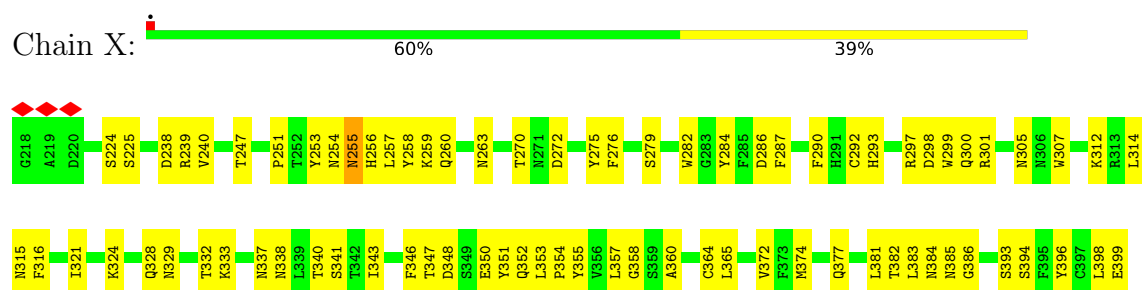


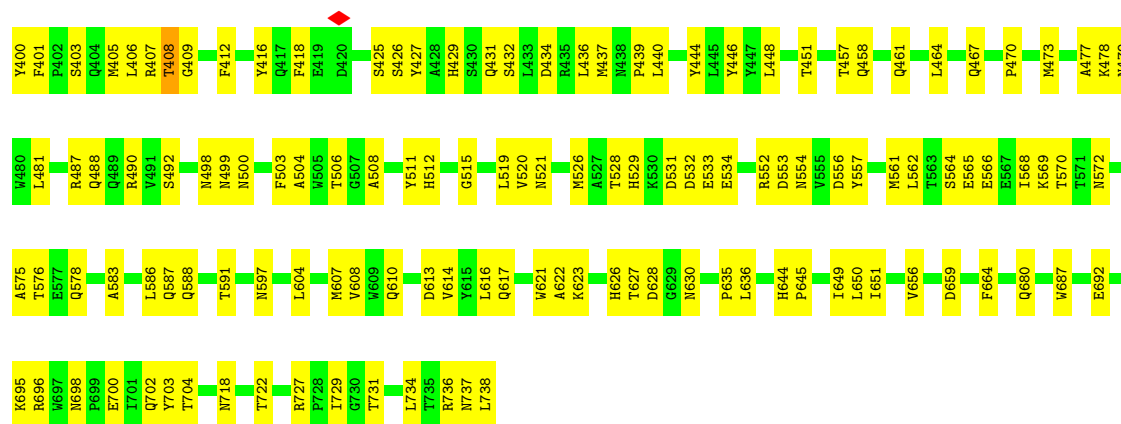


• Molecule 1: Capsid protein VP1

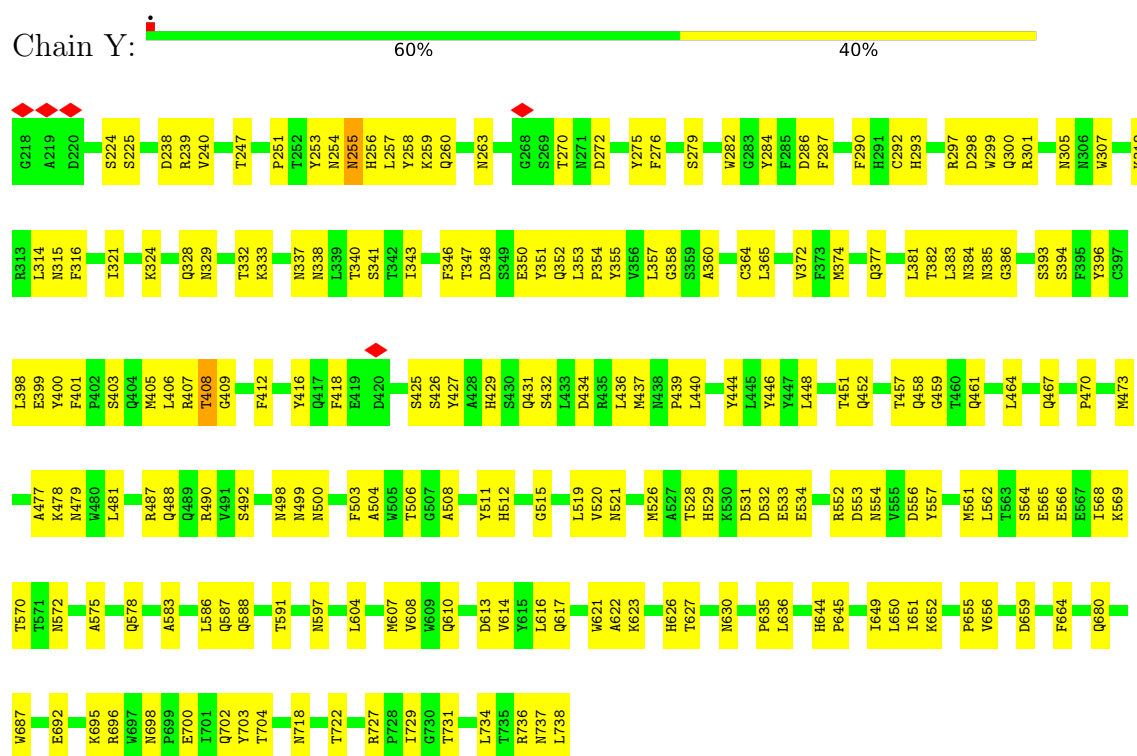


• Molecule 1: Capsid protein VP1

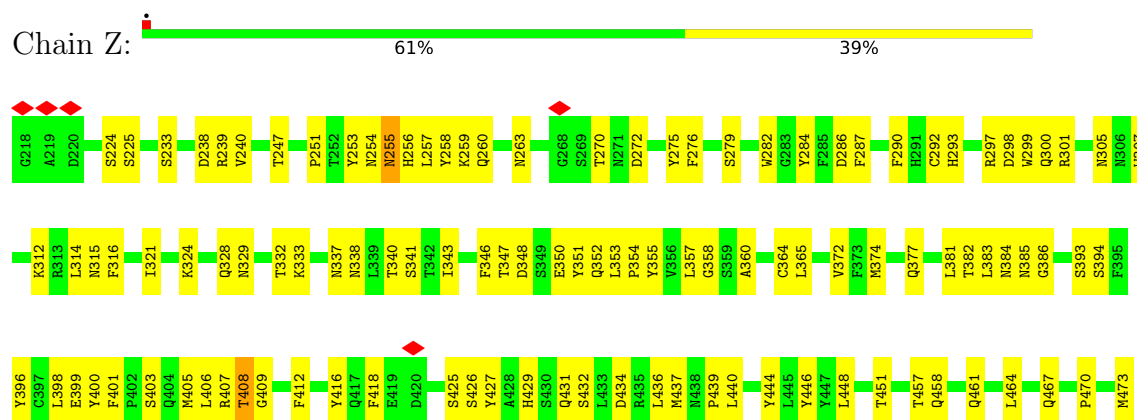


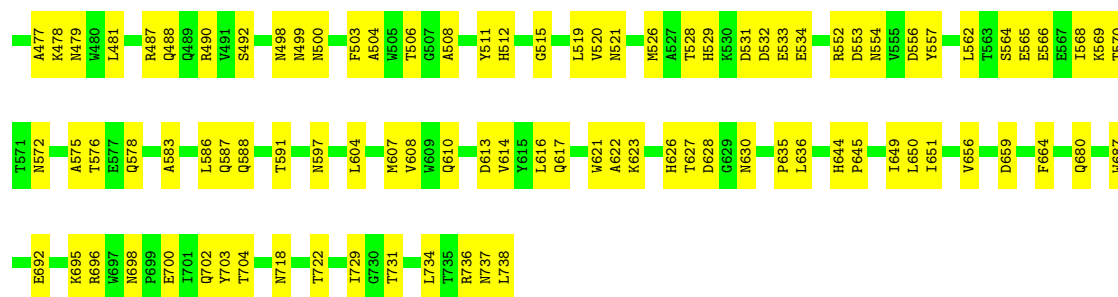


• Molecule 1: Capsid protein VP1

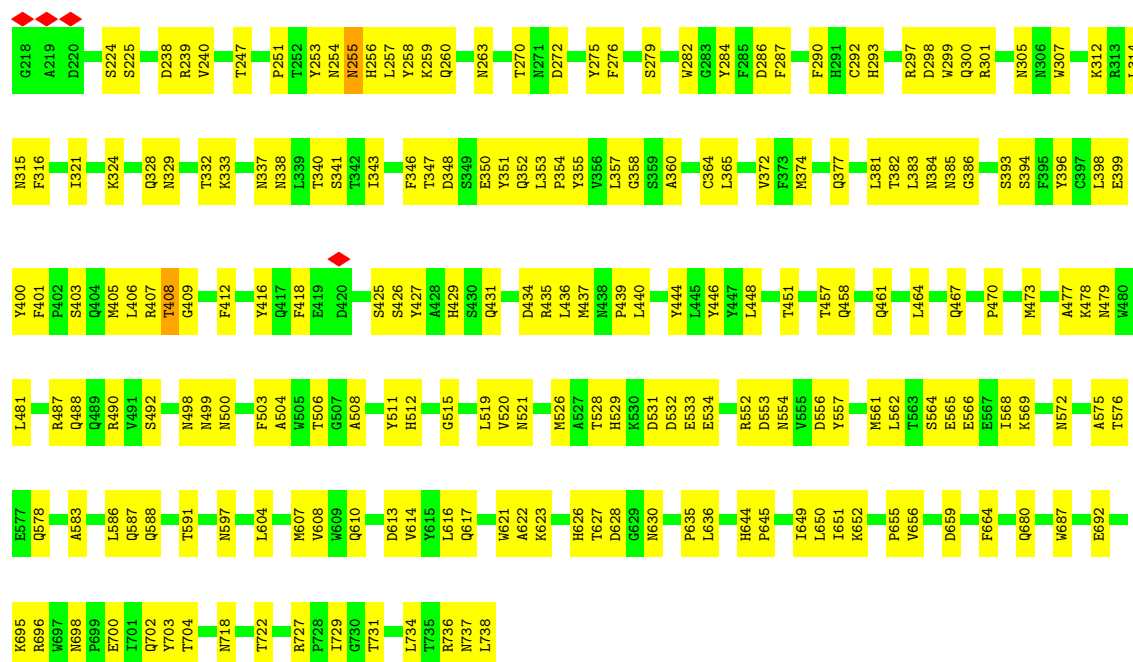


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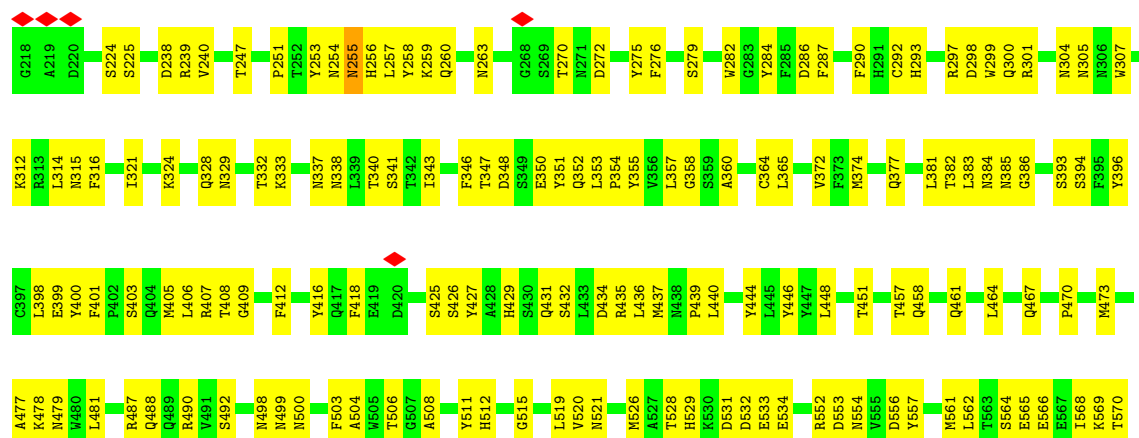


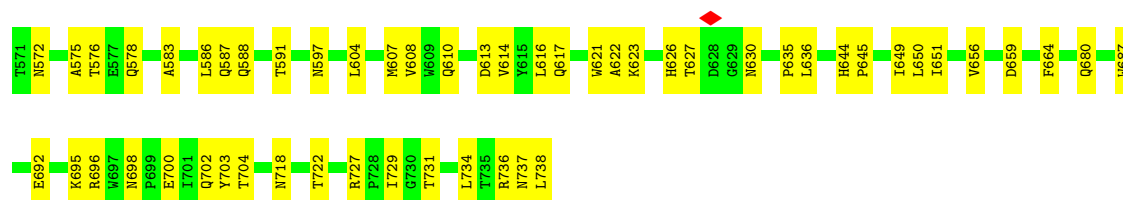


• Molecule 1: Capsid protein VP1

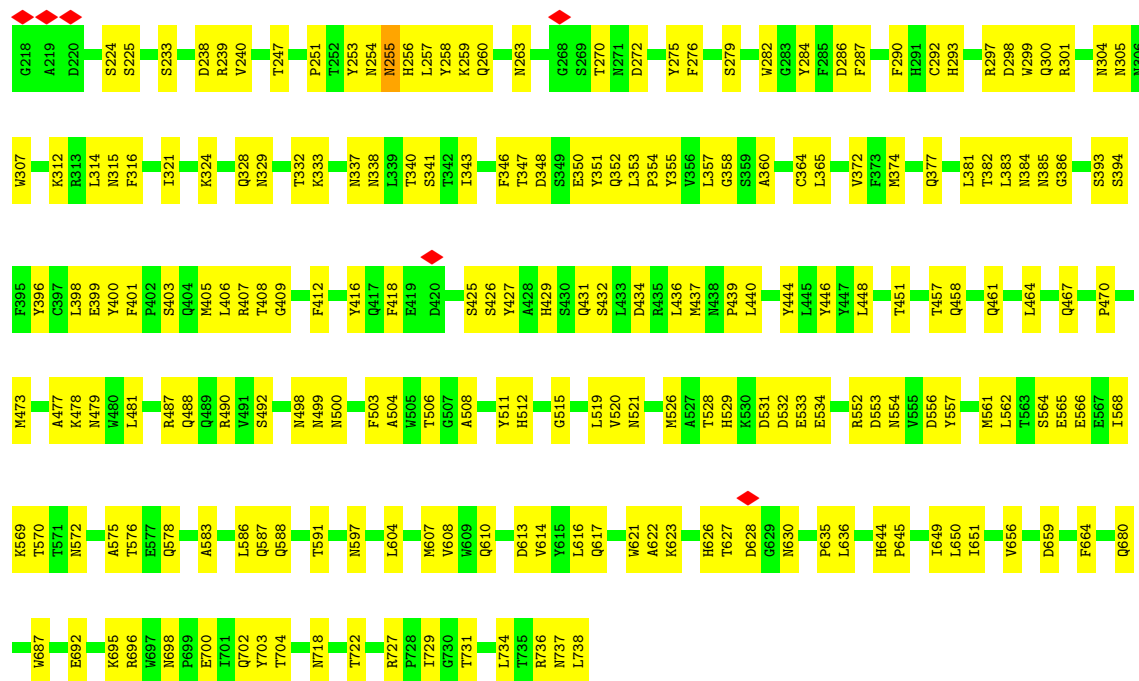


• Molecule 1: Capsid protein VP1

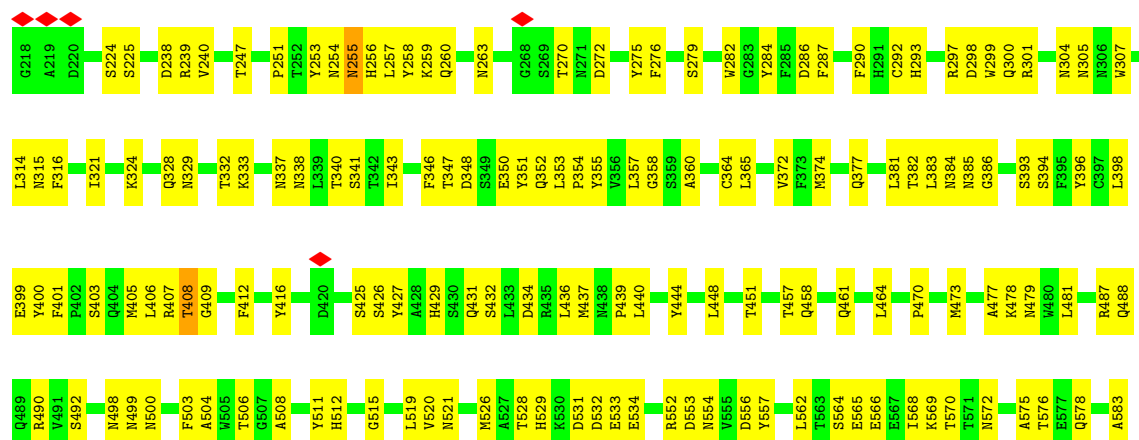


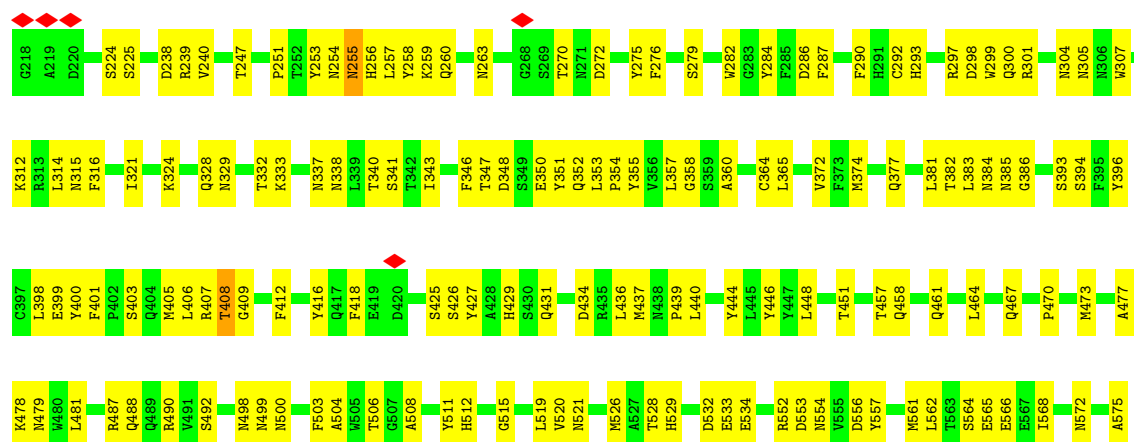


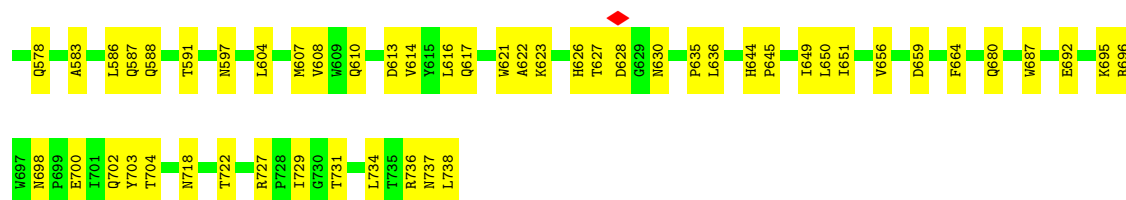
• Molecule 1: Capsid protein VP1



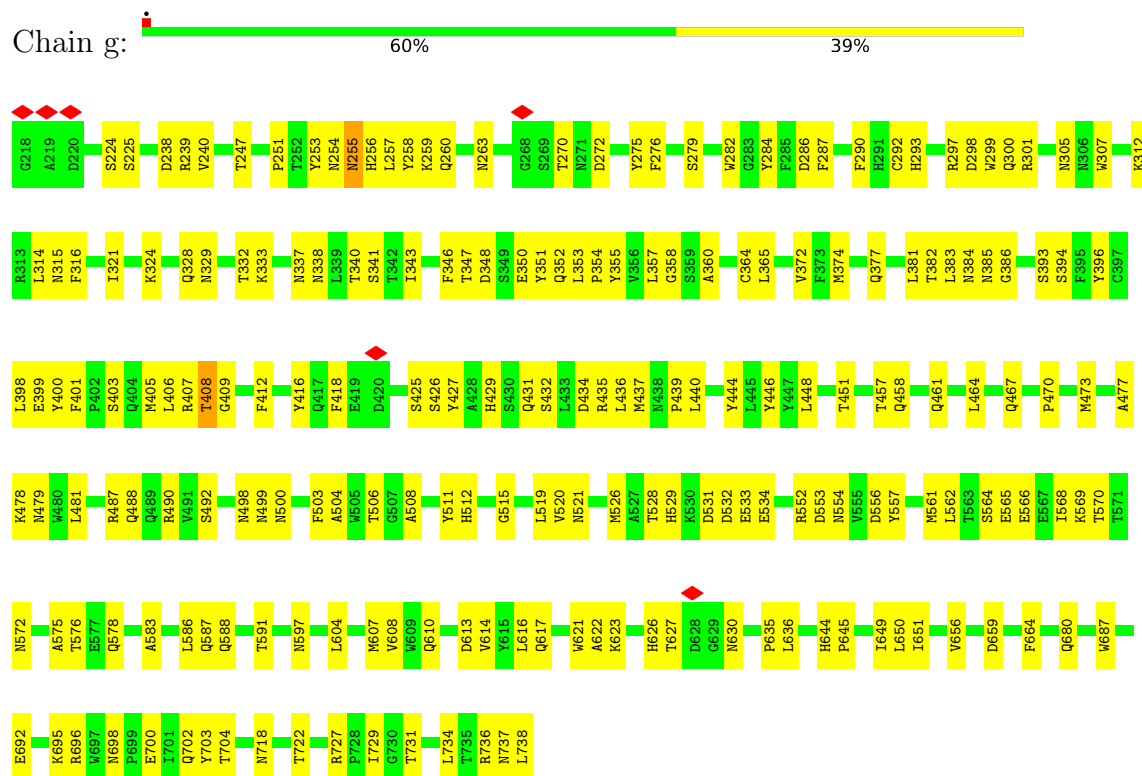
• Molecule 1: Capsid protein VP1



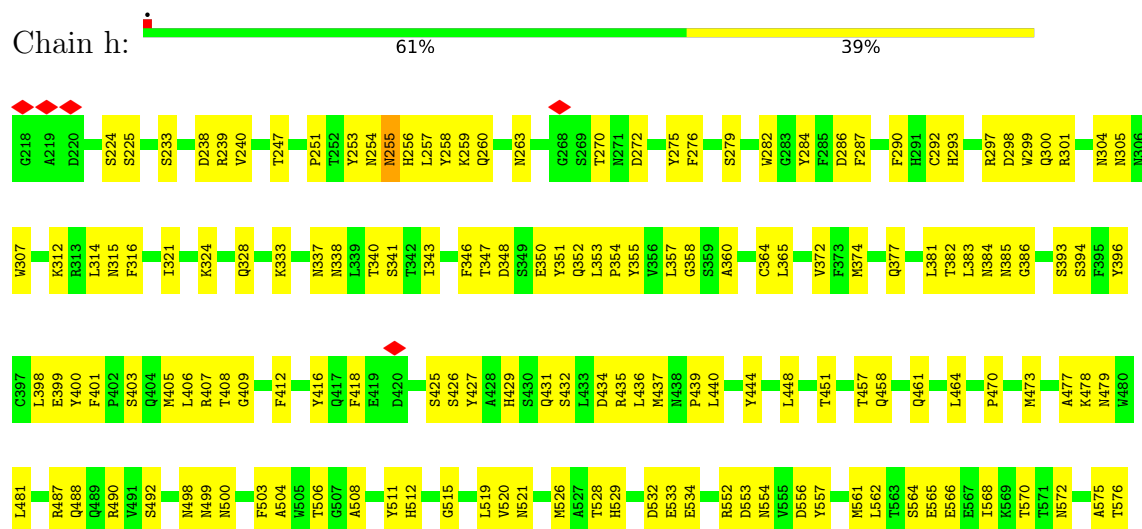


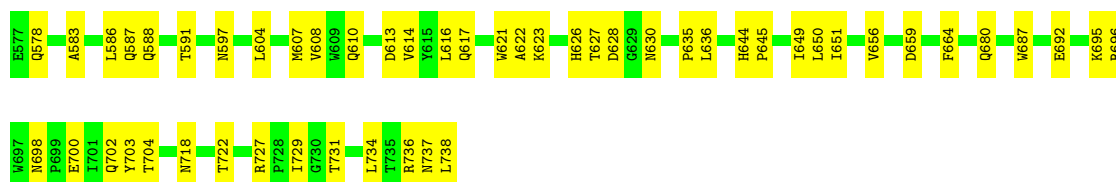


• Molecule 1: Capsid protein VP1

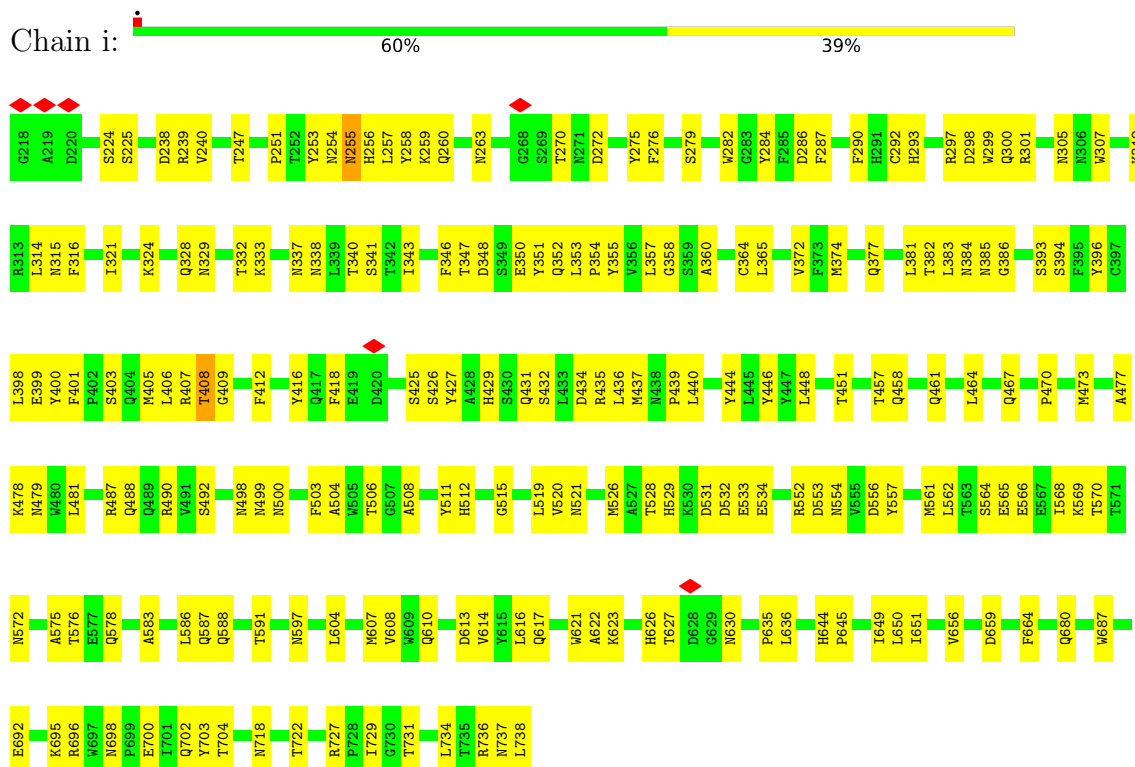


• Molecule 1: Capsid protein VP1

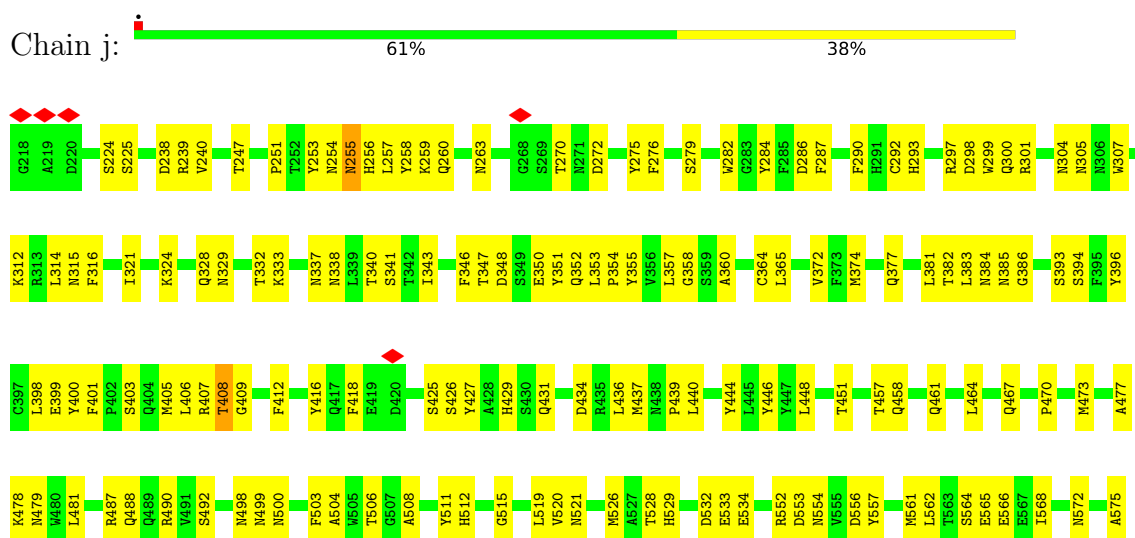


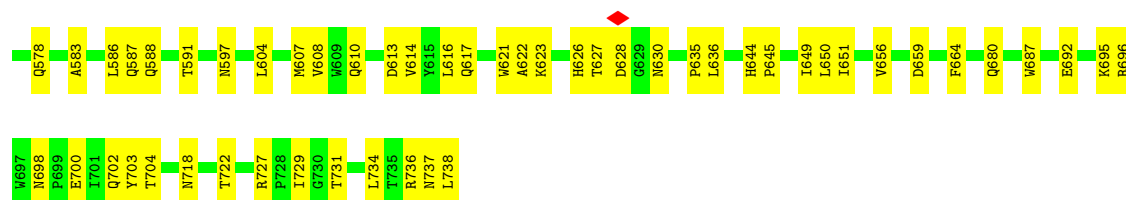


• Molecule 1: Capsid protein VP1

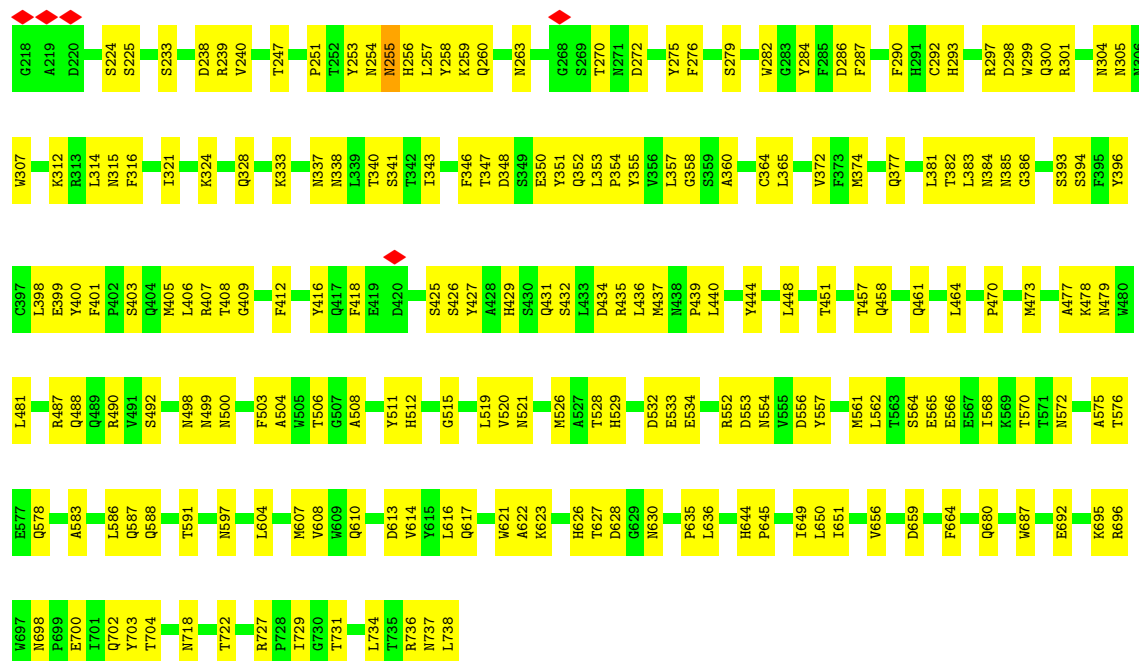


• Molecule 1: Capsid protein VP1

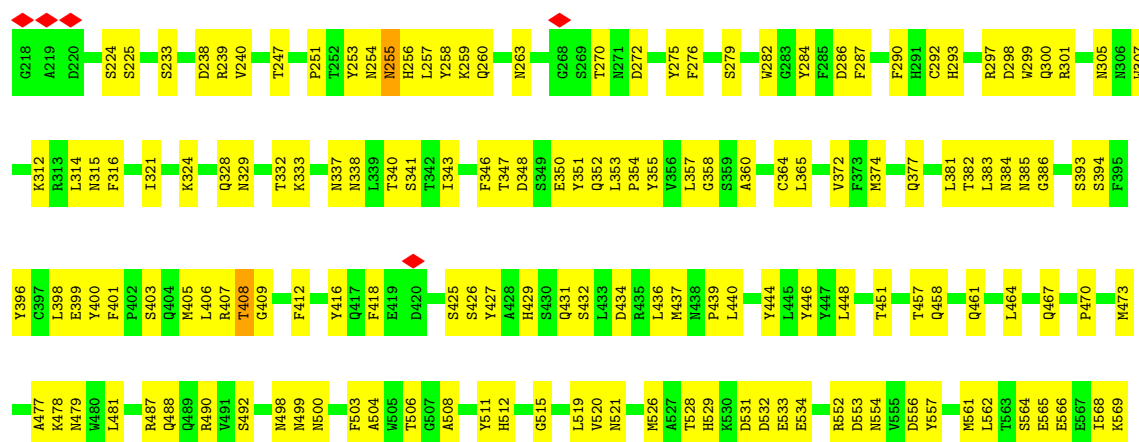


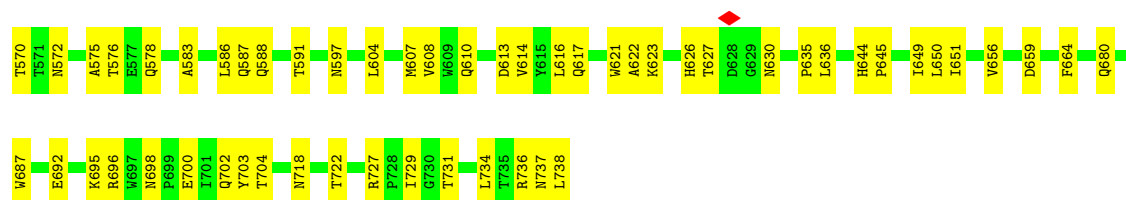


• Molecule 1: Capsid protein VP1

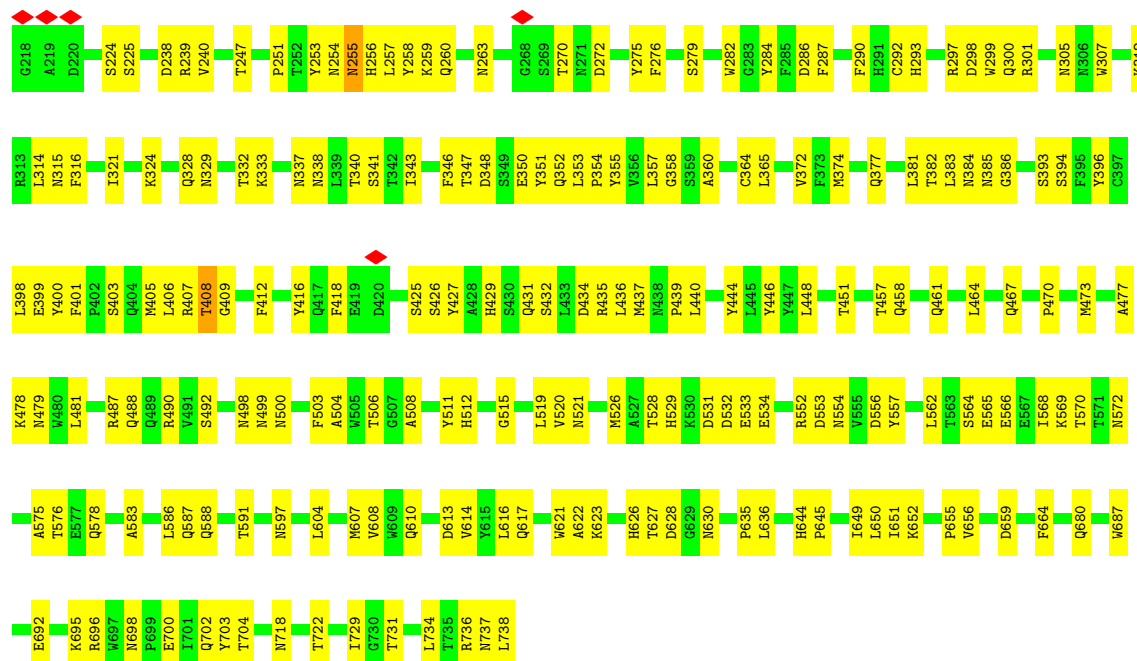


• Molecule 1: Capsid protein VP1

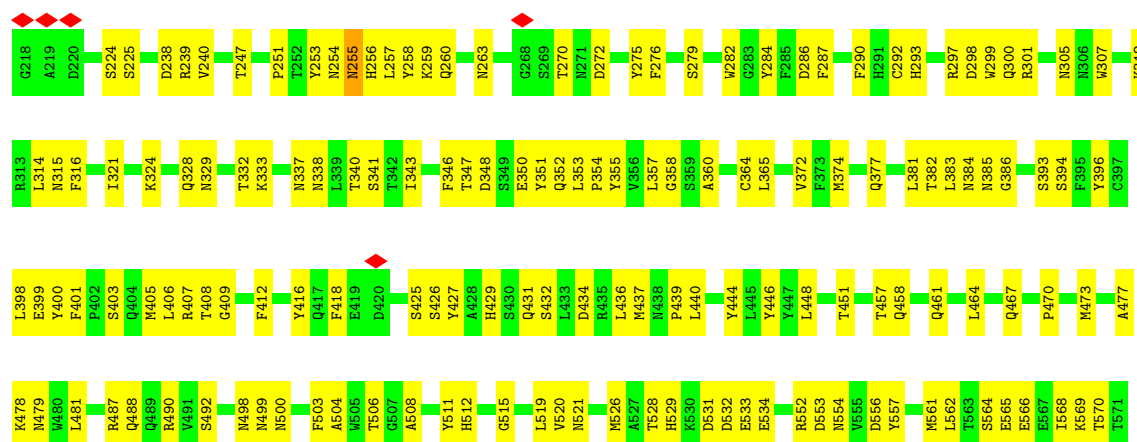


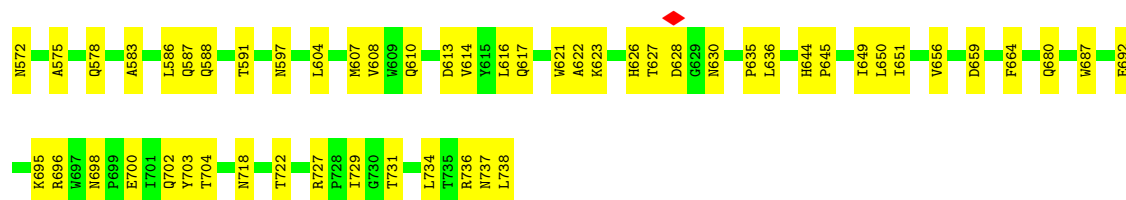


• Molecule 1: Capsid protein VP1

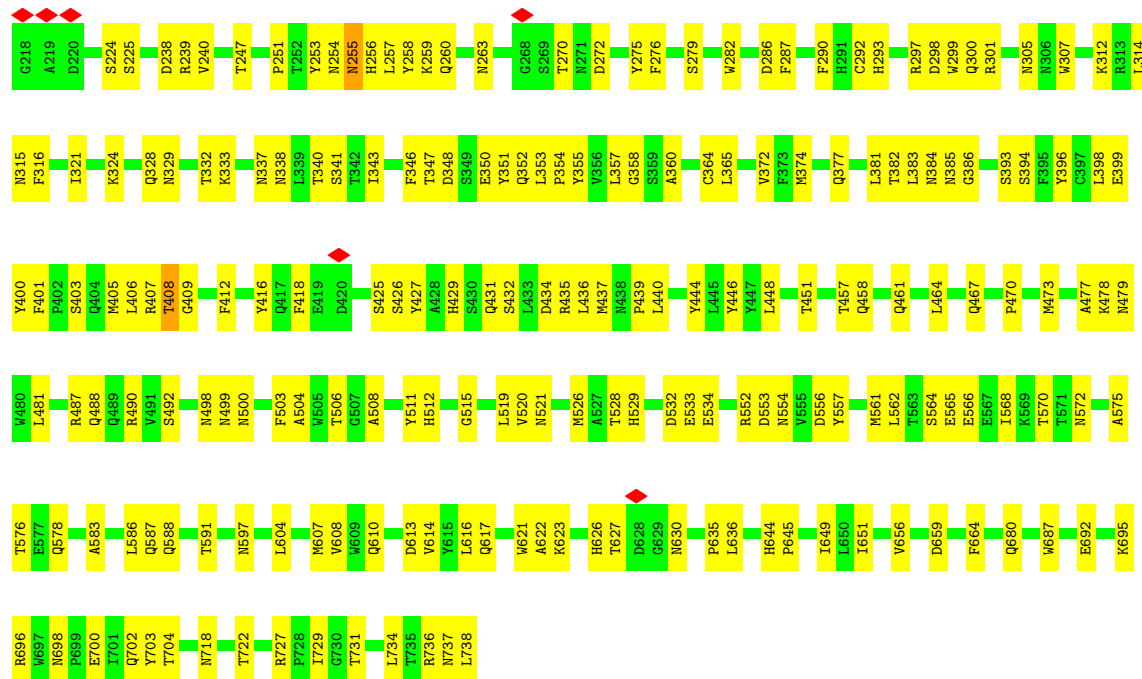


• Molecule 1: Capsid protein VP1

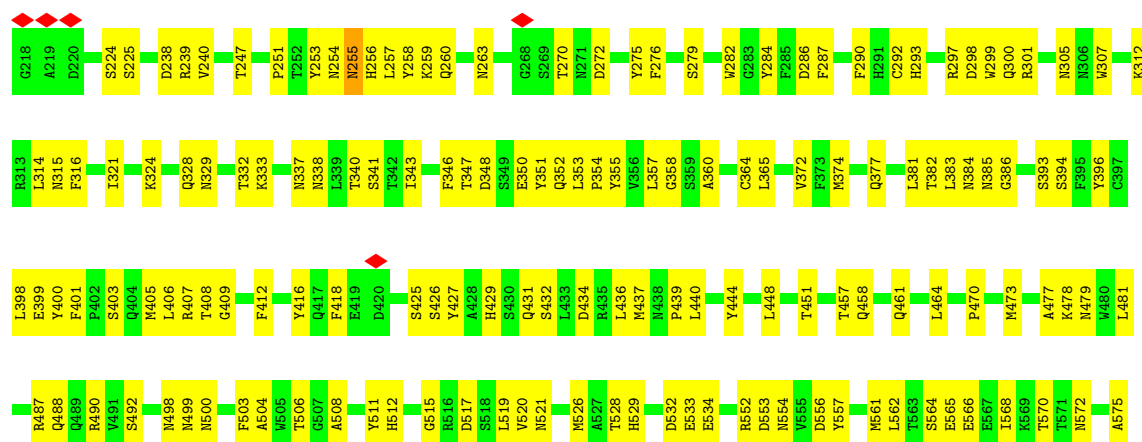


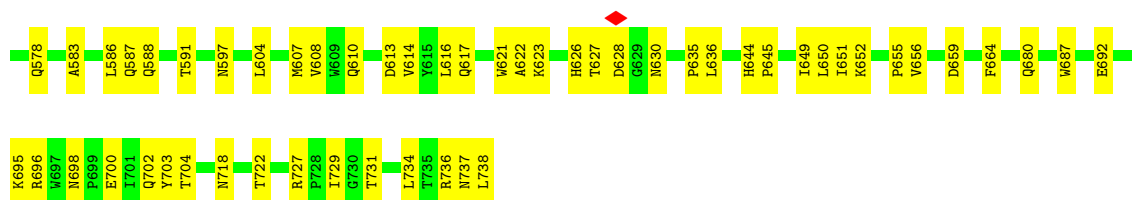


• Molecule 1: Capsid protein VP1

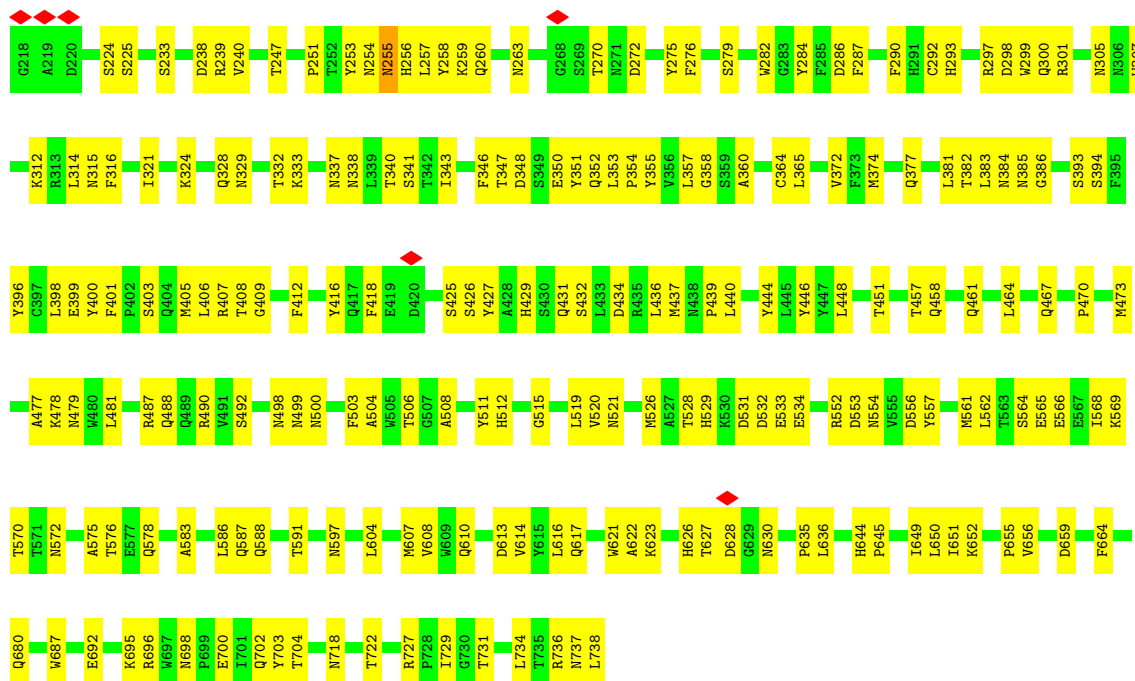


• Molecule 1: Capsid protein VP1

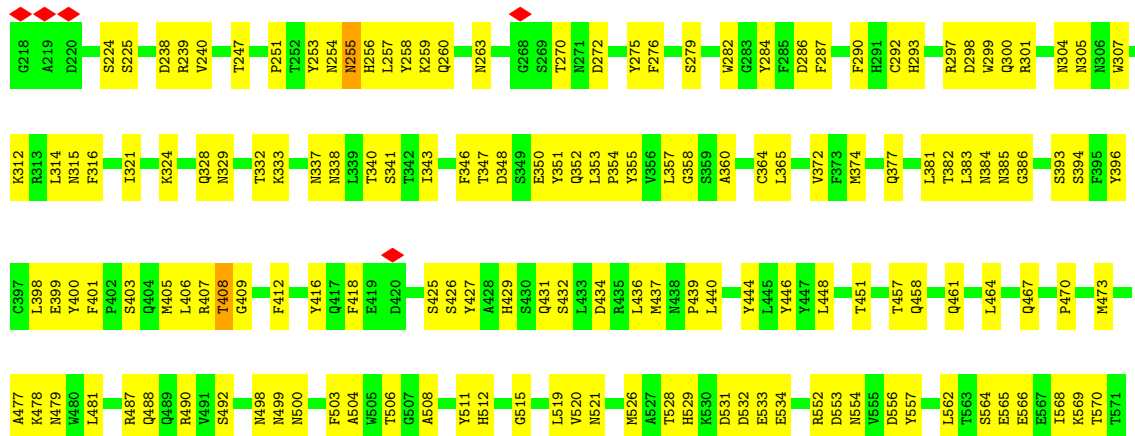


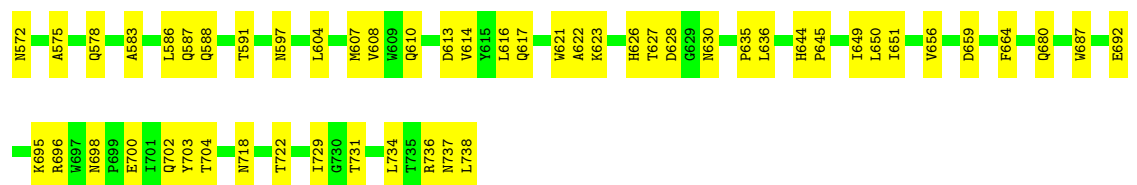


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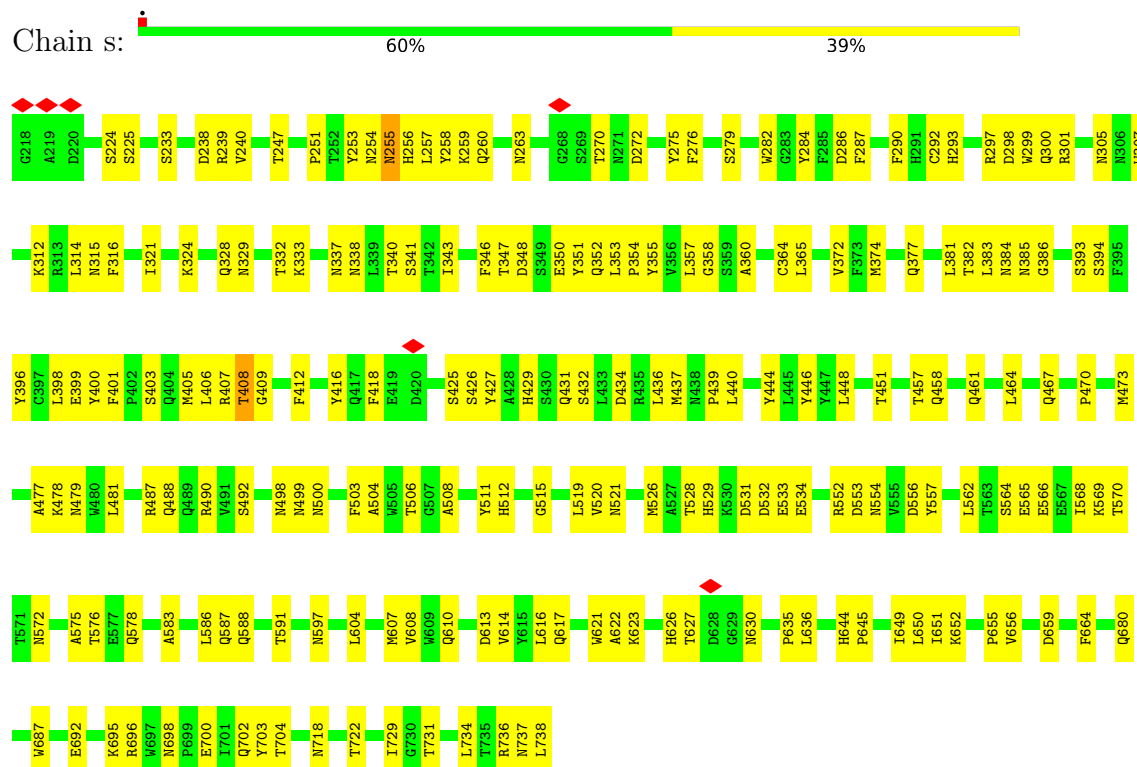


• Molecule 1: Capsid protein VP1

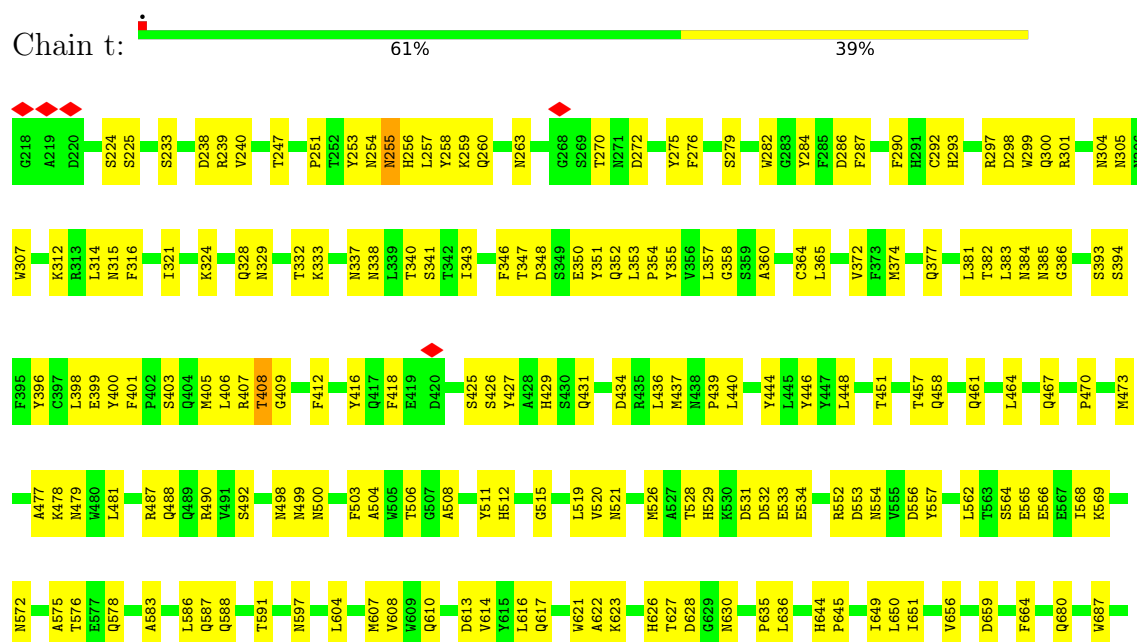




• Molecule 1: Capsid protein VP1

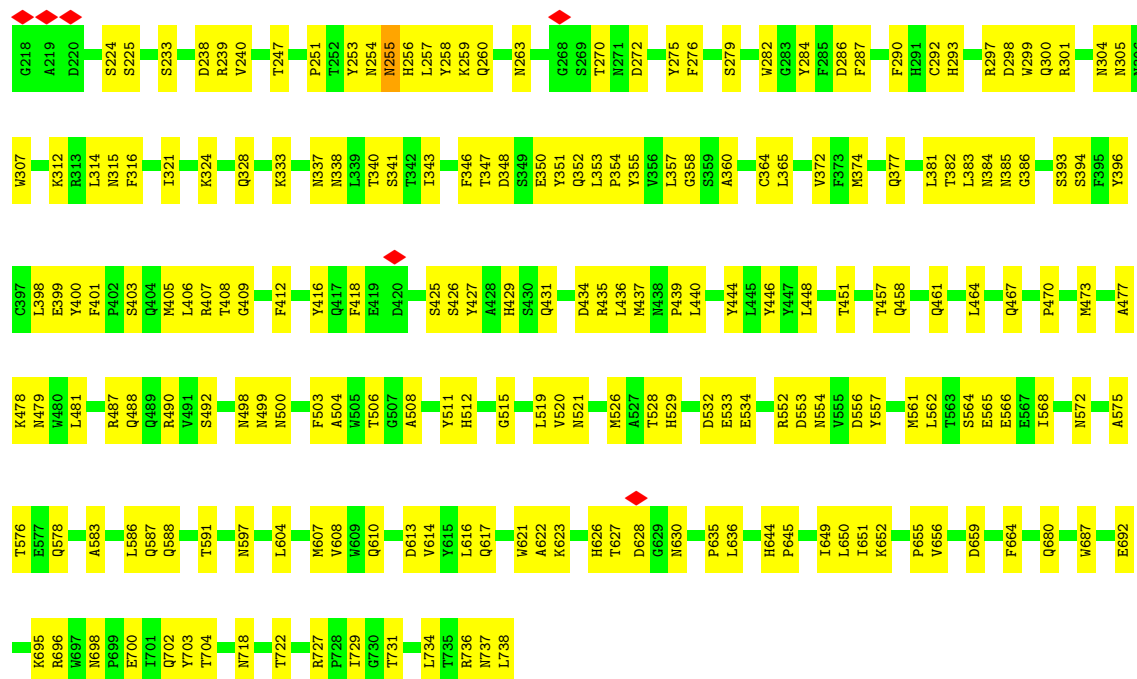


• Molecule 1: Capsid protein VP1

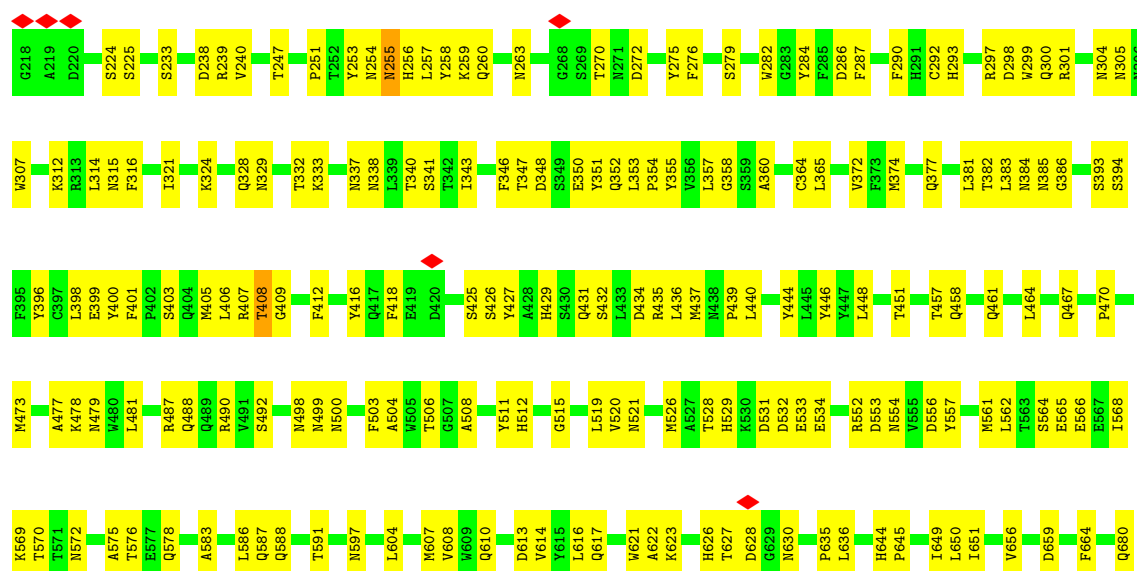


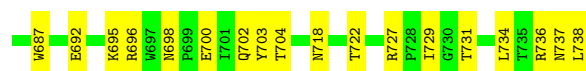


• Molecule 1: Capsid protein VP1

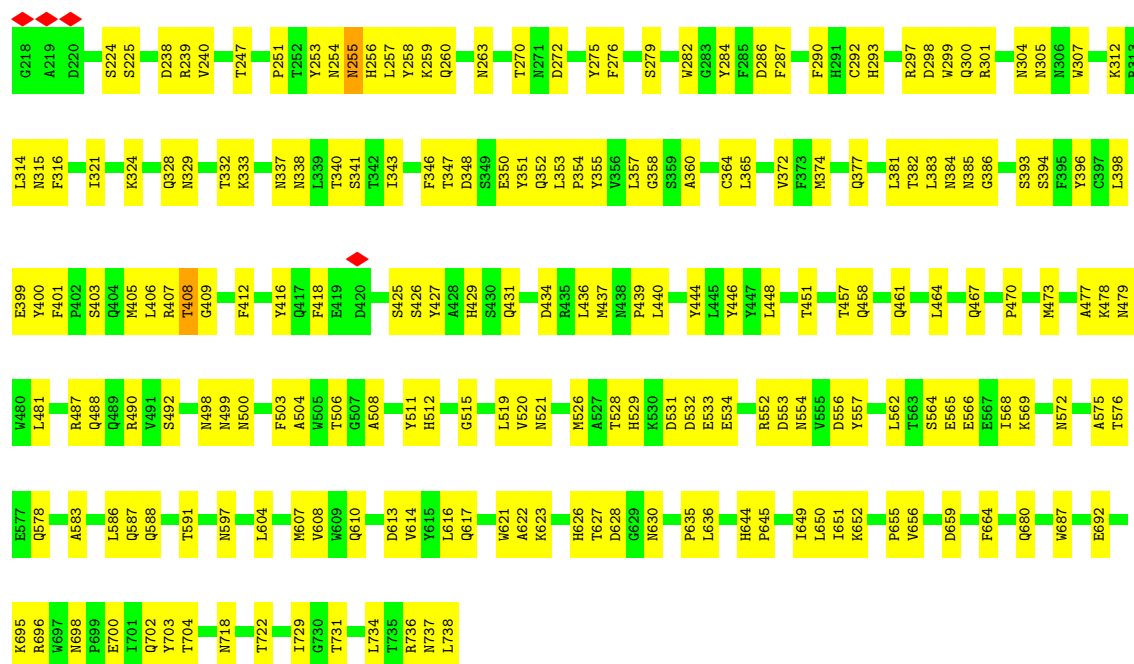


• Molecule 1: Capsid protein VP1

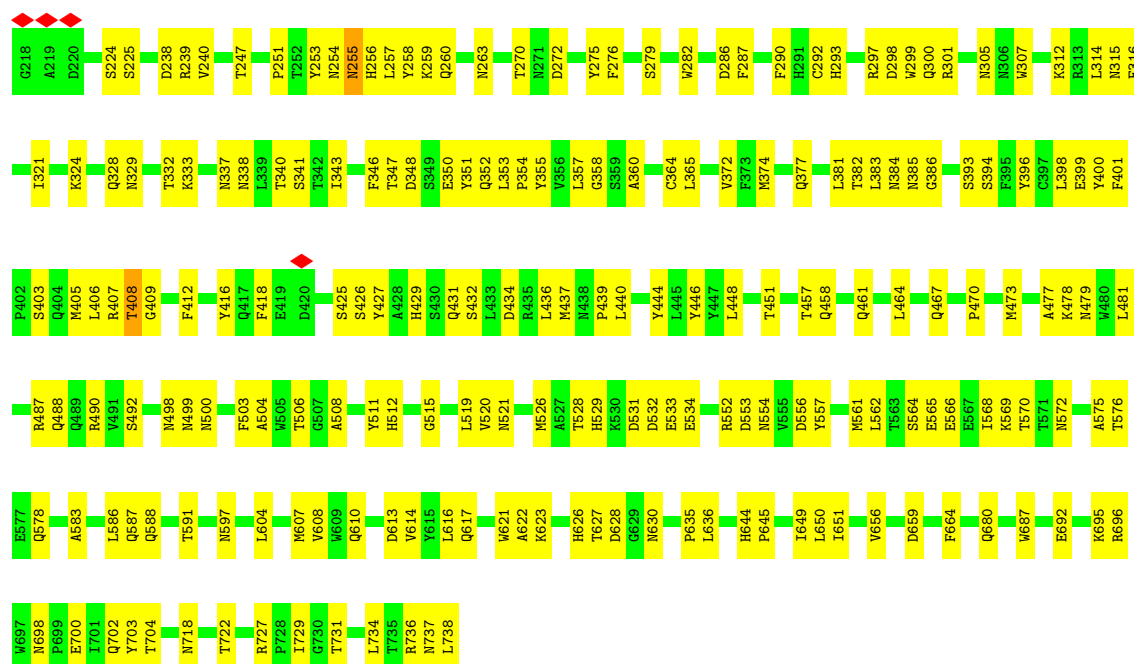




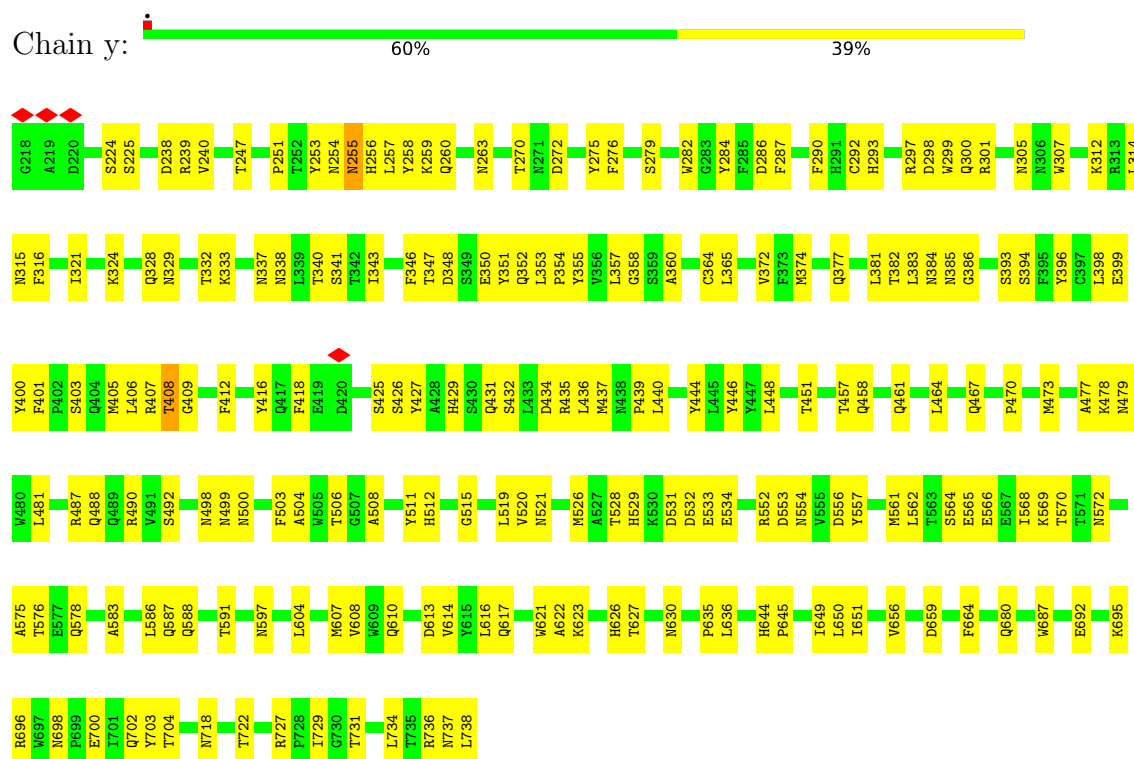
• Molecule 1: Capsid protein VP1



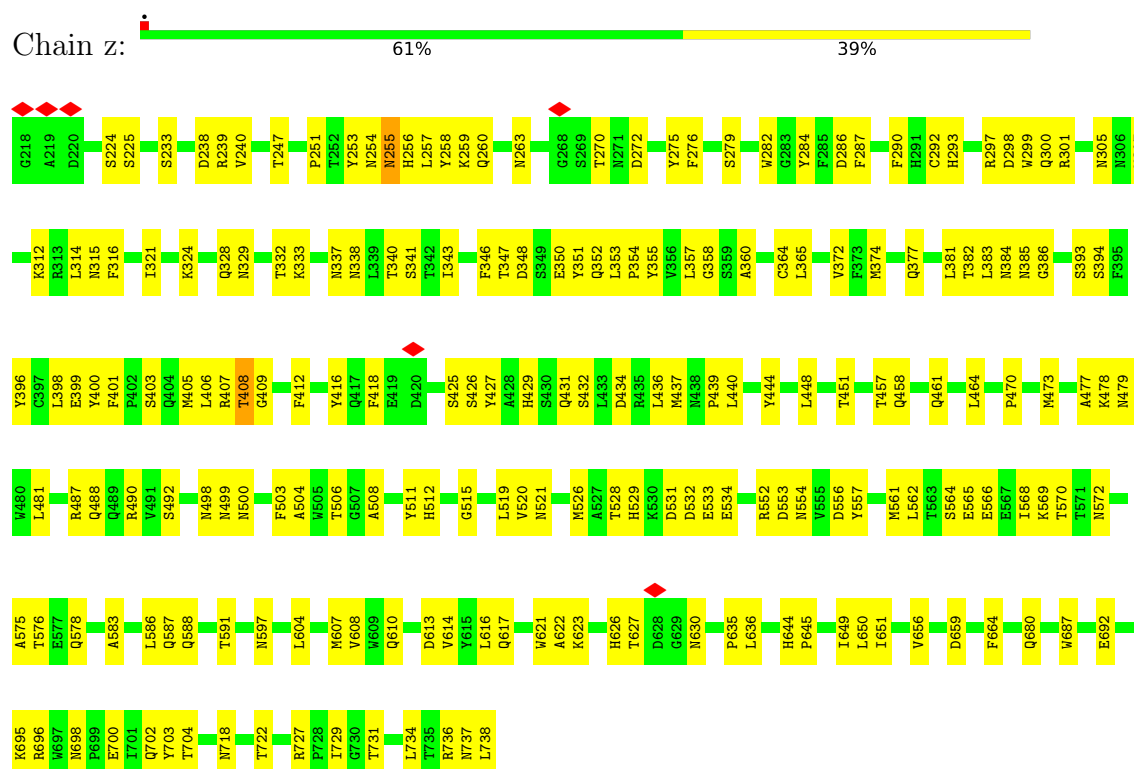
• Molecule 1: Capsid protein VP1



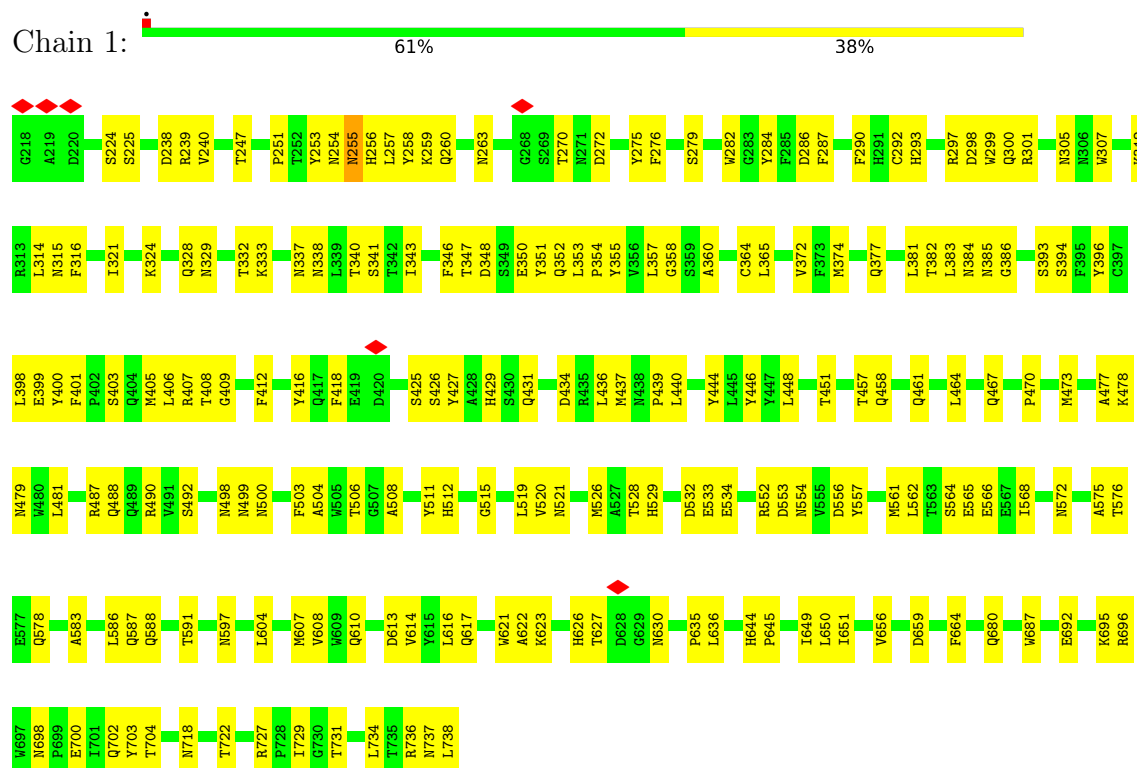
- Molecule 1: Capsid protein VP1



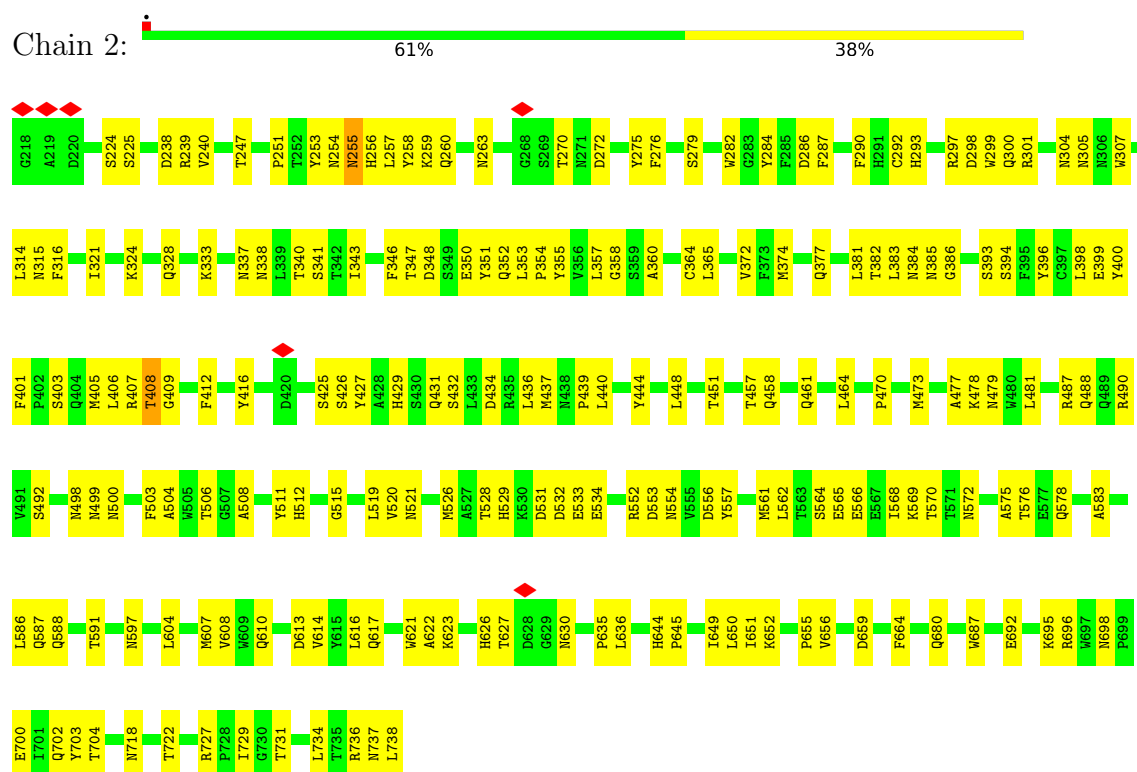
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

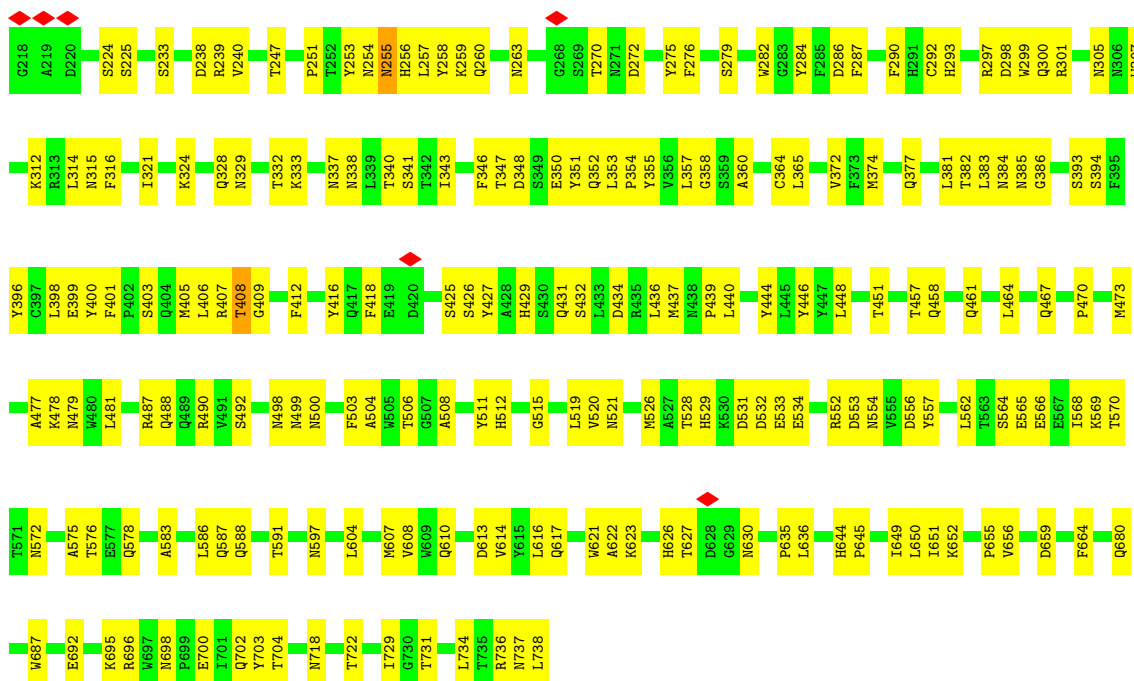


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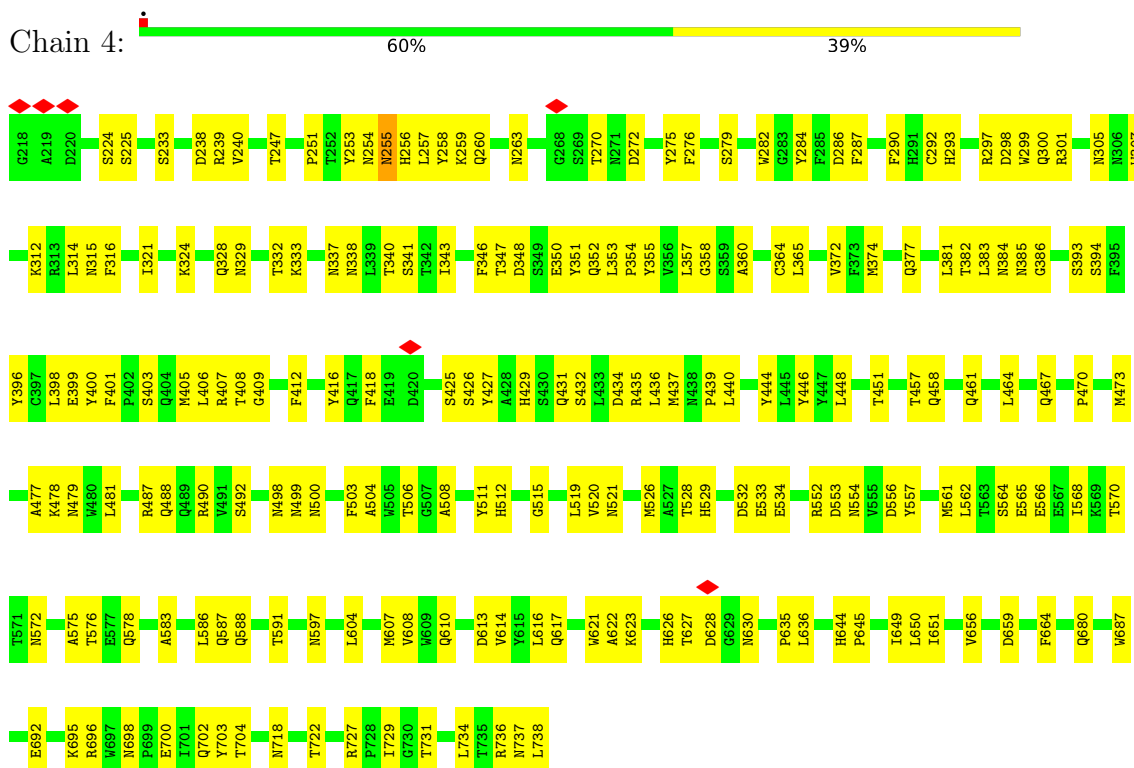


• Molecule 1: Capsid protein VP1



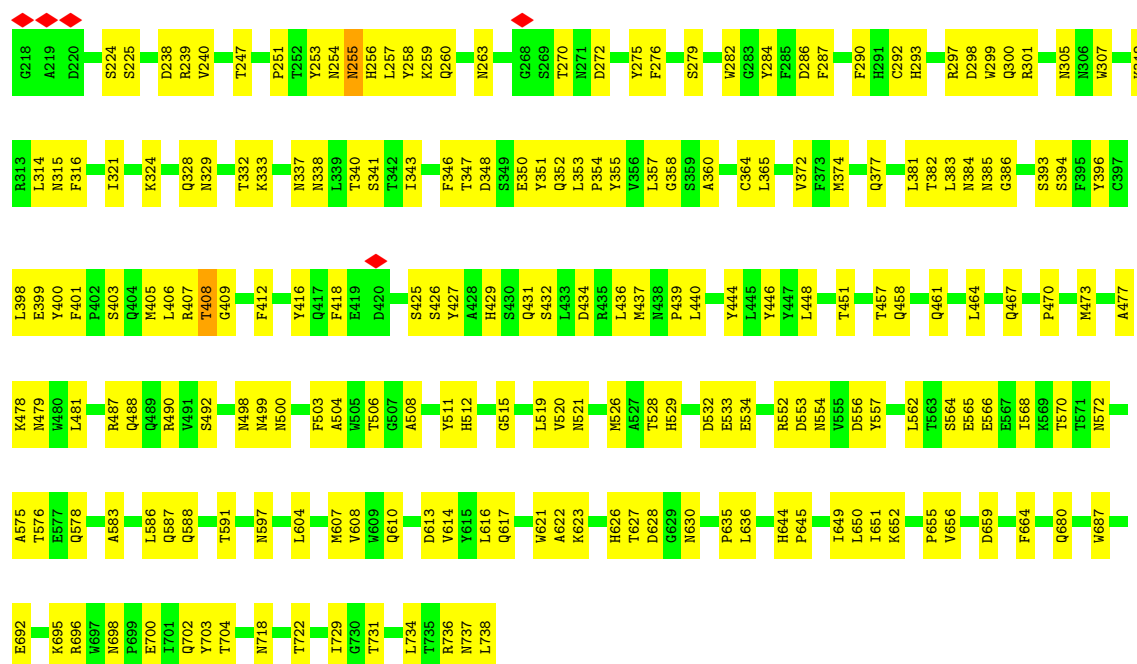


• Molecule 1: Capsid protein VP1

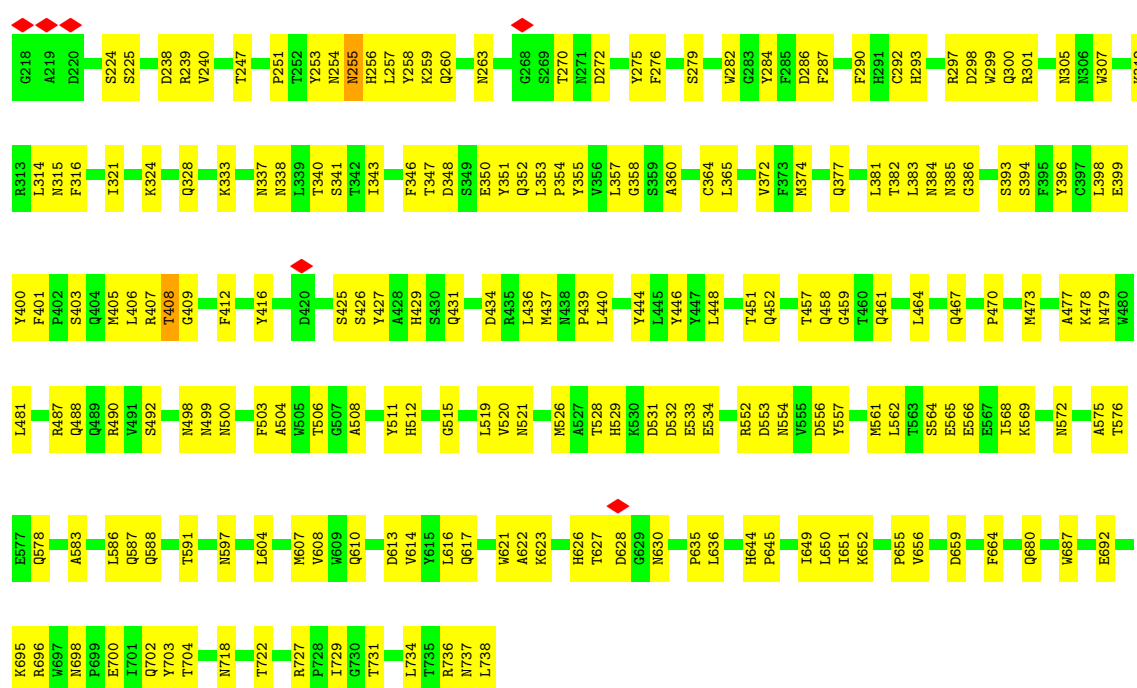


• Molecule 1: Capsid protein VP1



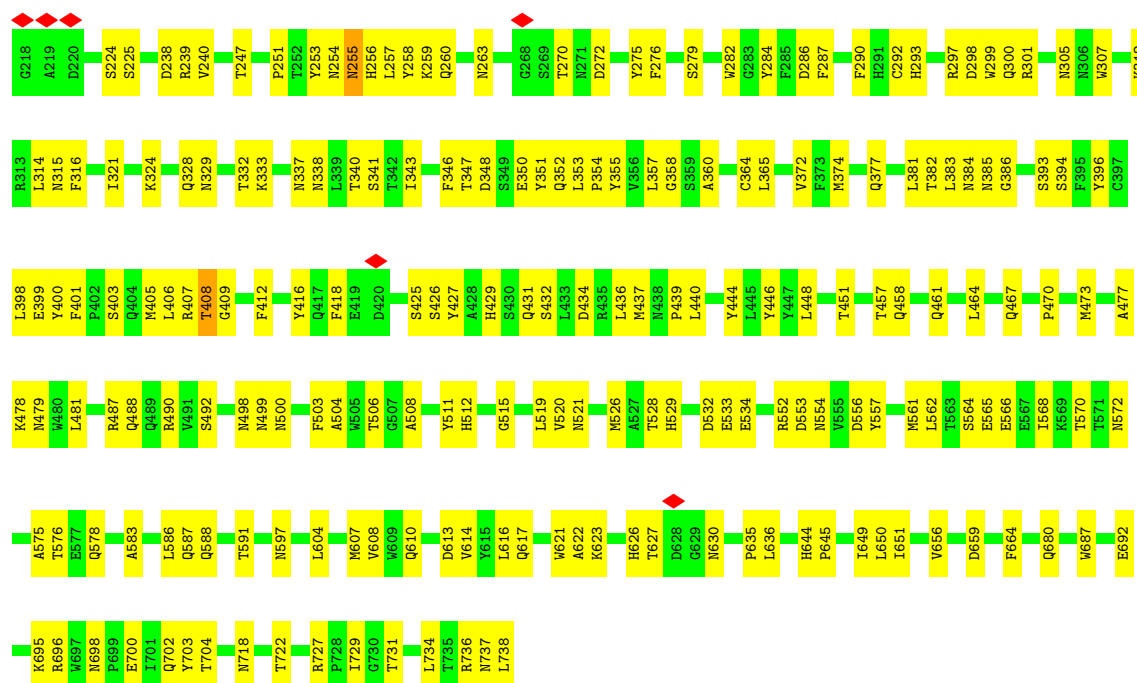


• Molecule 1: Capsid protein VP1

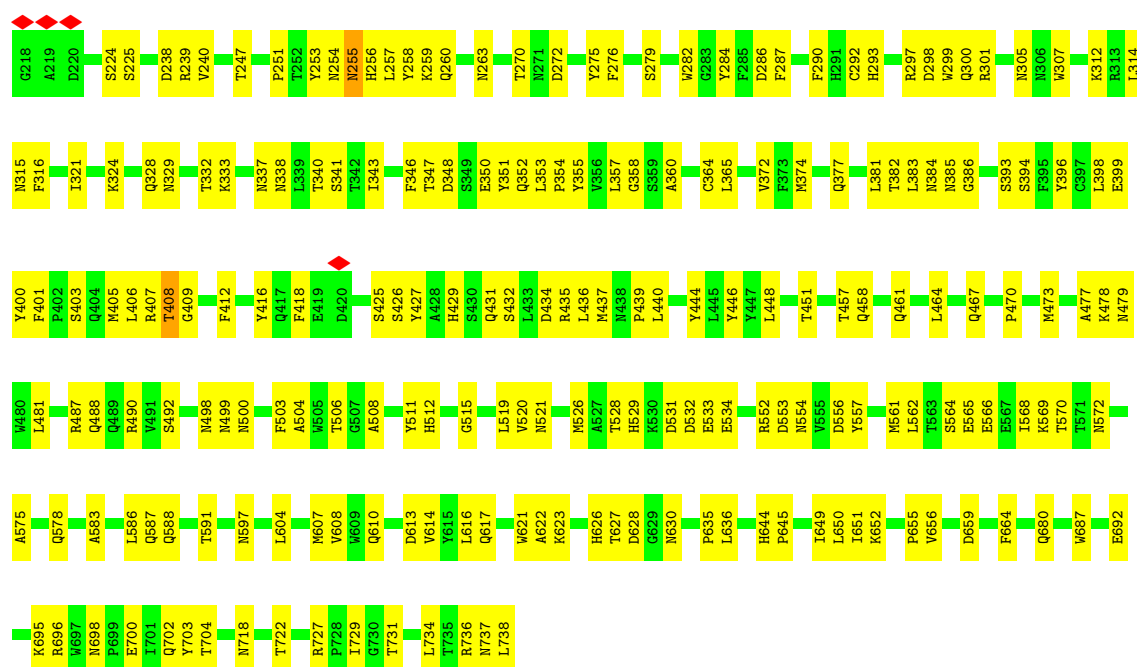


• Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

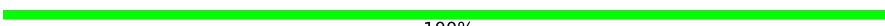


• Molecule 2: DNA (5'-D(*CP*A)-3')



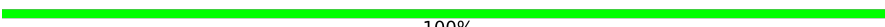
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain 9:  100%

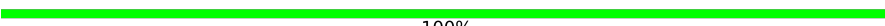
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain AA:  100%

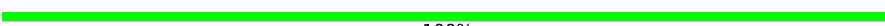
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain BA:  100%

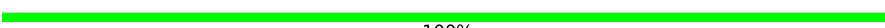
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain CA:  100%

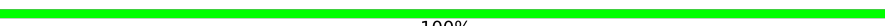
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain DA:  100%

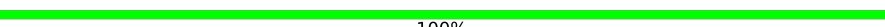
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain EA:  100%

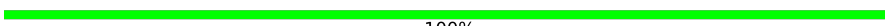
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain FA:  100%

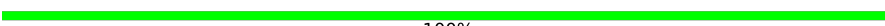
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain GA:  100%

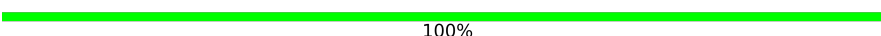
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain HA:  100%

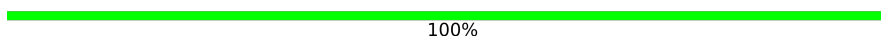
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain IA:  100%

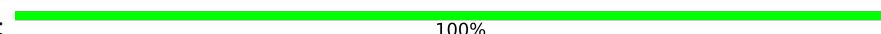
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain JA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain KA:  100%

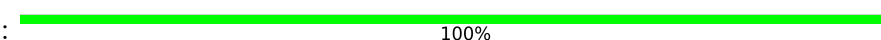
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain LA:  100%

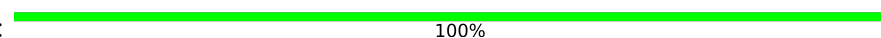
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain MA:  100%

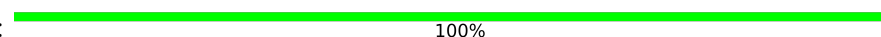
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain NA:  100%

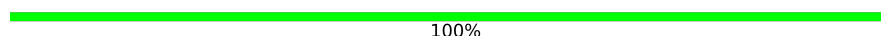
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain OA:  100%

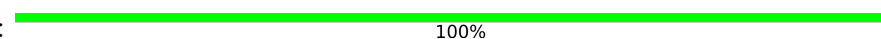
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain PA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain QA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain RA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain SA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain TA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain UA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain VA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain WA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain XA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain YA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain ZA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain aA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain bA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain cA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain dA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain eA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain fA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain gA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain hA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain iA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain jA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain kA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain lA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain mA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain nA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain oA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain pA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain qA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain rA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain sA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain tA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain uA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain vA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain wA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain xA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain yA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain zA:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain 0A:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain 1A:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain 2A:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain 3A:  100%

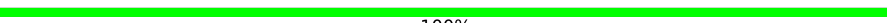
There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain 4A:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*A)-3')

Chain 5A:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	15.678	Depositor
Minimum map value	-9.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	384.237, 384.237, 384.237	wwPDB
Map dimensions	399, 399, 399	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.963, 0.963, 0.963	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.50	0/4272	0.54	0/5826
1	2	0.50	0/4272	0.54	0/5826
1	3	0.50	0/4272	0.54	0/5826
1	4	0.50	0/4272	0.54	0/5826
1	5	0.50	0/4272	0.54	0/5826
1	6	0.50	0/4272	0.54	0/5826
1	7	0.50	0/4272	0.54	0/5826
1	8	0.50	0/4272	0.54	0/5826
1	A	0.50	0/4272	0.54	0/5826
1	B	0.50	0/4272	0.54	0/5826
1	C	0.50	0/4272	0.54	0/5826
1	D	0.50	0/4272	0.54	0/5826
1	E	0.50	0/4272	0.54	0/5826
1	F	0.50	0/4272	0.54	0/5826
1	G	0.50	0/4272	0.54	0/5826
1	H	0.50	0/4272	0.54	0/5826
1	I	0.50	0/4272	0.54	0/5826
1	J	0.50	0/4272	0.54	0/5826
1	K	0.50	0/4272	0.54	0/5826
1	L	0.50	0/4272	0.54	0/5826
1	M	0.50	0/4272	0.54	0/5826
1	N	0.50	0/4272	0.54	0/5826
1	O	0.50	0/4272	0.54	0/5826
1	P	0.50	0/4272	0.54	0/5826
1	Q	0.50	0/4272	0.54	0/5826
1	R	0.50	0/4272	0.54	0/5826
1	S	0.50	0/4272	0.54	0/5826
1	T	0.50	0/4272	0.54	0/5826
1	U	0.50	0/4272	0.54	0/5826
1	V	0.50	0/4272	0.54	0/5826
1	W	0.50	0/4272	0.54	0/5826
1	X	0.50	0/4272	0.54	0/5826
1	Y	0.50	0/4272	0.54	0/5826
1	Z	0.50	0/4272	0.54	0/5826

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.50	0/4272	0.54	0/5826
1	b	0.50	0/4272	0.54	0/5826
1	c	0.50	0/4272	0.54	0/5826
1	d	0.50	0/4272	0.54	0/5826
1	e	0.50	0/4272	0.54	0/5826
1	f	0.50	0/4272	0.54	0/5826
1	g	0.50	0/4272	0.54	0/5826
1	h	0.50	0/4272	0.54	0/5826
1	i	0.50	0/4272	0.54	0/5826
1	j	0.50	0/4272	0.54	0/5826
1	k	0.50	0/4272	0.54	0/5826
1	l	0.50	0/4272	0.54	0/5826
1	m	0.50	0/4272	0.54	0/5826
1	n	0.50	0/4272	0.54	0/5826
1	o	0.50	0/4272	0.54	0/5826
1	p	0.50	0/4272	0.54	0/5826
1	q	0.50	0/4272	0.54	0/5826
1	r	0.50	0/4272	0.54	0/5826
1	s	0.50	0/4272	0.54	0/5826
1	t	0.50	0/4272	0.54	0/5826
1	u	0.50	0/4272	0.54	0/5826
1	v	0.50	0/4272	0.54	0/5826
1	w	0.50	0/4272	0.54	0/5826
1	x	0.50	0/4272	0.54	0/5826
1	y	0.50	0/4272	0.54	0/5826
1	z	0.50	0/4272	0.54	0/5826
2	0	0.24	0/41	0.36	0/61
2	0A	0.24	0/41	0.36	0/61
2	1A	0.24	0/41	0.36	0/61
2	2A	0.24	0/41	0.36	0/61
2	3A	0.24	0/41	0.36	0/61
2	4A	0.24	0/41	0.36	0/61
2	5A	0.23	0/41	0.36	0/61
2	9	0.24	0/41	0.36	0/61
2	AA	0.23	0/41	0.36	0/61
2	BA	0.24	0/41	0.36	0/61
2	CA	0.23	0/41	0.36	0/61
2	DA	0.24	0/41	0.36	0/61
2	EA	0.24	0/41	0.36	0/61
2	FA	0.24	0/41	0.36	0/61
2	GA	0.24	0/41	0.36	0/61
2	HA	0.24	0/41	0.36	0/61
2	IA	0.24	0/41	0.36	0/61

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
2	JA	0.23	0/41	0.36	0/61
2	KA	0.23	0/41	0.36	0/61
2	LA	0.24	0/41	0.36	0/61
2	MA	0.24	0/41	0.36	0/61
2	NA	0.23	0/41	0.36	0/61
2	OA	0.24	0/41	0.36	0/61
2	PA	0.23	0/41	0.36	0/61
2	QA	0.24	0/41	0.36	0/61
2	RA	0.24	0/41	0.36	0/61
2	SA	0.24	0/41	0.36	0/61
2	TA	0.24	0/41	0.36	0/61
2	UA	0.24	0/41	0.36	0/61
2	VA	0.23	0/41	0.36	0/61
2	WA	0.24	0/41	0.36	0/61
2	XA	0.24	0/41	0.36	0/61
2	YA	0.24	0/41	0.36	0/61
2	ZA	0.23	0/41	0.36	0/61
2	aA	0.24	0/41	0.36	0/61
2	bA	0.24	0/41	0.36	0/61
2	cA	0.24	0/41	0.36	0/61
2	dA	0.24	0/41	0.36	0/61
2	eA	0.24	0/41	0.36	0/61
2	fA	0.24	0/41	0.36	0/61
2	gA	0.23	0/41	0.36	0/61
2	hA	0.24	0/41	0.36	0/61
2	iA	0.24	0/41	0.36	0/61
2	jA	0.24	0/41	0.36	0/61
2	kA	0.23	0/41	0.36	0/61
2	lA	0.24	0/41	0.36	0/61
2	mA	0.24	0/41	0.36	0/61
2	nA	0.24	0/41	0.36	0/61
2	oA	0.24	0/41	0.36	0/61
2	pA	0.23	0/41	0.36	0/61
2	qA	0.24	0/41	0.36	0/61
2	rA	0.24	0/41	0.36	0/61
2	sA	0.24	0/41	0.36	0/61
2	tA	0.24	0/41	0.36	0/61
2	uA	0.24	0/41	0.36	0/61
2	vA	0.24	0/41	0.36	0/61
2	wA	0.24	0/41	0.36	0/61
2	xA	0.24	0/41	0.36	0/61
2	yA	0.24	0/41	0.36	0/61
2	zA	0.23	0/41	0.36	0/61

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.50	0/258780	0.54	0/353220

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](#)

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	1	4145	0	3907	182	0
1	2	4145	0	3907	180	0
1	3	4145	0	3907	183	0
1	4	4145	0	3907	185	0
1	5	4145	0	3907	183	0
1	6	4145	0	3907	183	0
1	7	4145	0	3907	180	0
1	8	4145	0	3907	185	0
1	A	4145	0	3907	182	0
1	B	4145	0	3907	185	0
1	C	4145	0	3907	181	0
1	D	4145	0	3907	181	0
1	E	4145	0	3907	181	0
1	F	4145	0	3907	183	0
1	G	4145	0	3907	183	0
1	H	4145	0	3907	188	0
1	I	4145	0	3907	185	0
1	J	4145	0	3907	185	0
1	K	4145	0	3907	181	0
1	L	4145	0	3907	179	0
1	M	4145	0	3907	183	0
1	N	4145	0	3907	184	0
1	O	4145	0	3907	183	0
1	P	4145	0	3907	183	0
1	Q	4145	0	3907	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	4145	0	3907	183	0
1	S	4145	0	3907	184	0
1	T	4145	0	3907	183	0
1	U	4145	0	3907	184	0
1	V	4145	0	3907	187	0
1	W	4145	0	3907	181	0
1	X	4145	0	3907	186	0
1	Y	4145	0	3907	185	0
1	Z	4145	0	3907	185	0
1	a	4145	0	3907	186	0
1	b	4145	0	3907	186	0
1	c	4145	0	3907	185	0
1	d	4145	0	3907	181	0
1	e	4145	0	3907	187	0
1	f	4145	0	3907	184	0
1	g	4145	0	3907	184	0
1	h	4145	0	3907	185	0
1	i	4145	0	3907	186	0
1	j	4145	0	3907	184	0
1	k	4145	0	3907	185	0
1	l	4145	0	3907	186	0
1	m	4145	0	3907	184	0
1	n	4145	0	3907	183	0
1	o	4145	0	3907	183	0
1	p	4145	0	3907	183	0
1	q	4145	0	3907	184	0
1	r	4145	0	3907	182	0
1	s	4145	0	3907	186	0
1	t	4145	0	3907	184	0
1	u	4145	0	3907	182	0
1	v	4145	0	3907	187	0
1	w	4145	0	3907	185	0
1	x	4145	0	3907	184	0
1	y	4145	0	3907	186	0
1	z	4145	0	3907	186	0
2	0	37	0	24	0	0
2	0A	37	0	24	0	0
2	1A	37	0	24	0	0
2	2A	37	0	24	0	0
2	3A	37	0	24	0	0
2	4A	37	0	24	0	0
2	5A	37	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	37	0	24	0	0
2	AA	37	0	24	0	0
2	BA	37	0	24	0	0
2	CA	37	0	24	0	0
2	DA	37	0	24	0	0
2	EA	37	0	24	0	0
2	FA	37	0	24	0	0
2	GA	37	0	24	0	0
2	HA	37	0	24	0	0
2	IA	37	0	24	0	0
2	JA	37	0	24	0	0
2	KA	37	0	24	0	0
2	LA	37	0	24	0	0
2	MA	37	0	24	0	0
2	NA	37	0	24	0	0
2	OA	37	0	24	0	0
2	PA	37	0	24	0	0
2	QA	37	0	24	0	0
2	RA	37	0	24	0	0
2	SA	37	0	24	0	0
2	TA	37	0	24	0	0
2	UA	37	0	24	0	0
2	VA	37	0	24	0	0
2	WA	37	0	24	0	0
2	XA	37	0	24	0	0
2	YA	37	0	24	0	0
2	ZA	37	0	24	0	0
2	aA	37	0	24	0	0
2	bA	37	0	24	0	0
2	cA	37	0	24	0	0
2	dA	37	0	24	0	0
2	eA	37	0	24	0	0
2	fA	37	0	24	0	0
2	gA	37	0	24	0	0
2	hA	37	0	24	0	0
2	iA	37	0	24	0	0
2	jA	37	0	24	0	0
2	kA	37	0	24	0	0
2	lA	37	0	24	0	0
2	mA	37	0	24	0	0
2	nA	37	0	24	0	0
2	oA	37	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	pA	37	0	24	0	0
2	qA	37	0	24	0	0
2	rA	37	0	24	0	0
2	sA	37	0	24	0	0
2	tA	37	0	24	0	0
2	uA	37	0	24	0	0
2	vA	37	0	24	0	0
2	wA	37	0	24	0	0
2	xA	37	0	24	0	0
2	yA	37	0	24	0	0
2	zA	37	0	24	0	0
All	All	250920	0	235860	8847	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 18.

The worst 5 of 8847 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:U:251:PRO:HG3	1:U:374:MET:HE3	1.56	0.88
1:A:251:PRO:HG3	1:A:374:MET:HE3	1.56	0.88
1:k:251:PRO:HG3	1:k:374:MET:HE3	1.56	0.88
1:v:251:PRO:HG3	1:v:374:MET:HE3	1.56	0.88
1:D:251:PRO:HG3	1:D:374:MET:HE3	1.56	0.88

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	1	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	3	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	4	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	5	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	6	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	7	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	8	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	A	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	B	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	C	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	D	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	E	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	F	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	G	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	H	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	I	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	J	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	K	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	L	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	M	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	N	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	O	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	P	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	Q	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	R	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	S	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	T	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	U	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	V	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	W	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	X	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	Z	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	a	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	b	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	c	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	d	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	e	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	f	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	g	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	h	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	i	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	j	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	k	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	l	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	m	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	n	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	o	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	p	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	q	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	r	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	s	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	t	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	u	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	v	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	w	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	x	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	y	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
1	z	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	30	60
All	All	31200/31260 (100%)	30240 (97%)	840 (3%)	120 (0%)	31	60

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	408	THR
1	B	255	ASN
1	B	408	THR
1	C	255	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	2	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	3	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	4	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	5	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	6	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	7	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	8	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	A	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	B	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	C	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	D	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	E	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	F	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	G	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	H	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	I	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	J	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	K	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	L	455/454 (100%)	453 (100%)	2 (0%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	N	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	O	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	P	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	Q	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	R	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	S	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	T	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	U	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	V	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	W	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	X	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	Y	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	Z	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	a	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	b	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	c	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	d	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	e	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	f	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	g	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	h	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	i	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	j	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	k	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	l	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	m	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	n	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	o	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	p	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	q	455/454 (100%)	453 (100%)	2 (0%)	84	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	s	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	t	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	u	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	v	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	w	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	x	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	y	455/454 (100%)	453 (100%)	2 (0%)	84	81
1	z	455/454 (100%)	453 (100%)	2 (0%)	84	81
All	All	27300/27240 (100%)	27180 (100%)	120 (0%)	81	81

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	586	LEU
1	4	448	LEU
1	j	586	LEU
1	3	586	LEU
1	8	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 869 such sidechains are listed below:

Mol	Chain	Res	Type
1	g	328	GLN
1	n	653	ASN
1	4	377	GLN
1	h	293	HIS
1	g	305	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

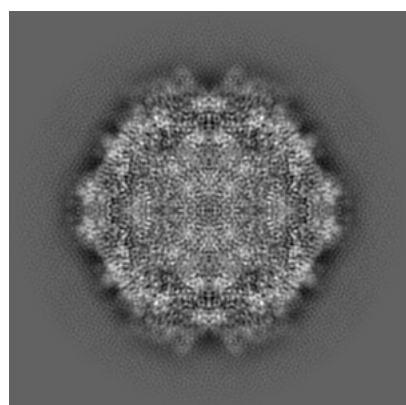
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21020. These allow visual inspection of the internal detail of the map and identification of artifacts.

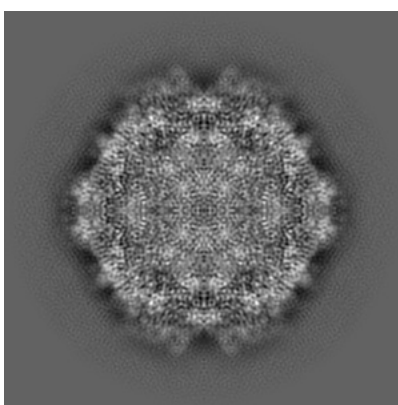
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

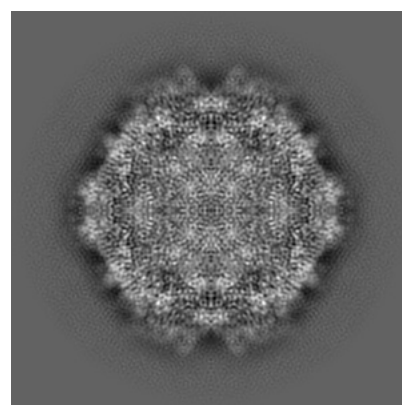
6.1.1 Primary map



X



Y

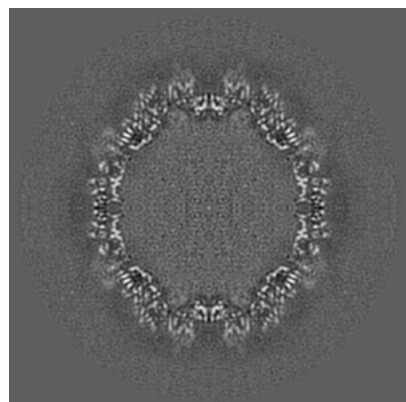


Z

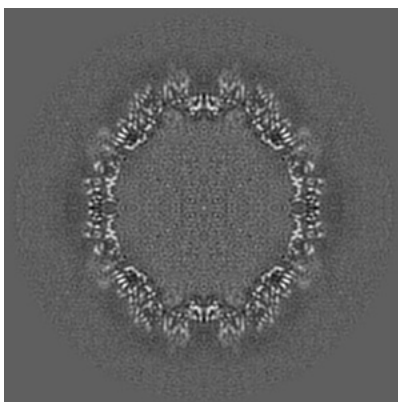
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

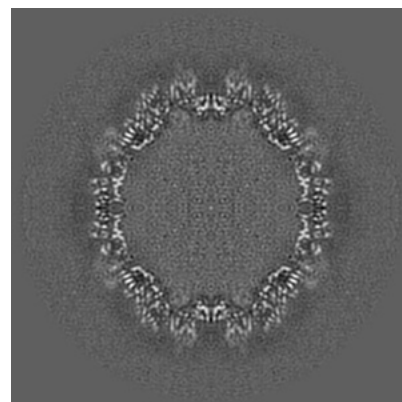
6.2.1 Primary map



X Index: 199



Y Index: 199

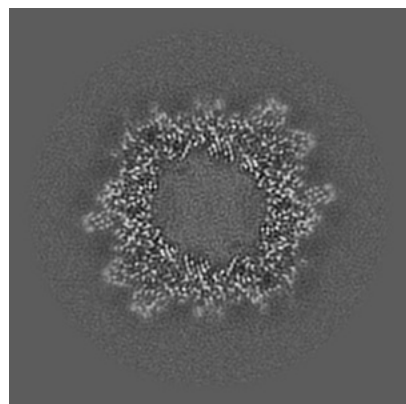


Z Index: 199

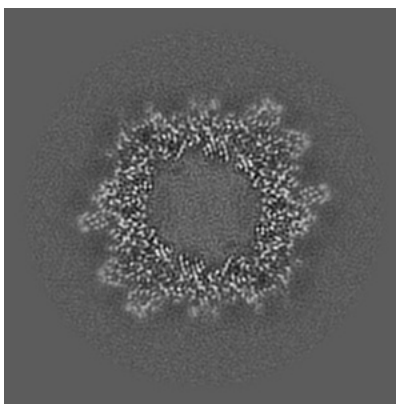
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

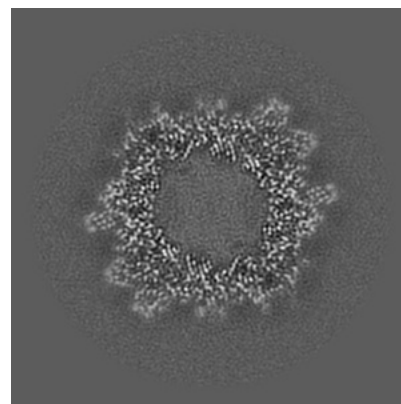
6.3.1 Primary map



X Index: 128



Y Index: 128

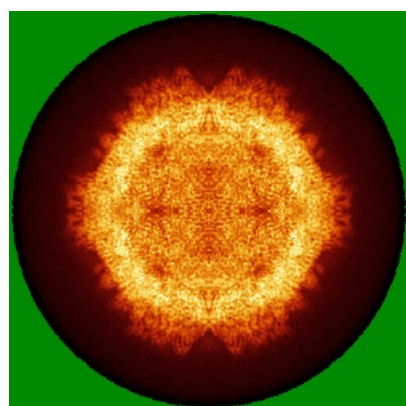


Z Index: 128

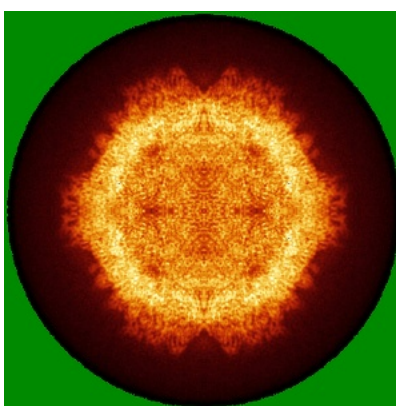
The images above show the largest variance slices of the map in three orthogonal directions.

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

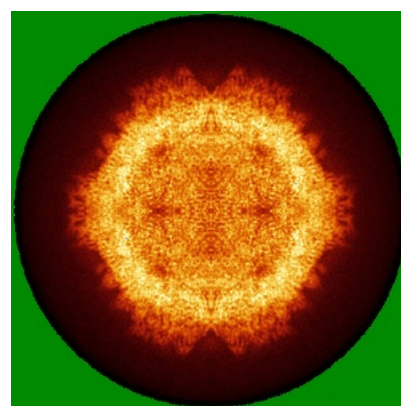
6.4.1 Primary map



X



Y

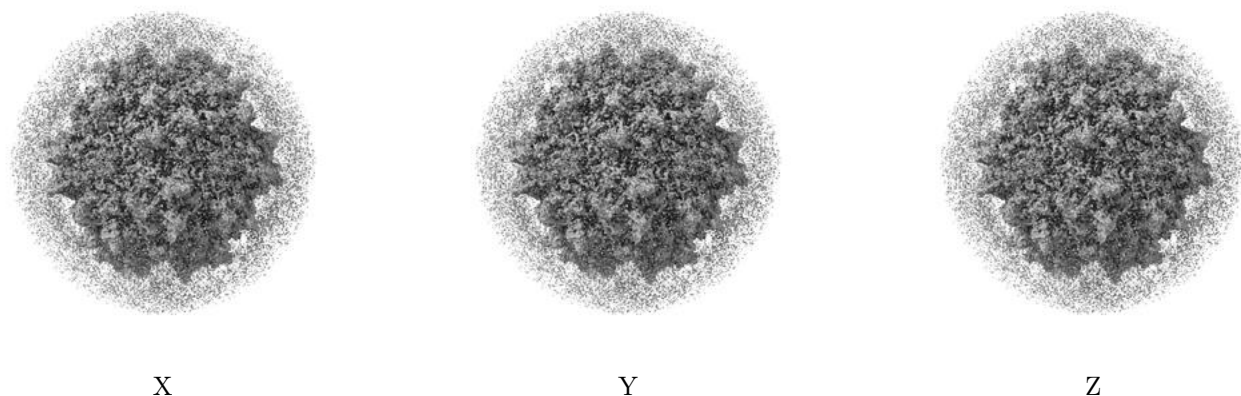


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

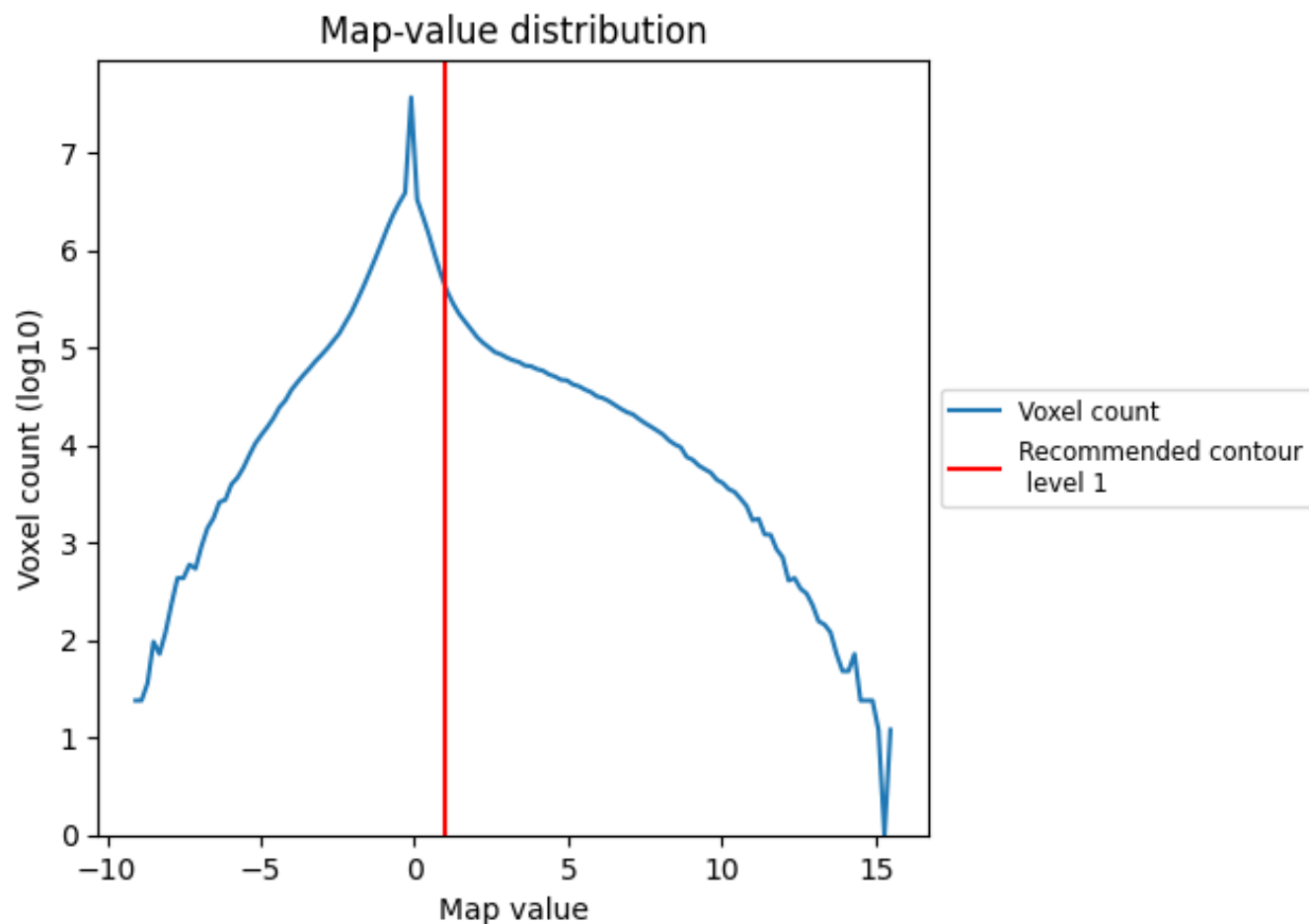
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

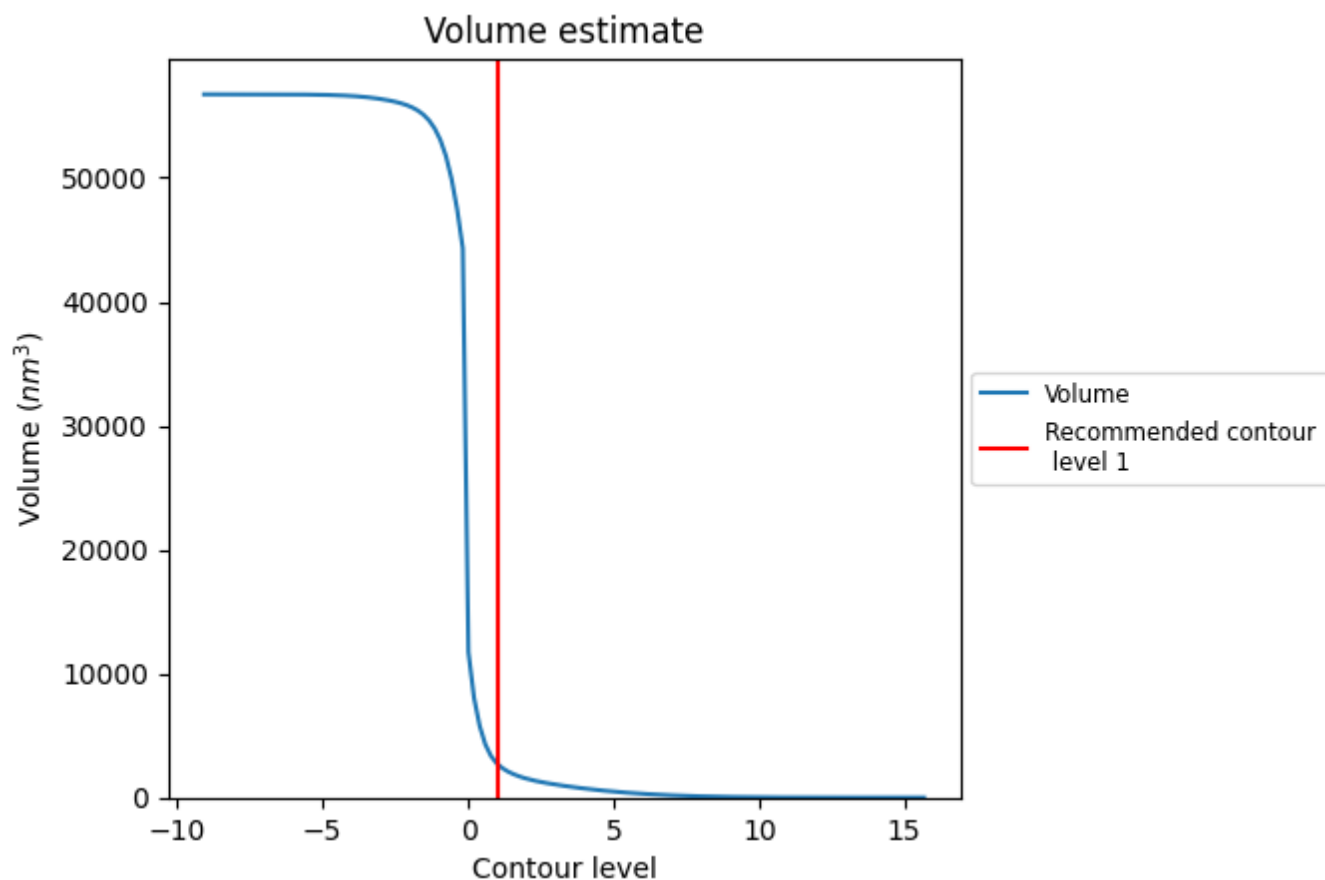
This section contains the results of statistical analysis of the map.

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.

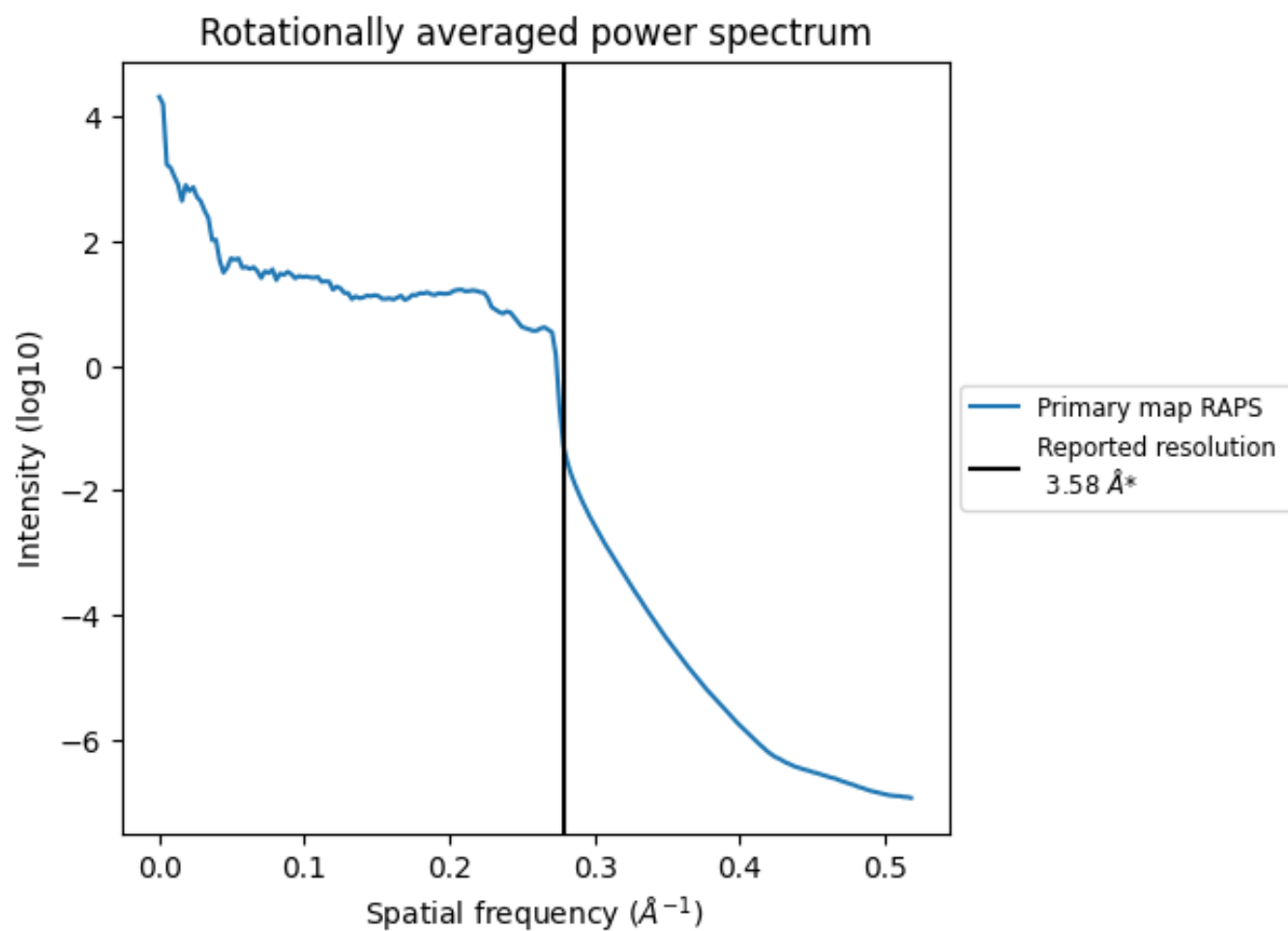
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2733 nm³; this corresponds to an approximate mass of 2469 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

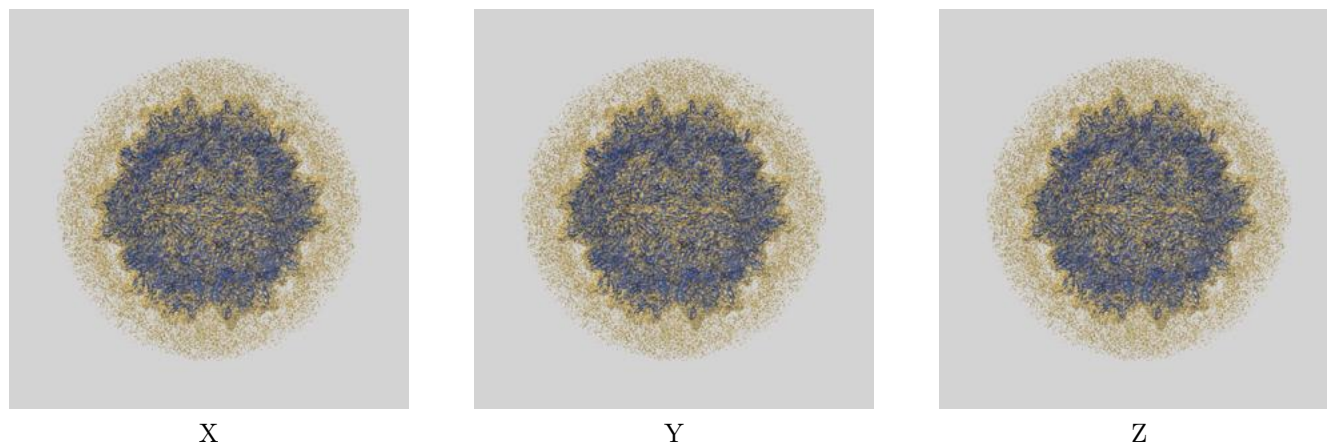
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

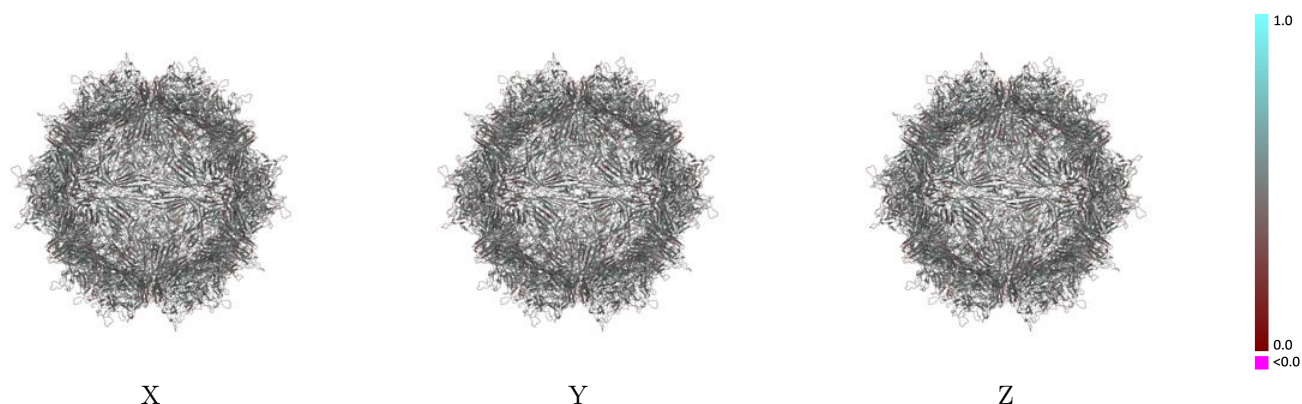
This section contains information regarding the fit between EMDB map EMD-21020 and PDB model 6V1Z. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



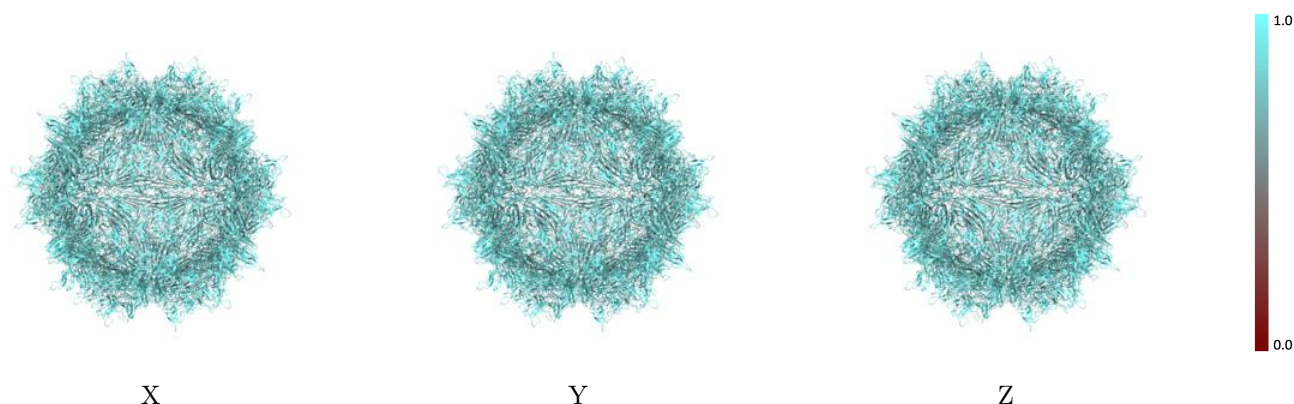
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



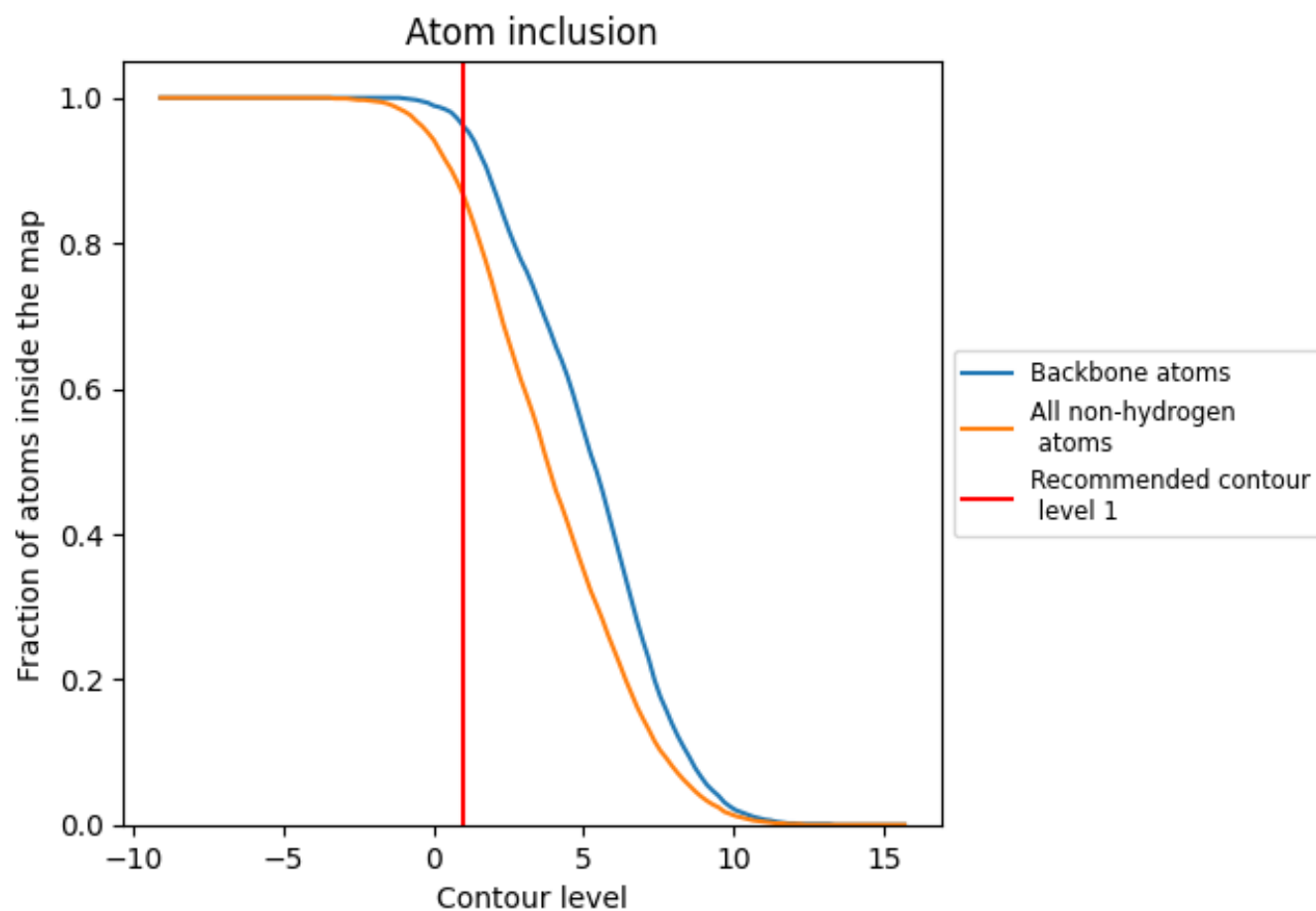
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.4670
0	 0.9190	 0.4840
0A	 0.9190	 0.4730
1	 0.8660	 0.4680
1A	 0.9190	 0.4780
2	 0.8650	 0.4670
2A	 0.9190	 0.4810
3	 0.8640	 0.4680
3A	 0.9190	 0.4840
4	 0.8660	 0.4670
4A	 0.9190	 0.4780
5	 0.8630	 0.4670
5A	 0.9190	 0.4730
6	 0.8650	 0.4680
7	 0.8650	 0.4670
8	 0.8670	 0.4670
9	 0.9190	 0.4860
A	 0.8650	 0.4670
AA	 0.9190	 0.4680
B	 0.8650	 0.4680
BA	 0.9190	 0.4810
C	 0.8620	 0.4660
CA	 0.9190	 0.4740
D	 0.8670	 0.4680
DA	 0.9190	 0.4830
E	 0.8650	 0.4680
EA	 0.9190	 0.4810
F	 0.8660	 0.4680
FA	 0.9190	 0.4720
G	 0.8650	 0.4670
GA	 0.9190	 0.4900
H	 0.8660	 0.4680
HA	 0.9190	 0.4800
I	 0.8660	 0.4670
IA	 0.9190	 0.4780



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Chain	Atom inclusion	Q-score
J	 0.8650	 0.4670
JA	 0.9190	 0.4660
K	 0.8670	 0.4670
KA	 0.9190	 0.4910
L	 0.8620	 0.4660
LA	 0.9190	 0.4710
M	 0.8650	 0.4670
MA	 0.9190	 0.4690
N	 0.8680	 0.4680
NA	 0.9190	 0.4760
O	 0.8640	 0.4660
OA	 0.9190	 0.4850
P	 0.8670	 0.4680
PA	 0.9190	 0.4770
Q	 0.8630	 0.4660
QA	 0.9190	 0.4770
R	 0.8630	 0.4670
RA	 0.9190	 0.4800
S	 0.8660	 0.4690
SA	 0.9190	 0.4740
T	 0.8660	 0.4670
TA	 0.9190	 0.4740
U	 0.8650	 0.4680
UA	 0.9190	 0.4760
V	 0.8670	 0.4680
VA	 0.9190	 0.4570
W	 0.8650	 0.4660
WA	 0.9190	 0.4650
X	 0.8680	 0.4690
XA	 0.9190	 0.4640
Y	 0.8620	 0.4670
YA	 0.9190	 0.4840
Z	 0.8630	 0.4650
ZA	 0.9190	 0.4810
a	 0.8670	 0.4670
aA	 0.9190	 0.4920
b	 0.8660	 0.4690
bA	 0.9190	 0.4700
c	 0.8660	 0.4670
cA	 0.9190	 0.4780
d	 0.8660	 0.4670
dA	 0.9190	 0.4880

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Chain	Atom inclusion	Q-score
e	 0.8670	 0.4690
eA	 0.9190	 0.4790
f	 0.8650	 0.4680
fA	 0.9190	 0.4630
g	 0.8650	 0.4680
gA	 0.9190	 0.4830
h	 0.8620	 0.4680
hA	 0.9190	 0.4860
i	 0.8650	 0.4680
iA	 0.9190	 0.4800
j	 0.8640	 0.4670
jA	 0.9190	 0.4810
k	 0.8620	 0.4670
kA	 0.9190	 0.4740
l	 0.8650	 0.4670
lA	 0.9190	 0.4830
m	 0.8630	 0.4660
mA	 0.9190	 0.4800
n	 0.8660	 0.4670
nA	 0.9190	 0.4760
o	 0.8660	 0.4670
oA	 0.9190	 0.4870
p	 0.8660	 0.4670
pA	 0.9190	 0.4740
q	 0.8650	 0.4660
qA	 0.9190	 0.4810
r	 0.8630	 0.4650
rA	 0.9190	 0.4670
s	 0.8650	 0.4670
sA	 0.9190	 0.4920
t	 0.8630	 0.4680
tA	 0.9190	 0.4700
u	 0.8650	 0.4680
uA	 0.9190	 0.4730
v	 0.8650	 0.4670
vA	 0.9190	 0.4700
w	 0.8670	 0.4680
wA	 0.9190	 0.4680
x	 0.8670	 0.4670
xA	 0.9190	 0.4870
y	 0.8670	 0.4680
yA	 0.9190	 0.4830

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Chain	Atom inclusion	Q-score
z	 0.8670	 0.4680
zA	 0.9190	 0.4810