



## wwPDB EM Validation Summary Report ⓘ

May 26, 2025 – 09:40 AM EDT

PDB ID : 5IPK / pdb\_00005ipk  
EMDB ID : EMD-8100  
Title : Structure of the R432A variant of Adeno-associated virus type 2 VLP  
Authors : Drouin, L.M.; Lins, B.; Janssen, M.E.; Bennet, A.; Chipman, P.; McKenna, R.; Chen, W.; Muzyczka, N.; Cardone, G.; Baker, T.S.; Agbandje-McKenna, M.  
Deposited on : 2016-03-09  
Resolution : 3.70 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

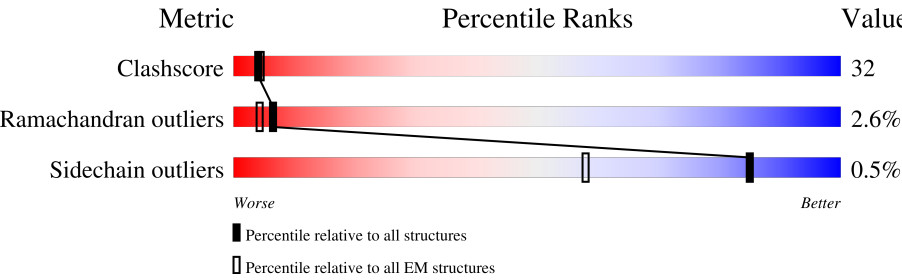
EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

# 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 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	735	<div> <div>16%</div> <div>29%</div> <div>36%</div> <div>32%</div> </div>
1	2	735	<div> <div>16%</div> <div>30%</div> <div>35%</div> <div>32%</div> </div>
1	3	735	<div> <div>15%</div> <div>30%</div> <div>36%</div> <div>32%</div> </div>
1	4	735	<div> <div>16%</div> <div>30%</div> <div>36%</div> <div>32%</div> </div>
1	5	735	<div> <div>16%</div> <div>30%</div> <div>36%</div> <div>32%</div> </div>
1	6	735	<div> <div>16%</div> <div>30%</div> <div>36%</div> <div>32%</div> </div>
1	7	735	<div> <div>15%</div> <div>30%</div> <div>36%</div> <div>32%</div> </div>
1	8	735	<div> <div>16%</div> <div>30%</div> <div>36%</div> <div>32%</div> </div>

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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	
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	

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Mol	Chain	Length	Quality of chain
1	y	735	<div><div><div>16%</div><div>30%</div><div>36%</div><div>32%</div></div></div>
1	z	735	<div><div><div>16%</div><div>30%</div><div>36%</div><div>32%</div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 240540 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	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	B	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	C	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	D	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	E	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	F	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	G	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	H	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	I	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	J	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	K	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	L	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	M	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	N	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	O	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	P	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	Q	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	S	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	T	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	U	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	V	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	W	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	X	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	Y	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	Z	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	a	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	b	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	c	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	d	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	e	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	f	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	g	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	h	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	i	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	j	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	k	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	l	500	Total 4009	C 2528	N 697	O 773	S 11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	n	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	o	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	p	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	q	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	r	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	s	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	t	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	u	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	v	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	w	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	x	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	y	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	z	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	1	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	2	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	3	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	4	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	5	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	6	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	7	500	Total 4009	C 2528	N 697	O 773	S 11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		

There are 60 discrepancies between the modelled and reference sequences:

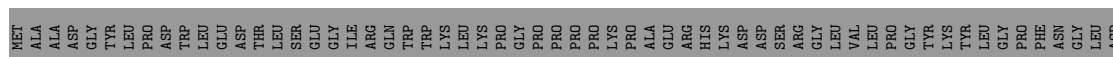
Chain	Residue	Modelled	Actual	Comment	Reference
A	432	ALA	ARG	engineered mutation	UNP P03135
B	432	ALA	ARG	engineered mutation	UNP P03135
C	432	ALA	ARG	engineered mutation	UNP P03135
D	432	ALA	ARG	engineered mutation	UNP P03135
E	432	ALA	ARG	engineered mutation	UNP P03135
F	432	ALA	ARG	engineered mutation	UNP P03135
G	432	ALA	ARG	engineered mutation	UNP P03135
H	432	ALA	ARG	engineered mutation	UNP P03135
I	432	ALA	ARG	engineered mutation	UNP P03135
J	432	ALA	ARG	engineered mutation	UNP P03135
K	432	ALA	ARG	engineered mutation	UNP P03135
L	432	ALA	ARG	engineered mutation	UNP P03135
M	432	ALA	ARG	engineered mutation	UNP P03135
N	432	ALA	ARG	engineered mutation	UNP P03135
O	432	ALA	ARG	engineered mutation	UNP P03135
P	432	ALA	ARG	engineered mutation	UNP P03135
Q	432	ALA	ARG	engineered mutation	UNP P03135
R	432	ALA	ARG	engineered mutation	UNP P03135
S	432	ALA	ARG	engineered mutation	UNP P03135
T	432	ALA	ARG	engineered mutation	UNP P03135
U	432	ALA	ARG	engineered mutation	UNP P03135
V	432	ALA	ARG	engineered mutation	UNP P03135
W	432	ALA	ARG	engineered mutation	UNP P03135
X	432	ALA	ARG	engineered mutation	UNP P03135
Y	432	ALA	ARG	engineered mutation	UNP P03135
Z	432	ALA	ARG	engineered mutation	UNP P03135
a	432	ALA	ARG	engineered mutation	UNP P03135
b	432	ALA	ARG	engineered mutation	UNP P03135
c	432	ALA	ARG	engineered mutation	UNP P03135
d	432	ALA	ARG	engineered mutation	UNP P03135
e	432	ALA	ARG	engineered mutation	UNP P03135
f	432	ALA	ARG	engineered mutation	UNP P03135
g	432	ALA	ARG	engineered mutation	UNP P03135
h	432	ALA	ARG	engineered mutation	UNP P03135
i	432	ALA	ARG	engineered mutation	UNP P03135
j	432	ALA	ARG	engineered mutation	UNP P03135

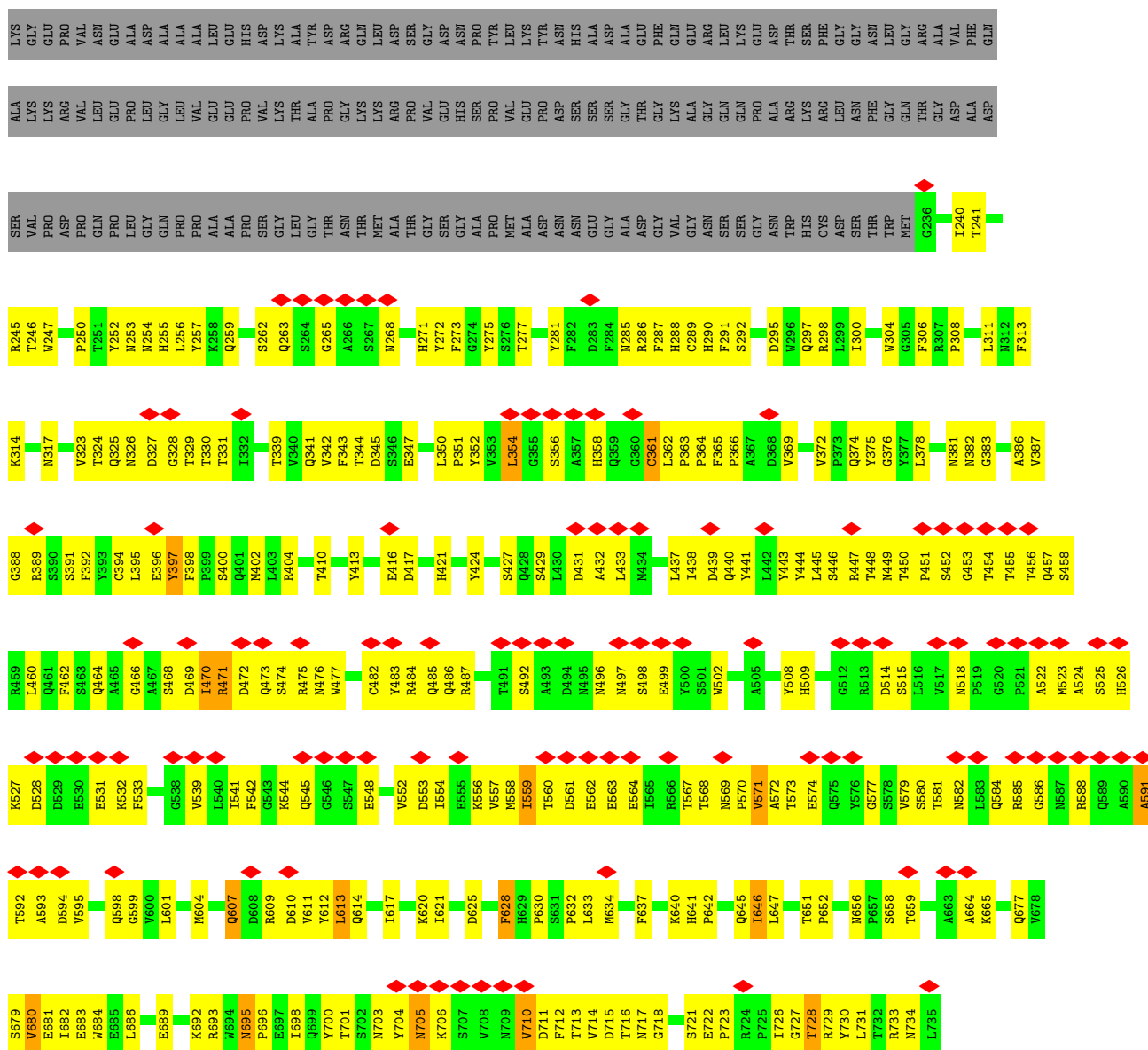
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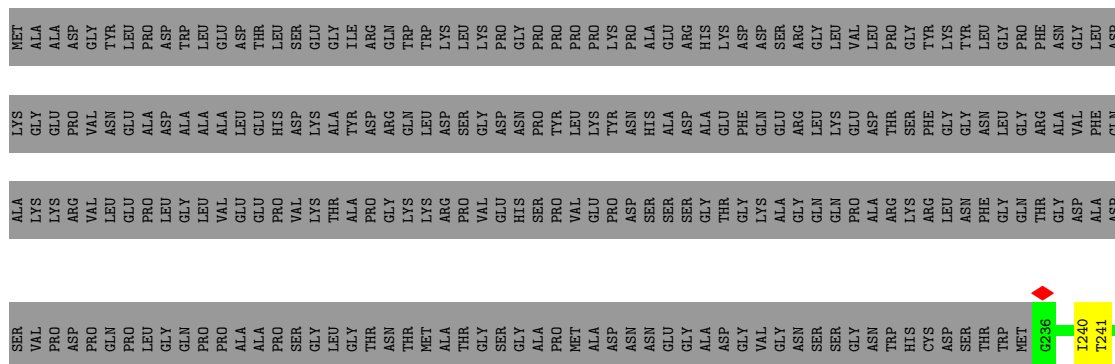
Chain	Residue	Modelled	Actual	Comment	Reference
k	432	ALA	ARG	engineered mutation	UNP P03135
l	432	ALA	ARG	engineered mutation	UNP P03135
m	432	ALA	ARG	engineered mutation	UNP P03135
n	432	ALA	ARG	engineered mutation	UNP P03135
o	432	ALA	ARG	engineered mutation	UNP P03135
p	432	ALA	ARG	engineered mutation	UNP P03135
q	432	ALA	ARG	engineered mutation	UNP P03135
r	432	ALA	ARG	engineered mutation	UNP P03135
s	432	ALA	ARG	engineered mutation	UNP P03135
t	432	ALA	ARG	engineered mutation	UNP P03135
u	432	ALA	ARG	engineered mutation	UNP P03135
v	432	ALA	ARG	engineered mutation	UNP P03135
w	432	ALA	ARG	engineered mutation	UNP P03135
x	432	ALA	ARG	engineered mutation	UNP P03135
y	432	ALA	ARG	engineered mutation	UNP P03135
z	432	ALA	ARG	engineered mutation	UNP P03135
1	432	ALA	ARG	engineered mutation	UNP P03135
2	432	ALA	ARG	engineered mutation	UNP P03135
3	432	ALA	ARG	engineered mutation	UNP P03135
4	432	ALA	ARG	engineered mutation	UNP P03135
5	432	ALA	ARG	engineered mutation	UNP P03135
6	432	ALA	ARG	engineered mutation	UNP P03135
7	432	ALA	ARG	engineered mutation	UNP P03135
8	432	ALA	ARG	engineered mutation	UNP P03135

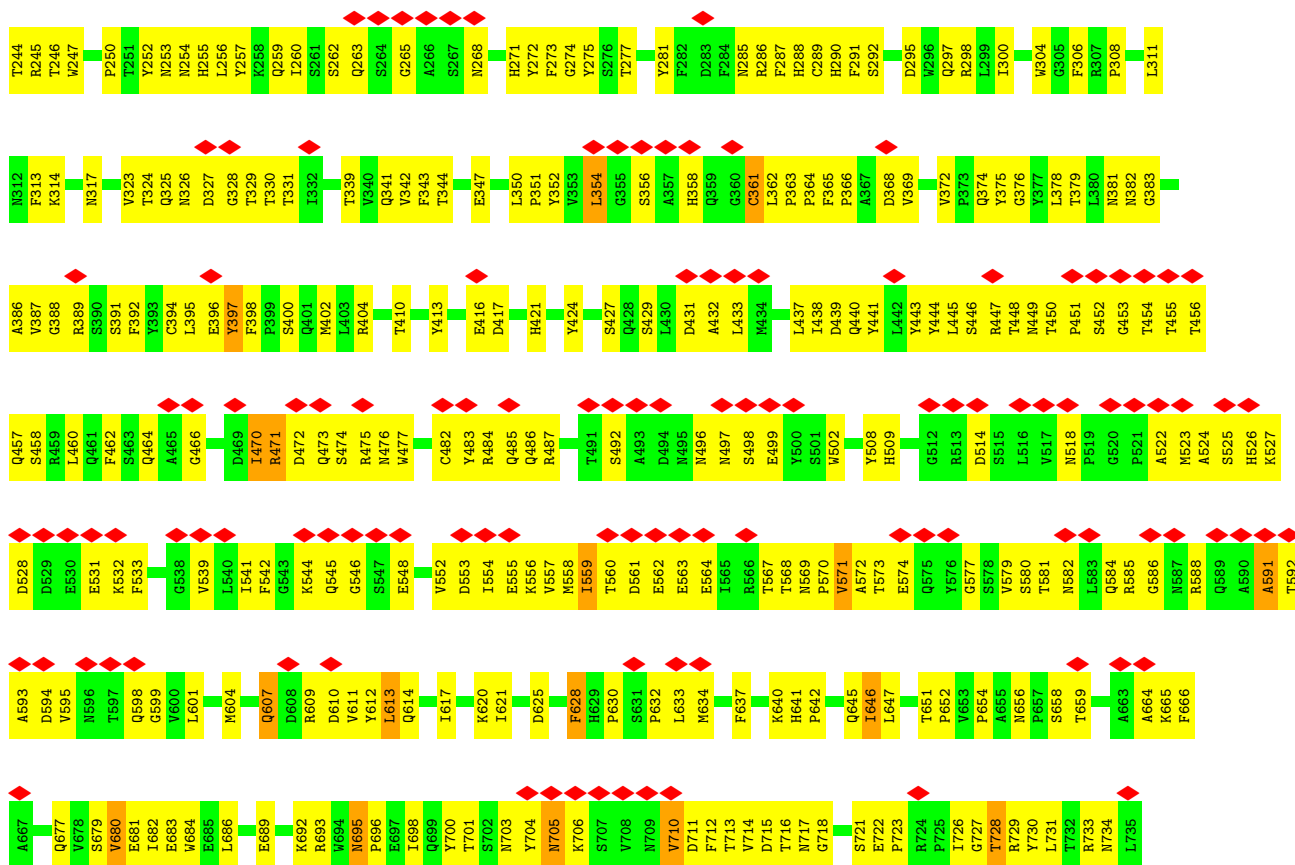




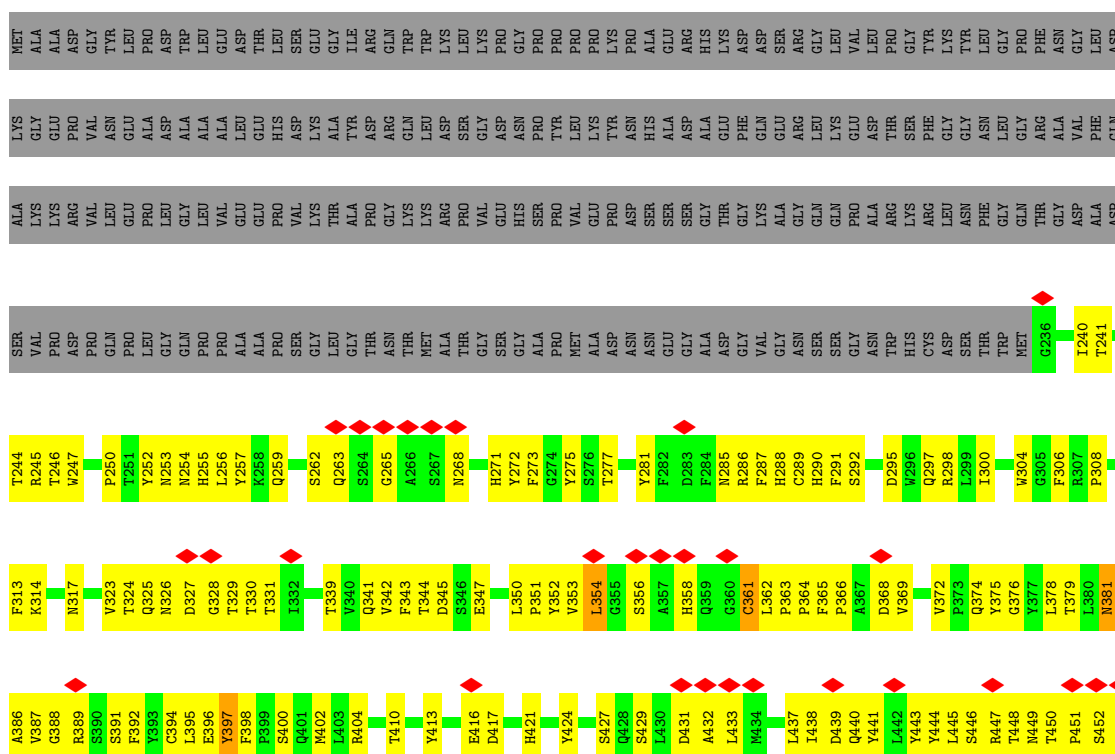


• Molecule 1: Capsid protein VP1

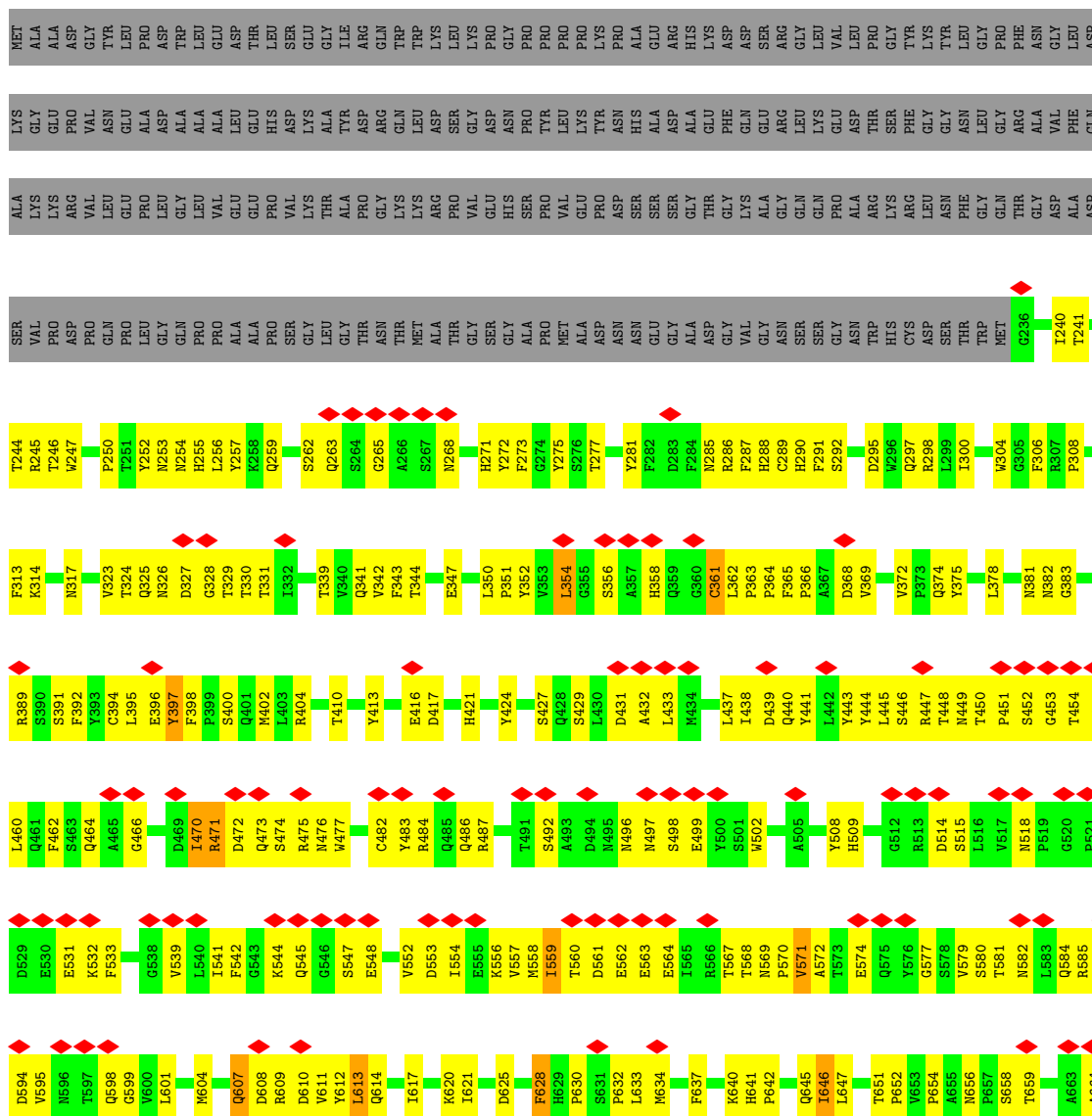




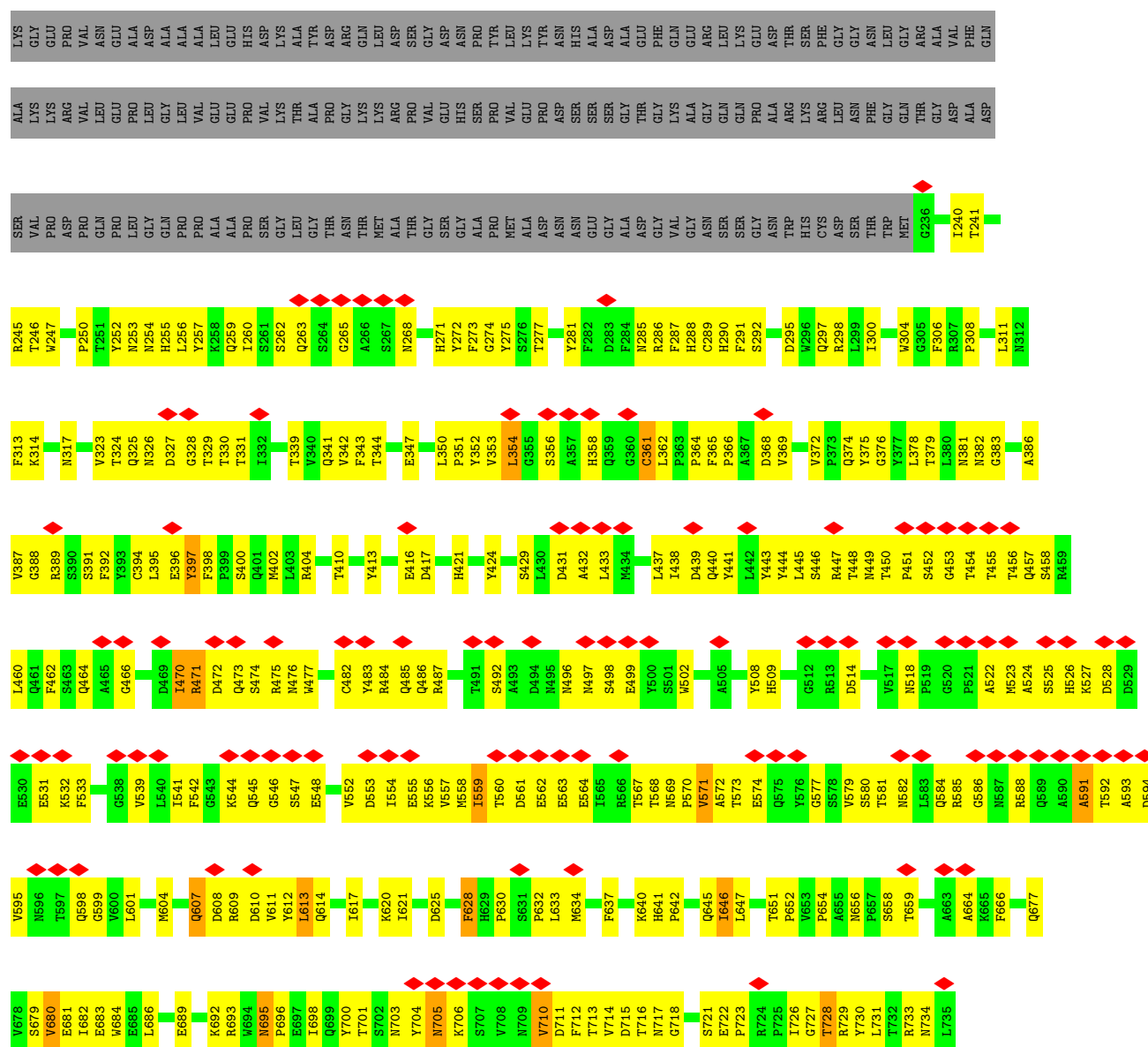
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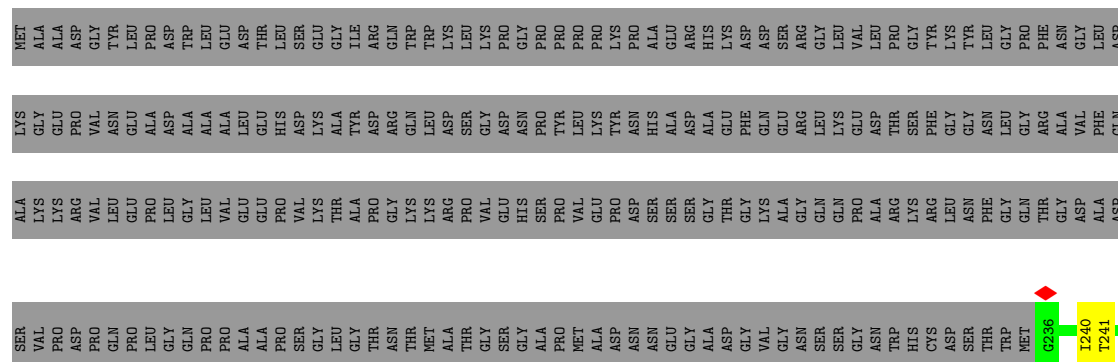
- Molecule 1: Capsid protein VP1



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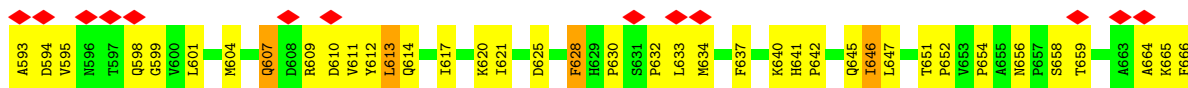
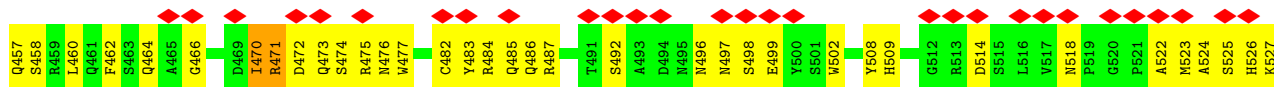
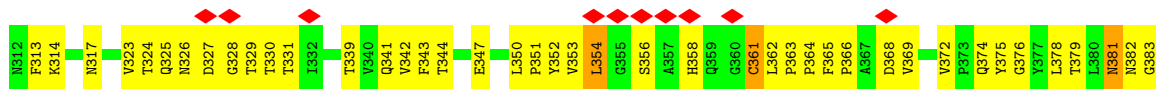
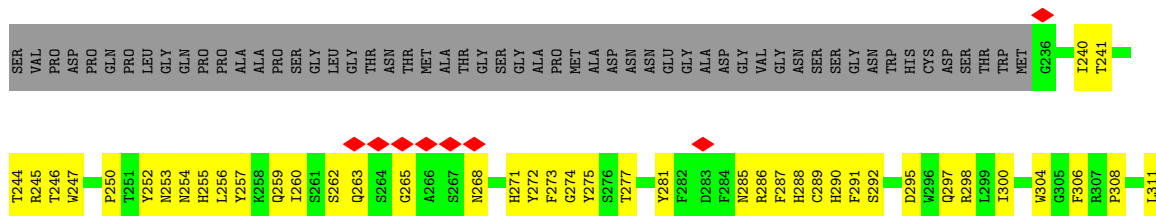
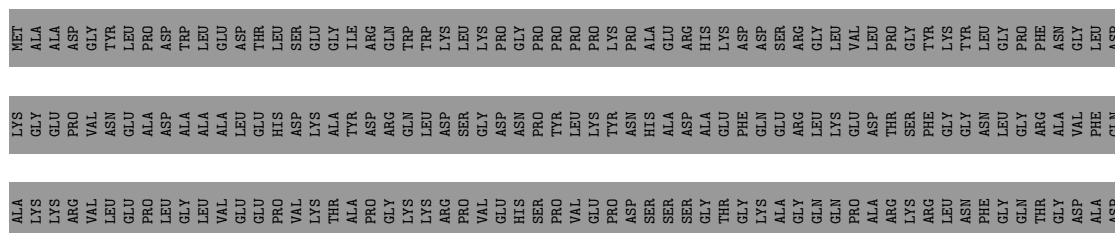


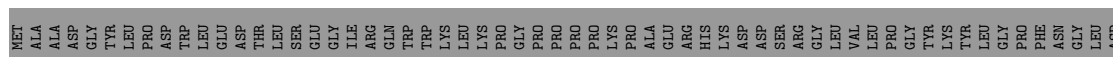
● Molecule 1: Capsid protein VP1

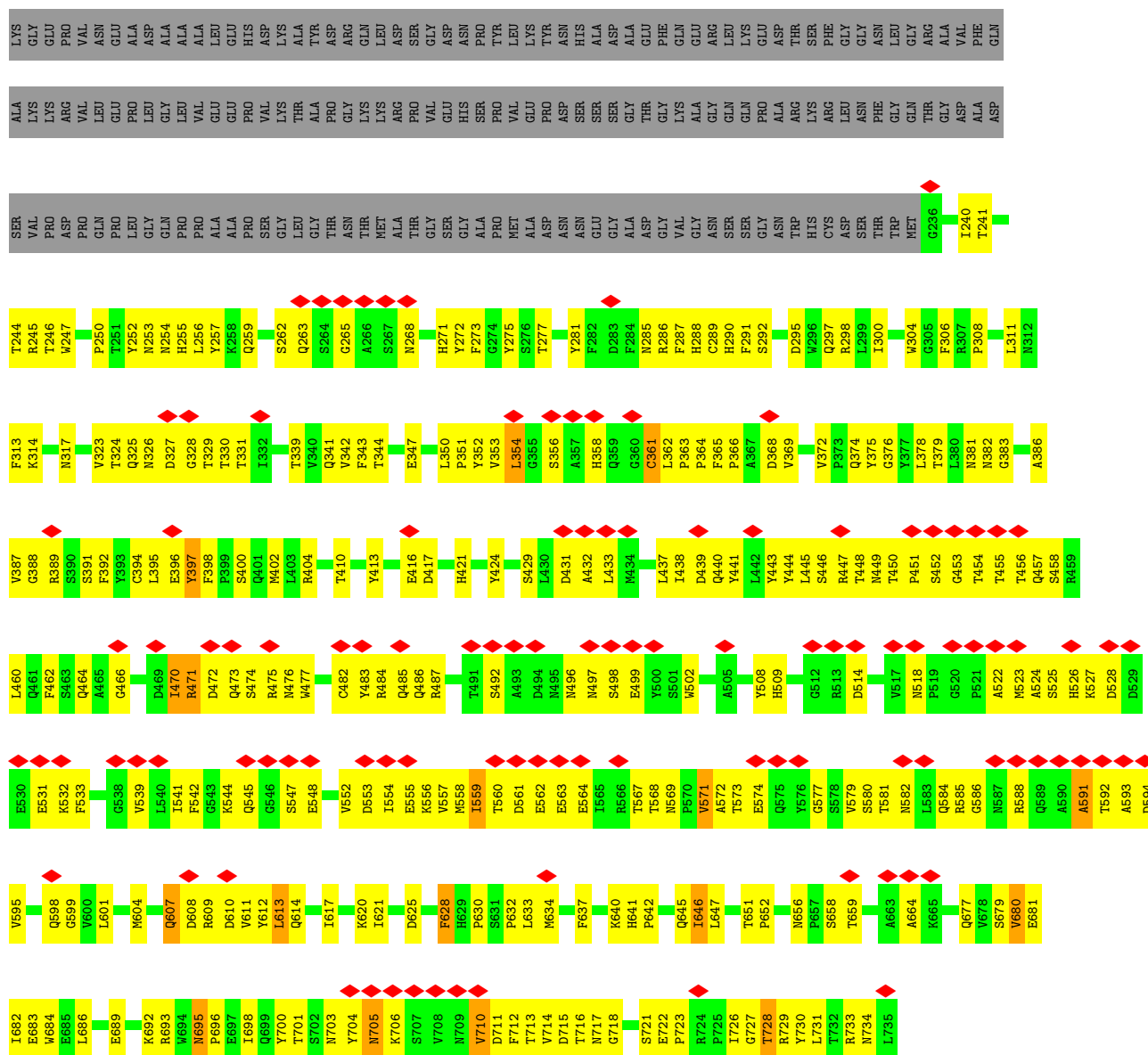




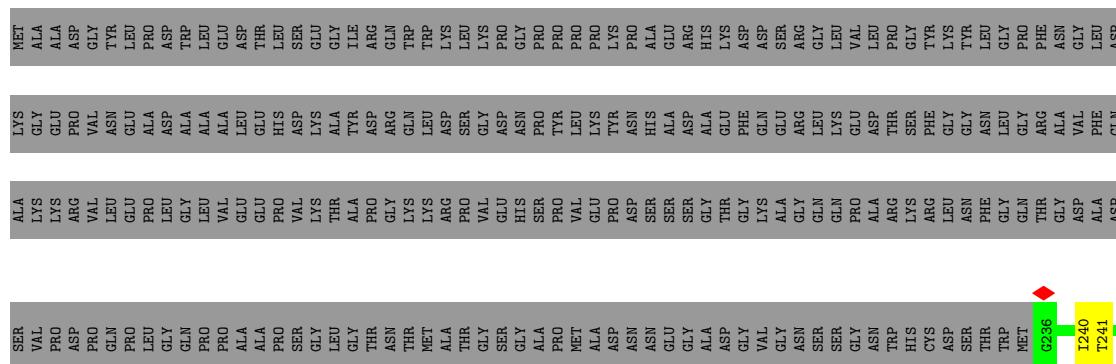
- Molecule 1: Capsid protein VP1

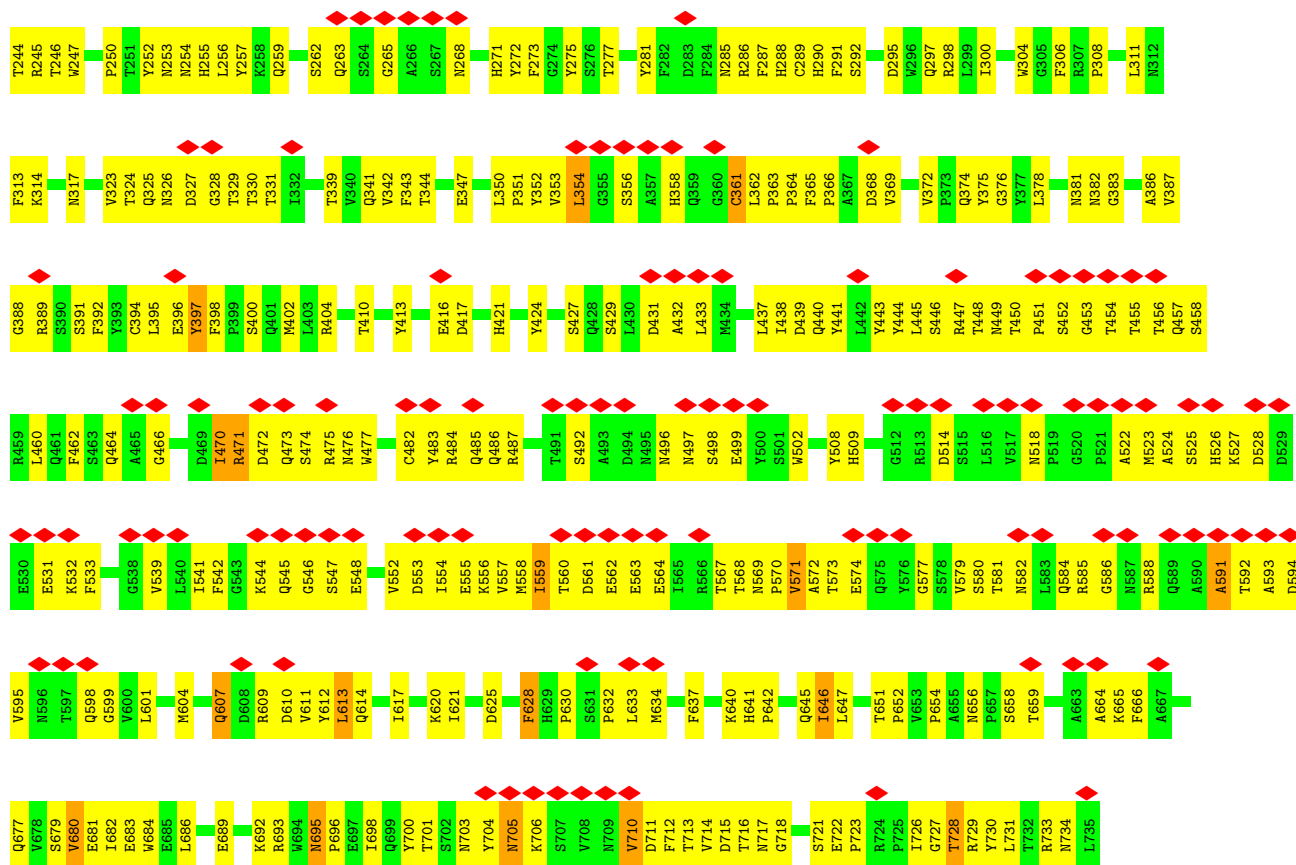




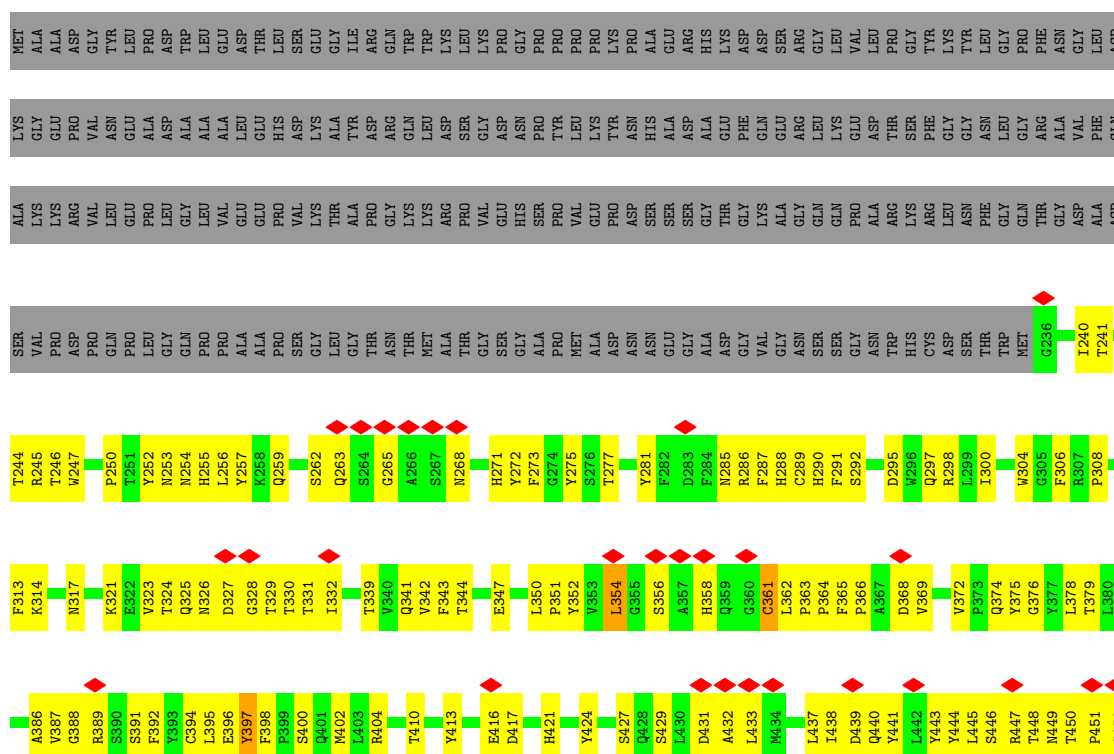


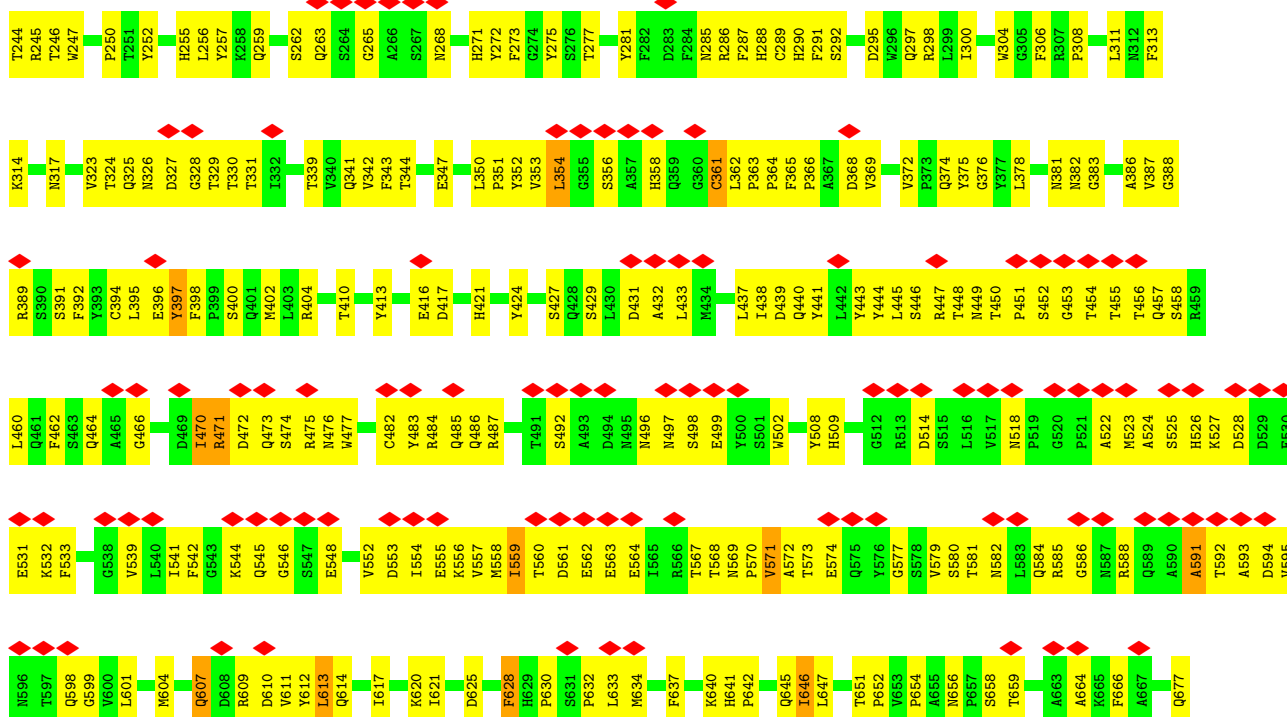
• Molecule 1: Capsid protein VP1

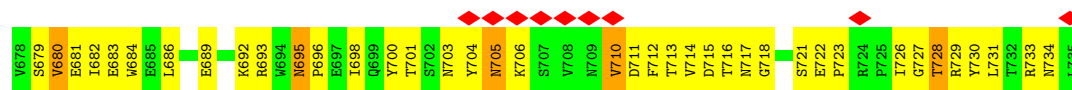




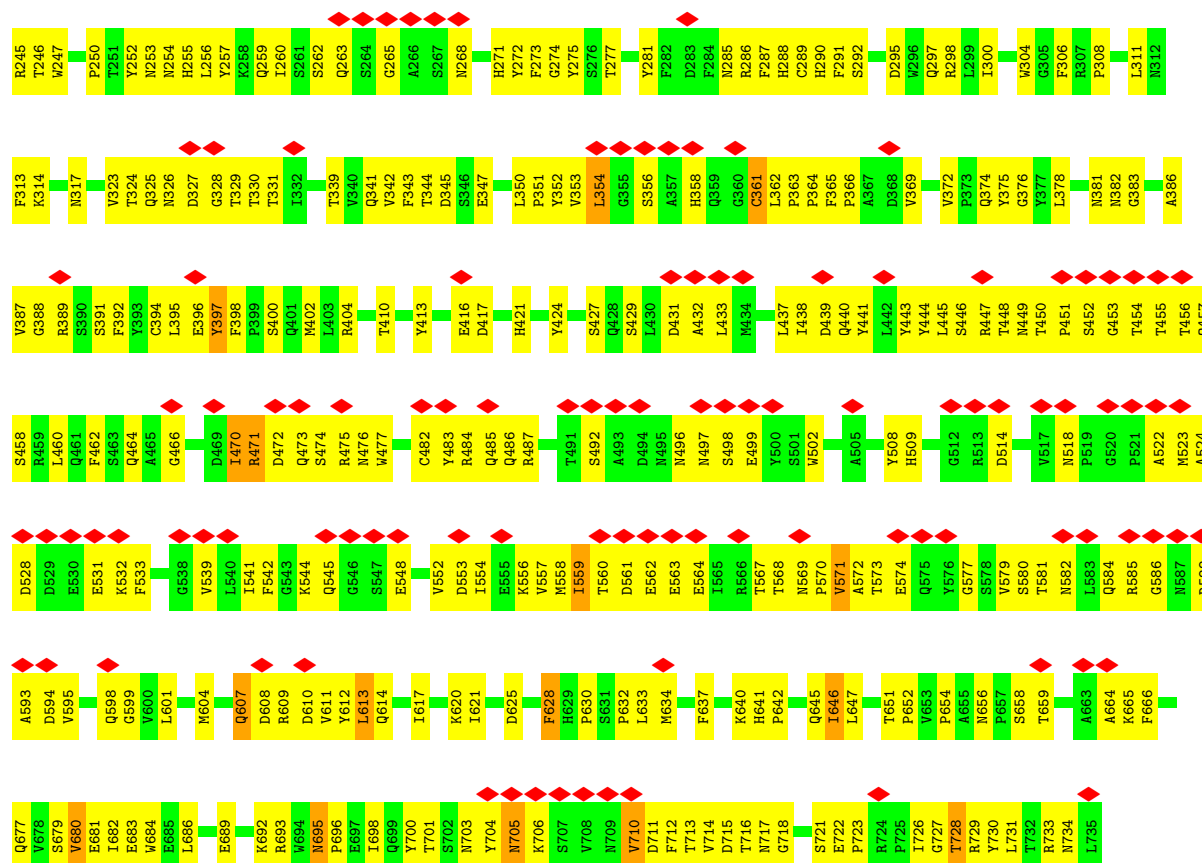
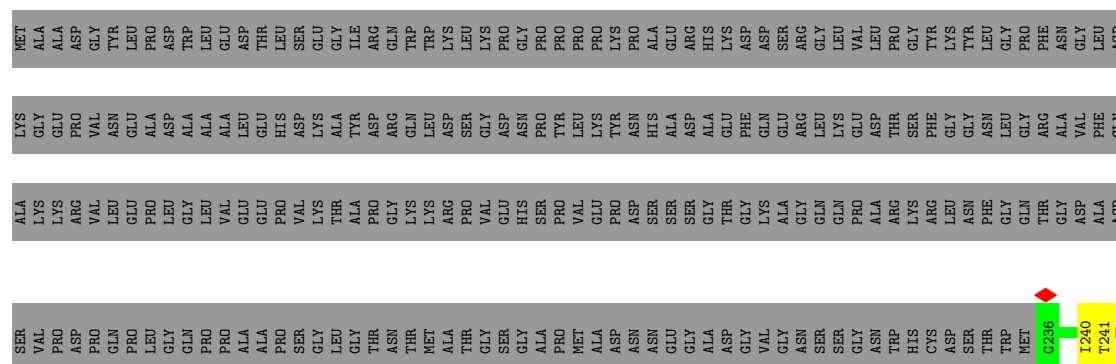
• Molecule 1: Capsid protein VP1



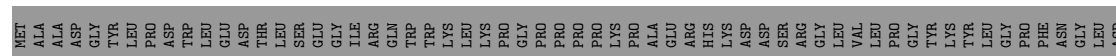


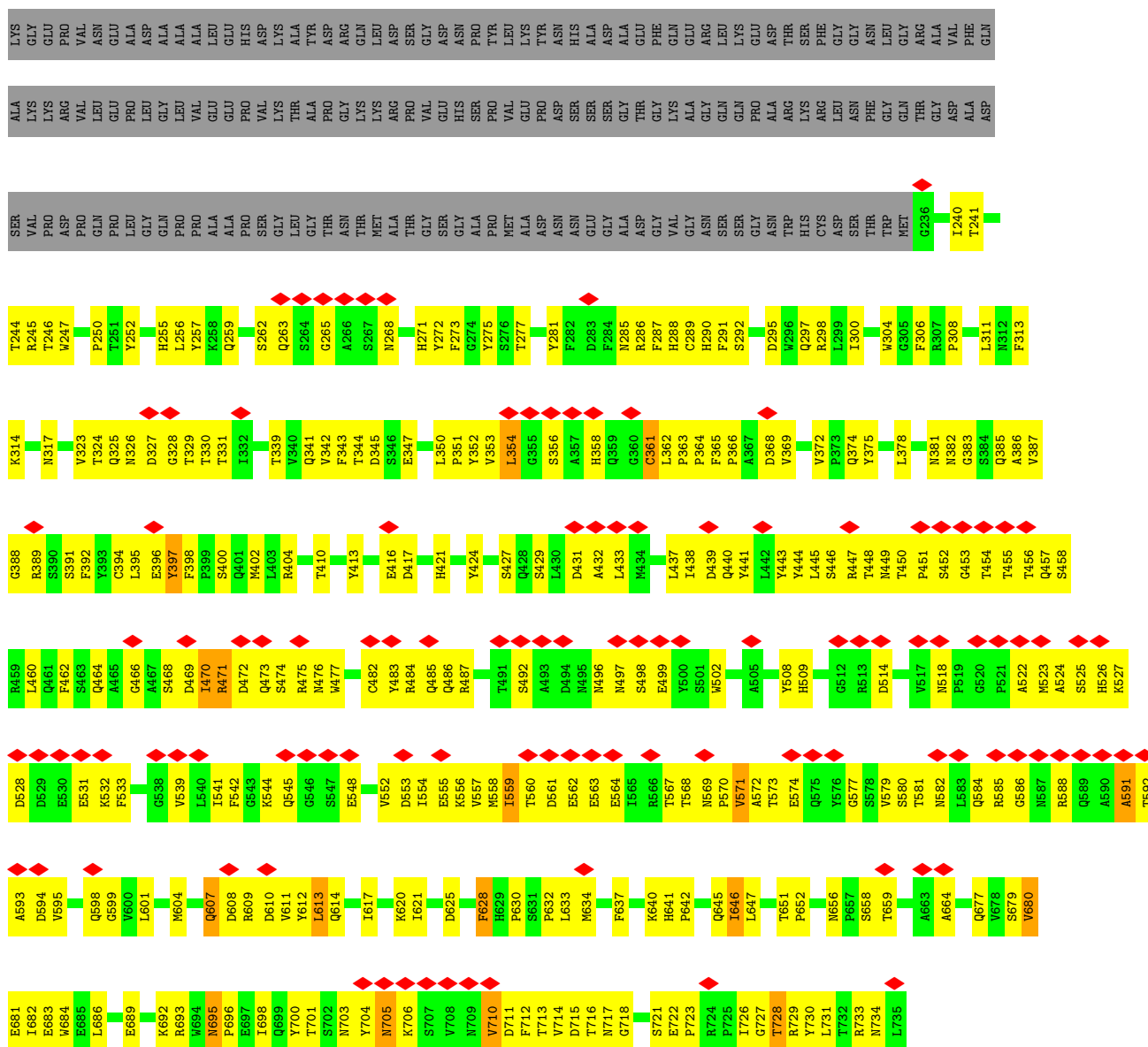


• Molecule 1: Capsid protein VP1

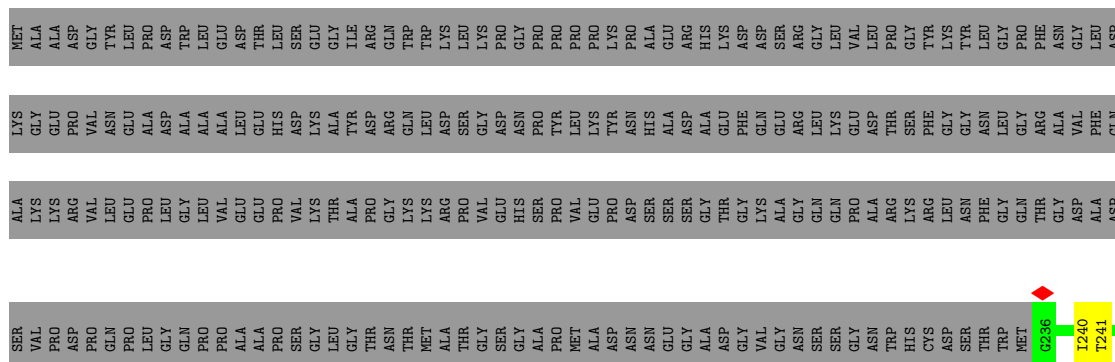


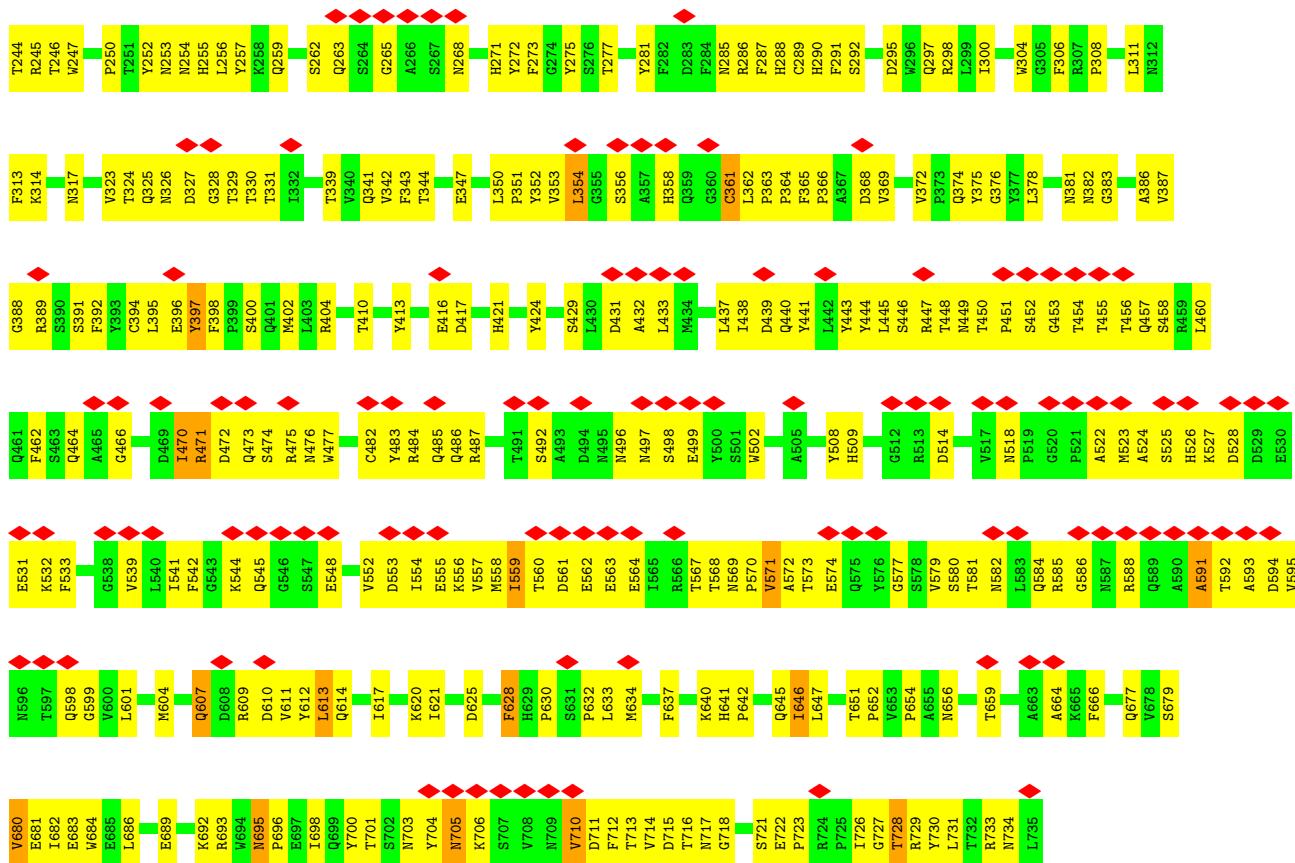
• Molecule 1: Capsid protein VP1



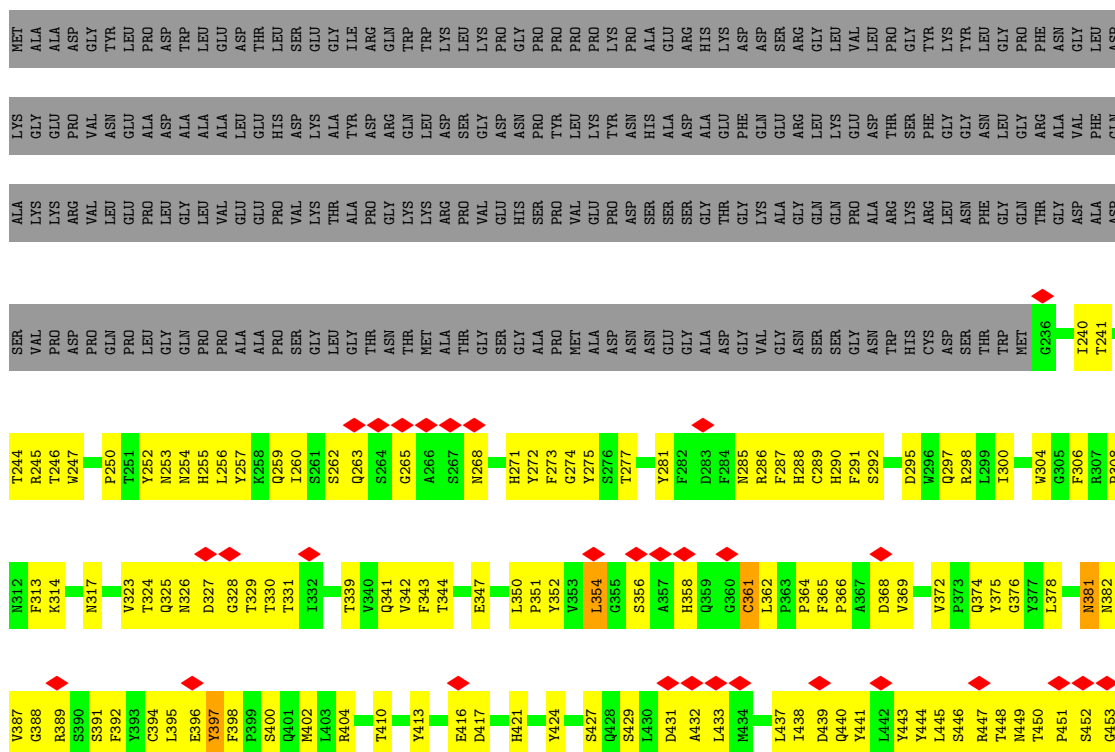


• Molecule 1: Capsid protein VP1



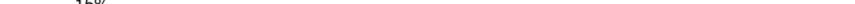


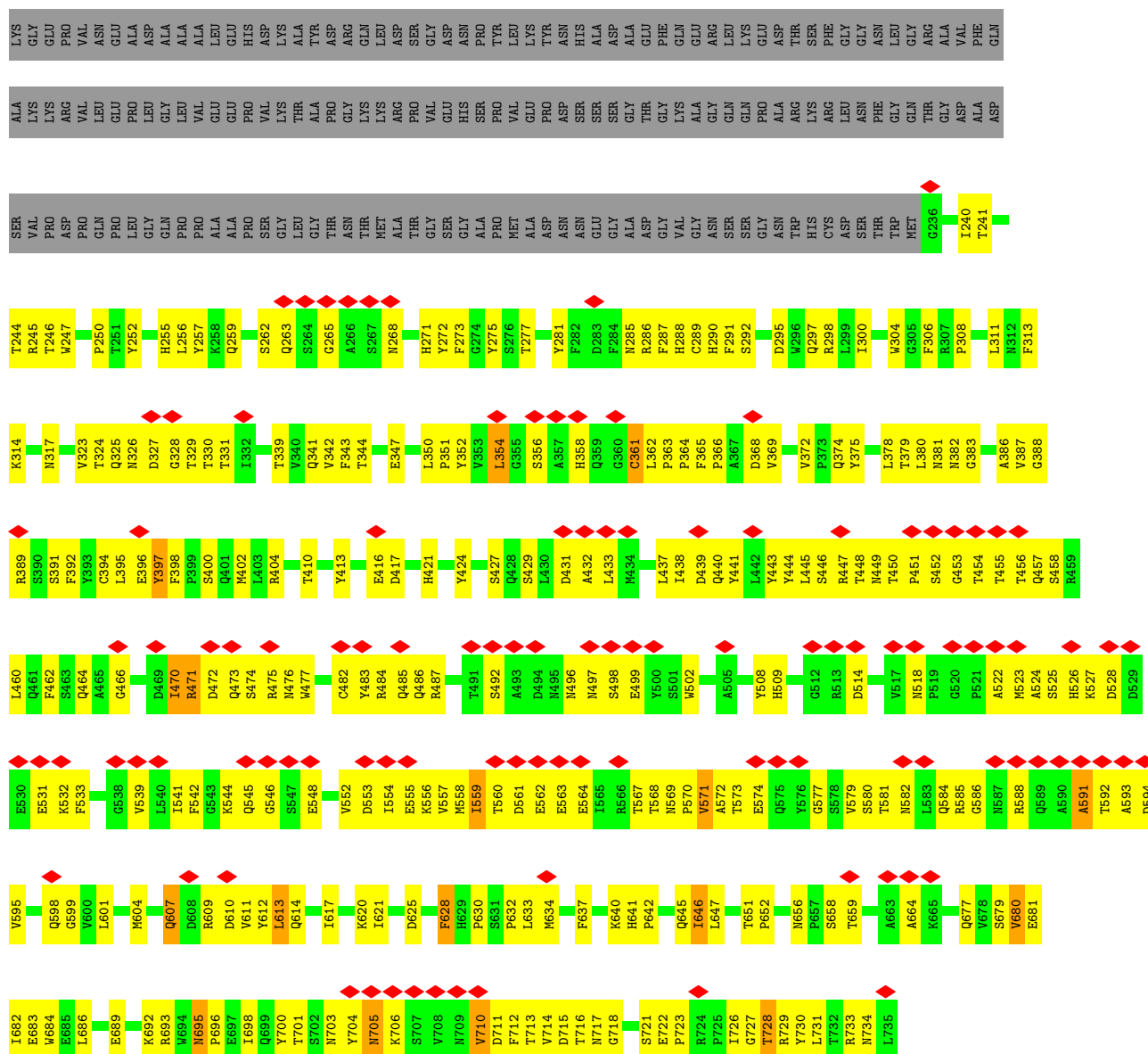
- Molecule 1: Capsid protein VP1



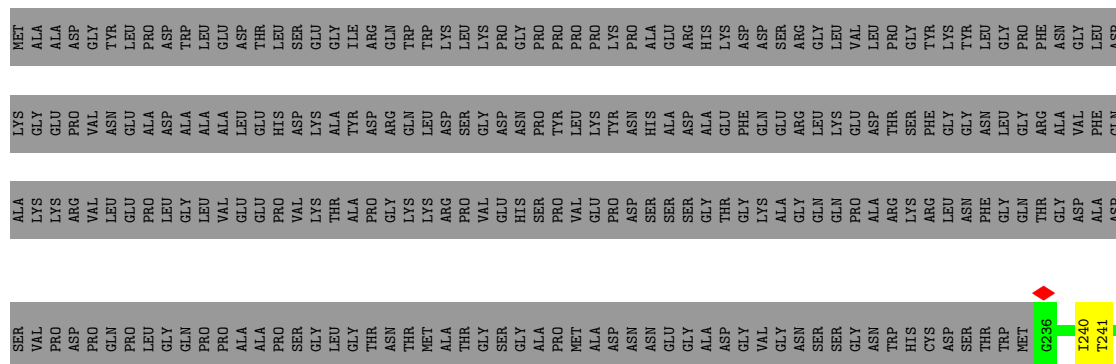


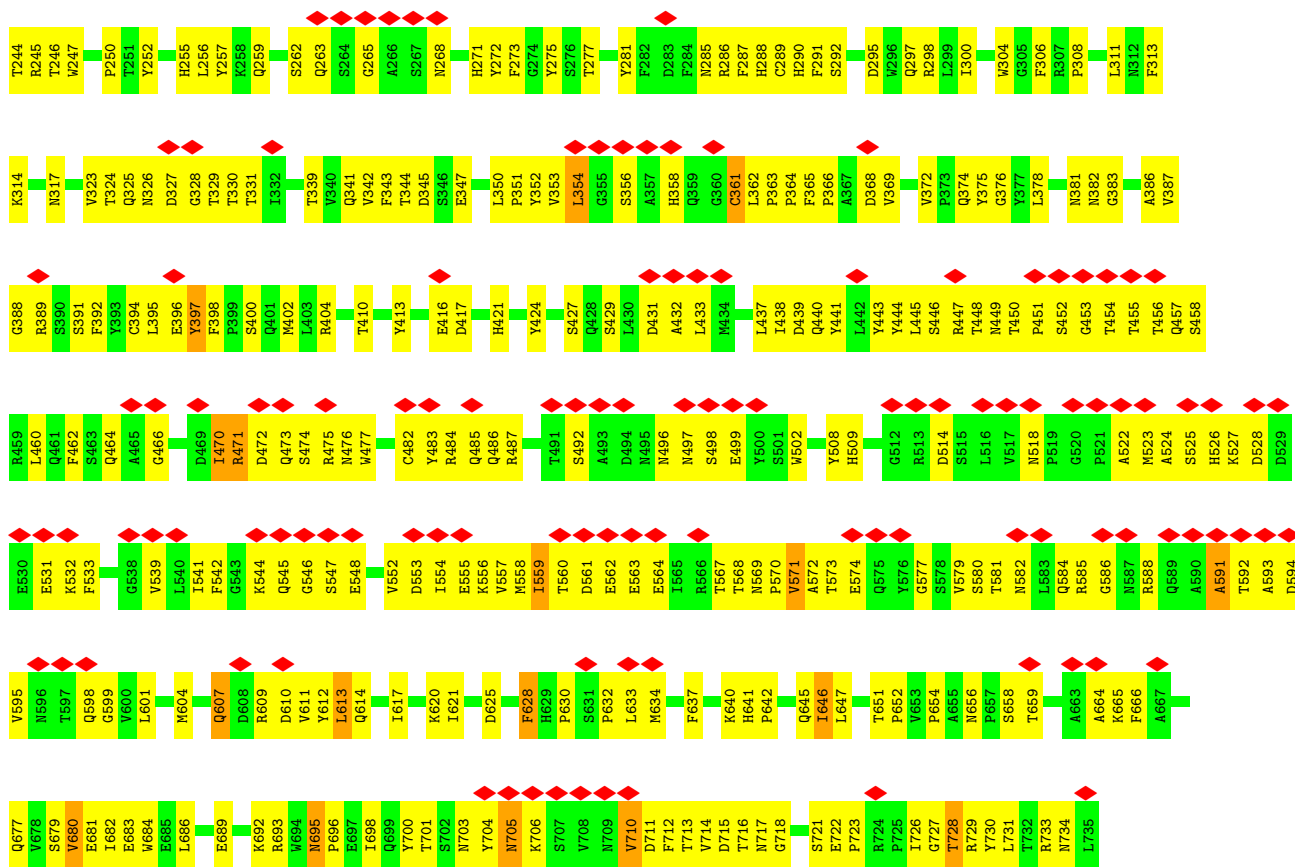
[illegible]

Chain W: 

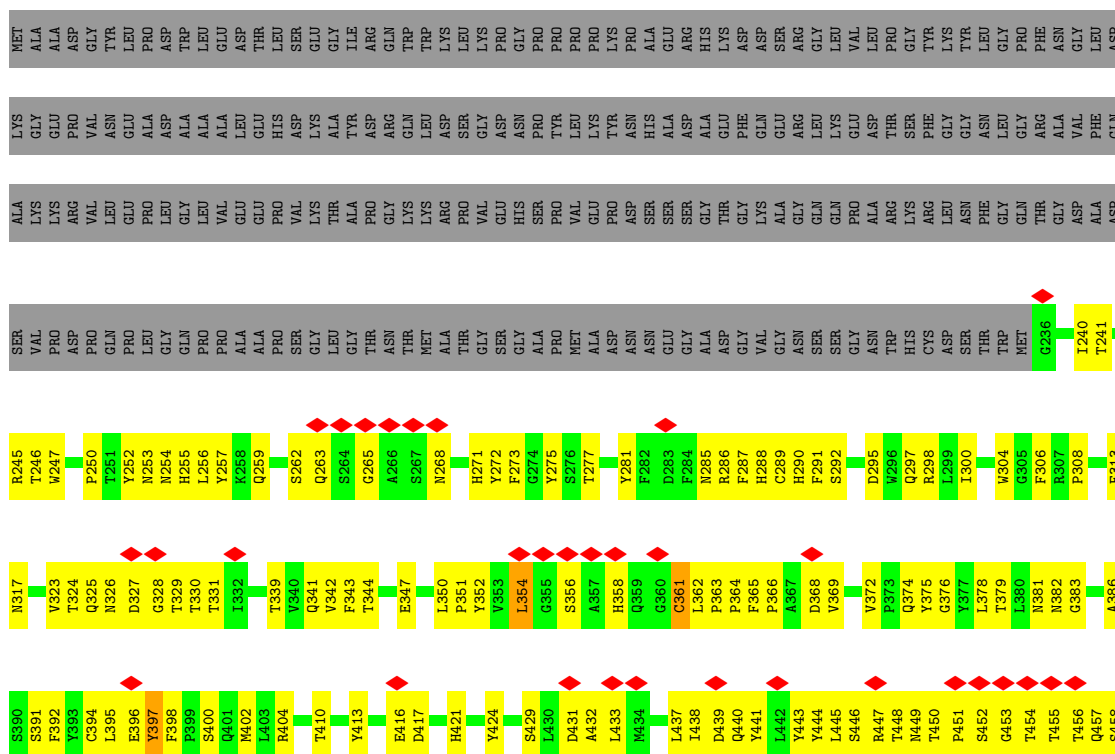


• Molecule 1: Capsid protein VP1

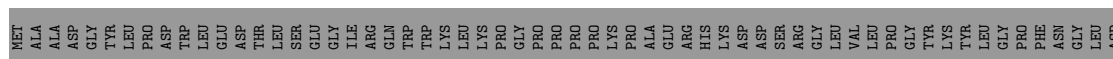


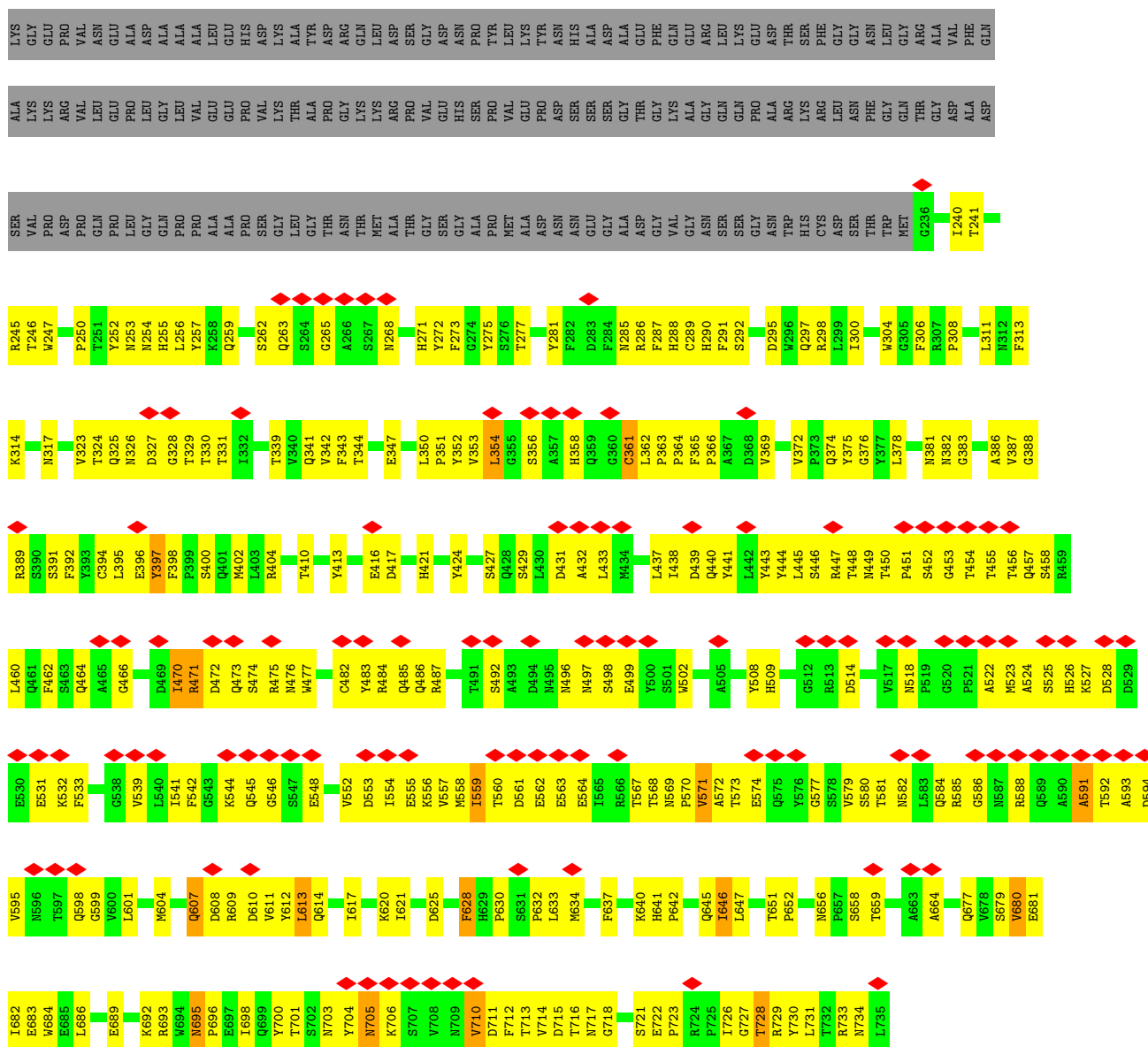


### • Molecule 1: Capsid protein VP1

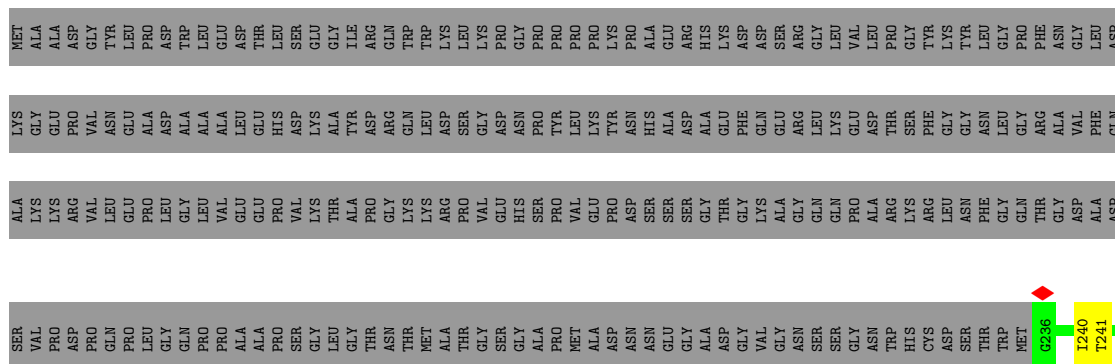




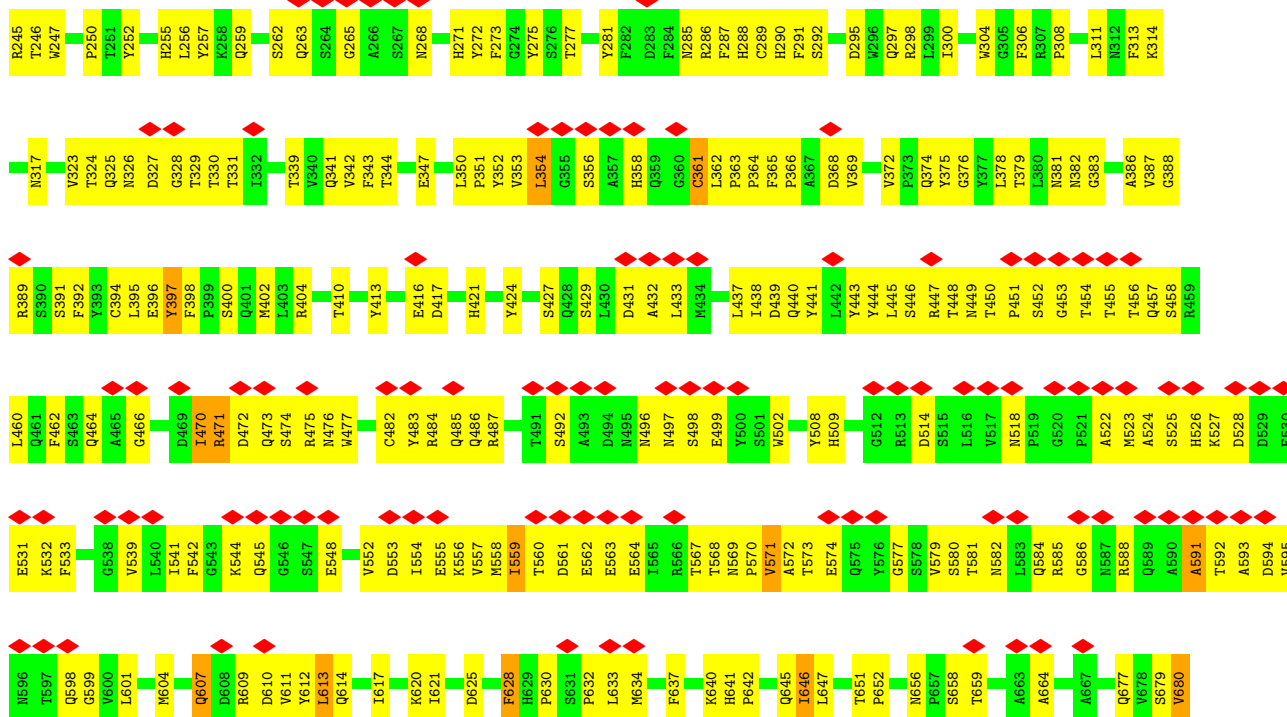


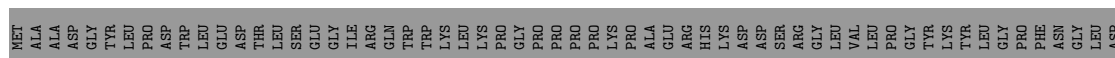


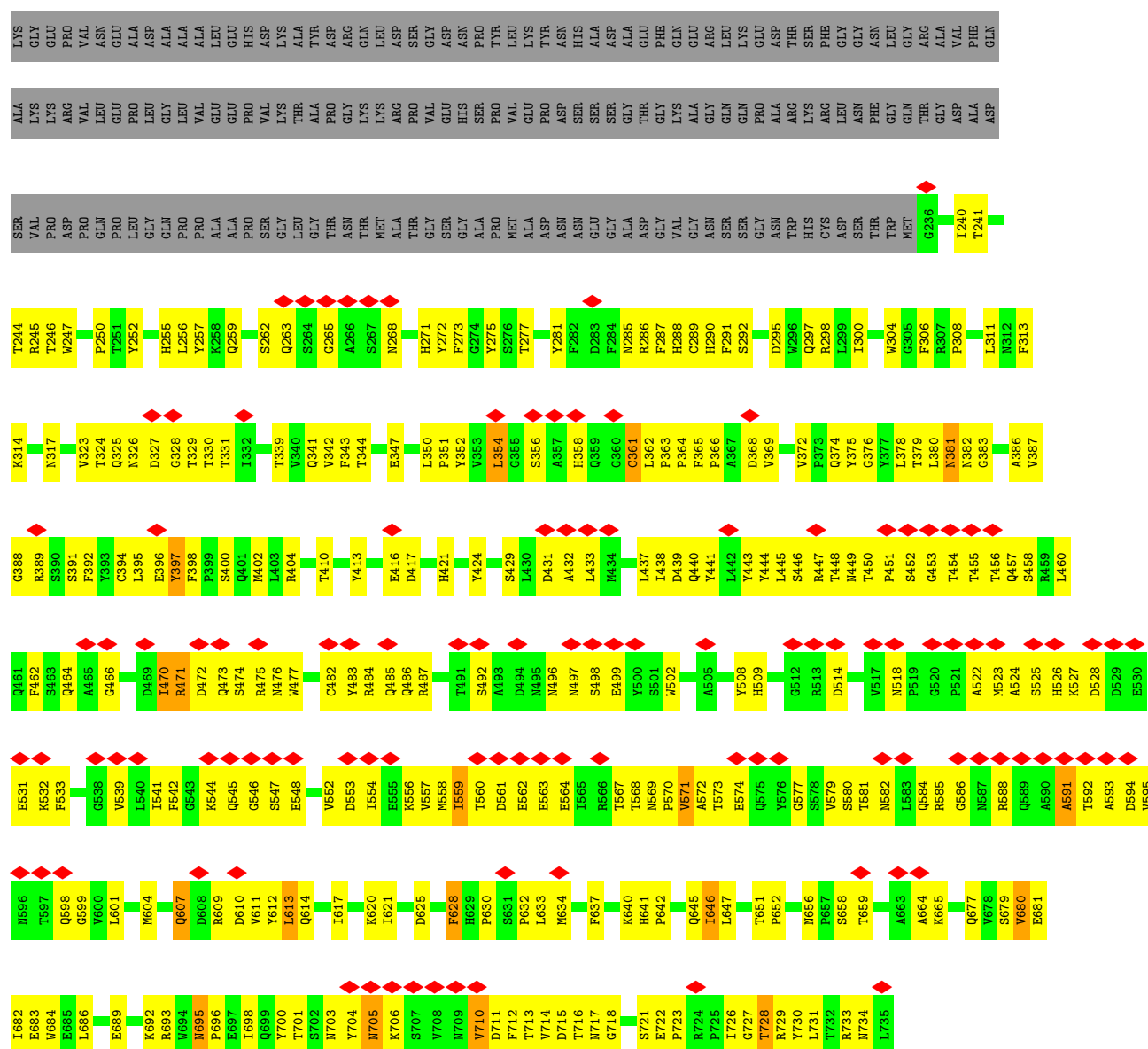
• Molecule 1: Capsid protein VP1



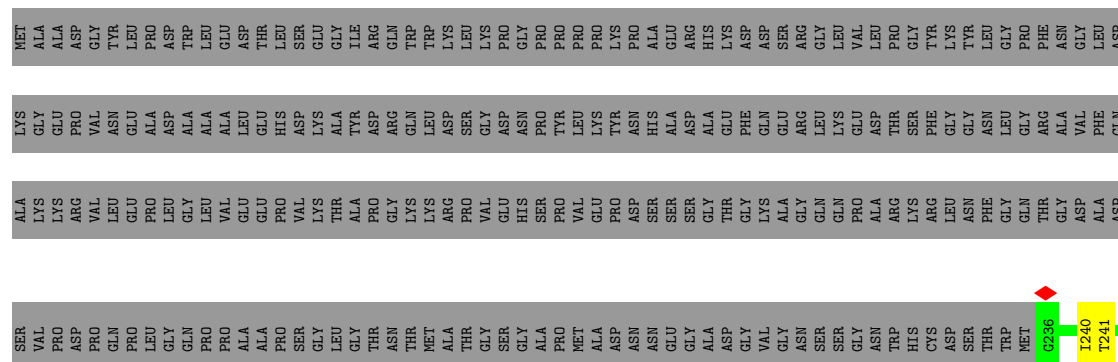


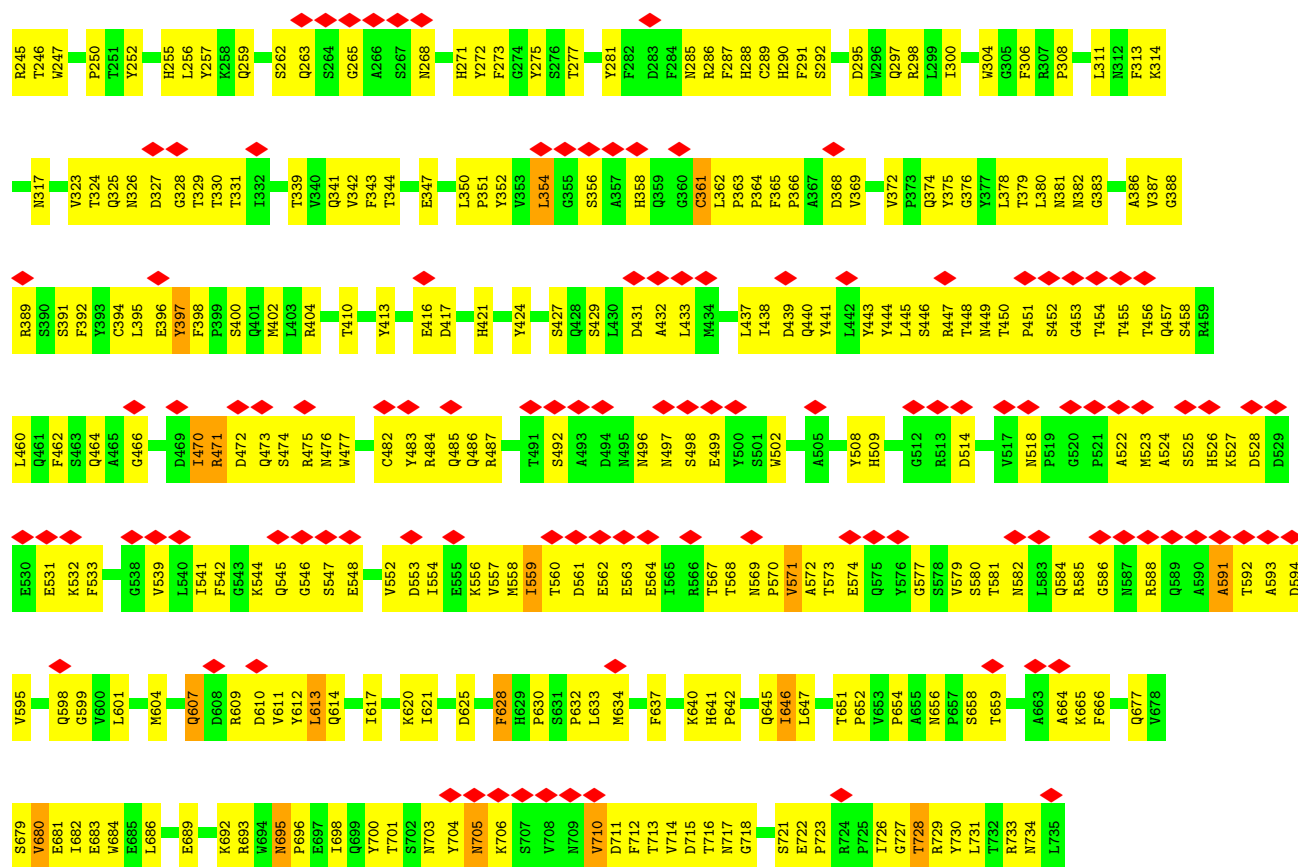




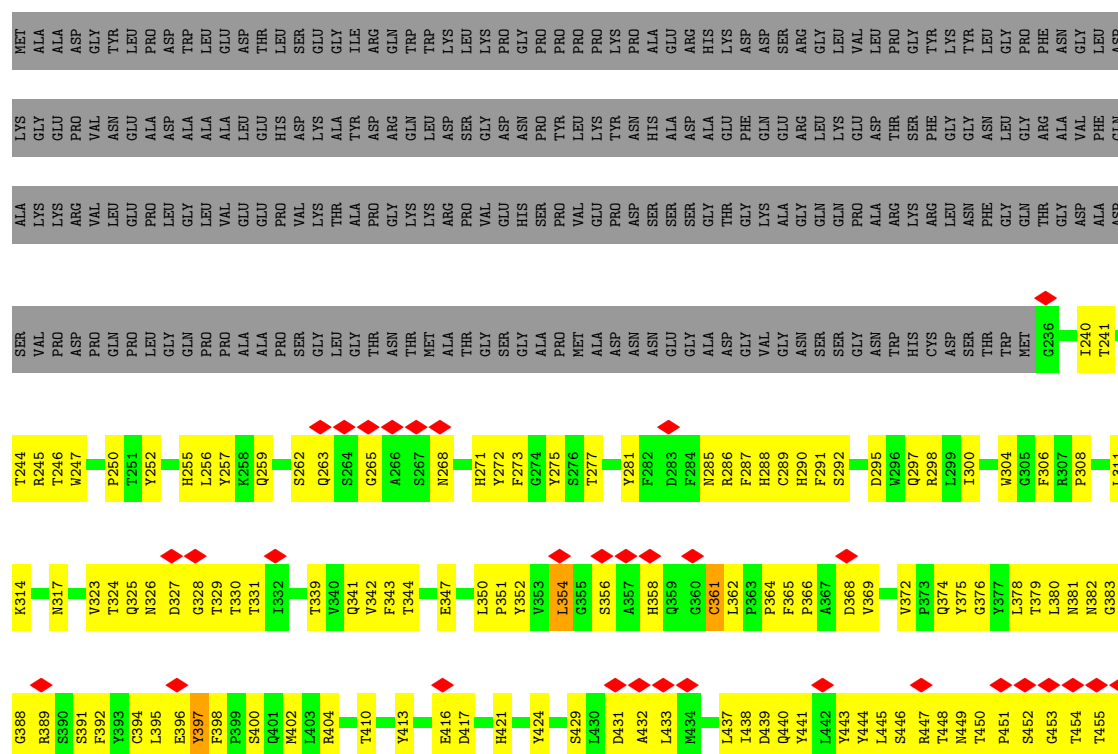


• Molecule 1: Capsid protein VP1





# • Molecule 1: Capsid protein VP1



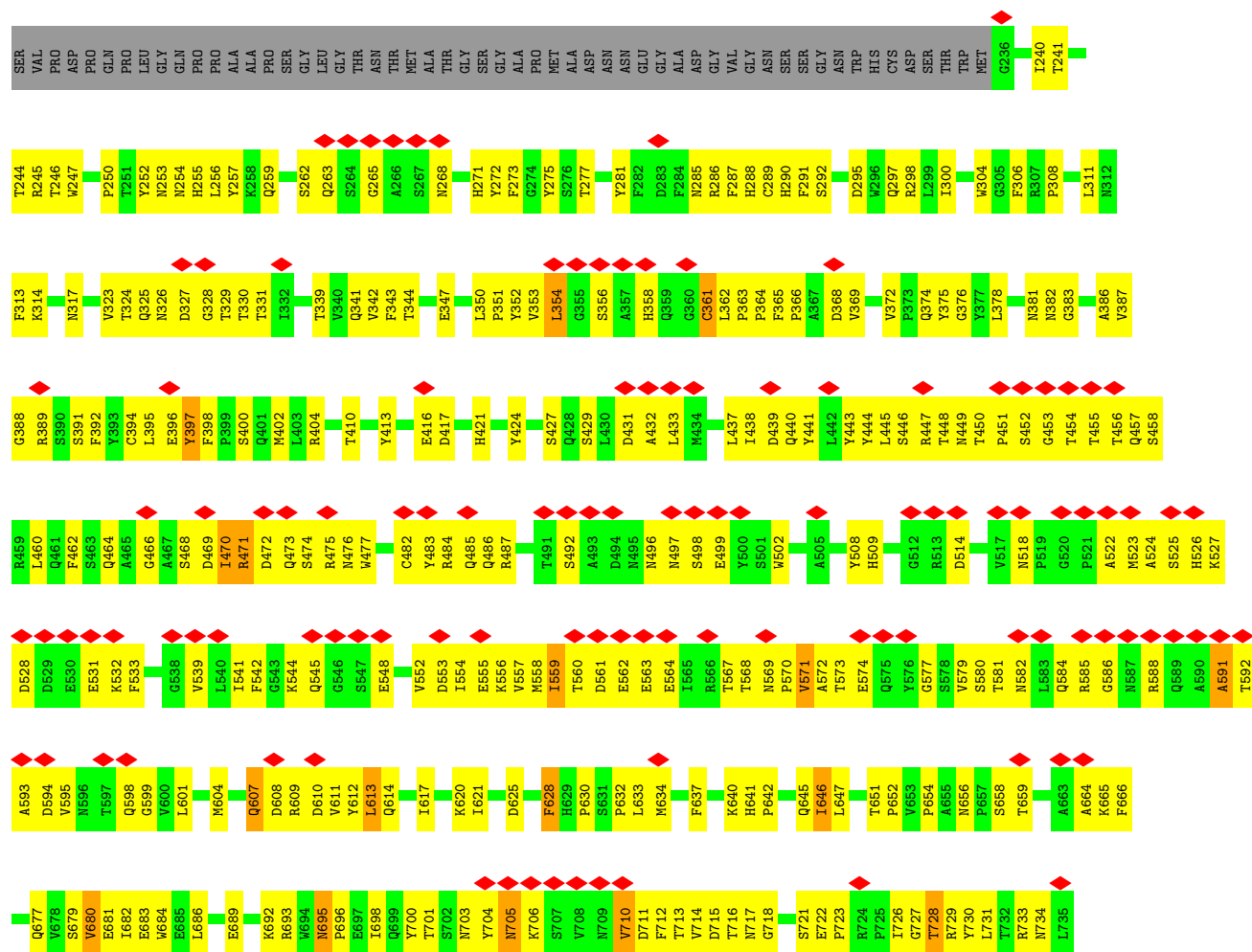




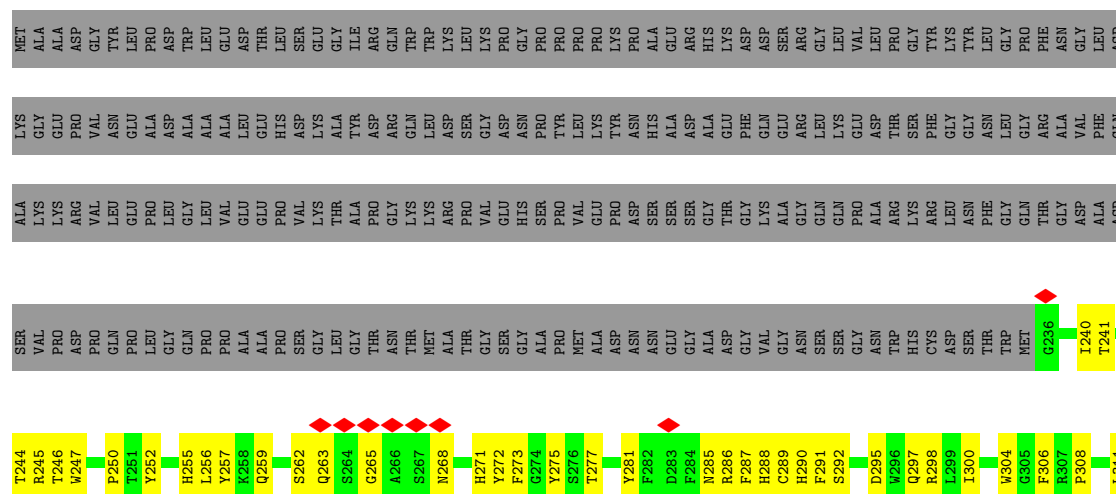
Chain 1:

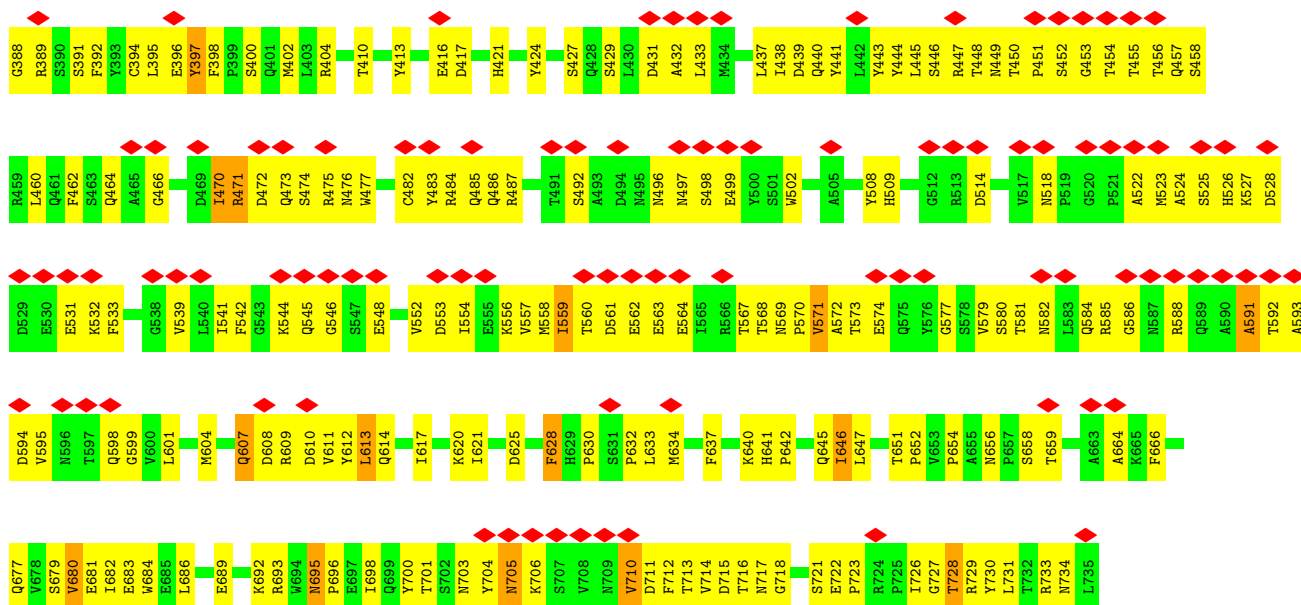
Chain m:



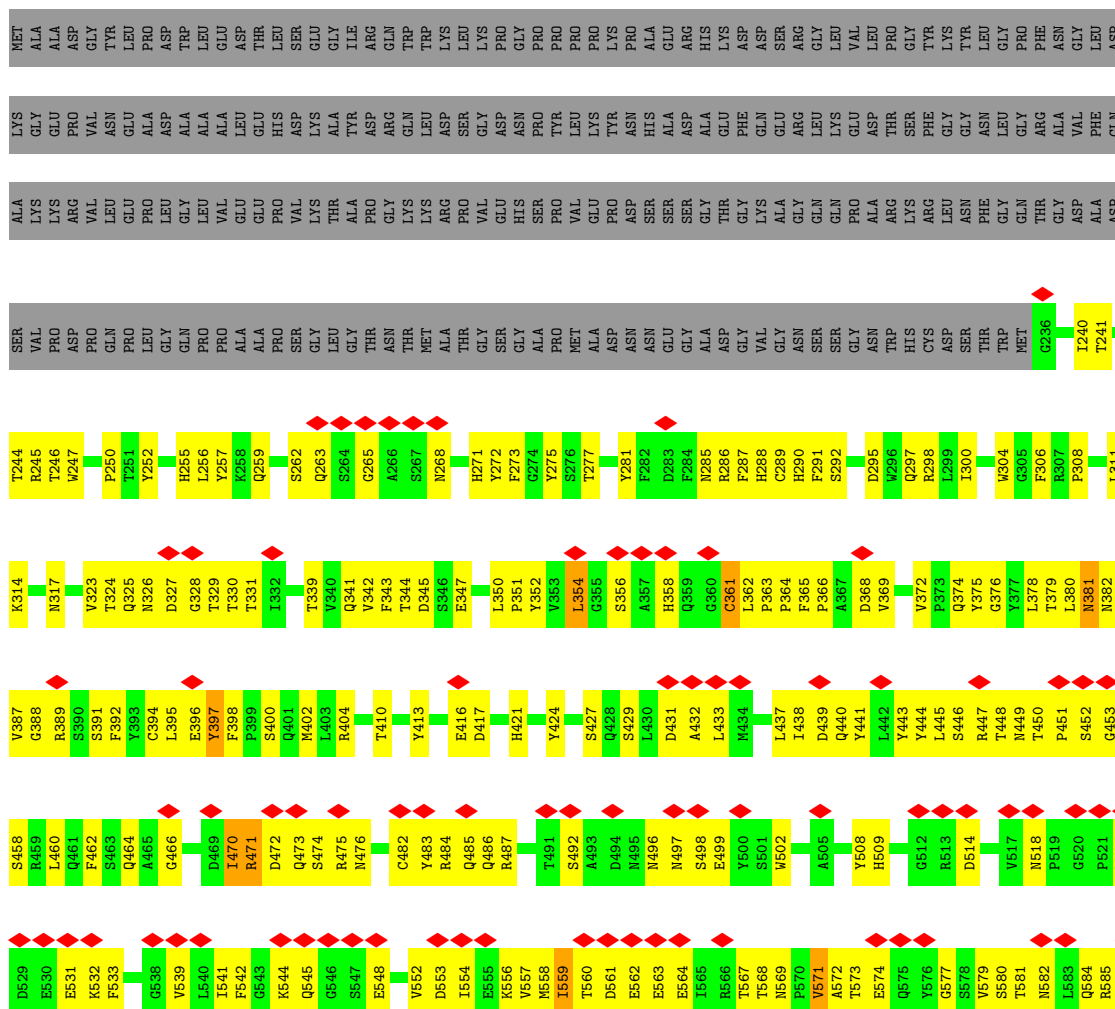


### • Molecule 1: Capsid protein VP1



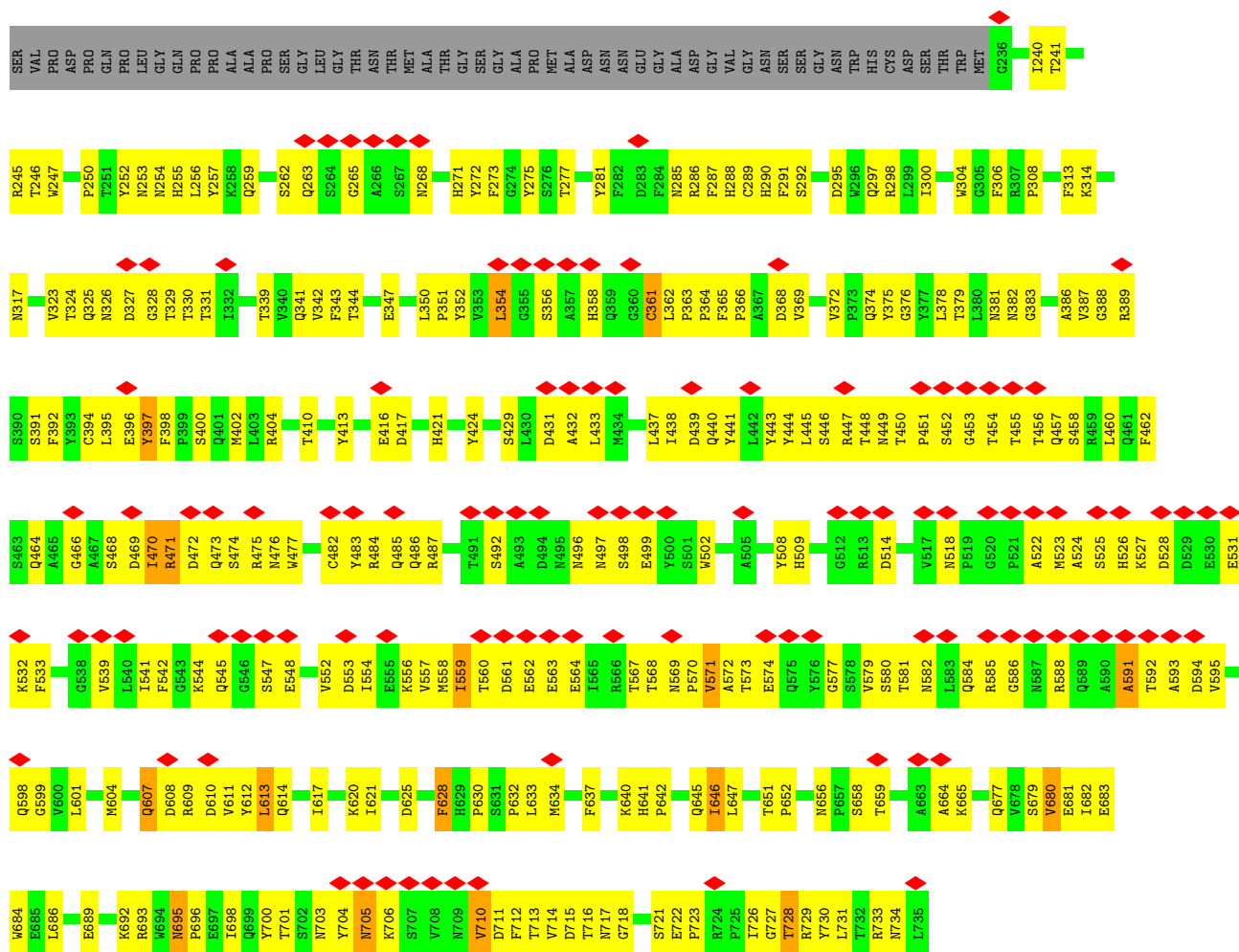


### • Molecule 1: Capsid protein VP1

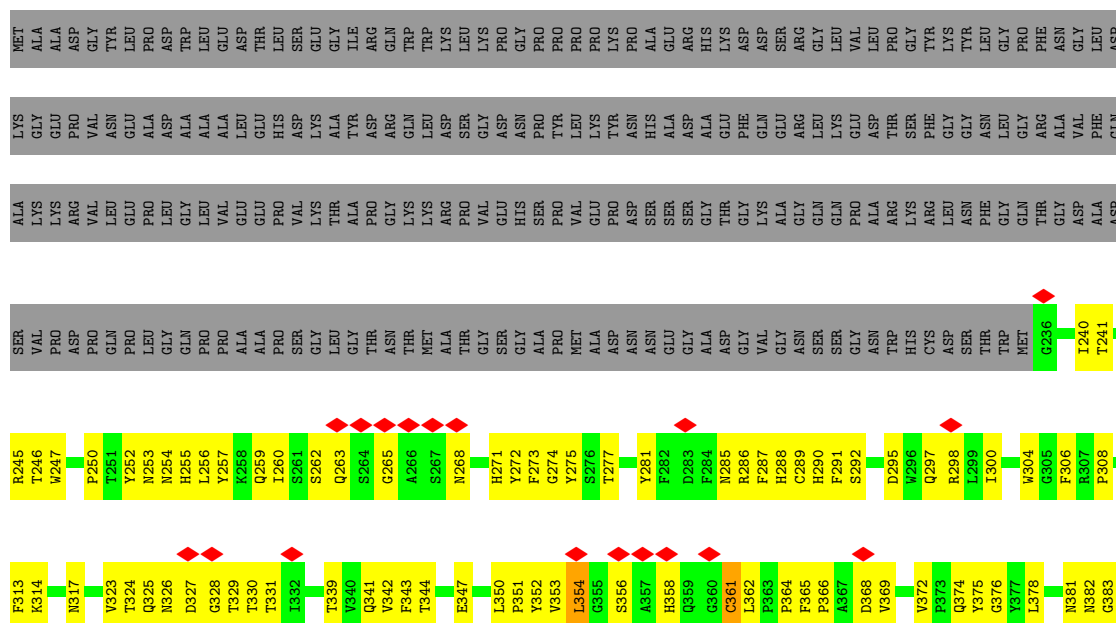




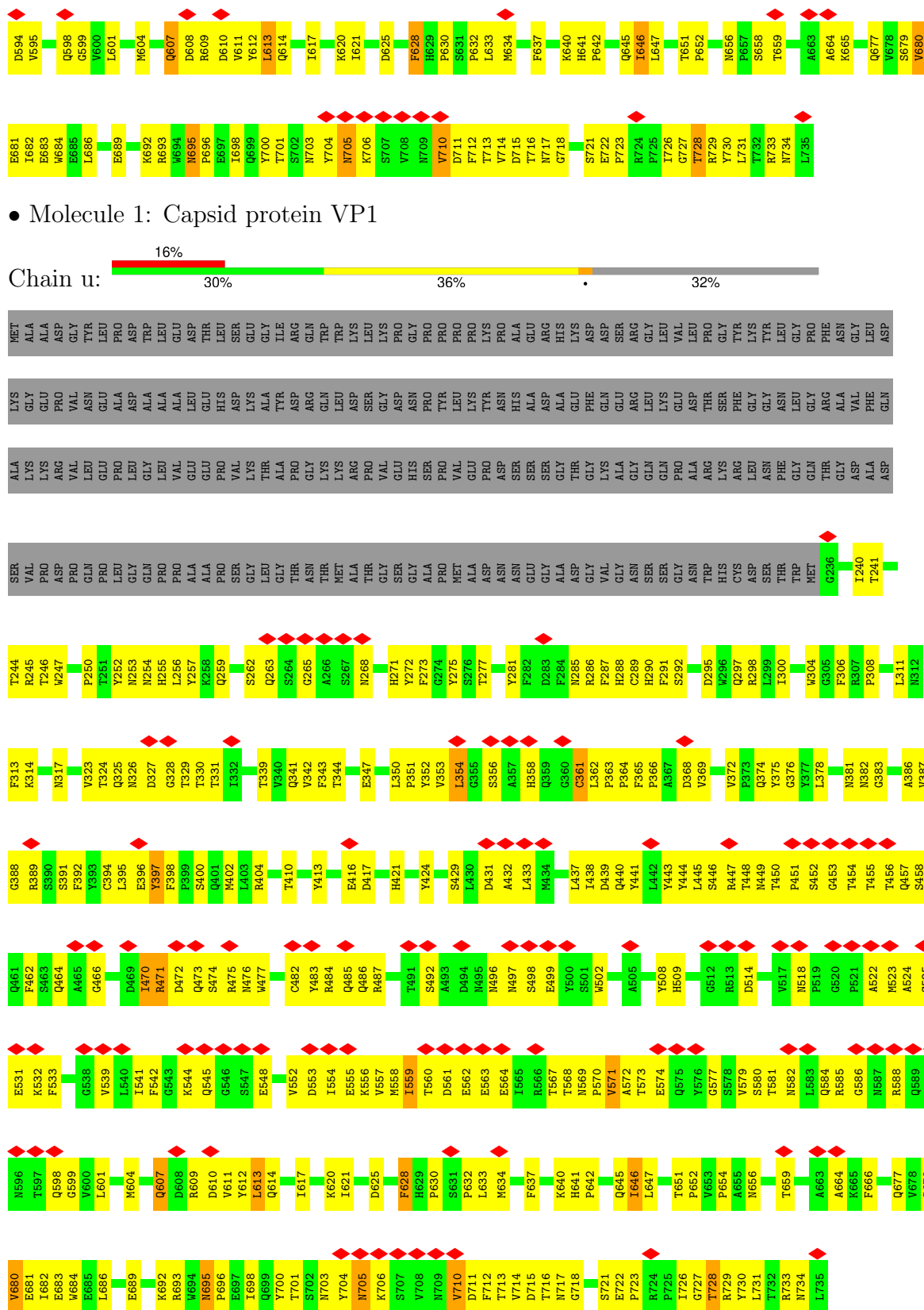




● Molecule 1: Capsid protein VP1

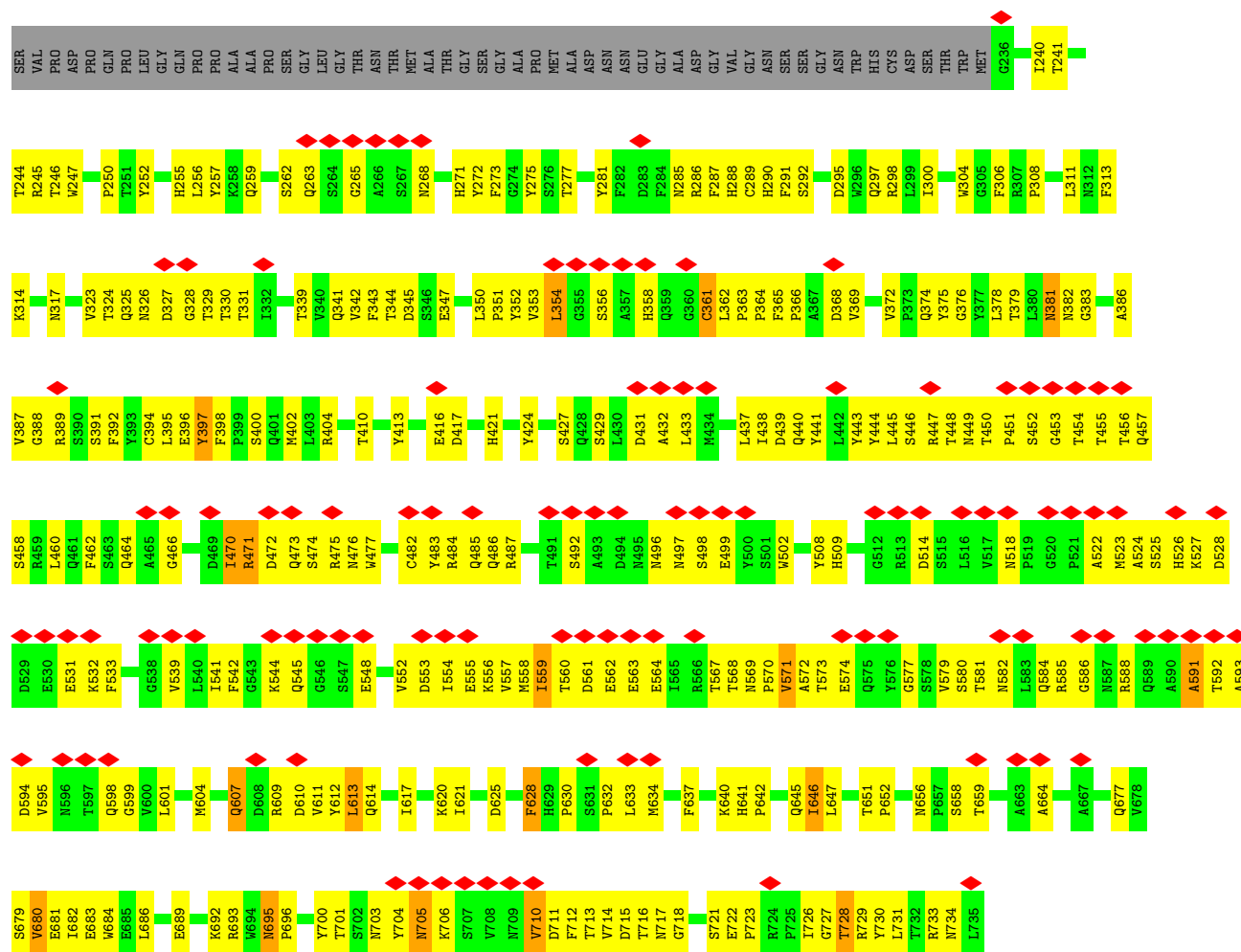




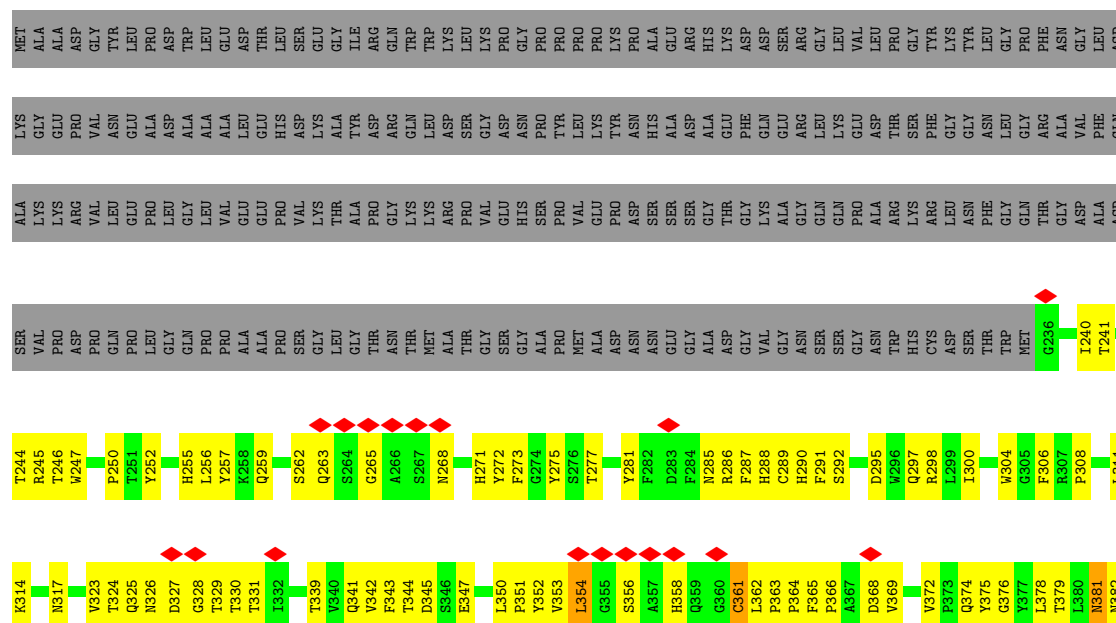


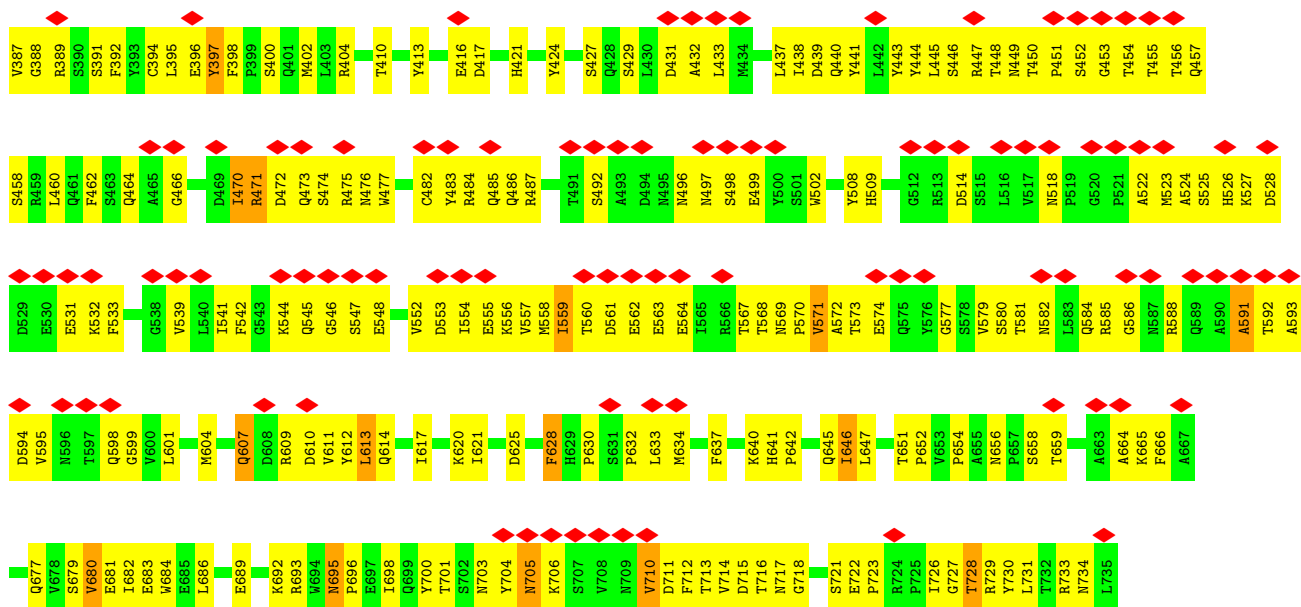
• Molecule 1: Capsid protein VP1



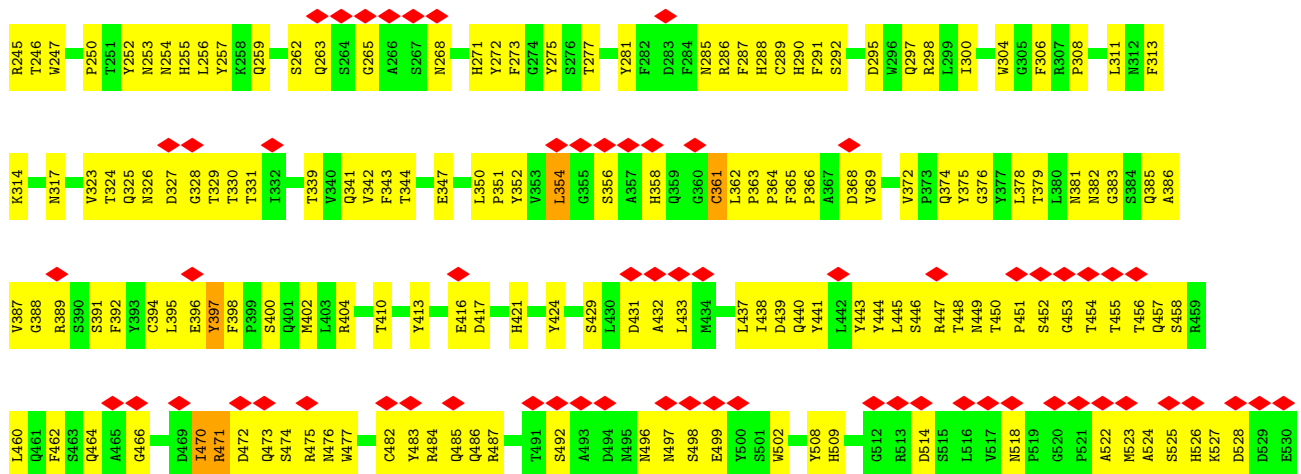
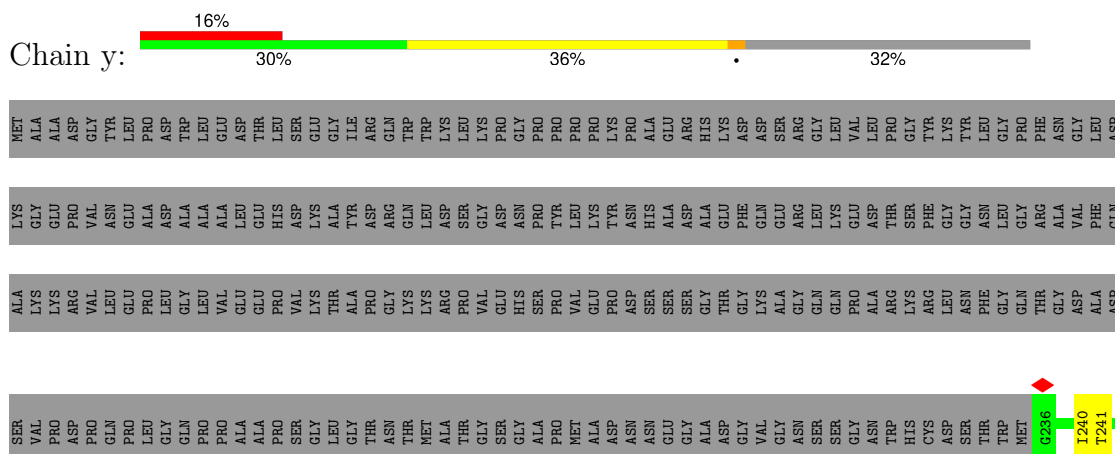


• Molecule 1: Capsid protein VP1



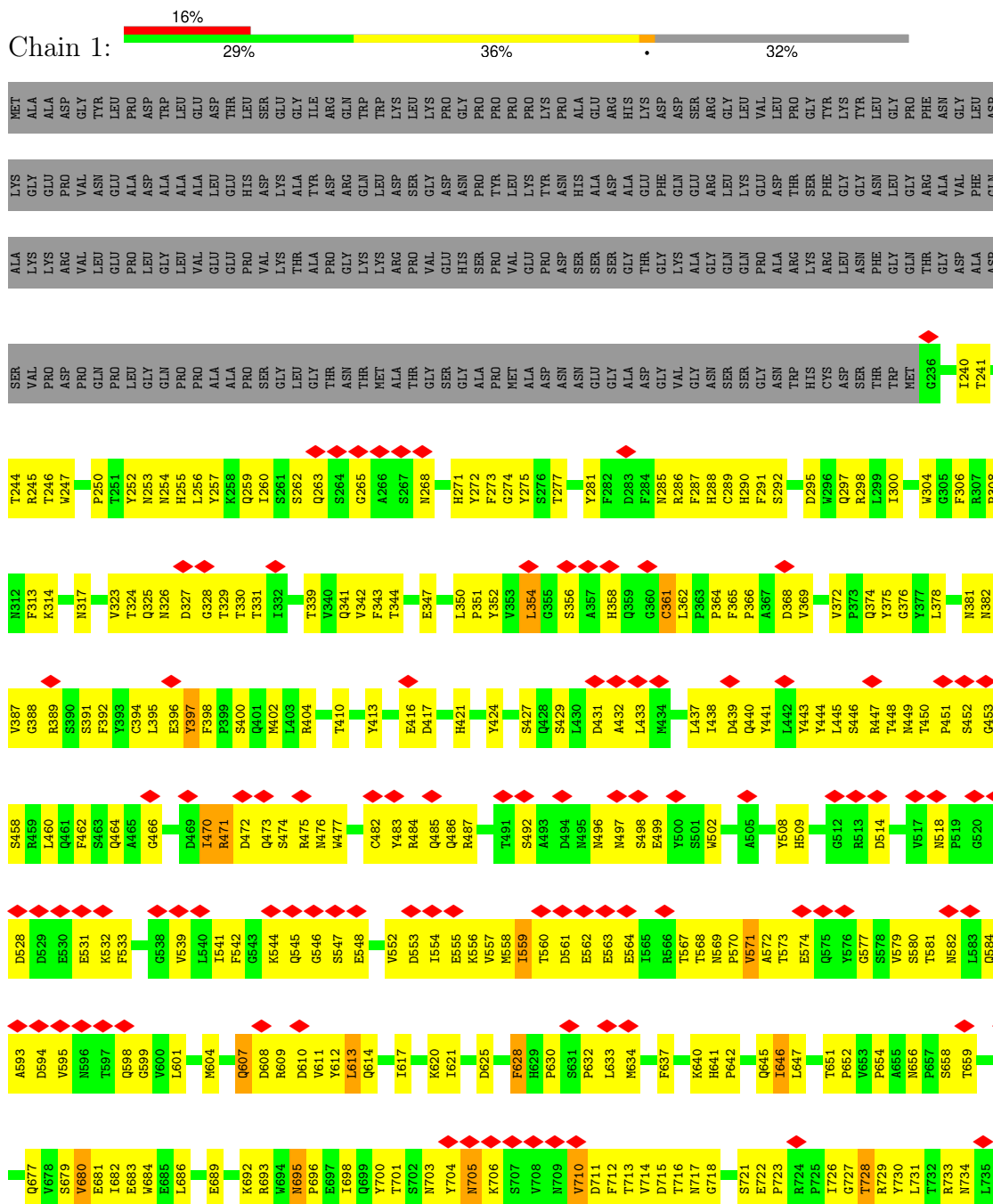


### • Molecule 1: Capsid protein VP1

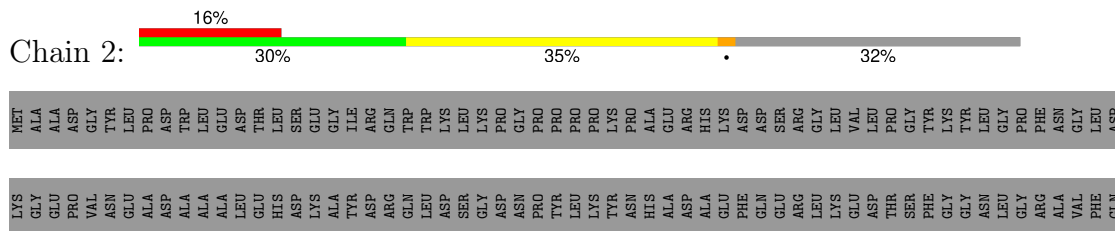


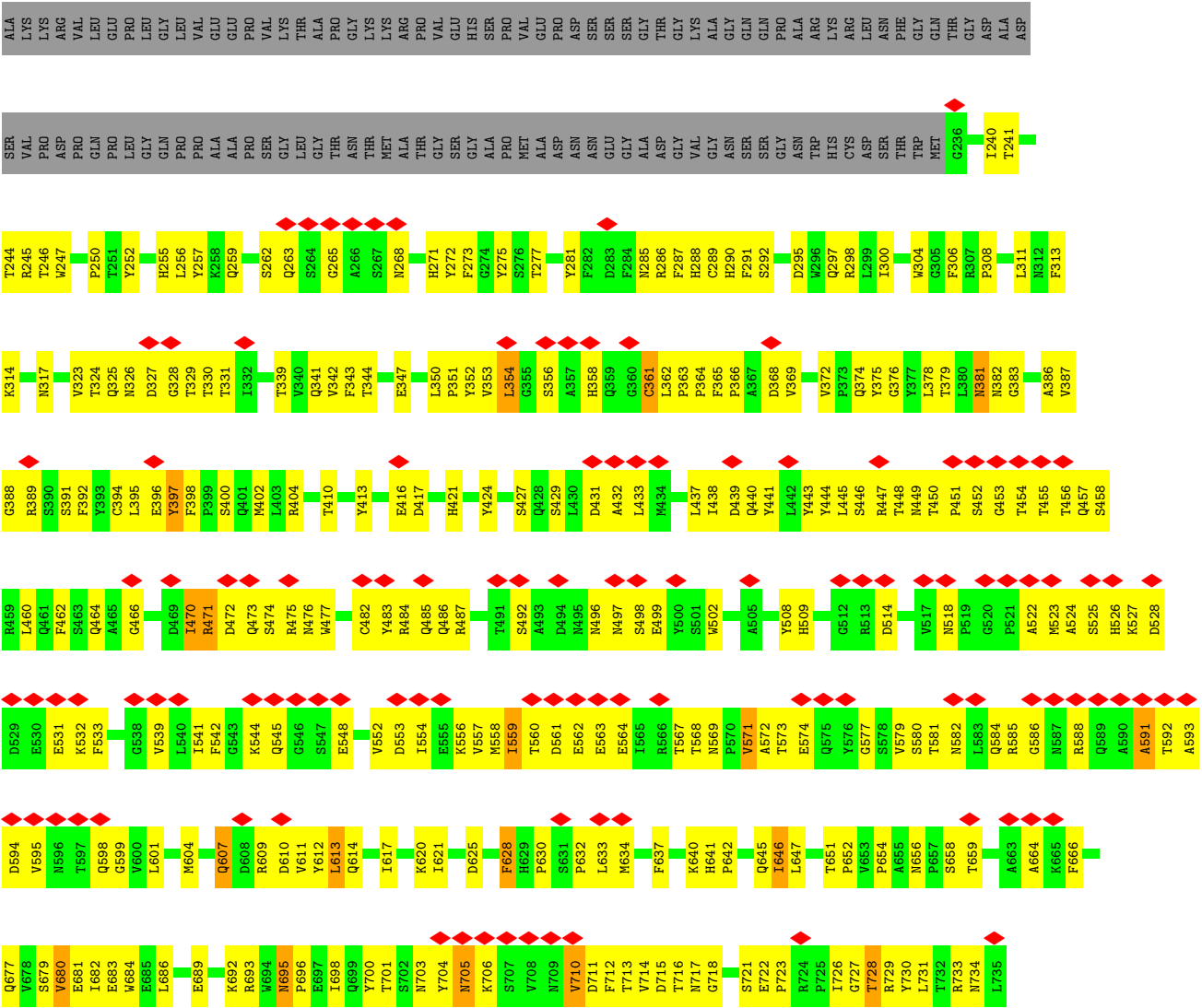


Chain 1:

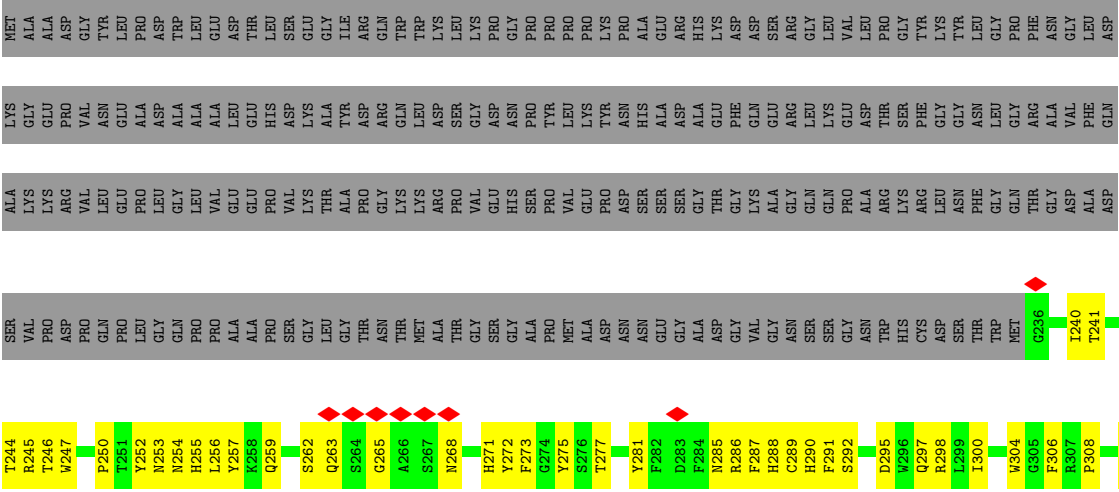
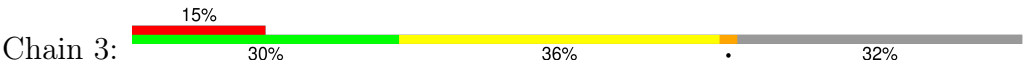


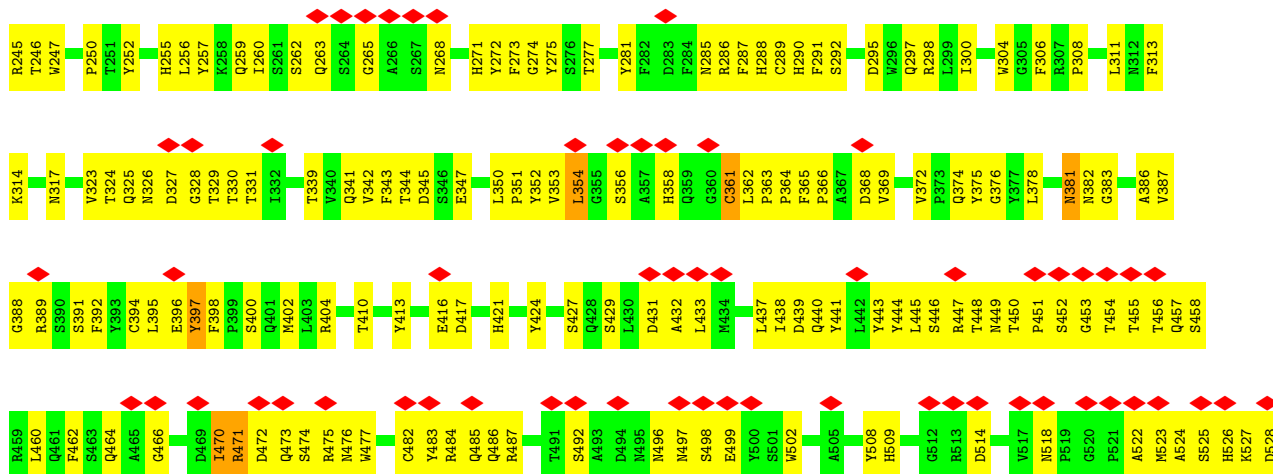
Chain 2:





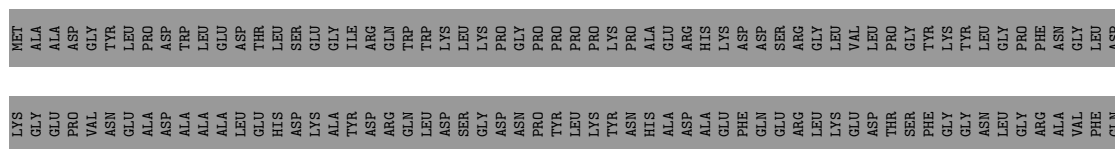
• Molecule 1: Capsid protein VP1



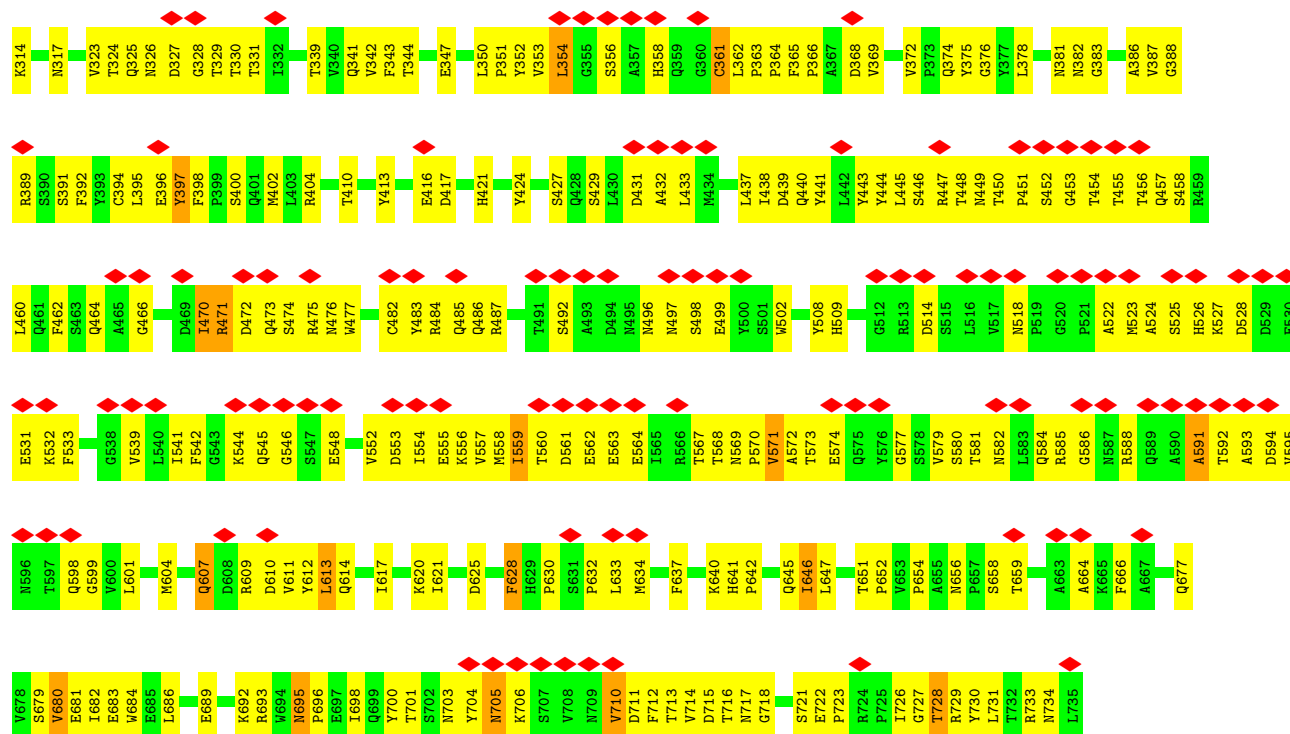




Chain 6: 16% 30% 36% 32%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19457	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	56924	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	14.966	Depositor
Minimum map value	-6.175	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.9	Depositor
Map size ( $\text{\AA}$ )	361.9, 361.9, 361.9	wwPDB
Map dimensions	329, 329, 329	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.51	0/4127	0.83	5/5626 (0.1%)
1	2	0.51	0/4127	0.83	5/5626 (0.1%)
1	3	0.51	0/4127	0.83	5/5626 (0.1%)
1	4	0.51	0/4127	0.83	5/5626 (0.1%)
1	5	0.51	0/4127	0.83	5/5626 (0.1%)
1	6	0.51	0/4127	0.83	5/5626 (0.1%)
1	7	0.51	0/4127	0.83	5/5626 (0.1%)
1	8	0.51	0/4127	0.83	5/5626 (0.1%)
1	A	0.51	0/4127	0.83	5/5626 (0.1%)
1	B	0.51	0/4127	0.83	5/5626 (0.1%)
1	C	0.51	0/4127	0.83	5/5626 (0.1%)
1	D	0.51	0/4127	0.83	5/5626 (0.1%)
1	E	0.51	0/4127	0.83	5/5626 (0.1%)
1	F	0.51	0/4127	0.83	5/5626 (0.1%)
1	G	0.51	0/4127	0.83	5/5626 (0.1%)
1	H	0.51	0/4127	0.83	5/5626 (0.1%)
1	I	0.51	0/4127	0.83	5/5626 (0.1%)
1	J	0.51	0/4127	0.83	5/5626 (0.1%)
1	K	0.51	0/4127	0.83	5/5626 (0.1%)
1	L	0.51	0/4127	0.83	5/5626 (0.1%)
1	M	0.51	0/4127	0.83	5/5626 (0.1%)
1	N	0.51	0/4127	0.83	5/5626 (0.1%)
1	O	0.51	0/4127	0.83	5/5626 (0.1%)
1	P	0.51	0/4127	0.83	5/5626 (0.1%)
1	Q	0.51	0/4127	0.83	5/5626 (0.1%)
1	R	0.51	0/4127	0.83	5/5626 (0.1%)
1	S	0.51	0/4127	0.83	5/5626 (0.1%)
1	T	0.51	0/4127	0.83	5/5626 (0.1%)
1	U	0.51	0/4127	0.83	5/5626 (0.1%)
1	V	0.51	0/4127	0.83	5/5626 (0.1%)
1	W	0.51	0/4127	0.83	5/5626 (0.1%)
1	X	0.51	0/4127	0.83	5/5626 (0.1%)
1	Y	0.51	0/4127	0.83	5/5626 (0.1%)
1	Z	0.51	0/4127	0.83	5/5626 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.51	0/4127	0.83	5/5626 (0.1%)
1	b	0.51	0/4127	0.83	5/5626 (0.1%)
1	c	0.51	0/4127	0.83	5/5626 (0.1%)
1	d	0.51	0/4127	0.83	5/5626 (0.1%)
1	e	0.51	0/4127	0.83	5/5626 (0.1%)
1	f	0.51	0/4127	0.83	5/5626 (0.1%)
1	g	0.51	0/4127	0.83	5/5626 (0.1%)
1	h	0.51	0/4127	0.83	5/5626 (0.1%)
1	i	0.51	0/4127	0.83	5/5626 (0.1%)
1	j	0.51	0/4127	0.83	5/5626 (0.1%)
1	k	0.51	0/4127	0.83	5/5626 (0.1%)
1	l	0.51	0/4127	0.83	5/5626 (0.1%)
1	m	0.51	0/4127	0.83	5/5626 (0.1%)
1	n	0.51	0/4127	0.83	5/5626 (0.1%)
1	o	0.51	0/4127	0.83	5/5626 (0.1%)
1	p	0.51	0/4127	0.83	5/5626 (0.1%)
1	q	0.51	0/4127	0.83	5/5626 (0.1%)
1	r	0.51	0/4127	0.83	5/5626 (0.1%)
1	s	0.51	0/4127	0.83	5/5626 (0.1%)
1	t	0.51	0/4127	0.83	5/5626 (0.1%)
1	u	0.51	0/4127	0.83	5/5626 (0.1%)
1	v	0.51	0/4127	0.83	5/5626 (0.1%)
1	w	0.51	0/4127	0.83	5/5626 (0.1%)
1	x	0.51	0/4127	0.83	5/5626 (0.1%)
1	y	0.51	0/4127	0.83	5/5626 (0.1%)
1	z	0.51	0/4127	0.83	5/5626 (0.1%)
All	All	0.51	0/247620	0.83	300/337560 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	5
1	2	0	6
1	3	0	5
1	4	0	6
1	5	0	5
1	6	0	5
1	7	0	6
1	8	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	6
1	F	0	5
1	G	0	5
1	H	0	5
1	I	0	5
1	J	0	5
1	K	0	6
1	L	0	5
1	M	0	5
1	N	0	5
1	O	0	6
1	P	0	5
1	Q	0	5
1	R	0	5
1	S	0	5
1	T	0	6
1	U	0	6
1	V	0	5
1	W	0	5
1	X	0	5
1	Y	0	5
1	Z	0	5
1	a	0	5
1	b	0	5
1	c	0	5
1	d	0	5
1	e	0	5
1	f	0	5
1	g	0	6
1	h	0	5
1	i	0	5
1	j	0	5
1	k	0	5
1	l	0	6
1	m	0	5
1	n	0	6
1	o	0	6
1	p	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	5
1	r	0	5
1	s	0	5
1	t	0	5
1	u	0	5
1	v	0	5
1	w	0	6
1	x	0	6
1	y	0	5
1	z	0	5
All	All	0	314

There are no bond length outliers.

The worst 5 of 300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	397	TYR	CA-C-N	7.85	132.61	120.60
1	X	397	TYR	C-N-CA	7.85	132.61	120.60
1	x	397	TYR	CA-C-N	7.85	132.61	120.60
1	x	397	TYR	C-N-CA	7.85	132.61	120.60
1	O	397	TYR	CA-C-N	7.83	132.57	120.60

There are no chirality outliers.

5 of 314 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	LEU	Peptide
1	A	607	GLN	Peptide
1	A	628	PHE	Peptide
1	A	705	ASN	Peptide
1	A	728	THR	Peptide

## 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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4009	0	3787	286	0
1	2	4009	0	3787	281	0
1	3	4009	0	3787	281	0
1	4	4009	0	3787	285	0
1	5	4009	0	3787	287	0
1	6	4009	0	3787	278	0
1	7	4009	0	3787	283	0
1	8	4009	0	3787	285	0
1	A	4009	0	3787	282	0
1	B	4009	0	3787	287	0
1	C	4009	0	3787	279	0
1	D	4009	0	3787	290	0
1	E	4009	0	3787	285	0
1	F	4009	0	3787	279	0
1	G	4009	0	3787	283	0
1	H	4009	0	3787	288	0
1	I	4009	0	3787	286	0
1	J	4009	0	3787	283	0
1	K	4009	0	3787	289	0
1	L	4009	0	3787	280	0
1	M	4009	0	3787	284	0
1	N	4009	0	3787	285	0
1	O	4009	0	3787	284	0
1	P	4009	0	3787	283	0
1	Q	4009	0	3787	288	0
1	R	4009	0	3787	283	0
1	S	4009	0	3787	281	0
1	T	4009	0	3787	284	0
1	U	4009	0	3787	284	0
1	V	4009	0	3787	283	0
1	W	4009	0	3787	284	0
1	X	4009	0	3787	287	0
1	Y	4009	0	3787	281	0
1	Z	4009	0	3787	289	0
1	a	4009	0	3787	285	0
1	b	4009	0	3787	284	0
1	c	4009	0	3787	290	0
1	d	4009	0	3787	282	0
1	e	4009	0	3787	283	0
1	f	4009	0	3787	285	0
1	g	4009	0	3787	281	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	4009	0	3787	286	0
1	i	4009	0	3787	279	0
1	j	4009	0	3787	283	0
1	k	4009	0	3787	286	0
1	l	4009	0	3787	282	0
1	m	4009	0	3787	288	0
1	n	4009	0	3787	280	0
1	o	4009	0	3787	282	0
1	p	4009	0	3787	293	0
1	q	4009	0	3787	289	0
1	r	4009	0	3787	281	0
1	s	4009	0	3787	289	0
1	t	4009	0	3787	281	0
1	u	4009	0	3787	282	0
1	v	4009	0	3787	285	0
1	w	4009	0	3787	283	0
1	x	4009	0	3787	287	0
1	y	4009	0	3787	284	0
1	z	4009	0	3787	284	0
All	All	240540	0	227220	15173	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 32.

The worst 5 of 15173 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:W:585:ARG:H	1:W:588:ARG:HB3	1.37	0.90
1:q:585:ARG:H	1:q:588:ARG:HB3	1.37	0.90
1:j:585:ARG:H	1:j:588:ARG:HB3	1.37	0.90
1:D:585:ARG:H	1:D:588:ARG:HB3	1.36	0.90
1:I:585:ARG:H	1:I:588:ARG:HB3	1.37	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	2	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	3	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	4	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	5	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	6	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	7	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	8	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	A	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	B	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	C	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	D	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	E	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	F	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	G	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	H	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	I	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	J	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	K	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	L	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	M	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	N	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	O	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	P	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	Q	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	S	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	T	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	U	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	V	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	W	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	X	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	Y	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	Z	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	a	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	b	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	c	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	d	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	e	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	f	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	g	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	h	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	i	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	j	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	k	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	l	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	m	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	n	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	o	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	p	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	q	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	r	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	s	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	t	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
1	u	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	v	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	x	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	y	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	4	29
1	z	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	4	29
All	All	29880/44100 (68%)	22656 (76%)	6444 (22%)	780 (3%)	6	29

5 of 780 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	680	VAL
1	B	680	VAL
1	C	680	VAL
1	D	680	VAL
1	E	680	VAL

### 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	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	2	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	3	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	4	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	5	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	6	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	7	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	8	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	A	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	B	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	C	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	D	444/629 (71%)	442 (100%)	2 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	F	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	G	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	H	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	I	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	J	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	K	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	L	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	M	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	N	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	O	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	P	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	Q	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	R	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	S	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	T	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	U	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	V	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	W	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	X	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	Y	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	Z	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	a	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	b	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	c	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	d	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	e	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	f	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	g	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	h	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	i	444/629 (71%)	442 (100%)	2 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	k	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	l	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	m	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	n	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	o	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	p	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	q	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	r	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	s	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	t	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	u	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	v	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	w	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	x	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	y	444/629 (71%)	442 (100%)	2 (0%)	86	92
1	z	444/629 (71%)	442 (100%)	2 (0%)	86	92
All	All	26640/37740 (71%)	26520 (100%)	120 (0%)	85	92

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

Mol	Chain	Res	Type
1	c	613	LEU
1	4	460	LEU
1	j	613	LEU
1	3	613	LEU
1	8	460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 801 such sidechains are listed below:

Mol	Chain	Res	Type
1	i	596	ASN
1	r	253	ASN
1	8	656	ASN
1	j	598	GLN

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Mol	Chain	Res	Type
1	i	589	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 oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

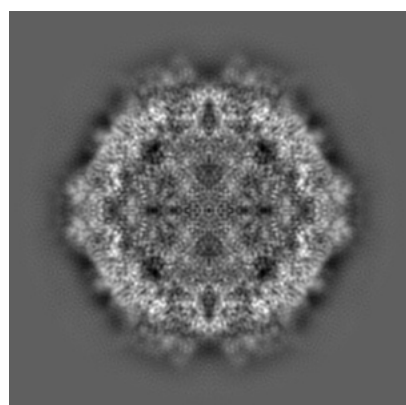
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8100. These allow visual inspection of the internal detail of the map and identification of artifacts.

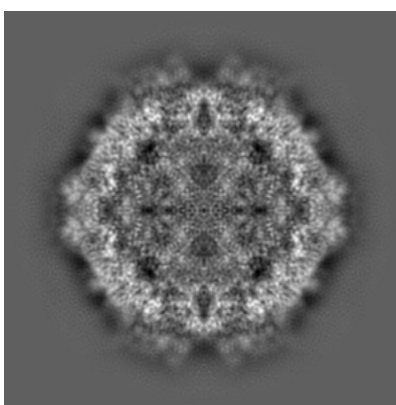
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

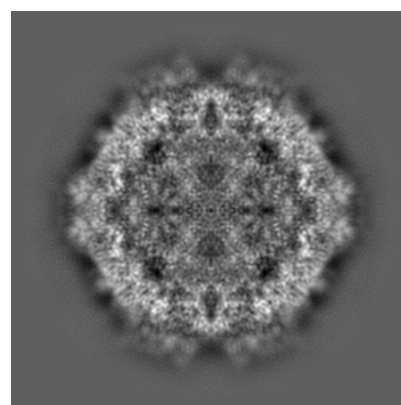
#### 6.1.1 Primary map



X



Y

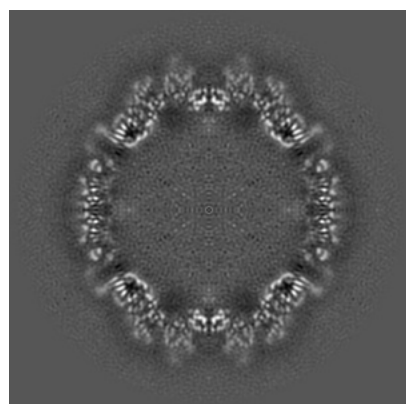


Z

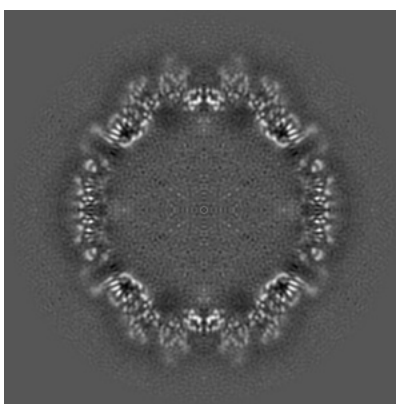
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

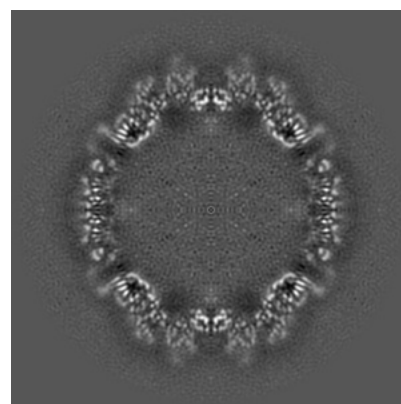
#### 6.2.1 Primary map



X Index: 164



Y Index: 164

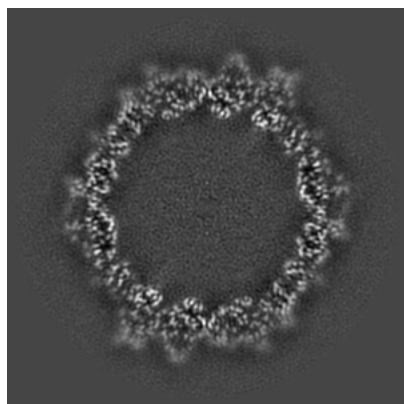


Z Index: 164

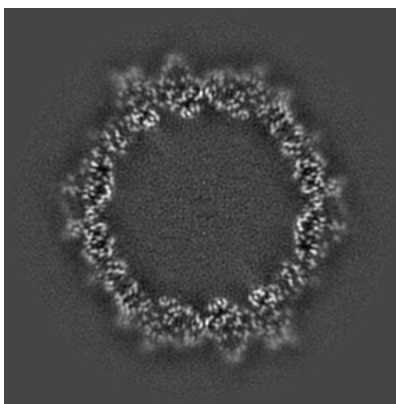
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

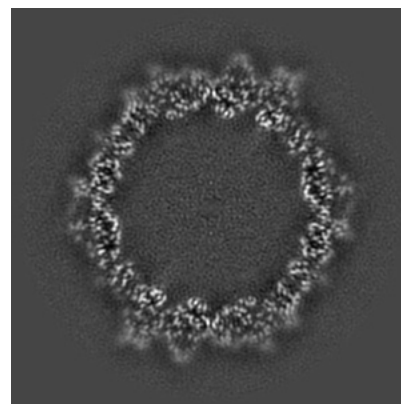
### 6.3.1 Primary map



X Index: 151



Y Index: 177

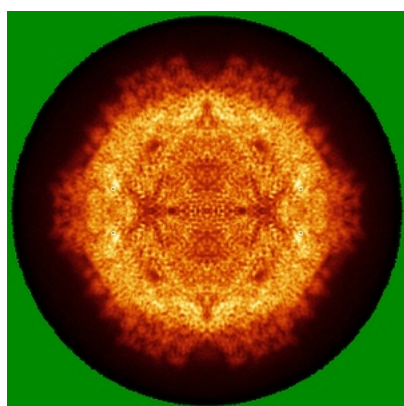


Z Index: 151

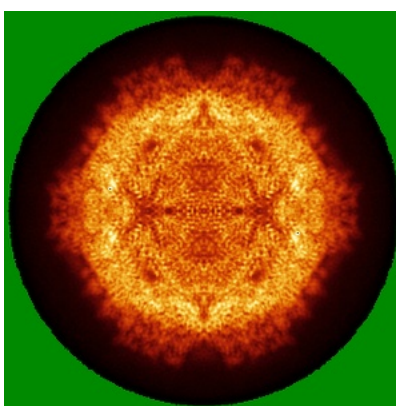
The images above show the largest variance slices of the map in three orthogonal directions.

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

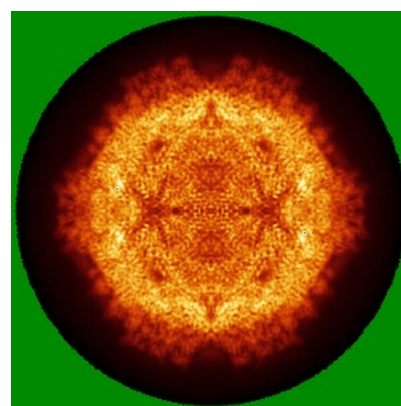
### 6.4.1 Primary map



X



Y

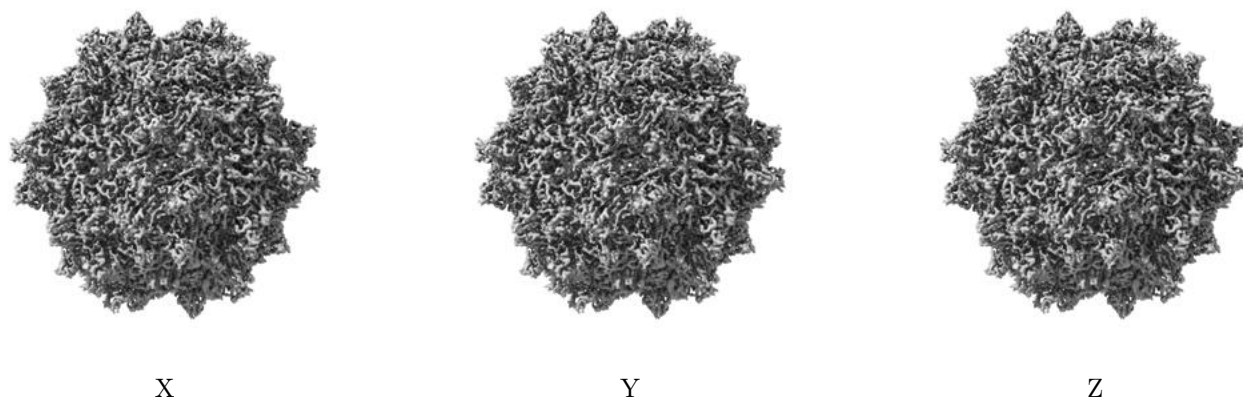


Z

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

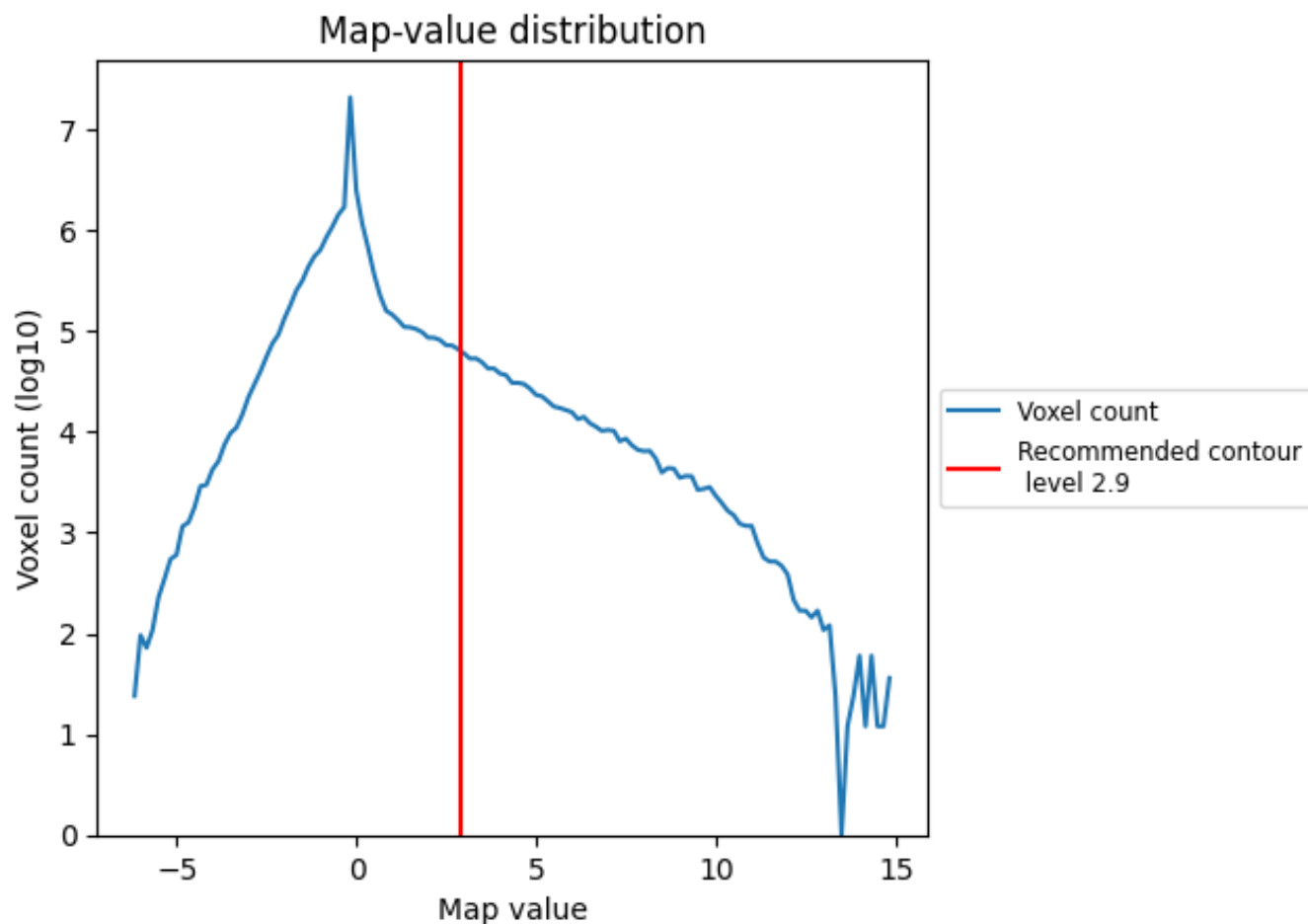
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

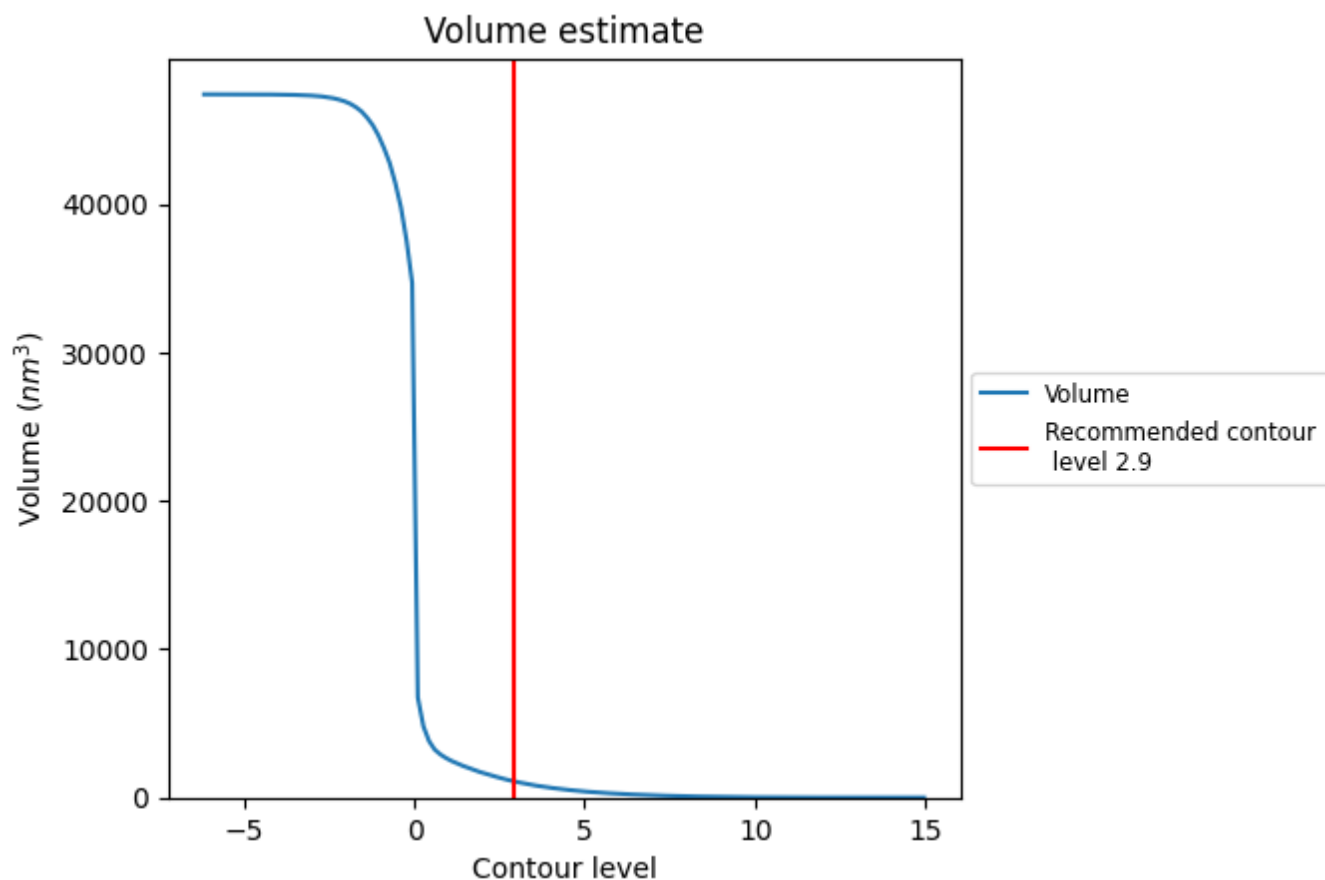
This section contains the results of statistical analysis of the map.

### 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.

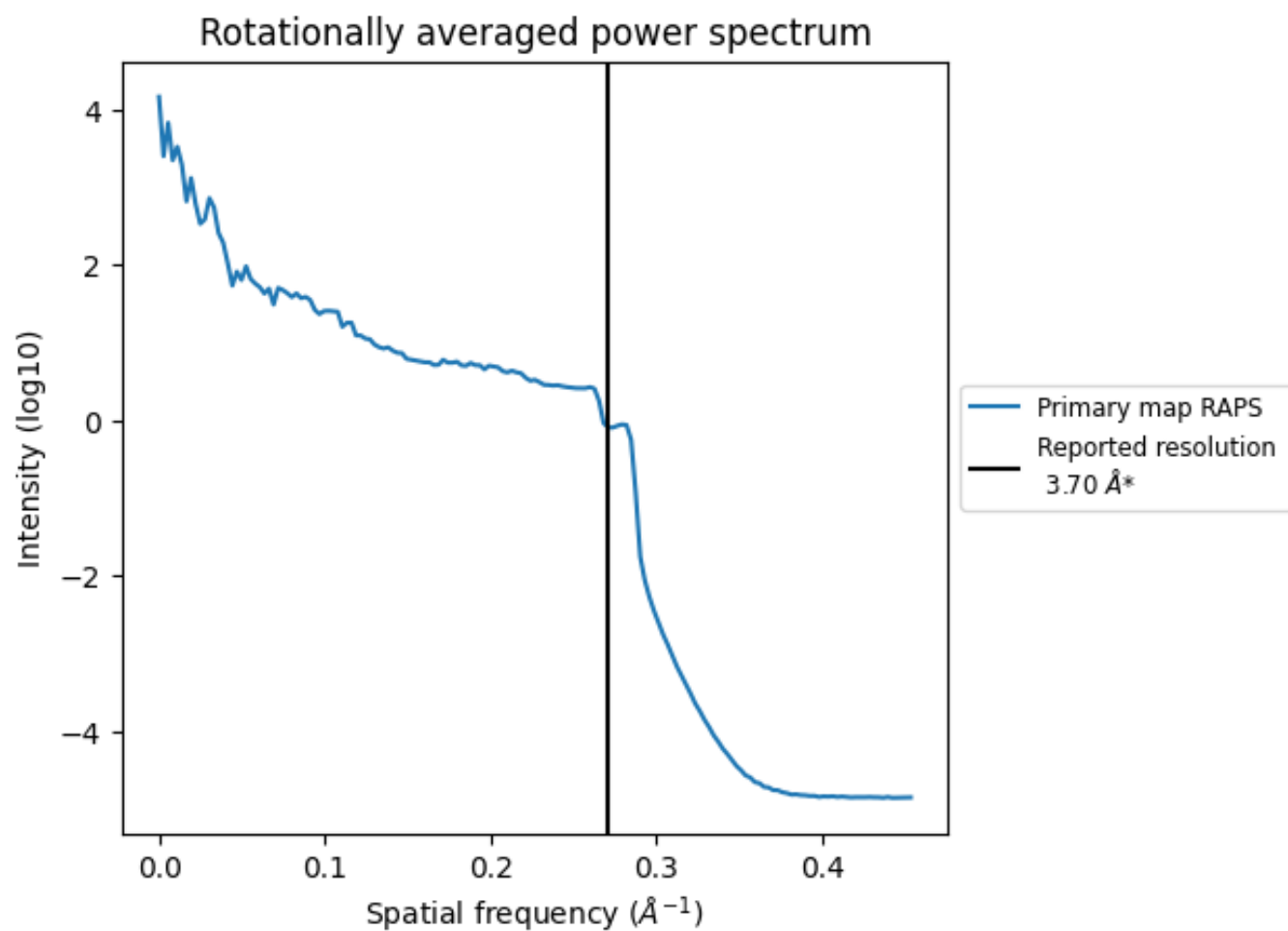
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1108 nm<sup>3</sup>; this corresponds to an approximate mass of 1001 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 0.270 Å<sup>-1</sup>

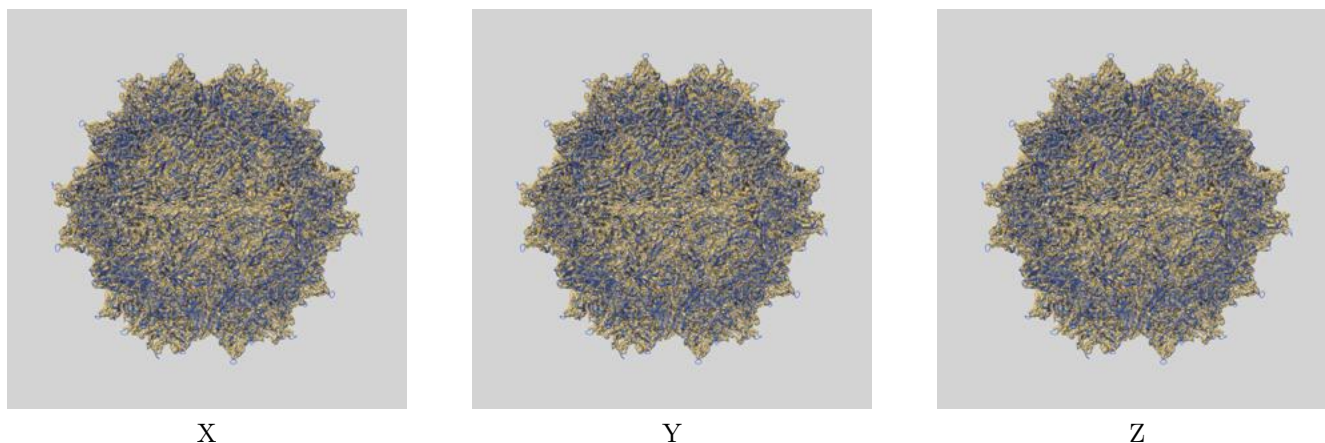
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

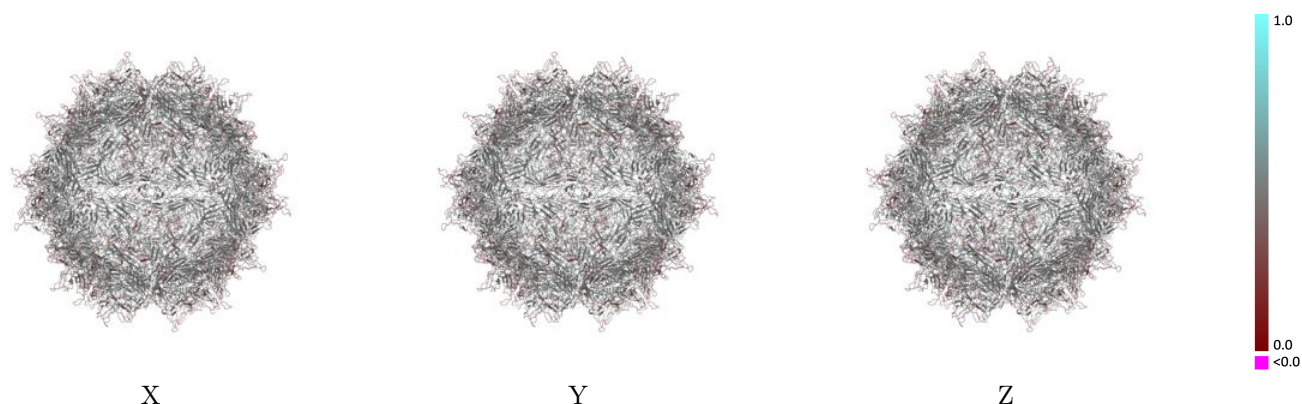
This section contains information regarding the fit between EMDB map EMD-8100 and PDB model 5IPK. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

### 9.1 Map-model overlay [i](#)



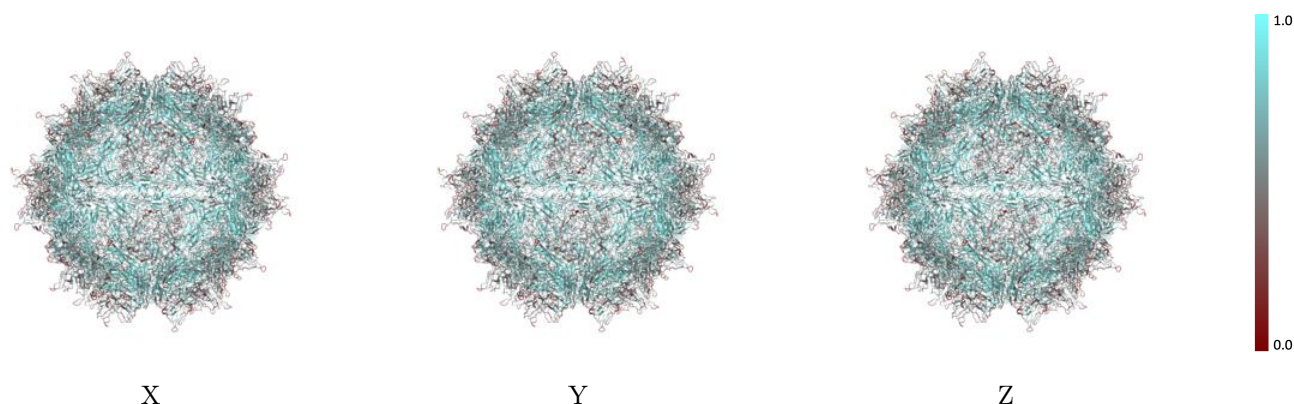
The images above show the 3D surface view of the map at the recommended contour level 2.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



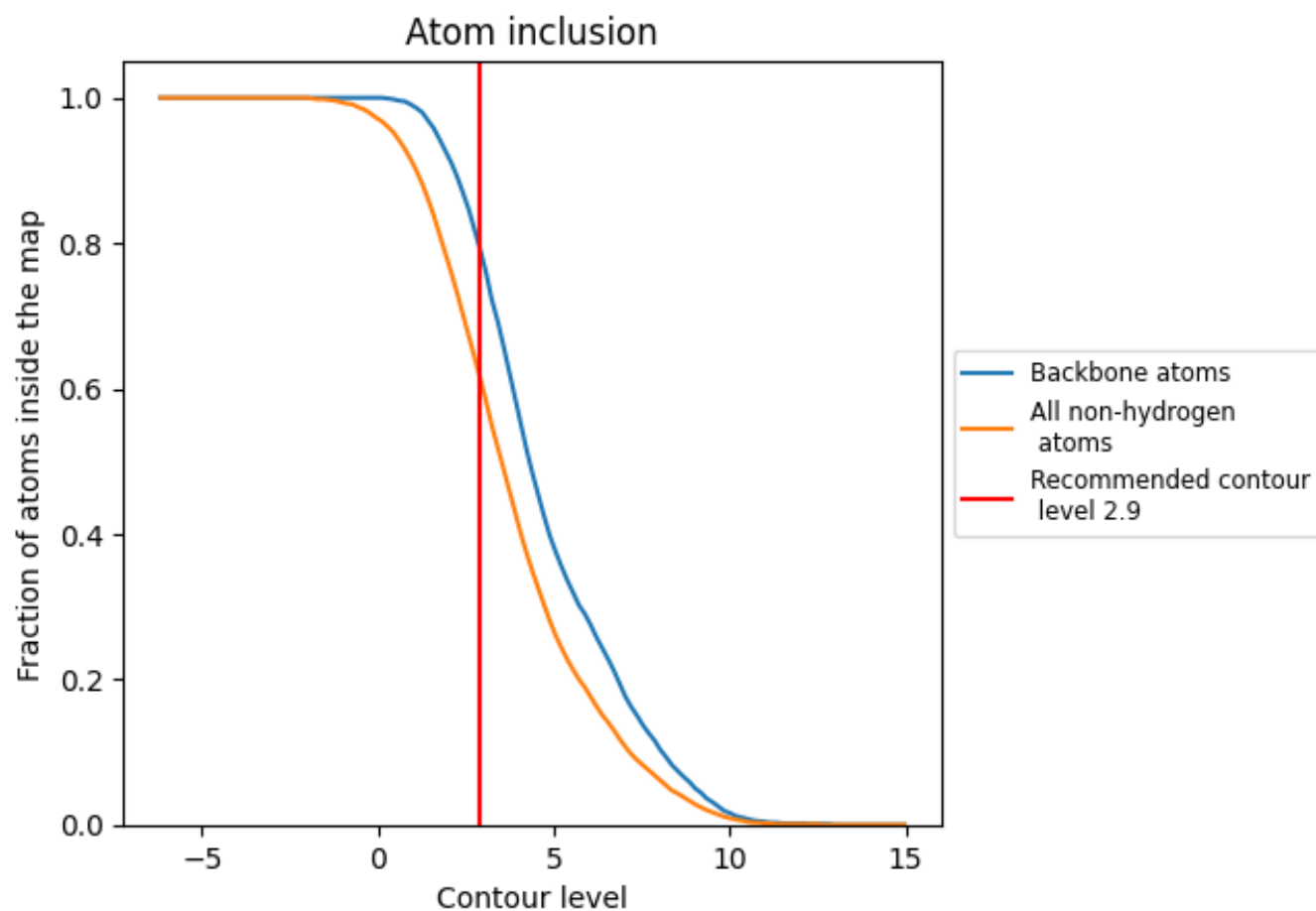
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.9).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































The table lists the average atom inclusion at the recommended contour level (2.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6160	 0.4490
1	 0.6190	 0.4500
2	 0.6190	 0.4490
3	 0.6190	 0.4480
4	 0.6130	 0.4490
5	 0.6140	 0.4490
6	 0.6130	 0.4490
7	 0.6190	 0.4500
8	 0.6160	 0.4490
A	 0.6180	 0.4490
B	 0.6120	 0.4490
C	 0.6140	 0.4490
D	 0.6160	 0.4500
E	 0.6190	 0.4490
F	 0.6120	 0.4480
G	 0.6180	 0.4500
H	 0.6130	 0.4480
I	 0.6180	 0.4480
J	 0.6190	 0.4480
K	 0.6160	 0.4500
L	 0.6140	 0.4480
M	 0.6190	 0.4490
N	 0.6160	 0.4490
O	 0.6190	 0.4490
P	 0.6160	 0.4500
Q	 0.6140	 0.4500
R	 0.6140	 0.4500
S	 0.6130	 0.4490
T	 0.6200	 0.4480
U	 0.6190	 0.4500
V	 0.6170	 0.4490
W	 0.6190	 0.4490
X	 0.6160	 0.4500
Y	 0.6140	 0.4490
Z	 0.6140	 0.4460



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Chain	Atom inclusion	Q-score
a	 0.6160	 0.4480
b	 0.6130	 0.4490
c	 0.6180	 0.4490
d	 0.6190	 0.4480
e	 0.6170	 0.4490
f	 0.6190	 0.4500
g	 0.6130	 0.4500
h	 0.6130	 0.4500
i	 0.6130	 0.4490
j	 0.6180	 0.4490
k	 0.6130	 0.4490
l	 0.6180	 0.4490
m	 0.6140	 0.4470
n	 0.6130	 0.4470
o	 0.6180	 0.4500
p	 0.6170	 0.4490
q	 0.6190	 0.4480
r	 0.6140	 0.4480
s	 0.6110	 0.4460
t	 0.6140	 0.4490
u	 0.6130	 0.4490
v	 0.6190	 0.4490
w	 0.6170	 0.4480
x	 0.6170	 0.4490
y	 0.6160	 0.4490
z	 0.6180	 0.4500