



## wwPDB EM Validation Summary Report ⓘ

Nov 1, 2022 – 06:43 PM EDT

PDB ID : 5IPK  
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:

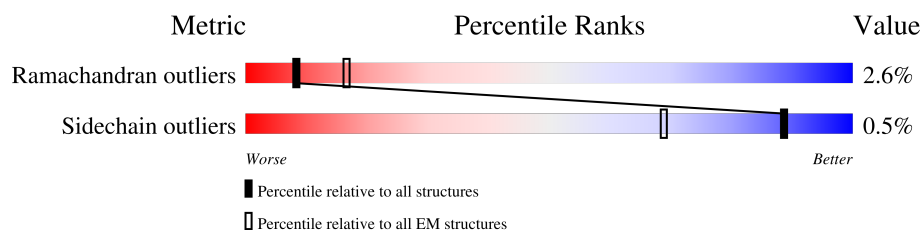
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	2	735	
1	3	735	
1	4	735	
1	5	735	
1	6	735	
1	7	735	
1	8	735	
1	A	735	

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

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

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Mol	Chain	Length	Quality of chain
1	z	735	<div><div></div><div>16%</div><div>65%</div><div></div><div>32%</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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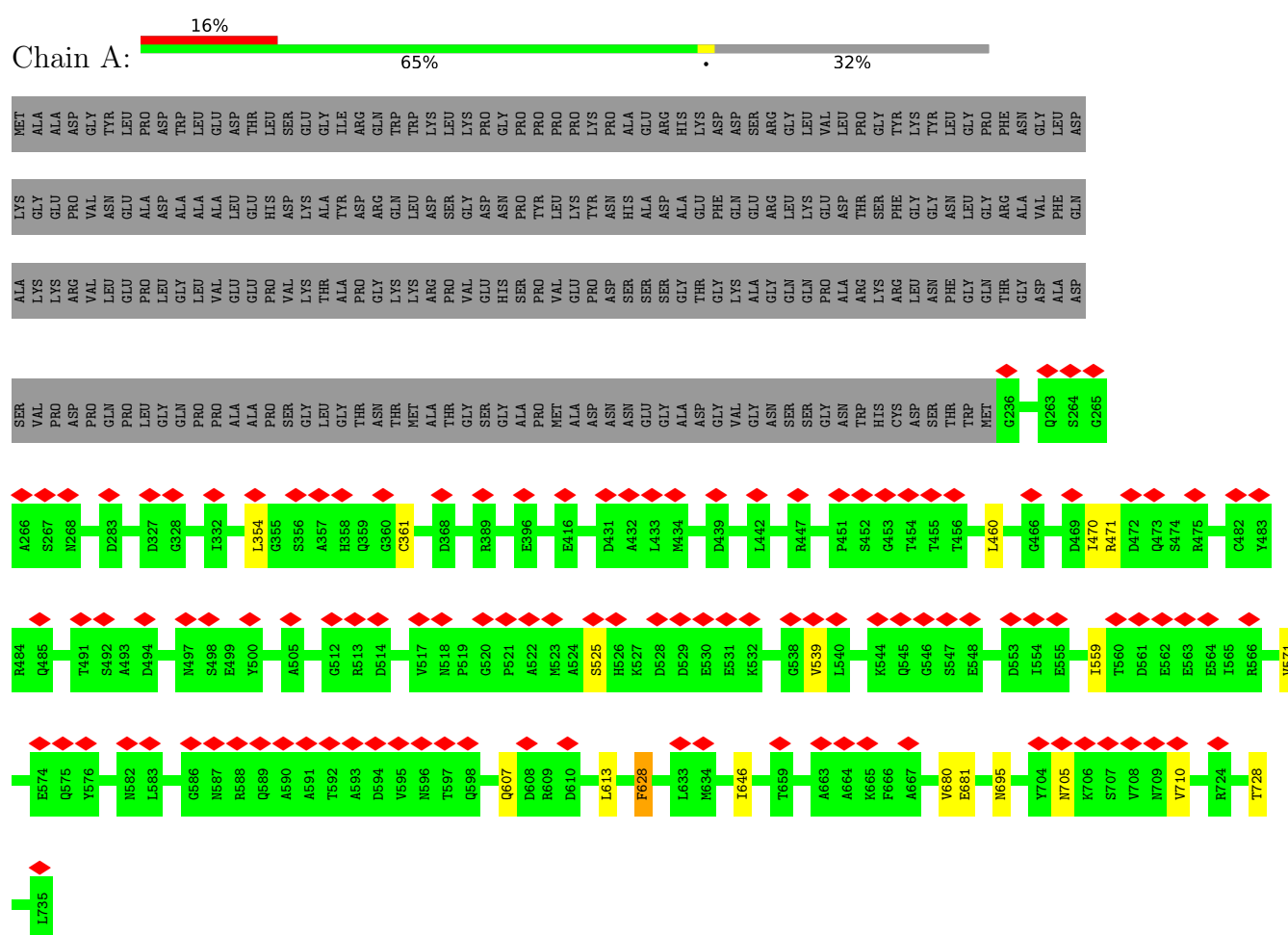
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Chain	Residue	Modelled	Actual	Comment	Reference
k	432	ALA	ARG	engineered mutation	UNP P03135
l	432	ALA	ARG	engineered mutation	UNP P03135
m	432	ALA	ARG	engineered mutation	UNP P03135
n	432	ALA	ARG	engineered mutation	UNP P03135
o	432	ALA	ARG	engineered 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

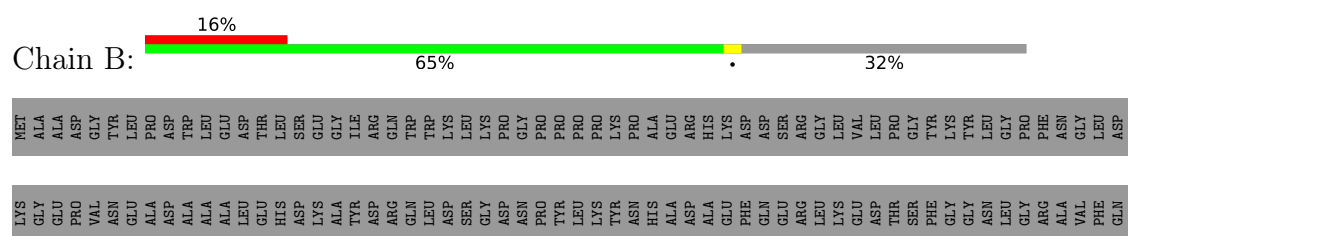
### 3 Residue-property plots

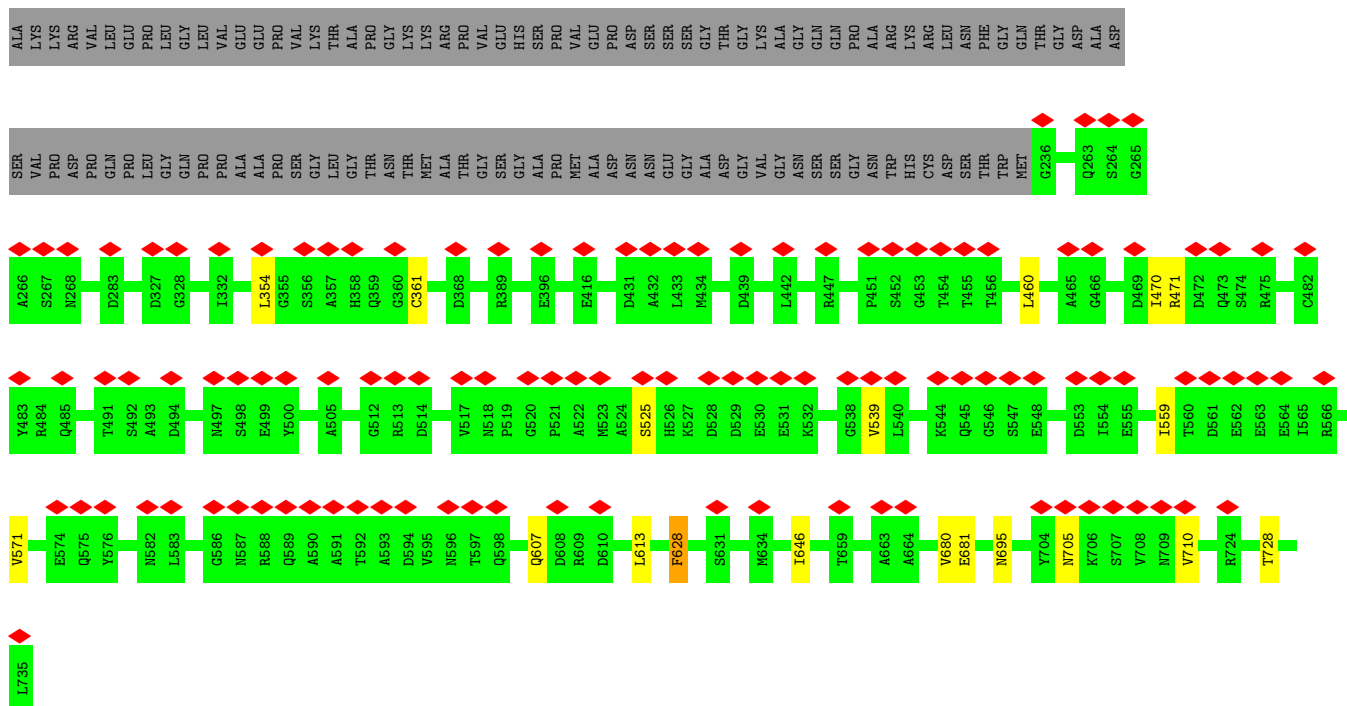
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

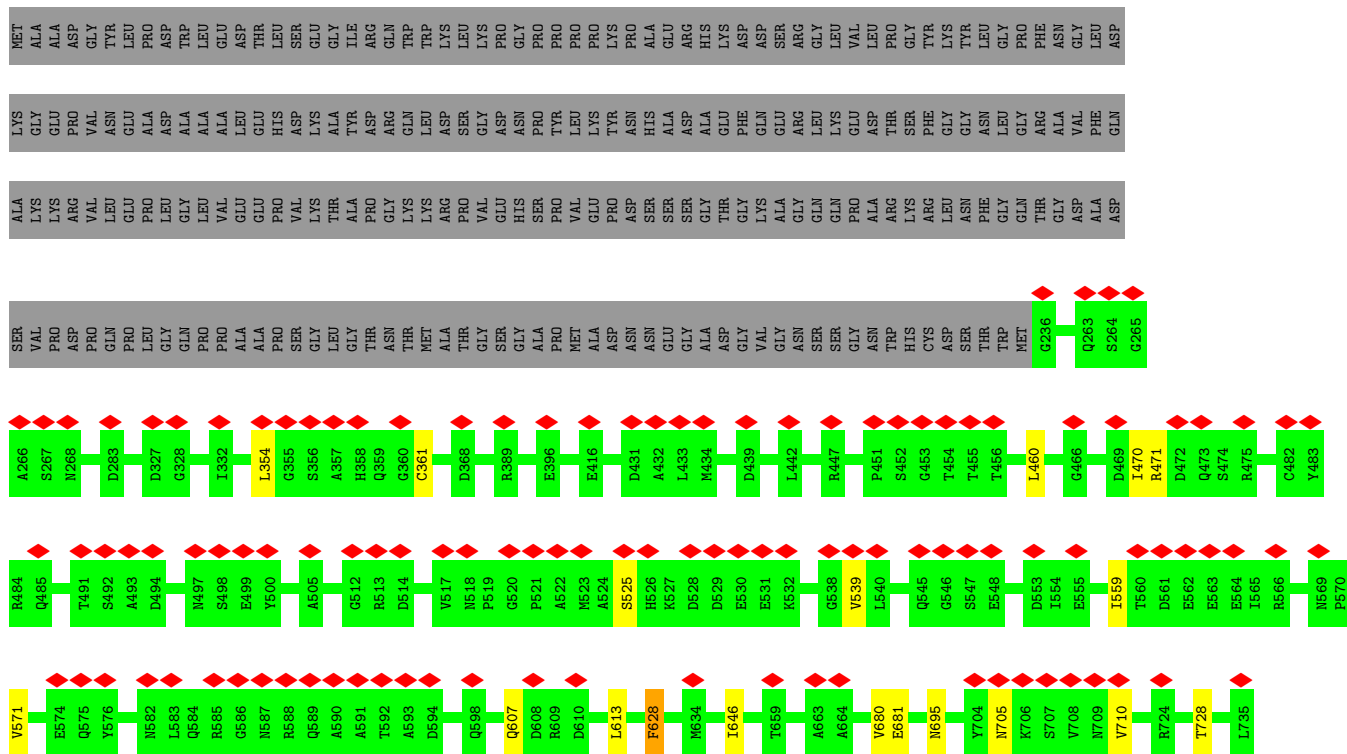


#### • Molecule 1: Capsid protein VP1



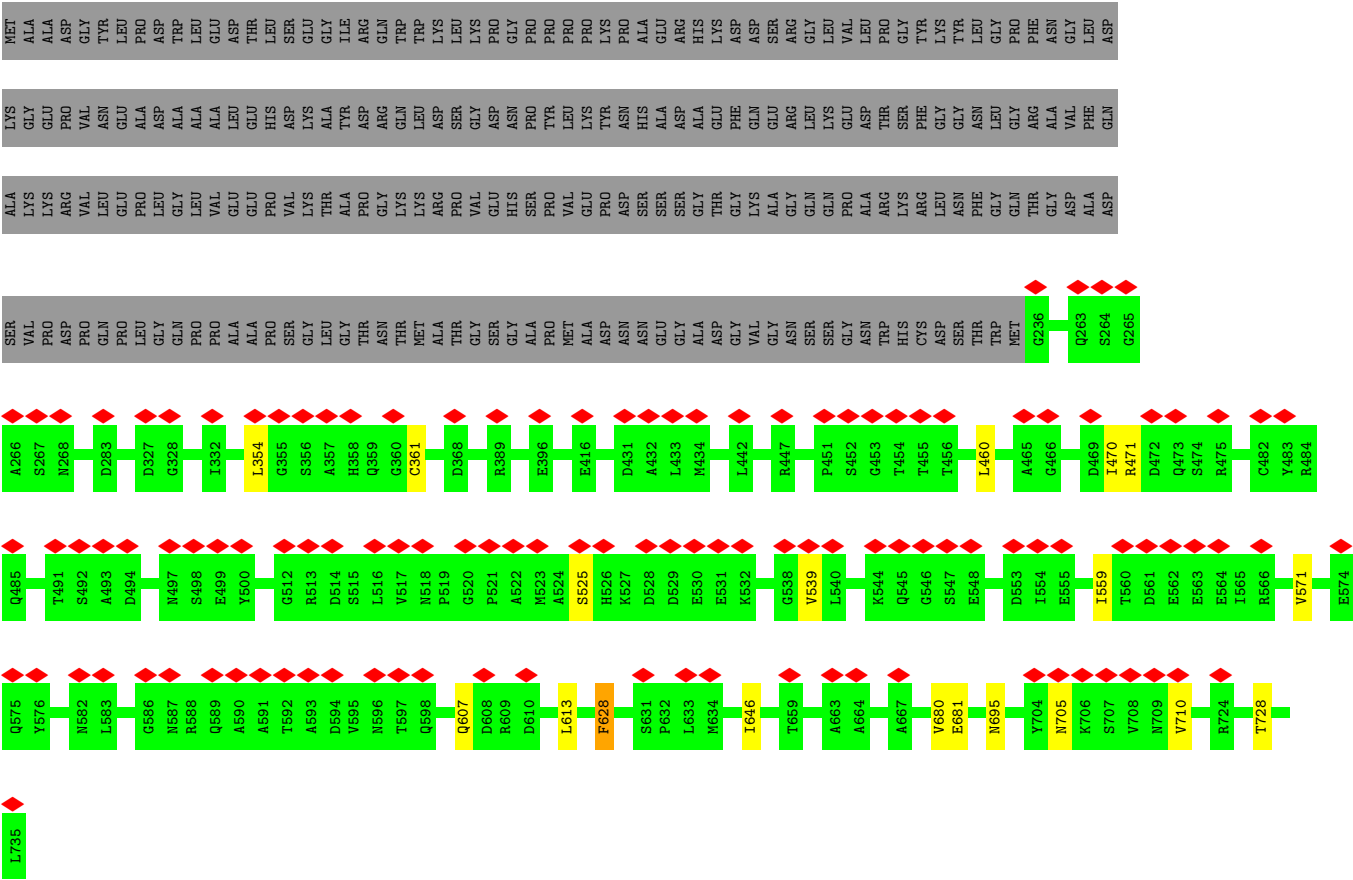


- Molecule 1: Capsid protein VP1

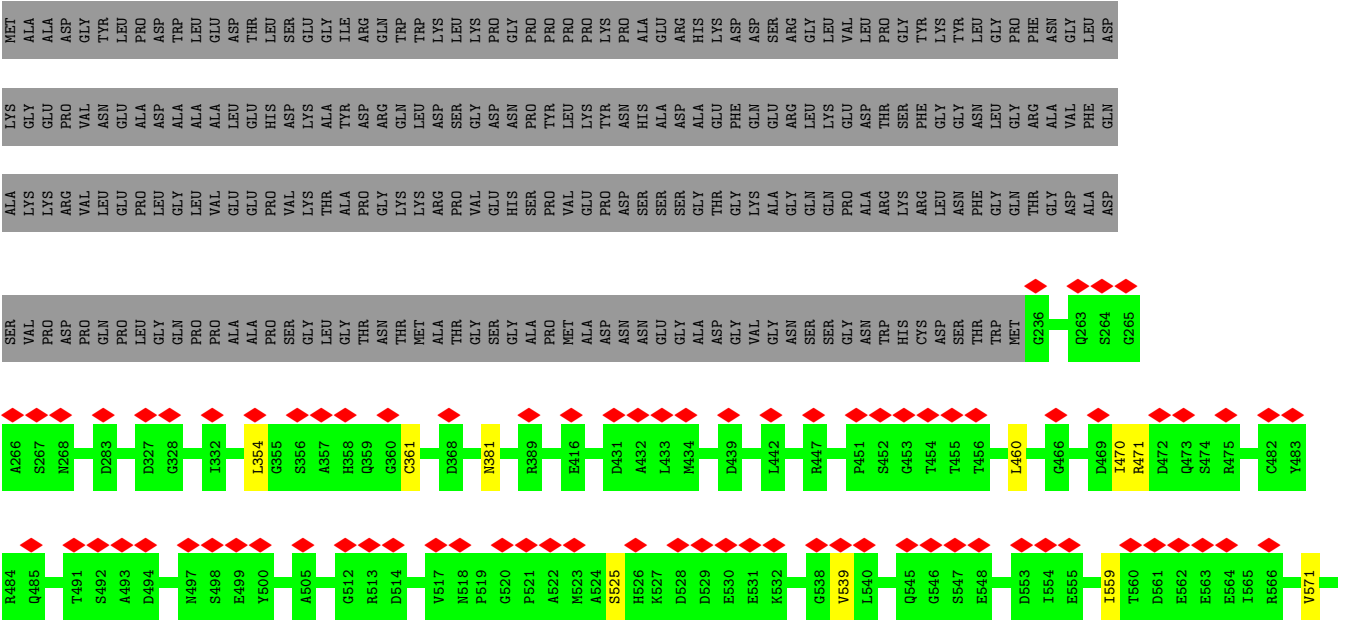


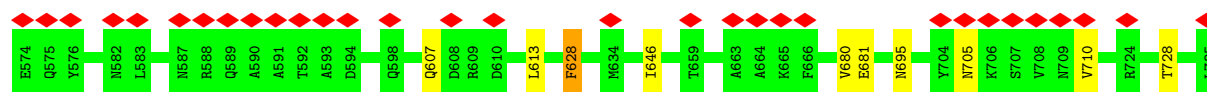
- Molecule 1: Capsid protein VP1



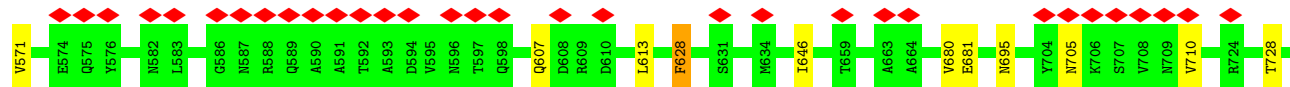
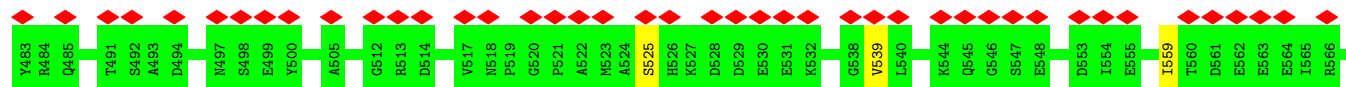
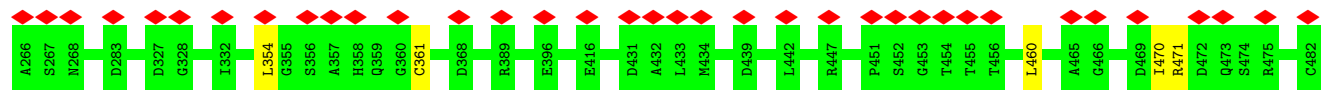
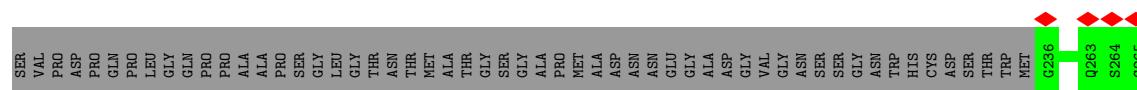
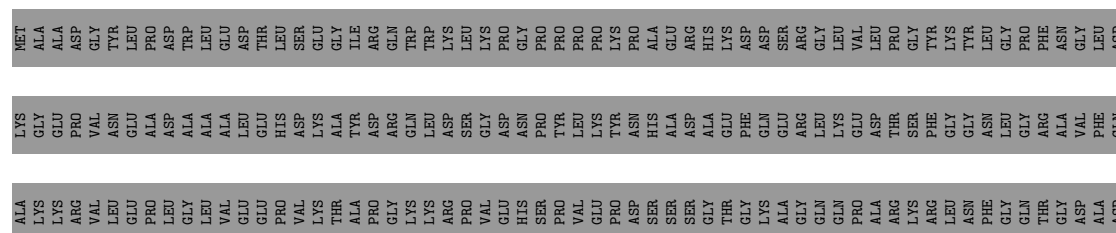


• Molecule 1: Capsid protein VP1

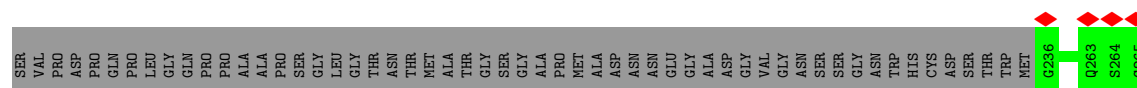
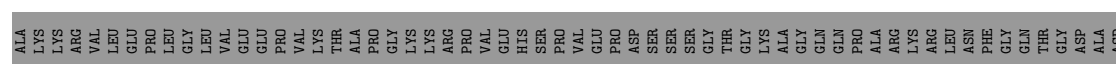
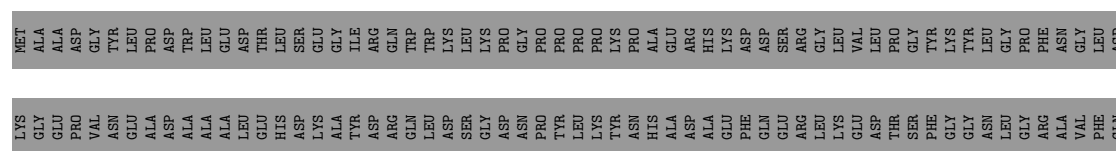


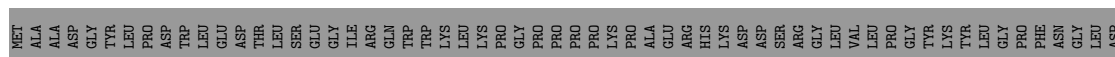


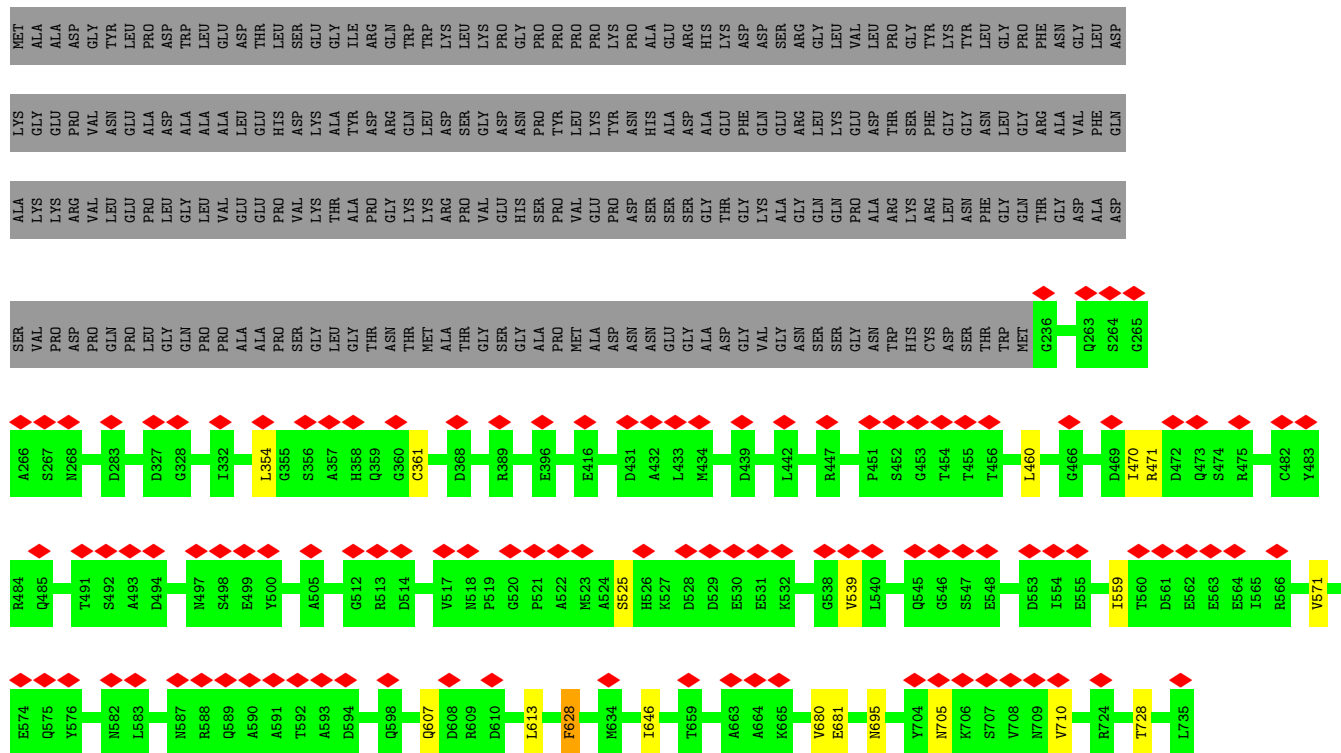
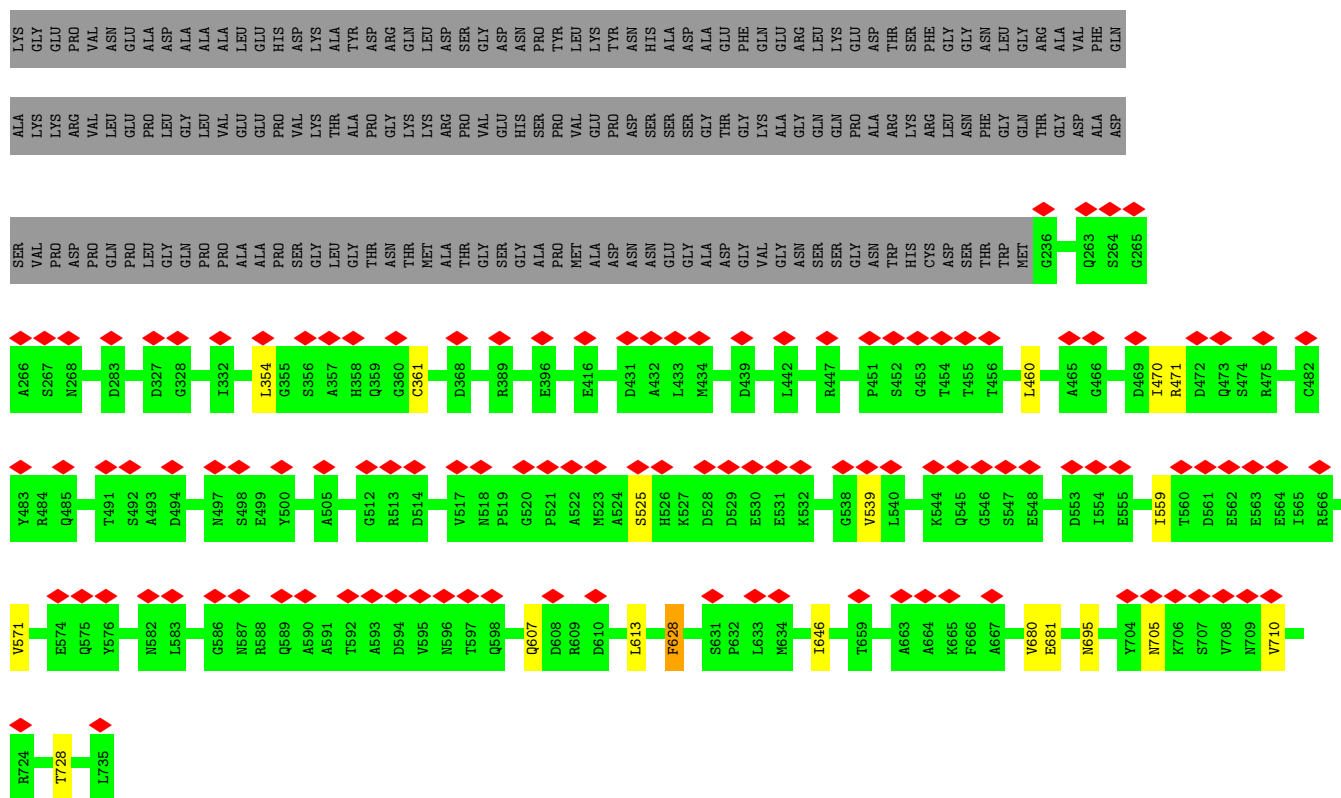
• Molecule 1: Capsid protein VP1



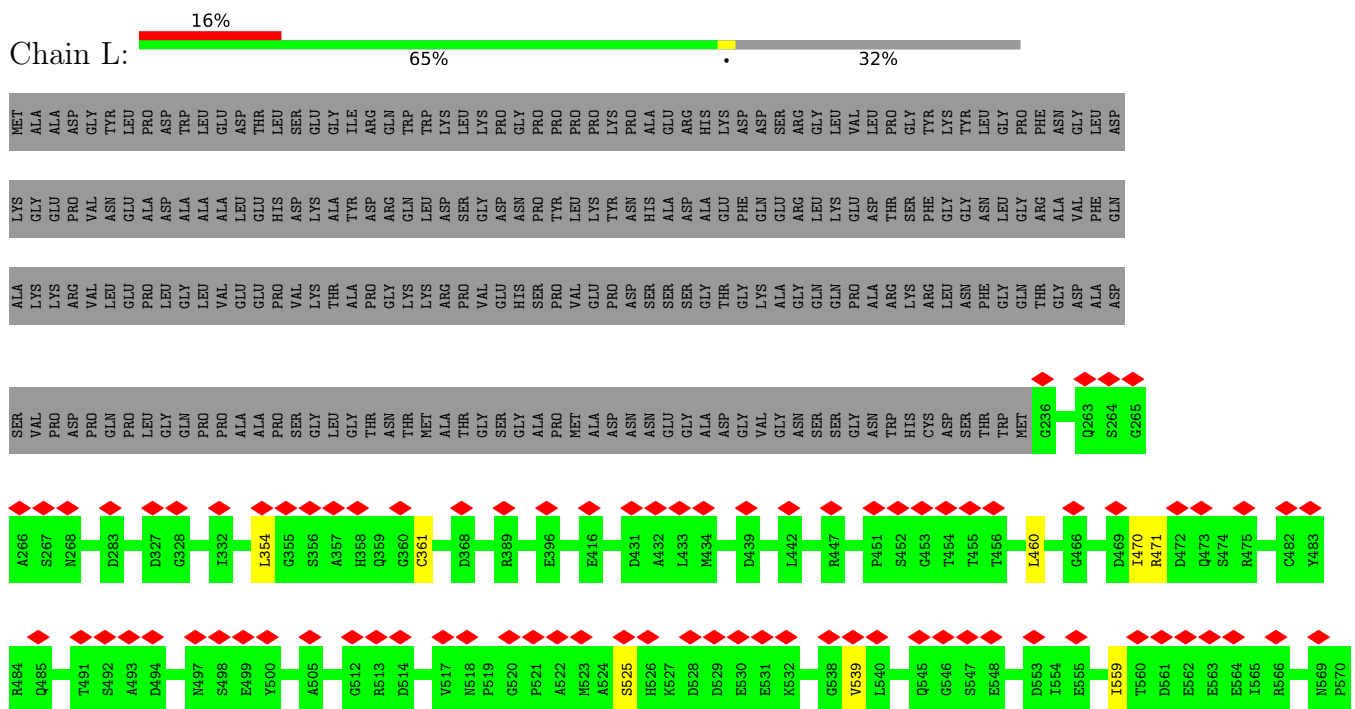
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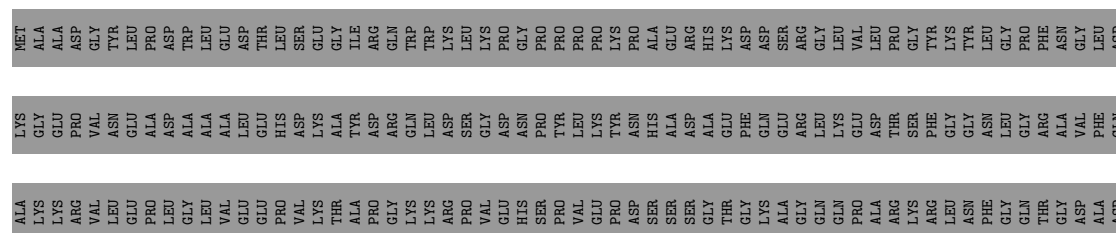


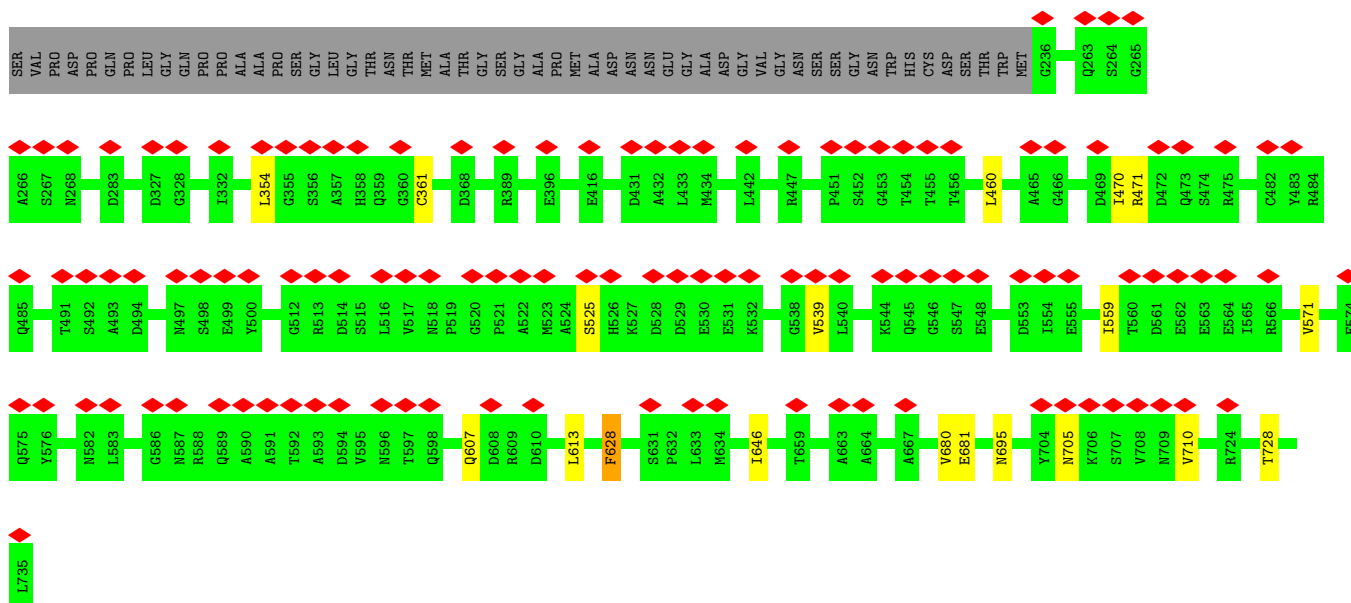




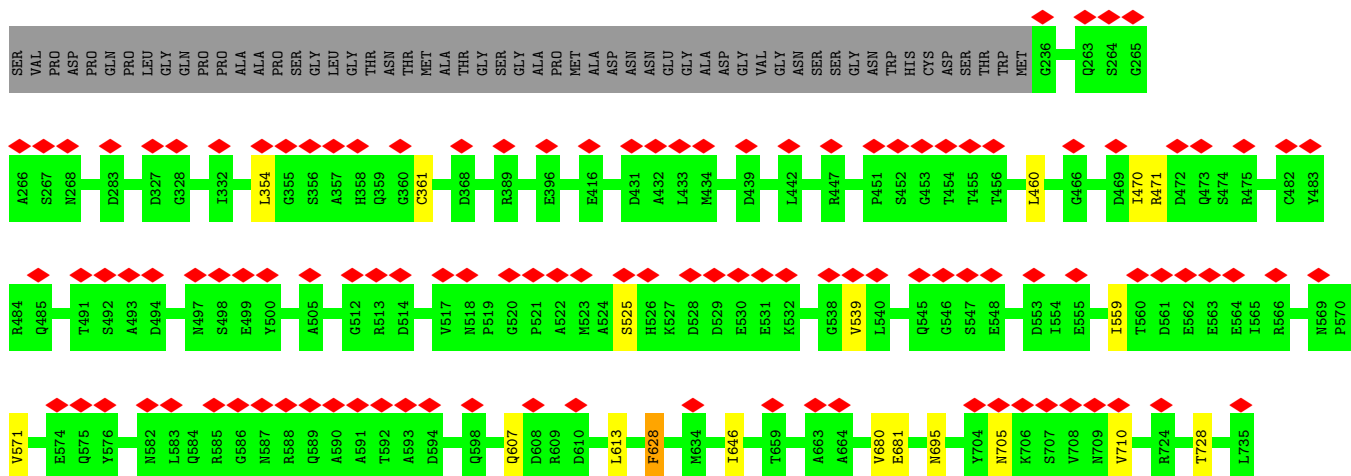
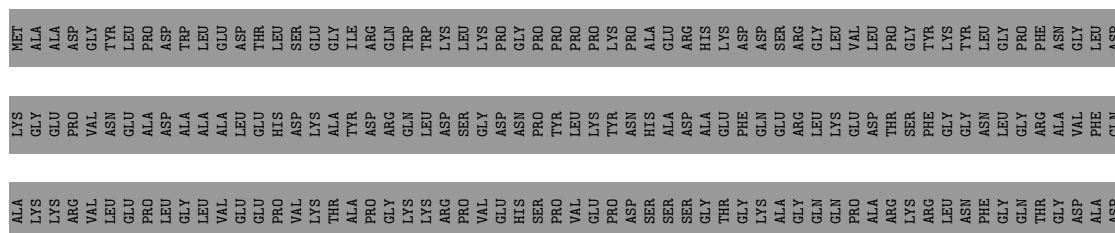




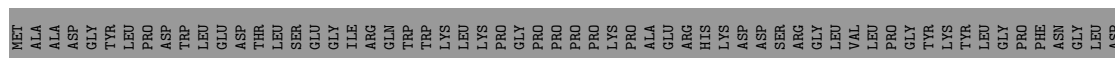




• Molecule 1: Capsid protein VP1



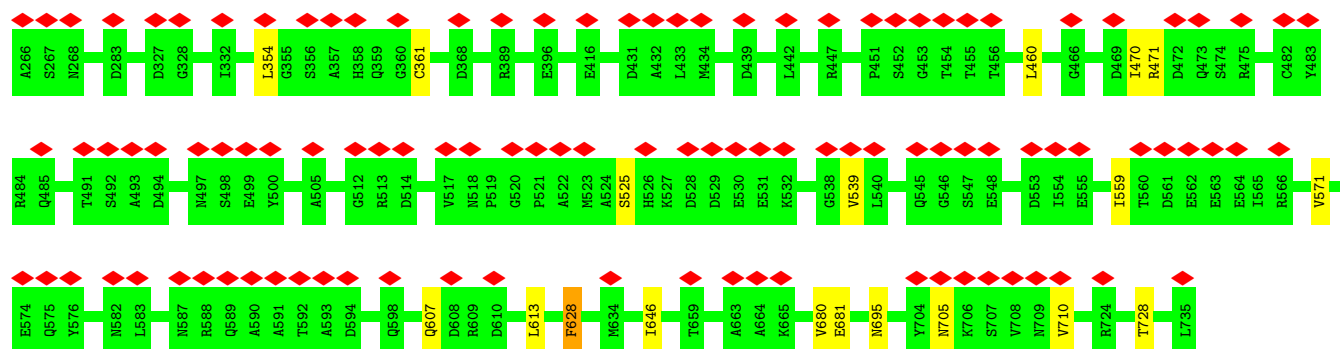
• Molecule 1: Capsid protein VP1



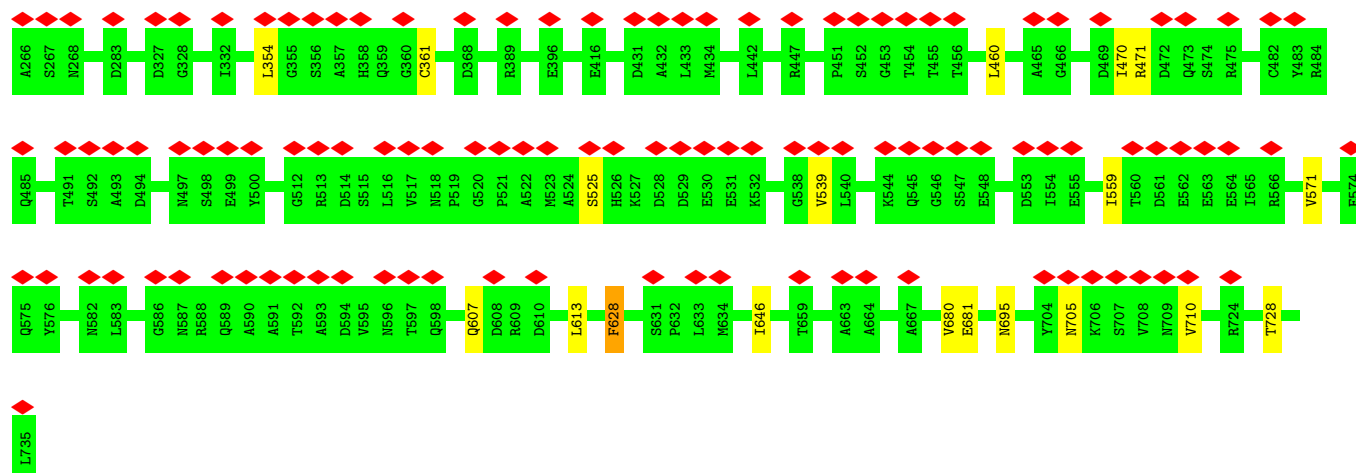
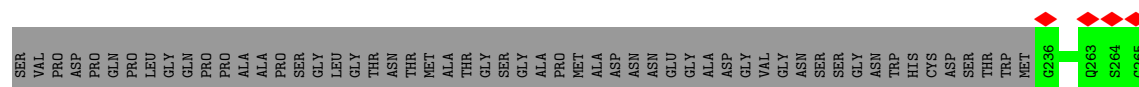
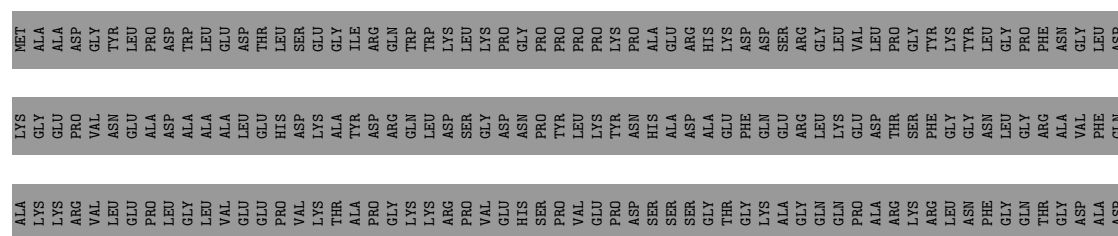




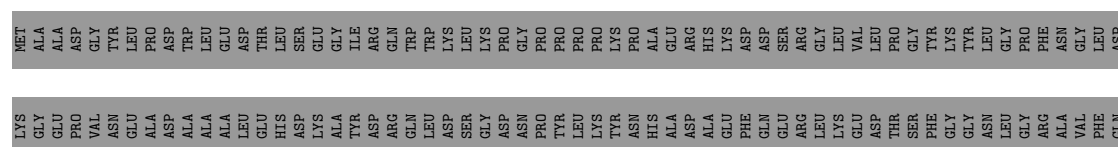




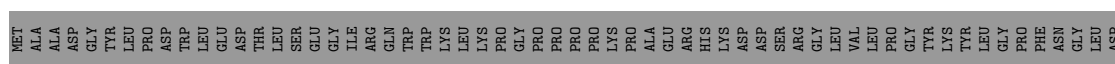
- Molecule 1: Capsid protein VP1

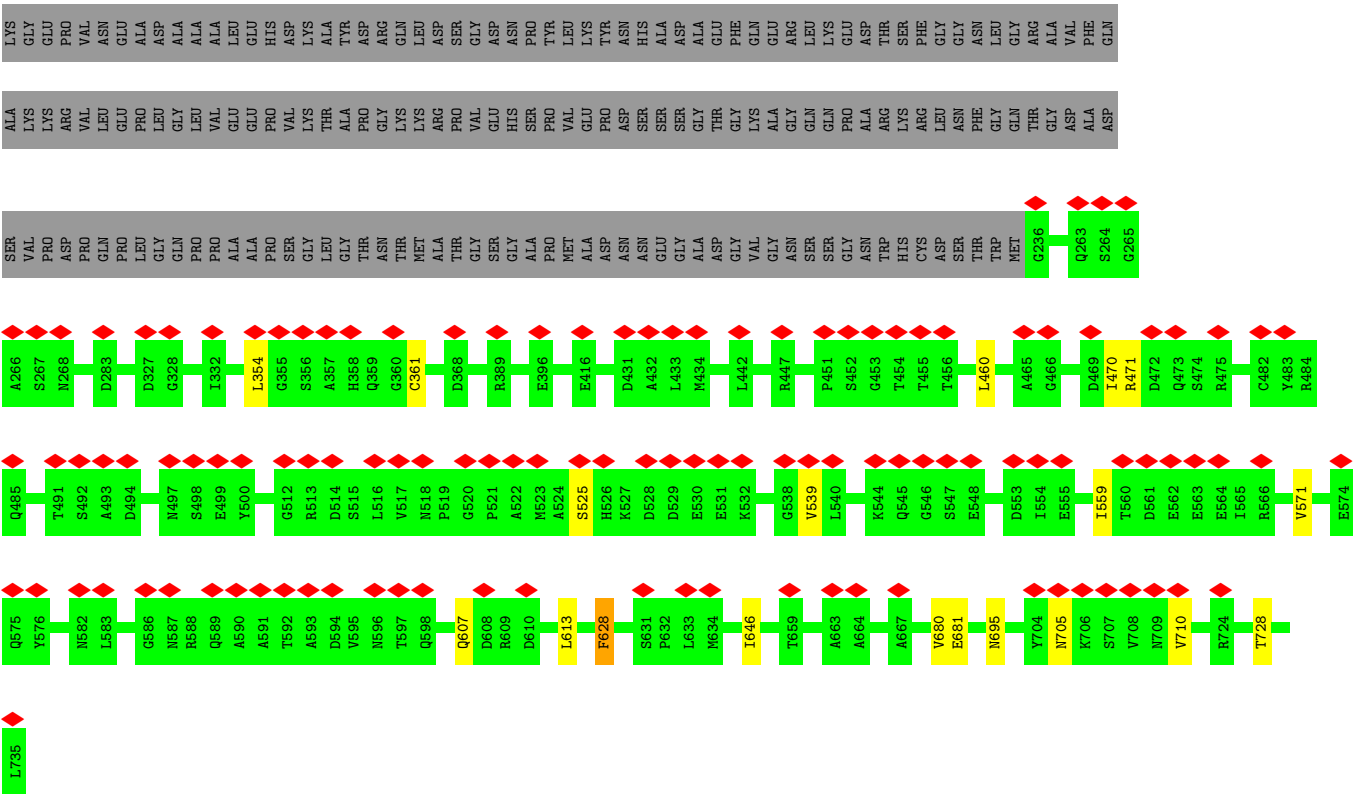


- Molecule 1: Capsid protein VP1

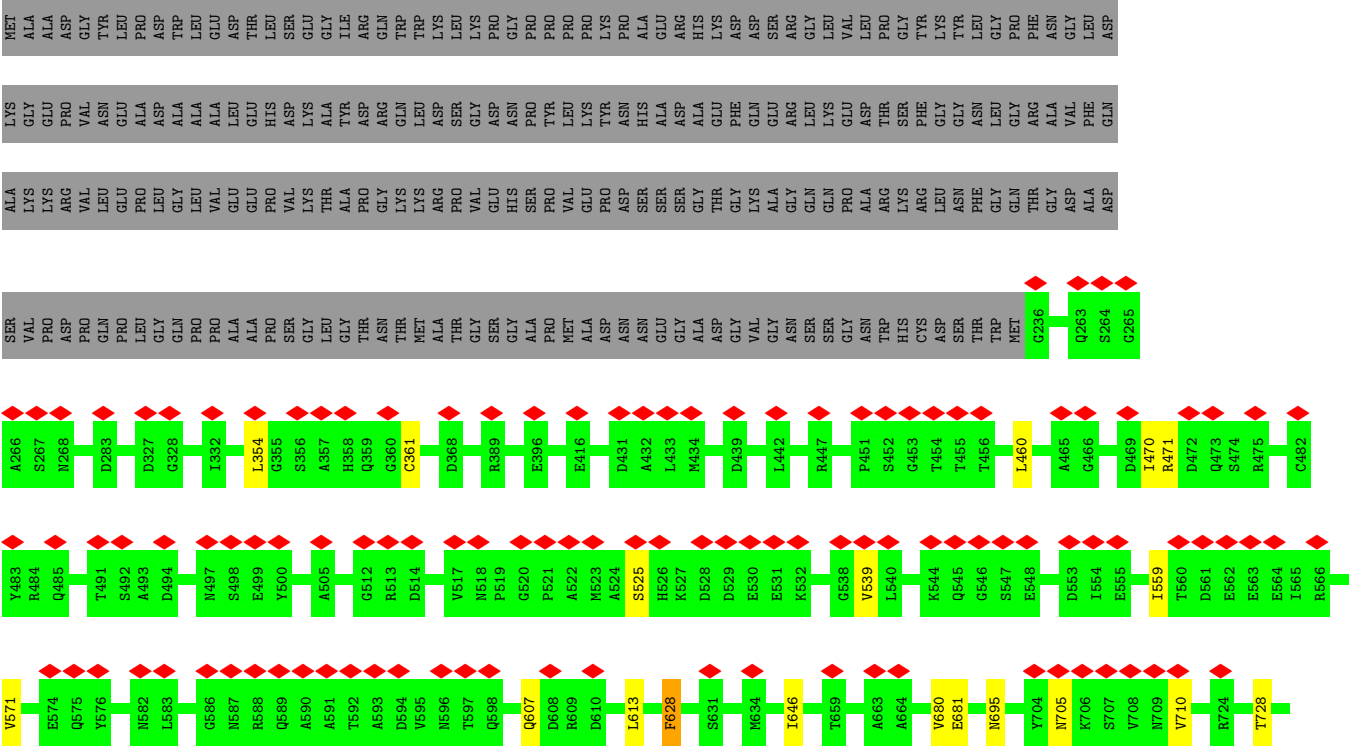








• Molecule 1: Capsid protein VP1



L735

- Molecule 1: Capsid protein VP1

Chain c:  16% 65% 32%

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

SER	VAL	PRO	PRO	ASP	PRO	GLN	PRO	LEU	GLY	GLN	PRO	PRO	ALA	ALA	PRO	SER	GLY	LEU	GLY	THR	ASN	THR	THR	MET	ALA	ALA	THR	GLY	SER	GLY	ALA	ALA	PRO	MET	ASP	ASN	ASN	GLU	GLY	ALA	ALA	ASP	GLY	VAL	GLY	ASN	ASN	SER	SER	SER	GLY	ASN	THR	THR	HIS	CYS	ASP	SER	SER	THR	THR	TRP	TRP	MET	G236	G235	G264	G265
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------

Category	Item	Value	Color
A	A266	100	Green
	A267	100	Green
	A268	100	Green
	A293	100	Green
	A327	100	Green
	A328	100	Green
	A332	100	Green
	A354	100	Yellow
	A355	100	Green
	A356	100	Green
B	B357	100	Green
	B358	100	Green
	B359	100	Green
	B360	100	Green
	B361	100	Yellow
	B368	100	Green
	B399	100	Green
	B396	100	Green
	B416	100	Green
	B431	100	Green
C	C432	100	Green
	C433	100	Green
	C434	100	Green
	C439	100	Green
	C442	100	Green
	C447	100	Green
	C451	100	Green
	C452	100	Green
	C453	100	Green
	C454	100	Green
D	D455	100	Green
	D456	100	Green
	D460	100	Yellow
	D466	100	Green
	D469	100	Green
	D470	100	Yellow
	D471	100	Green
	D472	100	Green
	D473	100	Green
	D475	100	Green
E	E482	100	Green
	E483	100	Green

R484	Q485	T491	S492	A493	D494	N497	S498	E499	Y500	A505	G512	R513	D514	V517	N518	P519	G520	P521	A522	M523	A524	S525	H526	K527	D528	D529	E530	E531	K532	G538	V539	L540	K544	Q545	G546	S547	E548	D553	E554	E555	L559	T560	D561	E562	E563	E564	L565	R566
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

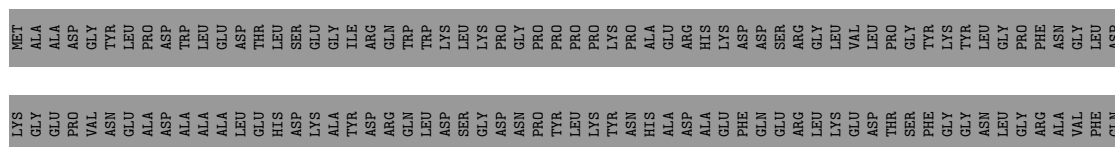
1

- Molecule 1: Capsid protein VP1

Chain d: 

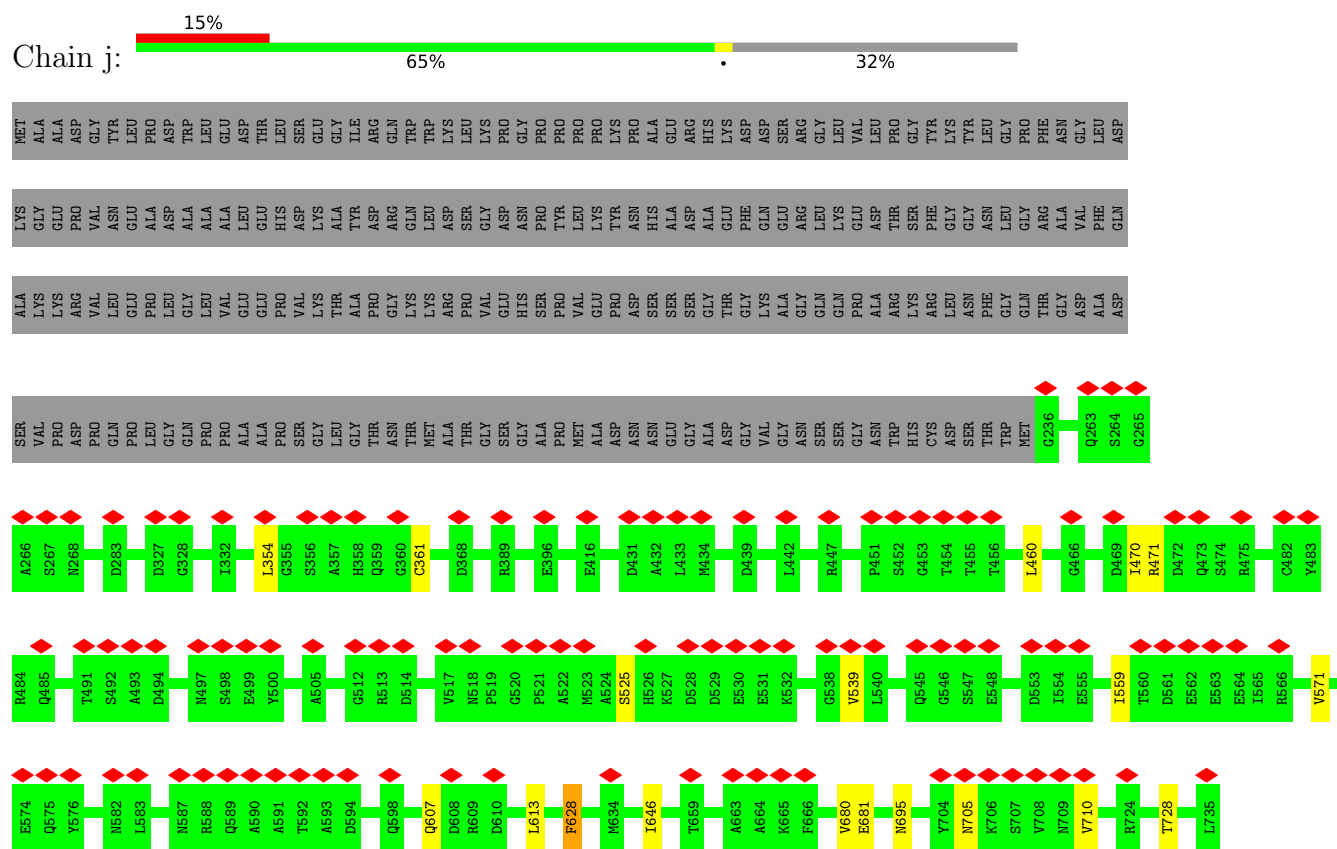
ALA	LYS	MET
LYS	GLY	ALA
LYS	GLU	ALA
ARG	PRO	ASP
VAL	VAL	GLY
LEU	ASN	TYR
GLU	GLU	LEU
PRO	ALA	PRO
LEU	ASP	ASP
GLY	ALA	TRP
LEU	ALA	LEU
VAL	ALA	GLU
GLU	LEU	ASP
GLU	GLU	THR
PRO	HIS	LEU
VAL	ASP	SER
LYS	LYS	GLU
THR	ALA	GLY
ALA	TYR	ILE
PRO	ASP	ARG
GLY	GLN	GLN
LYS	GLN	TRP
LYS	LEU	TRP
ARG	ASP	LYS
PRO	SER	LEU
VAL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

[illegible]

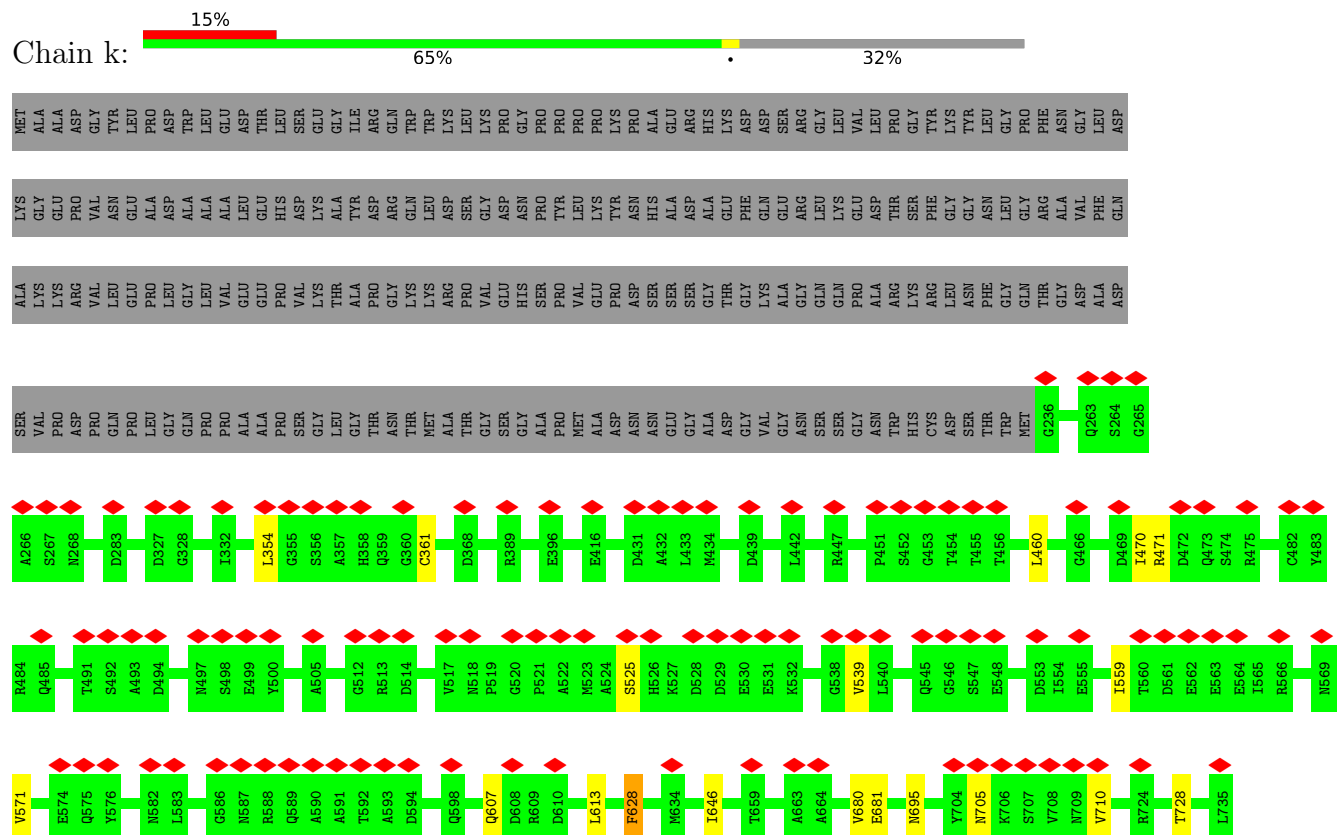






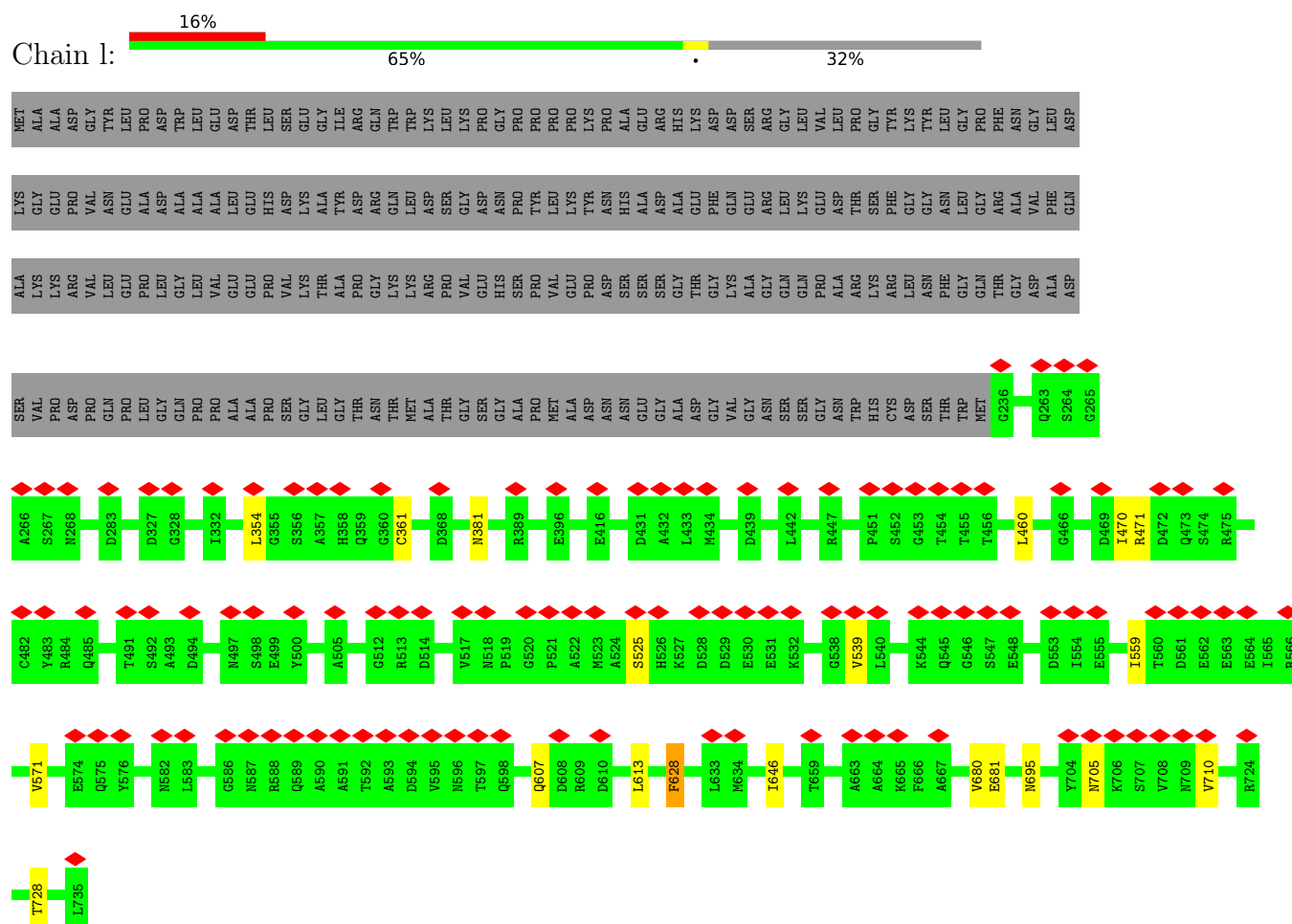


- Molecule 1: Capsid protein VP1



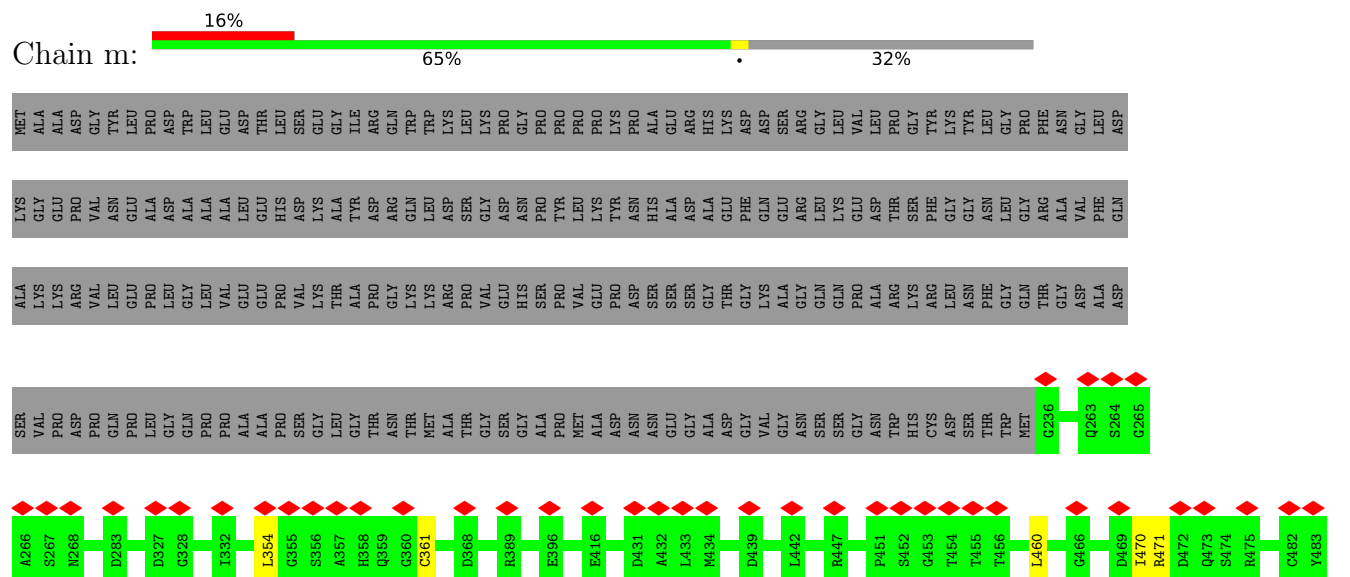
- Molecule 1: Capsid protein VP1

Chain l:

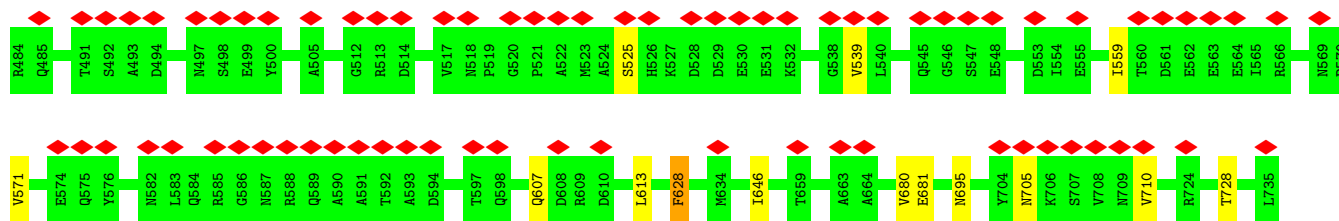


- Molecule 1: Capsid protein VP1

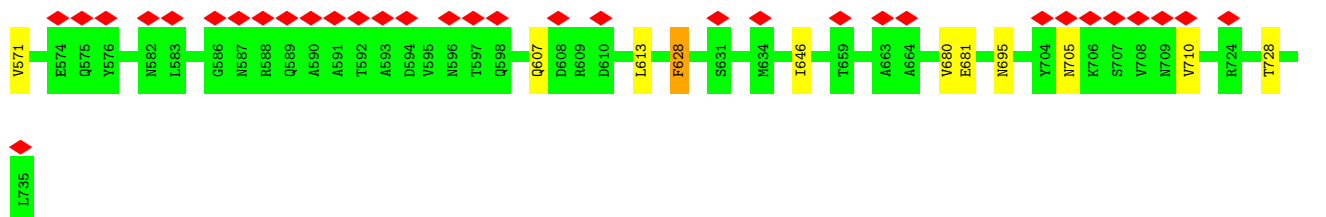
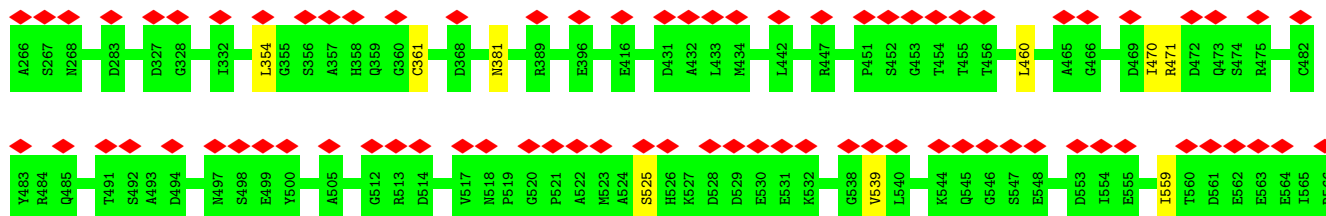
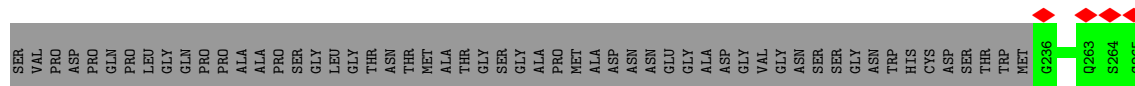
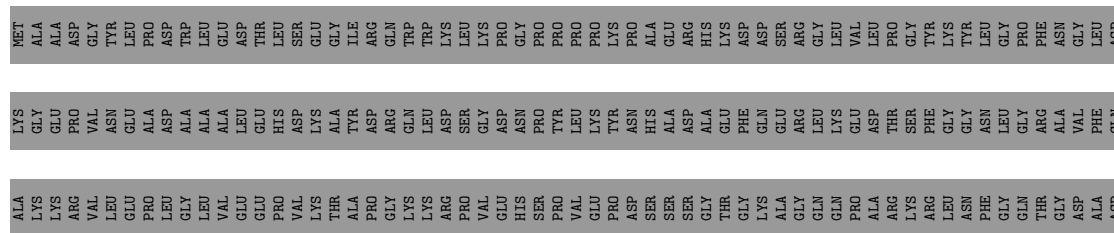
Chain m:



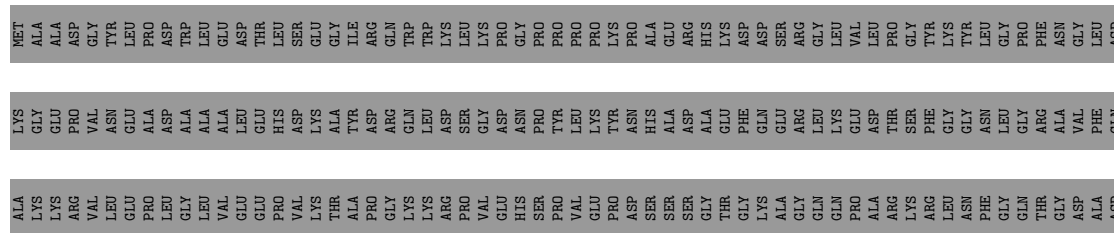


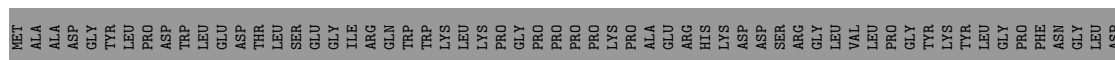


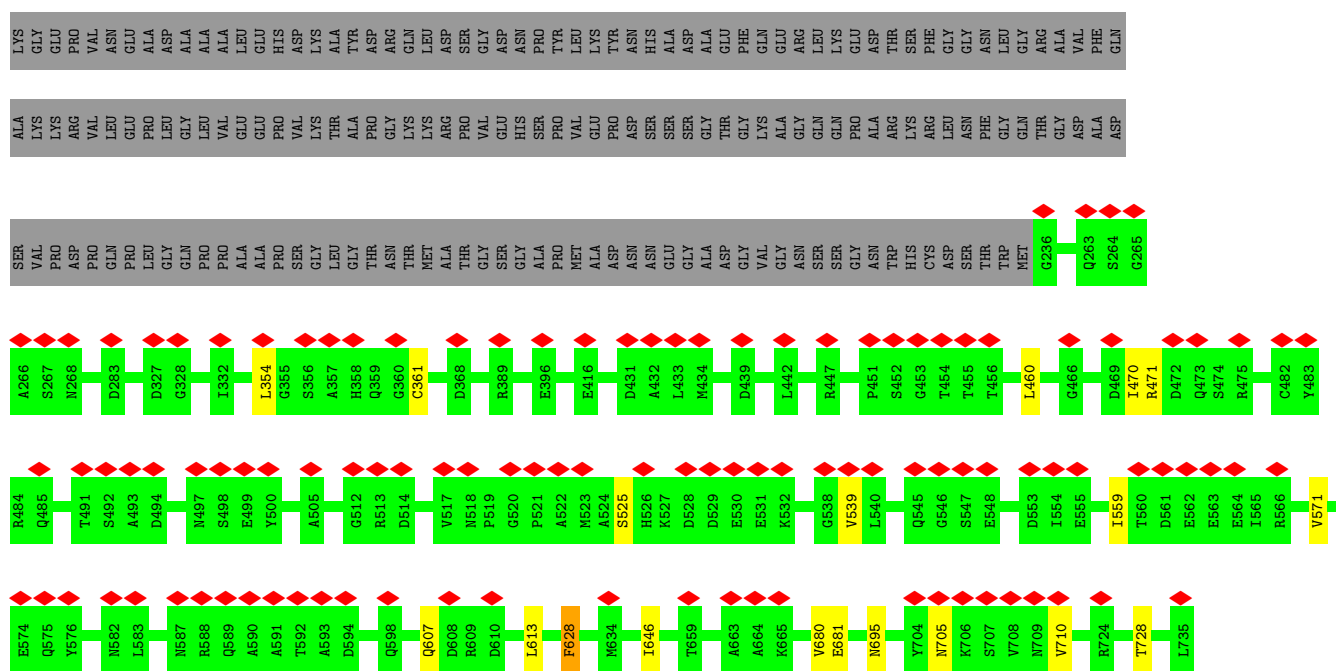
• Molecule 1: Capsid protein VP1



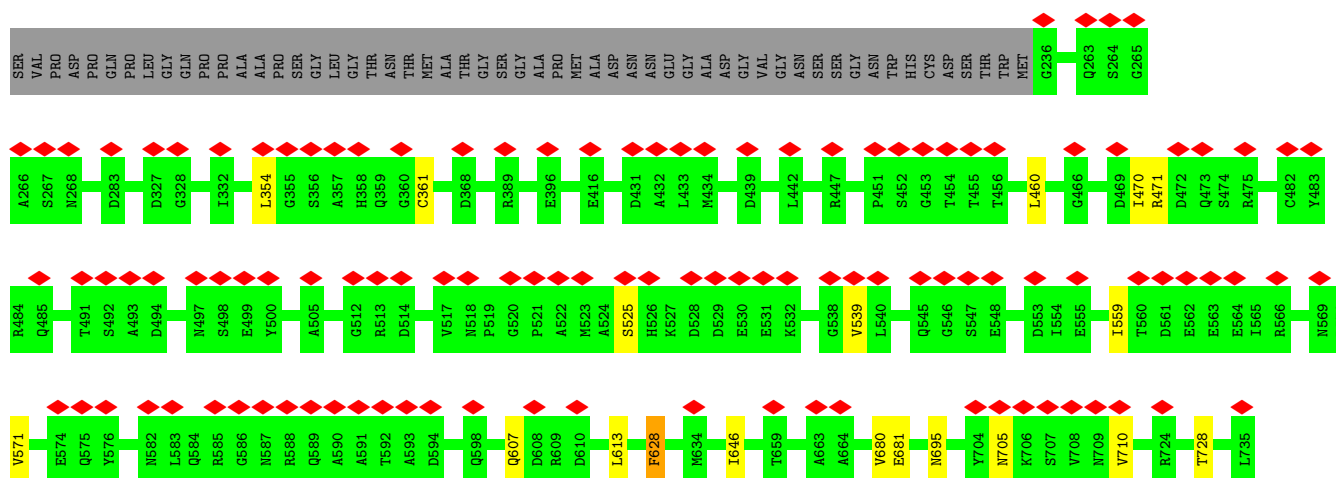
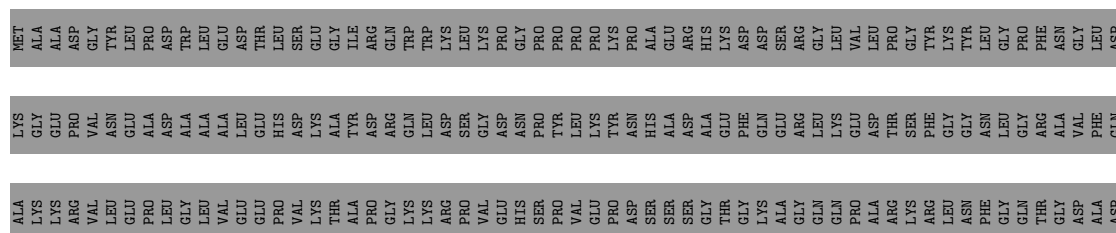
• Molecule 1: Capsid protein VP1





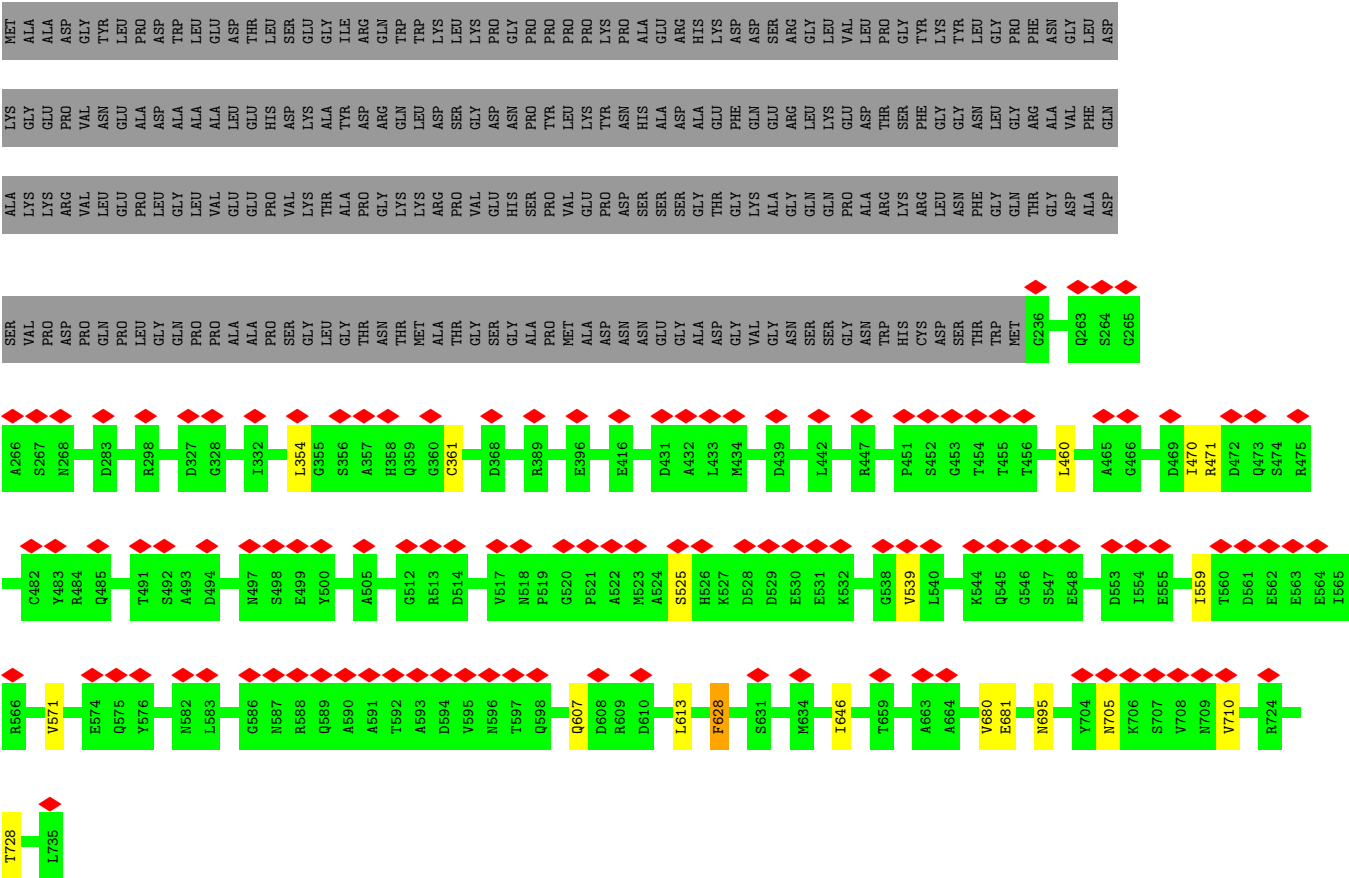


• Molecule 1: Capsid protein VP1

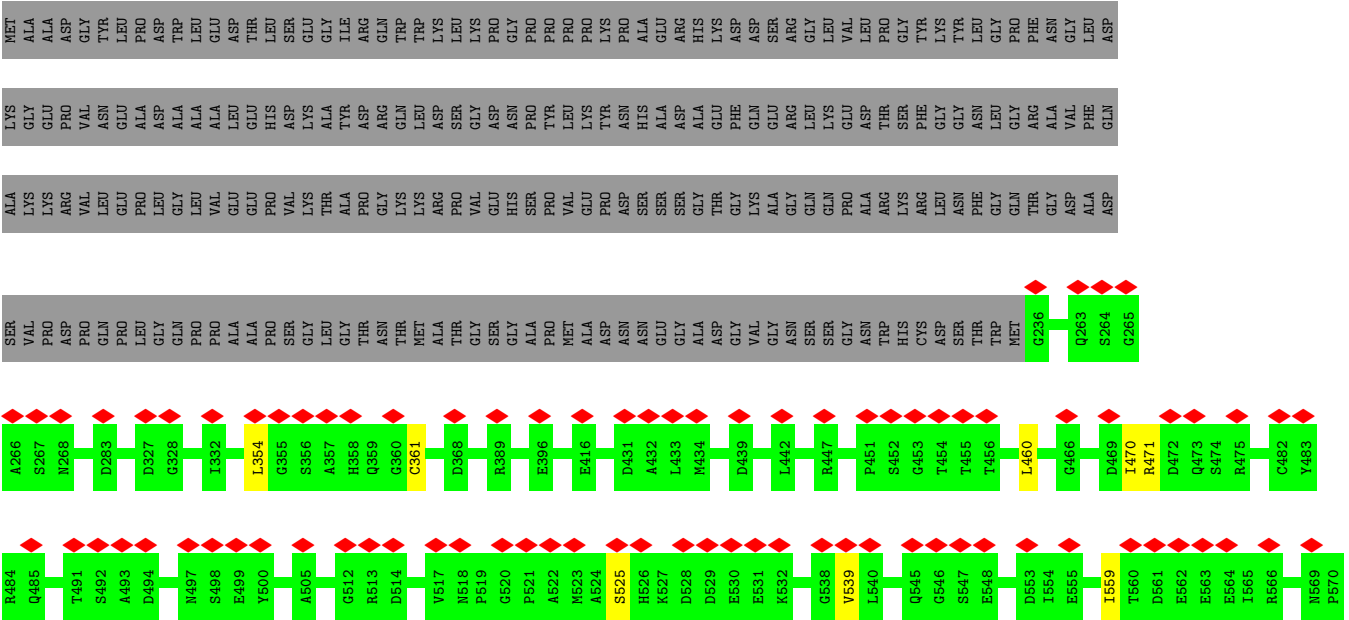


• Molecule 1: Capsid protein VP1

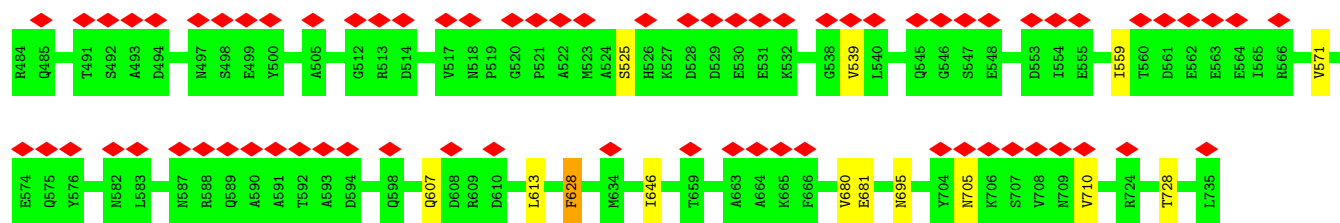




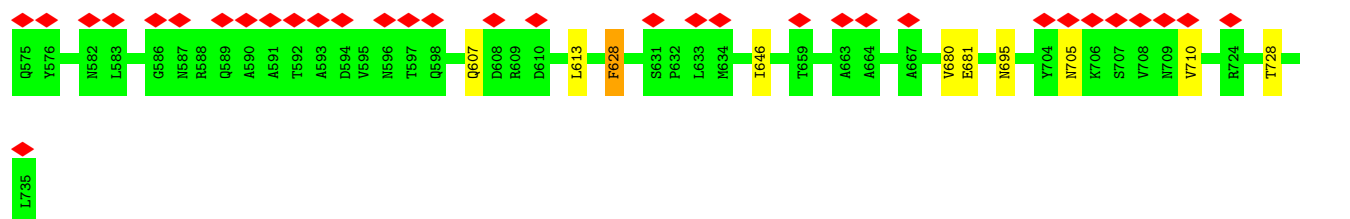
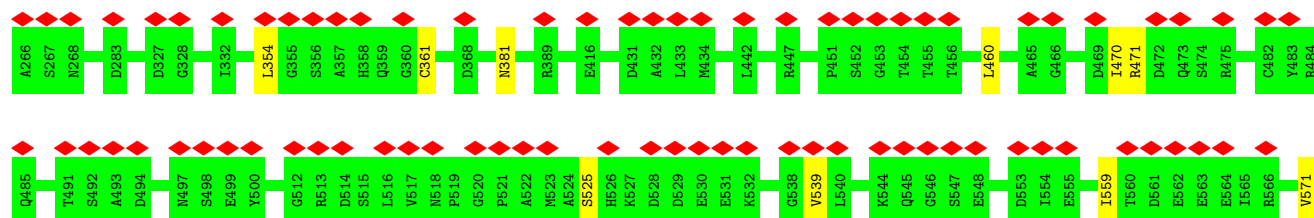
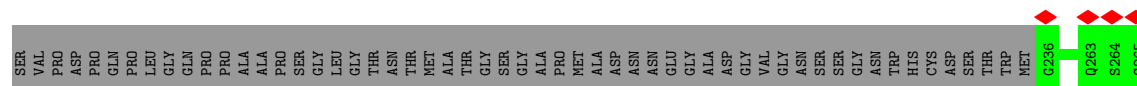
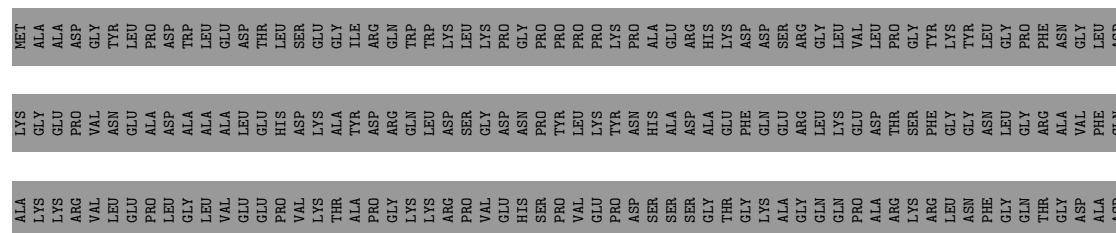
● Molecule 1: Capsid protein VP1



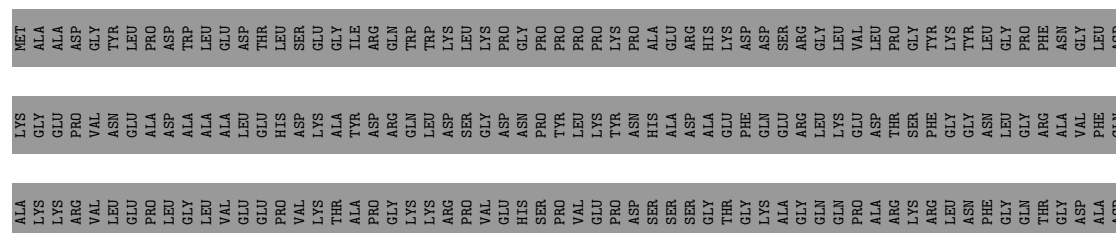




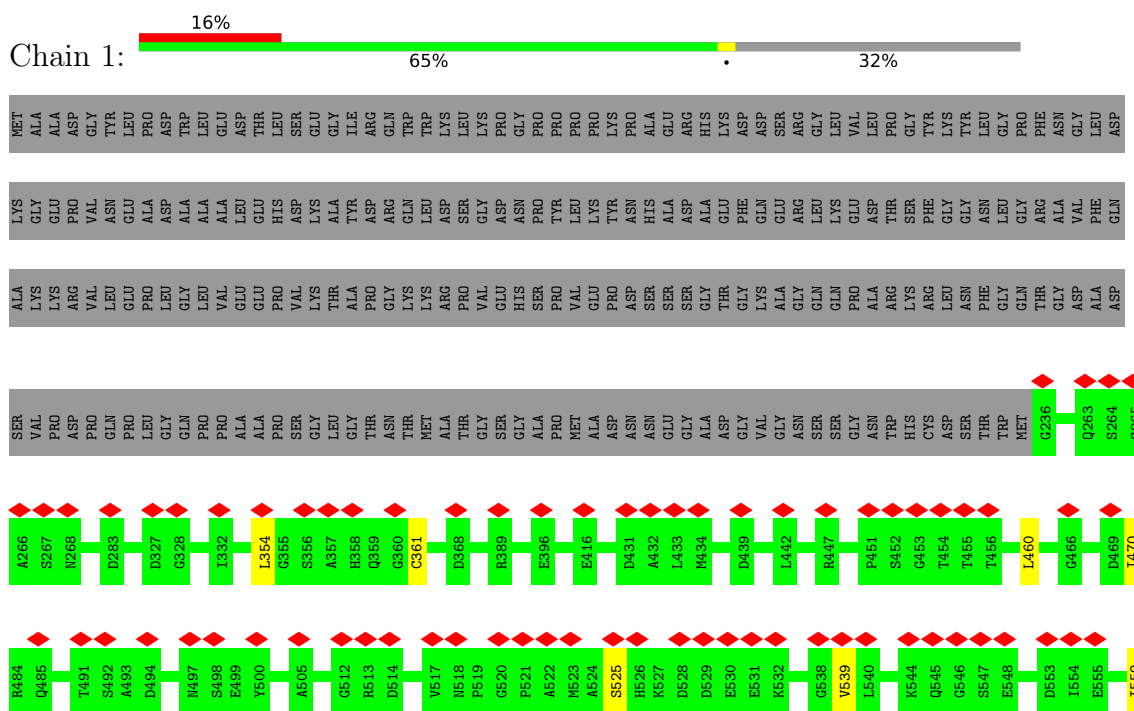
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

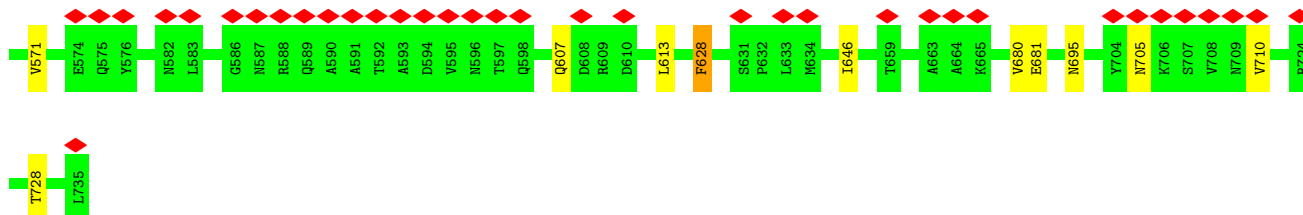
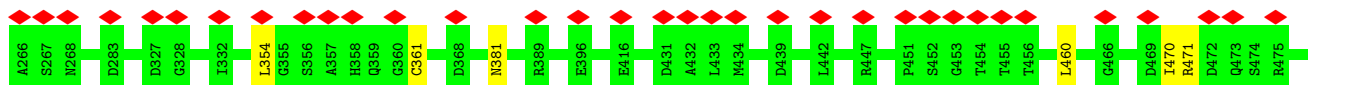
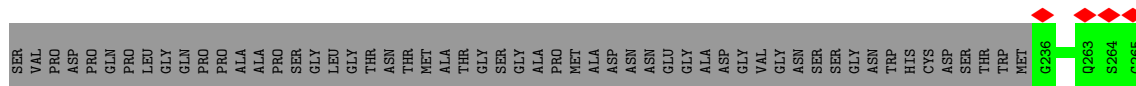
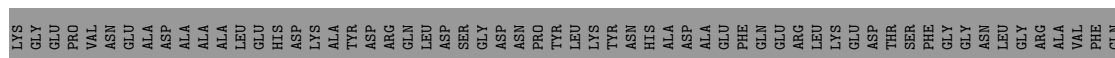




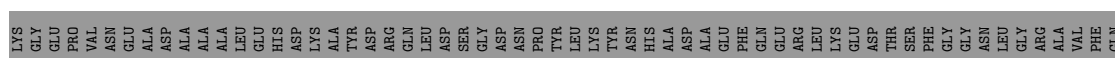
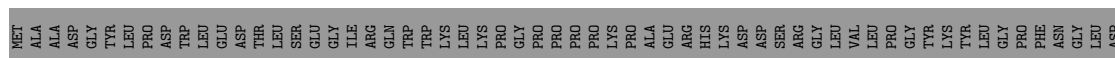


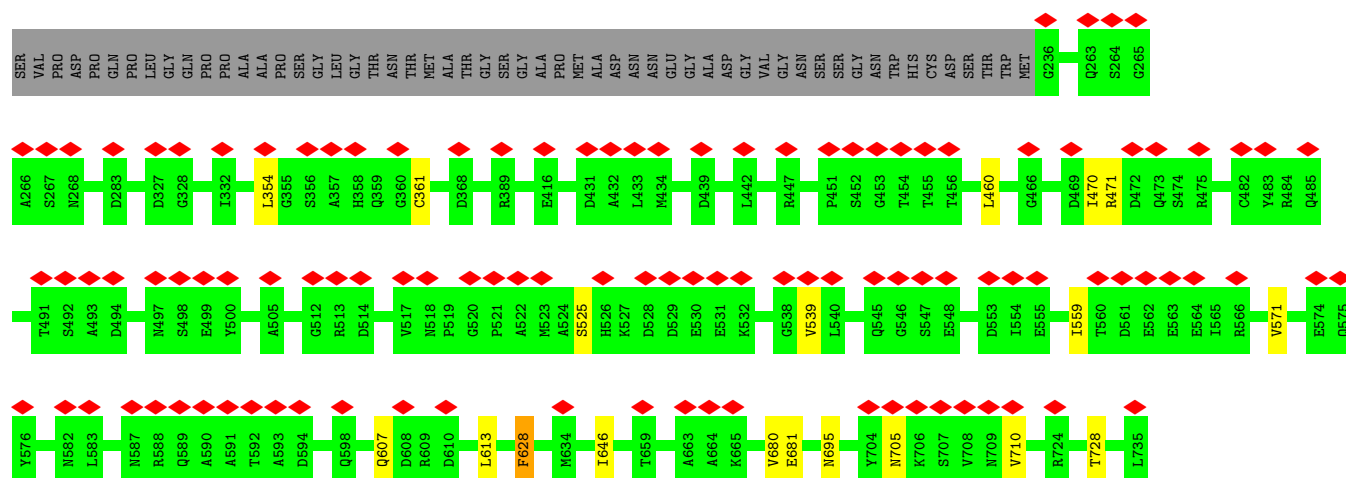


- Molecule 1: Capsid protein VP1

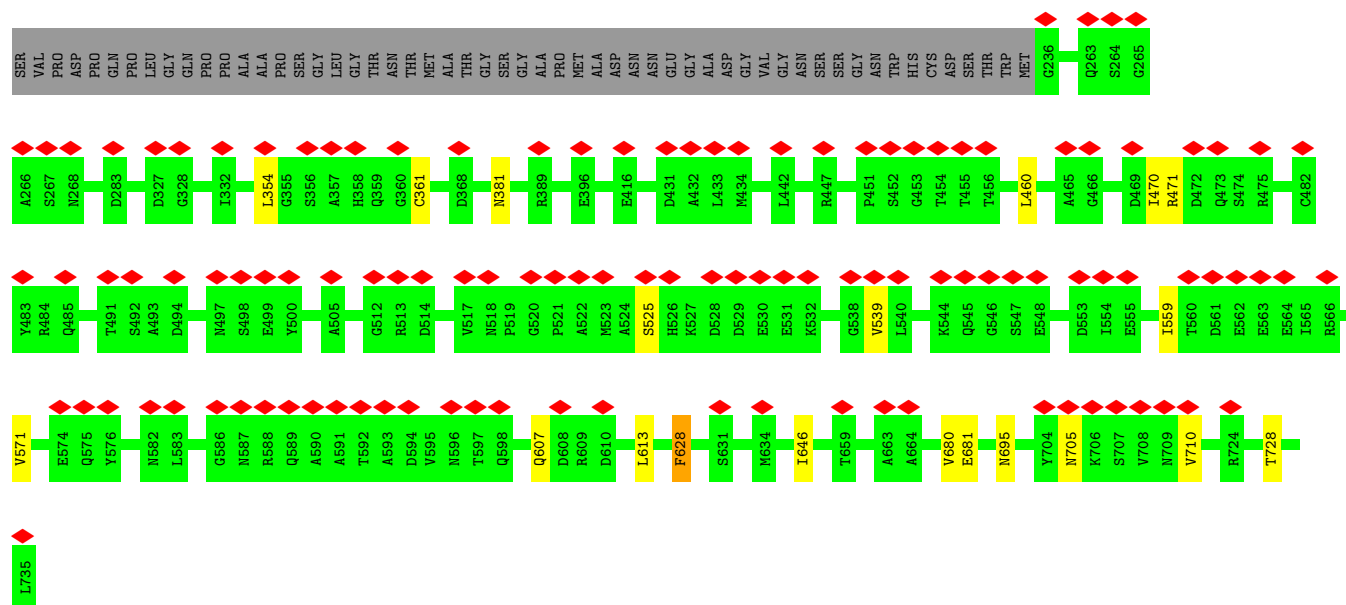
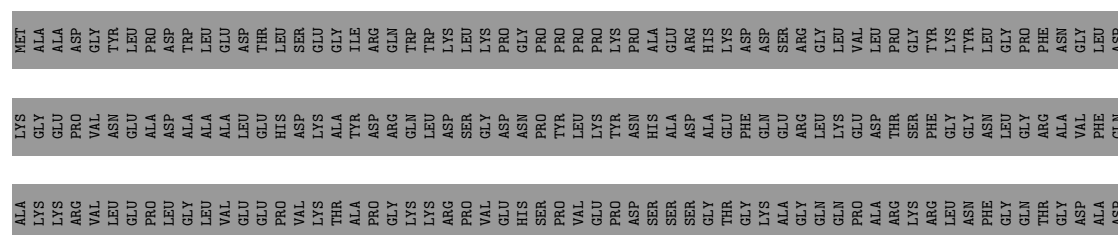


- Molecule 1: Capsid protein VP1

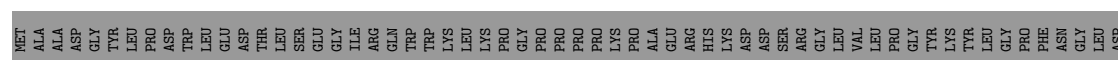




• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	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	0.57	0/4127	0.68	0/5626
1	2	0.57	0/4127	0.68	0/5626
1	3	0.57	0/4127	0.68	0/5626
1	4	0.57	0/4127	0.68	0/5626
1	5	0.57	0/4127	0.68	0/5626
1	6	0.57	0/4127	0.68	0/5626
1	7	0.57	0/4127	0.68	0/5626
1	8	0.57	0/4127	0.68	0/5626
1	A	0.57	0/4127	0.68	0/5626
1	B	0.57	0/4127	0.68	0/5626
1	C	0.57	0/4127	0.68	0/5626
1	D	0.57	0/4127	0.68	0/5626
1	E	0.57	0/4127	0.68	0/5626
1	F	0.57	0/4127	0.68	0/5626
1	G	0.57	0/4127	0.68	0/5626
1	H	0.57	0/4127	0.68	0/5626
1	I	0.57	0/4127	0.68	0/5626
1	J	0.57	0/4127	0.68	0/5626
1	K	0.57	0/4127	0.68	0/5626
1	L	0.57	0/4127	0.68	0/5626
1	M	0.57	0/4127	0.68	0/5626
1	N	0.57	0/4127	0.68	0/5626
1	O	0.57	0/4127	0.68	0/5626
1	P	0.57	0/4127	0.68	0/5626
1	Q	0.57	0/4127	0.68	0/5626
1	R	0.57	0/4127	0.67	0/5626
1	S	0.57	0/4127	0.68	0/5626
1	T	0.57	0/4127	0.68	0/5626
1	U	0.57	0/4127	0.68	0/5626
1	V	0.57	0/4127	0.68	0/5626
1	W	0.57	0/4127	0.68	0/5626
1	X	0.57	0/4127	0.68	0/5626
1	Y	0.57	0/4127	0.68	0/5626
1	Z	0.57	0/4127	0.68	0/5626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.57	0/4127	0.68	0/5626
1	b	0.57	0/4127	0.68	0/5626
1	c	0.57	0/4127	0.68	0/5626
1	d	0.57	0/4127	0.68	0/5626
1	e	0.57	0/4127	0.68	0/5626
1	f	0.57	0/4127	0.68	0/5626
1	g	0.57	0/4127	0.68	0/5626
1	h	0.57	0/4127	0.68	0/5626
1	i	0.57	0/4127	0.68	0/5626
1	j	0.57	0/4127	0.68	0/5626
1	k	0.57	0/4127	0.68	0/5626
1	l	0.57	0/4127	0.68	0/5626
1	m	0.57	0/4127	0.68	0/5626
1	n	0.57	0/4127	0.68	0/5626
1	o	0.57	0/4127	0.68	0/5626
1	p	0.57	0/4127	0.68	0/5626
1	q	0.57	0/4127	0.68	0/5626
1	r	0.57	0/4127	0.68	0/5626
1	s	0.57	0/4127	0.68	0/5626
1	t	0.57	0/4127	0.68	0/5626
1	u	0.57	0/4127	0.68	0/5626
1	v	0.57	0/4127	0.68	0/5626
1	w	0.57	0/4127	0.68	0/5626
1	x	0.57	0/4127	0.68	0/5626
1	y	0.57	0/4127	0.68	0/5626
1	z	0.57	0/4127	0.68	0/5626
All	All	0.57	0/247620	0.68	0/337560

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

*Continued on next page...*



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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

*Continued on next page...*

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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.

There are no bond angle outliers.

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](#)

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

## 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	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	2	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	3	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	4	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	5	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	6	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	7	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	8	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	A	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	B	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	C	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	D	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	E	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	F	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	G	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	H	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	I	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	J	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	K	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	L	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	M	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	N	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	O	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	P	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	Q	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	R	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	S	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	T	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	U	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	V	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	W	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	X	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	Z	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	a	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	b	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	c	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	d	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	e	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	f	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	g	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	h	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	i	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	j	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	k	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	l	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	m	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	n	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	o	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	p	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	q	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	r	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	s	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	t	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	u	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	v	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	w	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	x	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	y	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	z	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
All	All	29880/44100 (68%)	22656 (76%)	6444 (22%)	780 (3%)	8	34

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%)	88	94
1	2	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	3	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	4	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	5	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	6	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	7	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	8	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	A	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	B	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	C	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	D	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	E	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	F	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	G	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	H	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	I	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	J	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	K	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	L	444/629 (71%)	442 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	N	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	O	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	P	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	Q	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	R	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	S	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	T	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	U	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	V	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	W	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	X	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	Y	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	Z	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	a	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	b	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	c	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	d	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	e	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	f	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	g	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	h	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	i	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	j	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	k	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	l	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	m	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	n	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	o	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	p	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	q	444/629 (71%)	442 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	s	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	t	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	u	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	v	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	w	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	x	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	y	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	z	444/629 (71%)	442 (100%)	2 (0%)	88	94
All	All	26640/37740 (71%)	26520 (100%)	120 (0%)	89	94

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 558 such sidechains are listed below:

Mol	Chain	Res	Type
1	x	473	GLN
1	z	253	ASN
1	x	461	GLN
1	4	607	GLN
1	U	598	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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



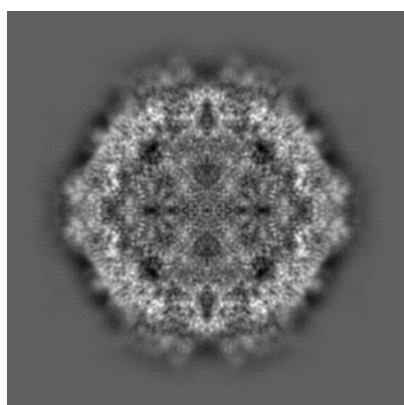
## 6 Map visualisation [i](#)

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

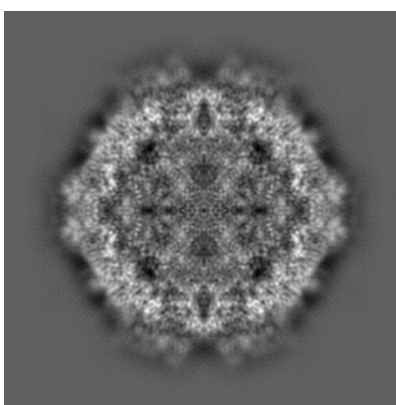
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

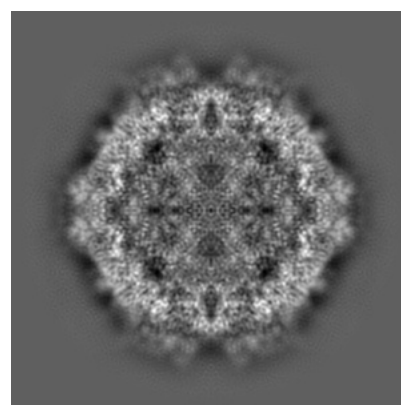
#### 6.1.1 Primary map



X



Y

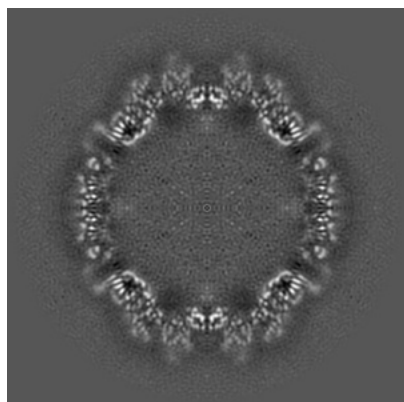


Z

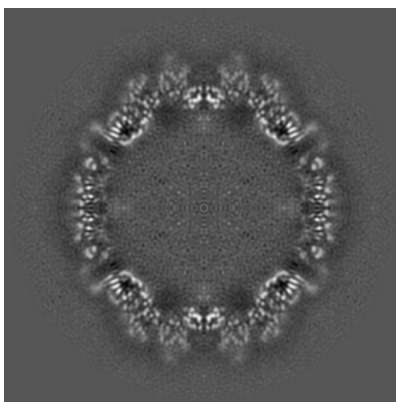
The images above show the map projected in three orthogonal directions.

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

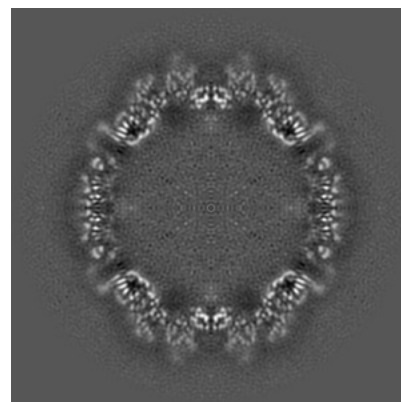
#### 6.2.1 Primary map



X Index: 164



Y Index: 164

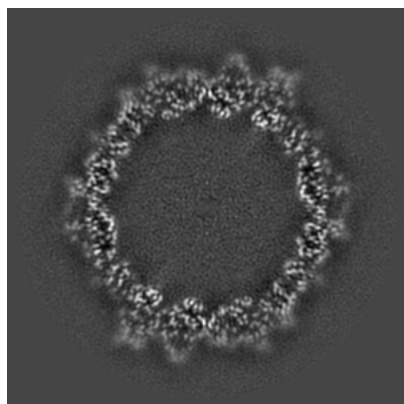


Z Index: 164

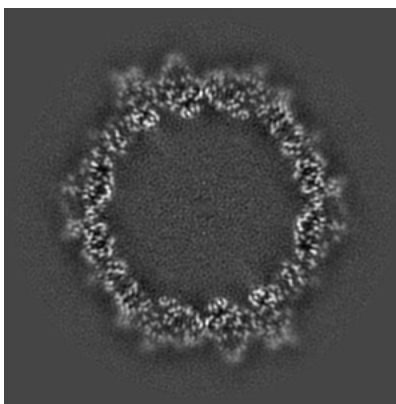
The images above show central slices of the map in three orthogonal directions.

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

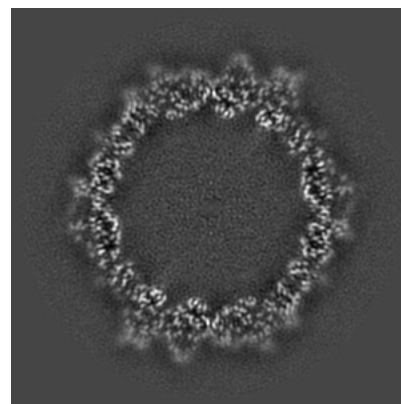
### 6.3.1 Primary map



X Index: 151



Y Index: 177

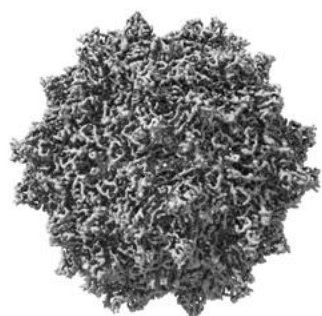


Z Index: 151

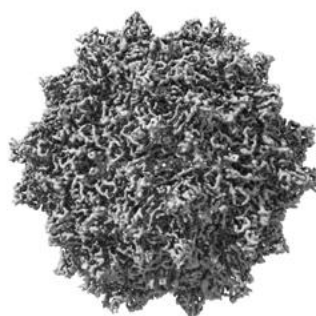
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

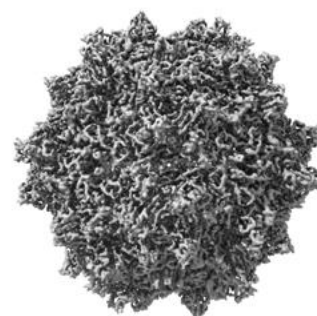
### 6.4.1 Primary map



X



Y



Z

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.

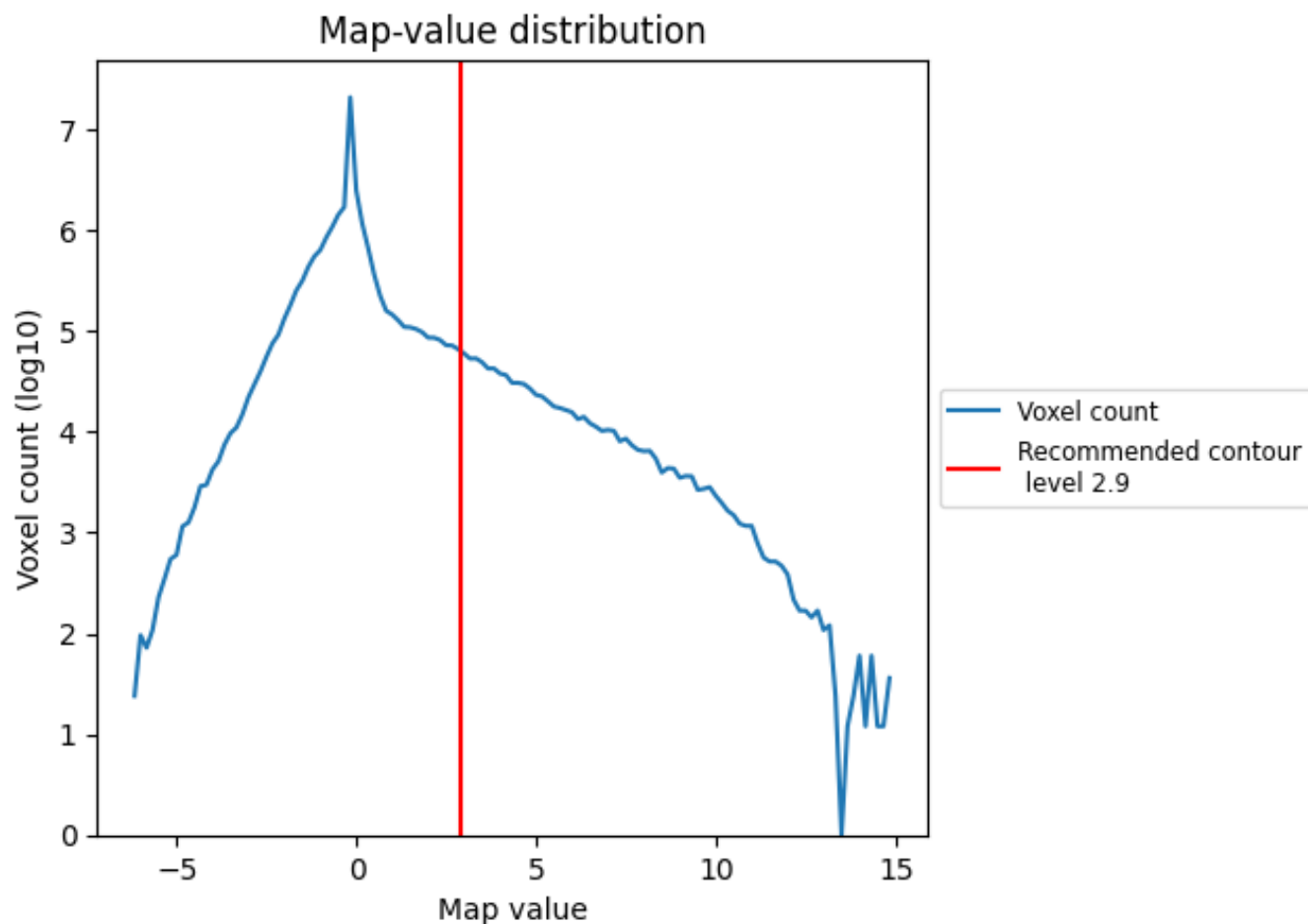
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

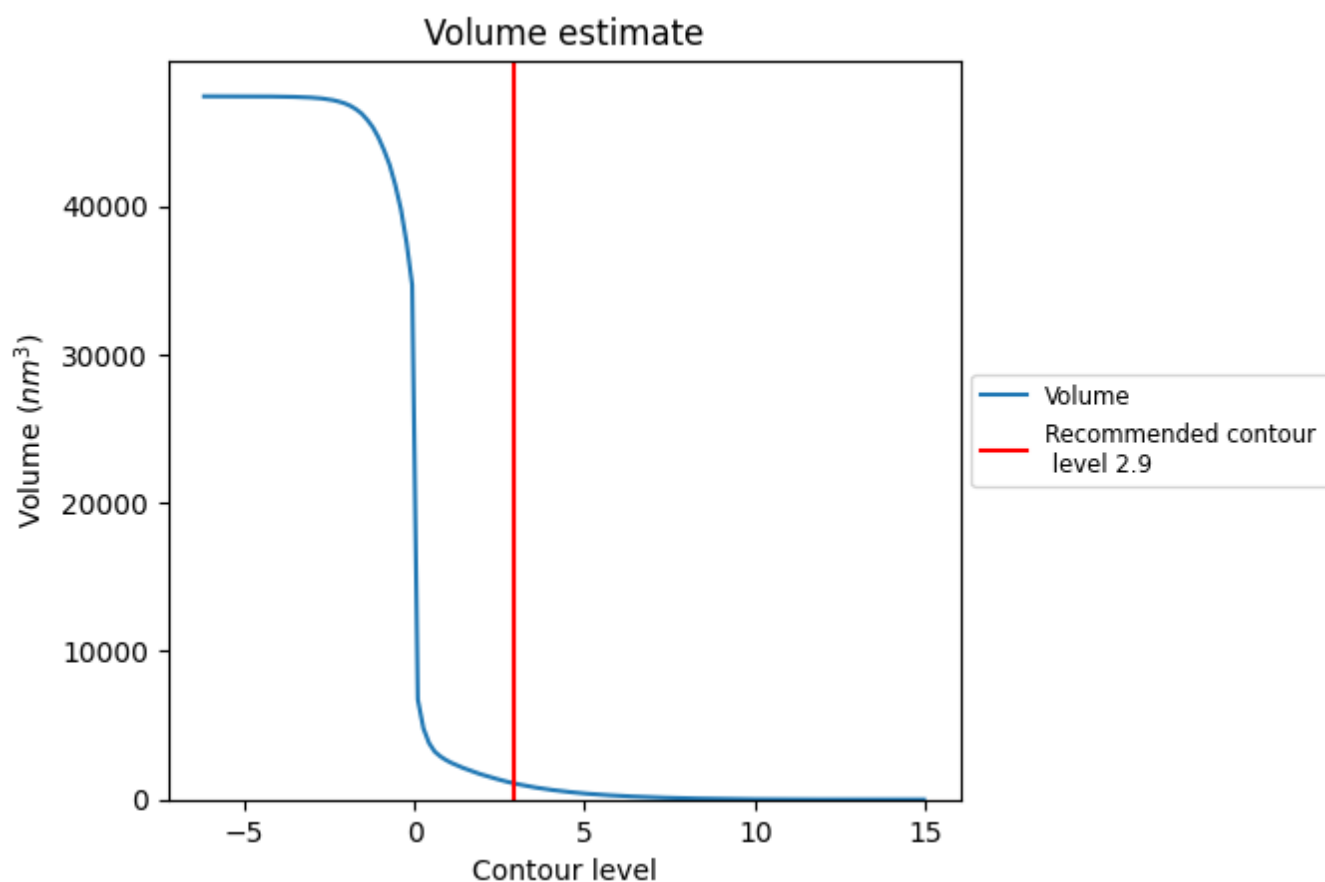
This section contains the results of statistical analysis of the map.

### 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.

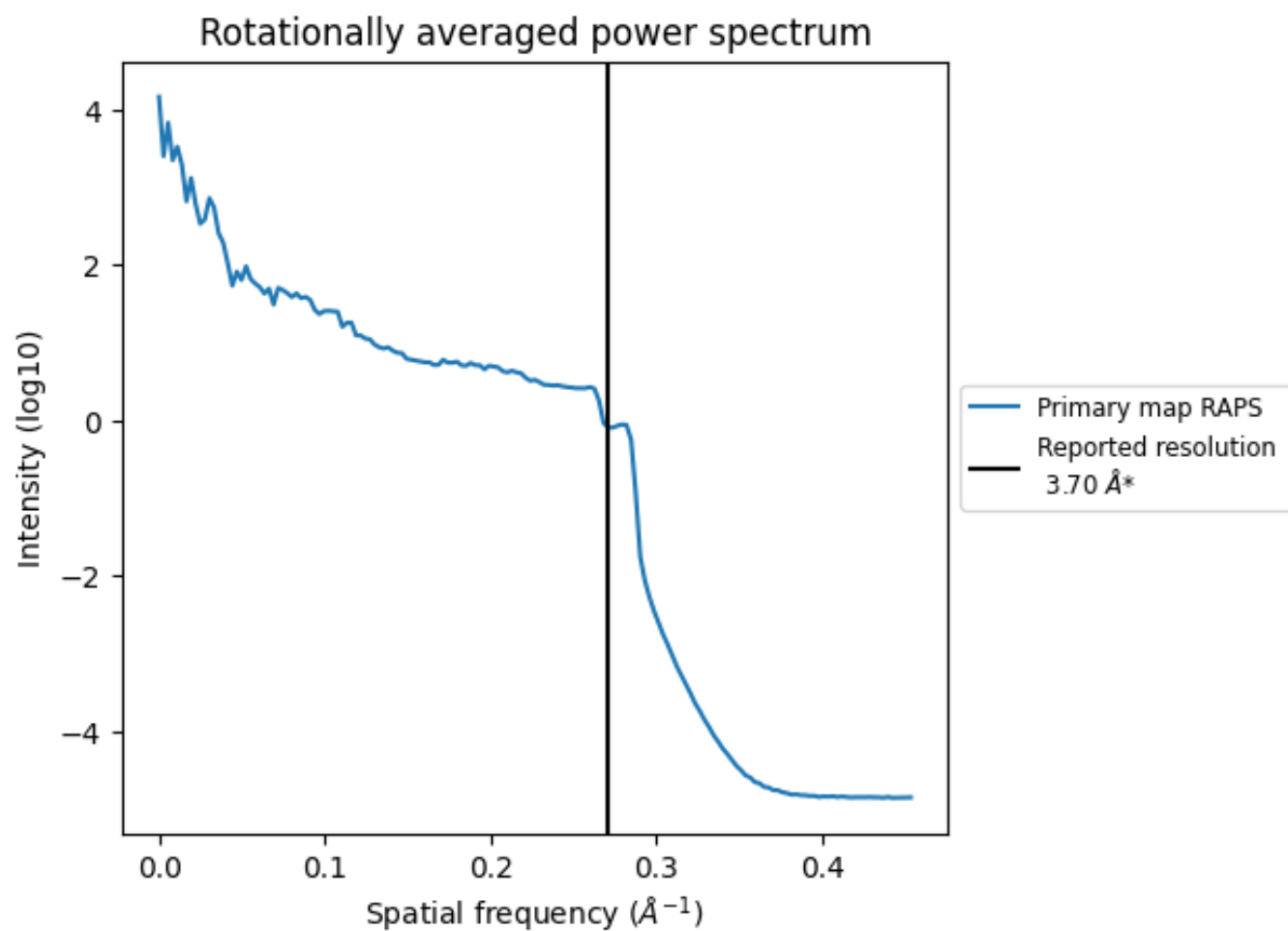
## 7.2 Volume estimate [i](#)



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>

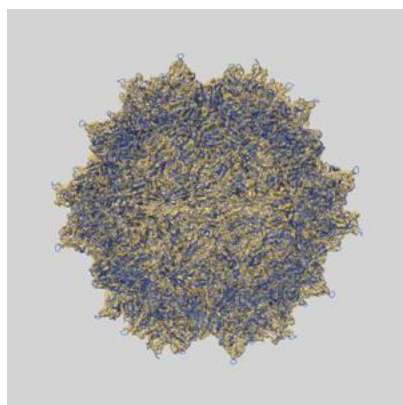
## 8 Fourier-Shell correlation

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

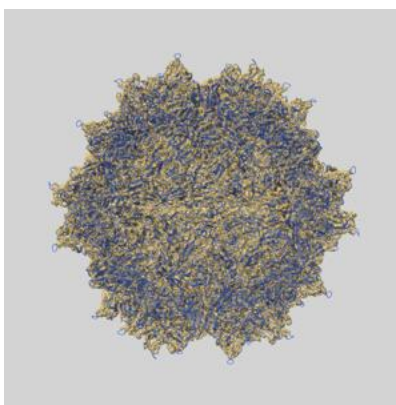
## 9 Map-model fit [i](#)

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](#).

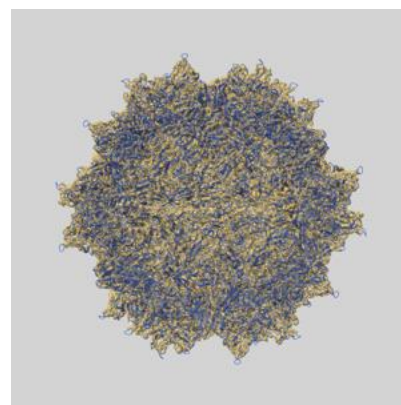
### 9.1 Map-model overlay [i](#)



X



Y

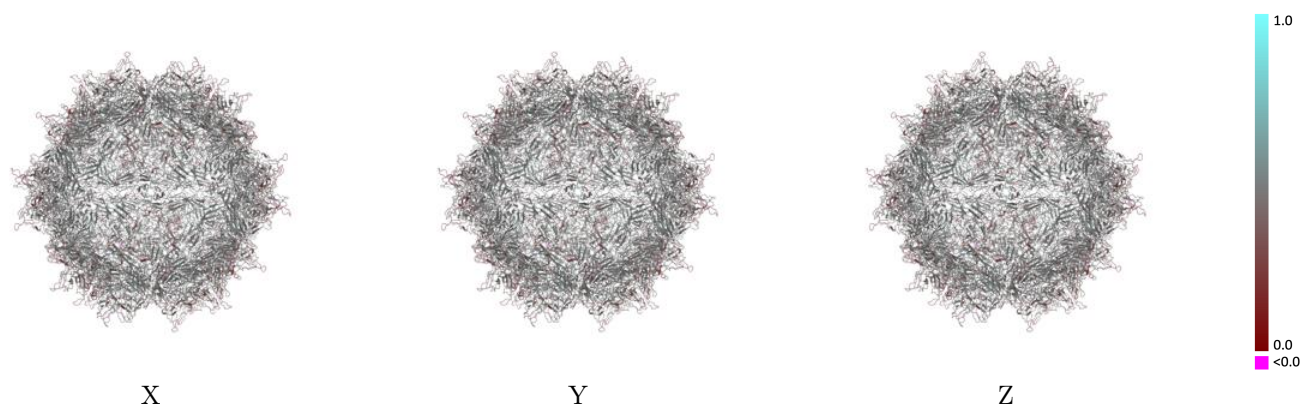


Z

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.

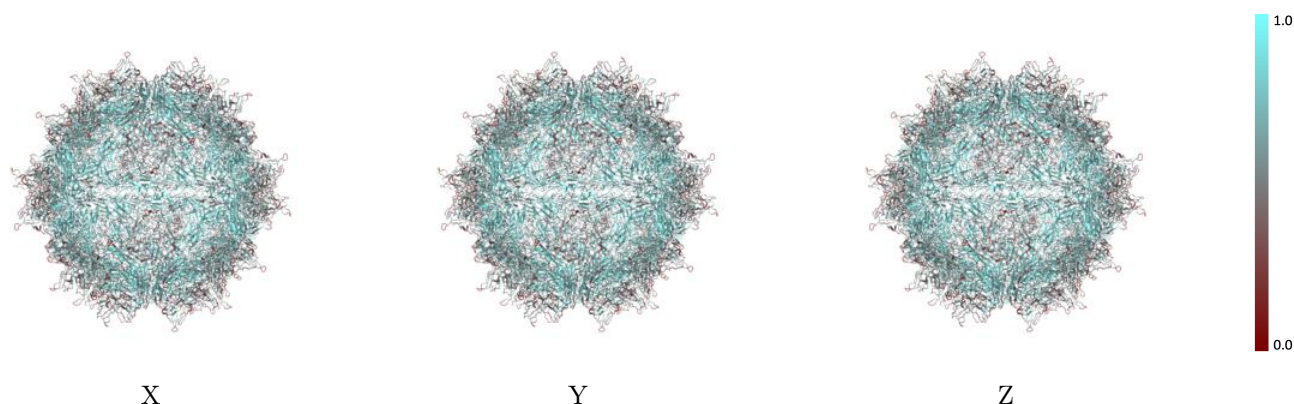


## 9.2 Q-score mapped to coordinate model [i](#)



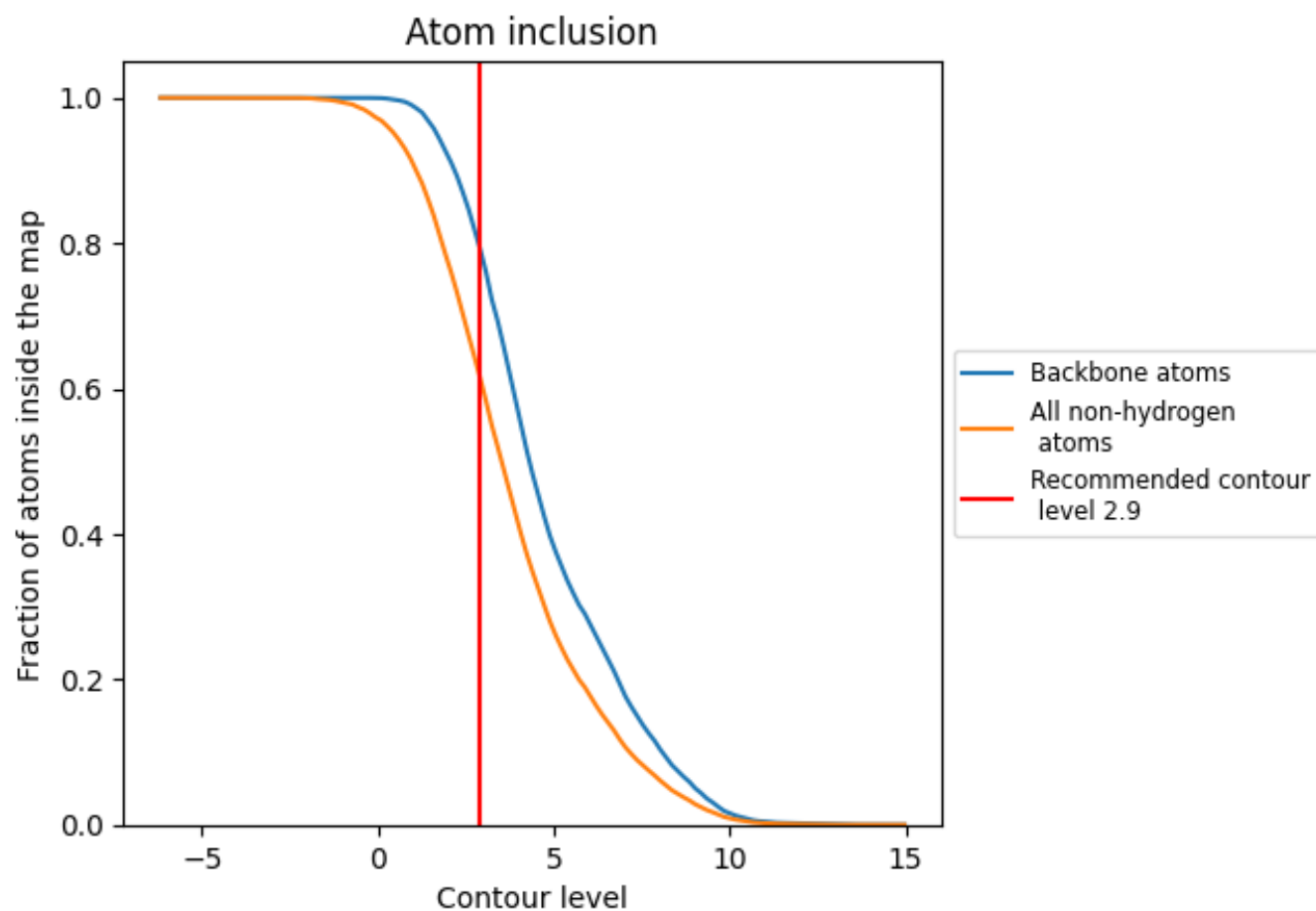
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.6191	 0.4500
2	 0.6186	 0.4490
3	 0.6194	 0.4480
4	 0.6127	 0.4490
5	 0.6135	 0.4490
6	 0.6127	 0.4490
7	 0.6194	 0.4500
8	 0.6161	 0.4490
A	 0.6181	 0.4490
B	 0.6122	 0.4490
C	 0.6135	 0.4490
D	 0.6163	 0.4500
E	 0.6191	 0.4490
F	 0.6122	 0.4480
G	 0.6183	 0.4500
H	 0.6125	 0.4480
I	 0.6176	 0.4480
J	 0.6189	 0.4480
K	 0.6163	 0.4500
L	 0.6138	 0.4480
M	 0.6189	 0.4490
N	 0.6163	 0.4490
O	 0.6189	 0.4490
P	 0.6161	 0.4500
Q	 0.6138	 0.4500
R	 0.6138	 0.4500
S	 0.6125	 0.4490
T	 0.6196	 0.4480
U	 0.6191	 0.4500
V	 0.6166	 0.4490
W	 0.6191	 0.4490
X	 0.6163	 0.4500
Y	 0.6138	 0.4490
Z	 0.6138	 0.4460



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Chain	Atom inclusion	Q-score
a	 0.6161	 0.4480
b	 0.6125	 0.4490
c	 0.6183	 0.4490
d	 0.6189	 0.4480
e	 0.6168	 0.4490
f	 0.6186	 0.4500
g	 0.6130	 0.4500
h	 0.6132	 0.4500
i	 0.6132	 0.4490
j	 0.6183	 0.4490
k	 0.6132	 0.4490
l	 0.6178	 0.4490
m	 0.6138	 0.4470
n	 0.6127	 0.4470
o	 0.6181	 0.4500
p	 0.6168	 0.4490
q	 0.6189	 0.4480
r	 0.6140	 0.4480
s	 0.6110	 0.4460
t	 0.6135	 0.4490
u	 0.6127	 0.4490
v	 0.6189	 0.4490
w	 0.6173	 0.4480
x	 0.6168	 0.4490
y	 0.6163	 0.4490
z	 0.6181	 0.4500