



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 07:40 PM EDT

PDB ID : 5IPI
EMDB ID: : EMD-8099
Title : Structure 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 : unknown
Resolution : 3.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

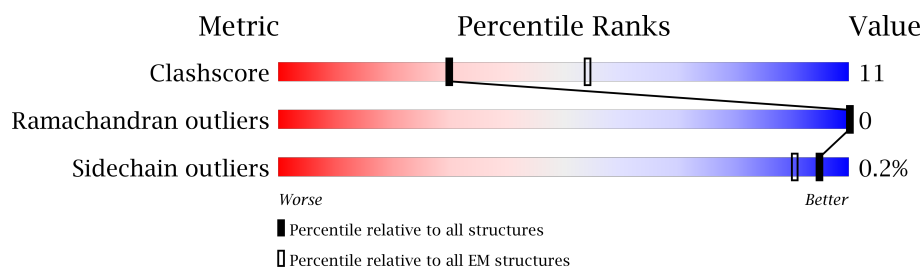
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	735	45% 24% 30%
1	2	735	45% 24% 30%
1	3	735	45% 24% 30%
1	4	735	45% 24% 30%
1	5	735	45% 24% 30%
1	6	735	45% 24% 30%
1	7	735	44% 25% 30%
1	8	735	45% 24% 30%
1	A	735	43% 26% 30%


























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Mol	Chain	Length	Quality of chain		
1	B	735	44%	25%	30%
1	C	735	44%	25%	30%
1	D	735	44%	25%	30%
1	E	735	44%	25%	30%
1	F	735	45%	24%	30%
1	G	735	44%	26%	30%
1	H	735	43%	26%	30%
1	I	735	44%	25%	30%
1	J	735	44%	25%	30%
1	K	735	44%	25%	30%
1	L	735	44%	25%	30%
1	M	735	44%	25%	30%
1	N	735	44%	25%	30%
1	O	735	44%	25%	30%
1	P	735	44%	25%	30%
1	Q	735	44%	25%	30%
1	R	735	44%	25%	30%
1	S	735	43%	26%	30%
1	T	735	44%	25%	30%
1	U	735	44%	25%	30%
1	V	735	44%	25%	30%
1	W	735	45%	24%	30%
1	X	735	46%	24%	30%
1	Y	735	43%	26%	30%
1	Z	735	45%	24%	30%

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Mol	Chain	Length	Quality of chain	
1	a	735		69% 30%
1	b	735		69% 30%
1	c	735		69% 30%
1	d	735		69% 30%
1	e	735		69% 30%
1	f	735		69% 30%
1	g	735		69% 30%
1	h	735		69% 30%
1	i	735		69% 30%
1	j	735		69% 30%
1	k	735		69% 30%
1	l	735		69% 30%
1	m	735		69% 30%
1	n	735		69% 30%
1	o	735		69% 30%
1	p	735		69% 30%
1	q	735		69% 30%
1	r	735		69% 30%
1	s	735		69% 30%
1	t	735		69% 30%
1	u	735		69% 30%
1	v	735		69% 30%
1	w	735		69% 30%
1	x	735		69% 30%
1	y	735		69% 30%

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Mol	Chain	Length	Quality of chain
1	z	735	<div><div></div><div>69%</div><div>30%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 246360 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	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	B	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	C	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	D	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	E	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	F	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	G	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	H	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	I	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	J	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	K	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	L	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	M	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	N	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	O	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	P	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	Q	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	S	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	T	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	U	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	V	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	W	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	X	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	Y	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	Z	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	a	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	b	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	c	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	d	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	e	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	f	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	g	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	h	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	i	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	j	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	k	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	l	511	Total 4106	C 2588	N 716	O 789	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	n	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	o	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	p	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	q	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	r	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	s	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	t	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	u	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	v	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	w	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	x	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	y	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	z	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	1	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	2	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	3	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	4	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	5	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	6	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	7	511	Total 4106	C 2588	N 716	O 789	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	THR	SER	conflict	UNP P03135
B	452	THR	SER	conflict	UNP P03135
C	452	THR	SER	conflict	UNP P03135
D	452	THR	SER	conflict	UNP P03135
E	452	THR	SER	conflict	UNP P03135
F	452	THR	SER	conflict	UNP P03135
G	452	THR	SER	conflict	UNP P03135
H	452	THR	SER	conflict	UNP P03135
I	452	THR	SER	conflict	UNP P03135
J	452	THR	SER	conflict	UNP P03135
K	452	THR	SER	conflict	UNP P03135
L	452	THR	SER	conflict	UNP P03135
M	452	THR	SER	conflict	UNP P03135
N	452	THR	SER	conflict	UNP P03135
O	452	THR	SER	conflict	UNP P03135
P	452	THR	SER	conflict	UNP P03135
Q	452	THR	SER	conflict	UNP P03135
R	452	THR	SER	conflict	UNP P03135
S	452	THR	SER	conflict	UNP P03135
T	452	THR	SER	conflict	UNP P03135
U	452	THR	SER	conflict	UNP P03135
V	452	THR	SER	conflict	UNP P03135
W	452	THR	SER	conflict	UNP P03135
X	452	THR	SER	conflict	UNP P03135
Y	452	THR	SER	conflict	UNP P03135
Z	452	THR	SER	conflict	UNP P03135
a	452	THR	SER	conflict	UNP P03135
b	452	THR	SER	conflict	UNP P03135
c	452	THR	SER	conflict	UNP P03135
d	452	THR	SER	conflict	UNP P03135
e	452	THR	SER	conflict	UNP P03135
f	452	THR	SER	conflict	UNP P03135
g	452	THR	SER	conflict	UNP P03135
h	452	THR	SER	conflict	UNP P03135
i	452	THR	SER	conflict	UNP P03135
j	452	THR	SER	conflict	UNP P03135

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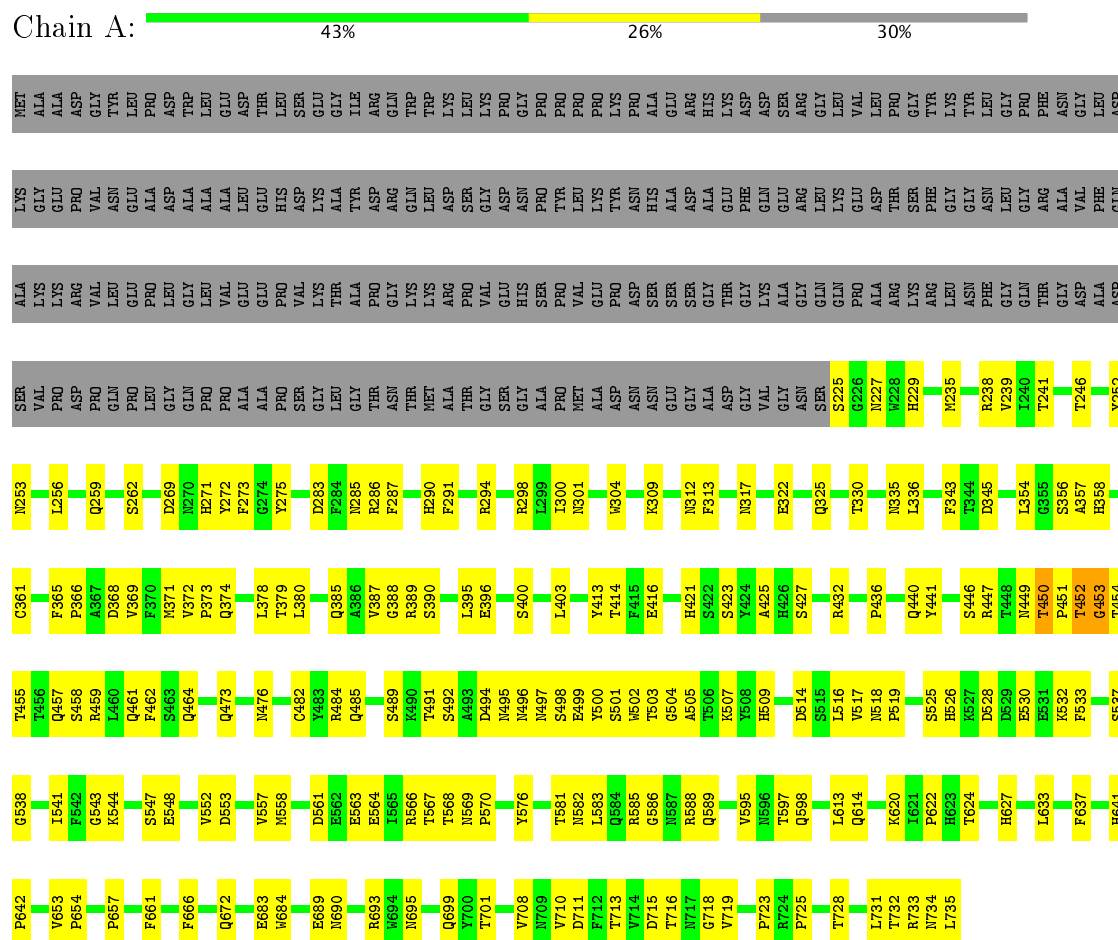
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Chain	Residue	Modelled	Actual	Comment	Reference
k	452	THR	SER	conflict	UNP P03135
l	452	THR	SER	conflict	UNP P03135
m	452	THR	SER	conflict	UNP P03135
n	452	THR	SER	conflict	UNP P03135
o	452	THR	SER	conflict	UNP P03135
p	452	THR	SER	conflict	UNP P03135
q	452	THR	SER	conflict	UNP P03135
r	452	THR	SER	conflict	UNP P03135
s	452	THR	SER	conflict	UNP P03135
t	452	THR	SER	conflict	UNP P03135
u	452	THR	SER	conflict	UNP P03135
v	452	THR	SER	conflict	UNP P03135
w	452	THR	SER	conflict	UNP P03135
x	452	THR	SER	conflict	UNP P03135
y	452	THR	SER	conflict	UNP P03135
z	452	THR	SER	conflict	UNP P03135
1	452	THR	SER	conflict	UNP P03135
2	452	THR	SER	conflict	UNP P03135
3	452	THR	SER	conflict	UNP P03135
4	452	THR	SER	conflict	UNP P03135
5	452	THR	SER	conflict	UNP P03135
6	452	THR	SER	conflict	UNP P03135
7	452	THR	SER	conflict	UNP P03135
8	452	THR	SER	conflict	UNP P03135

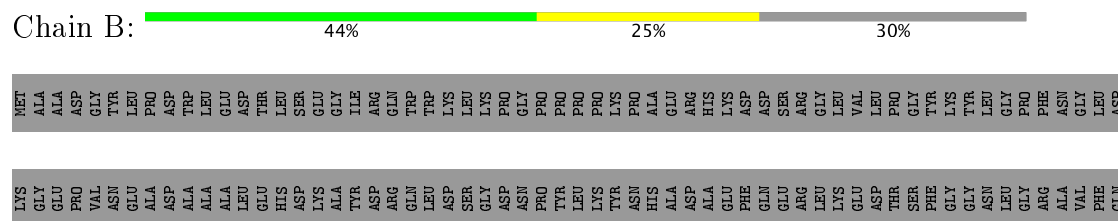
3 Residue-property plots

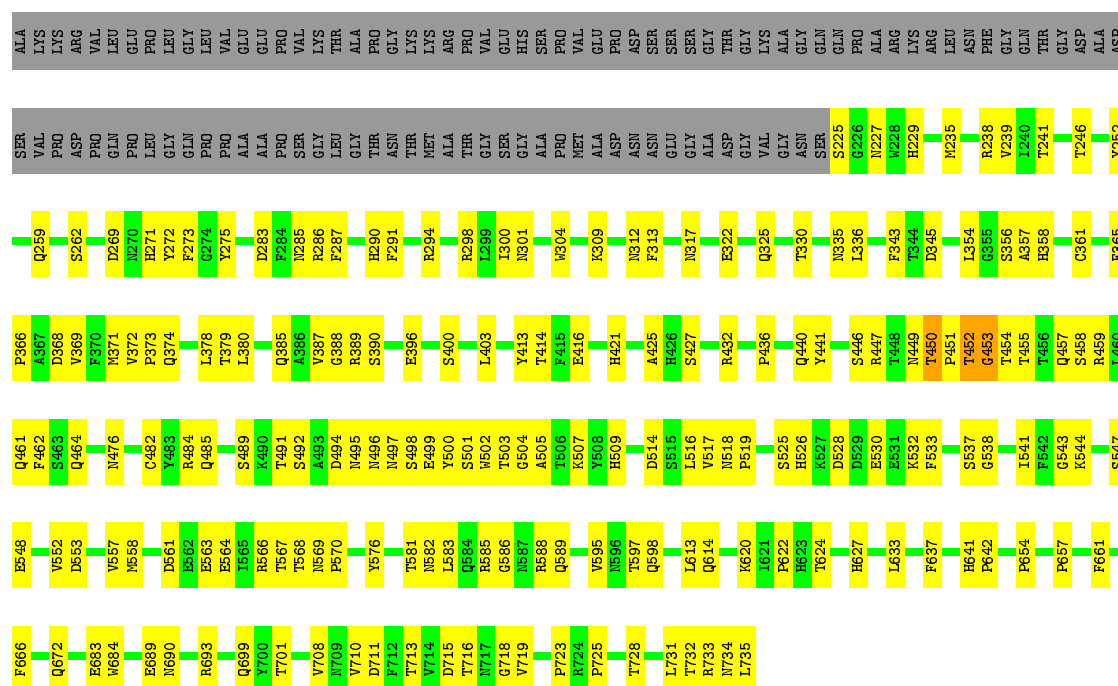
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

• Molecule 1: Capsid protein VP1



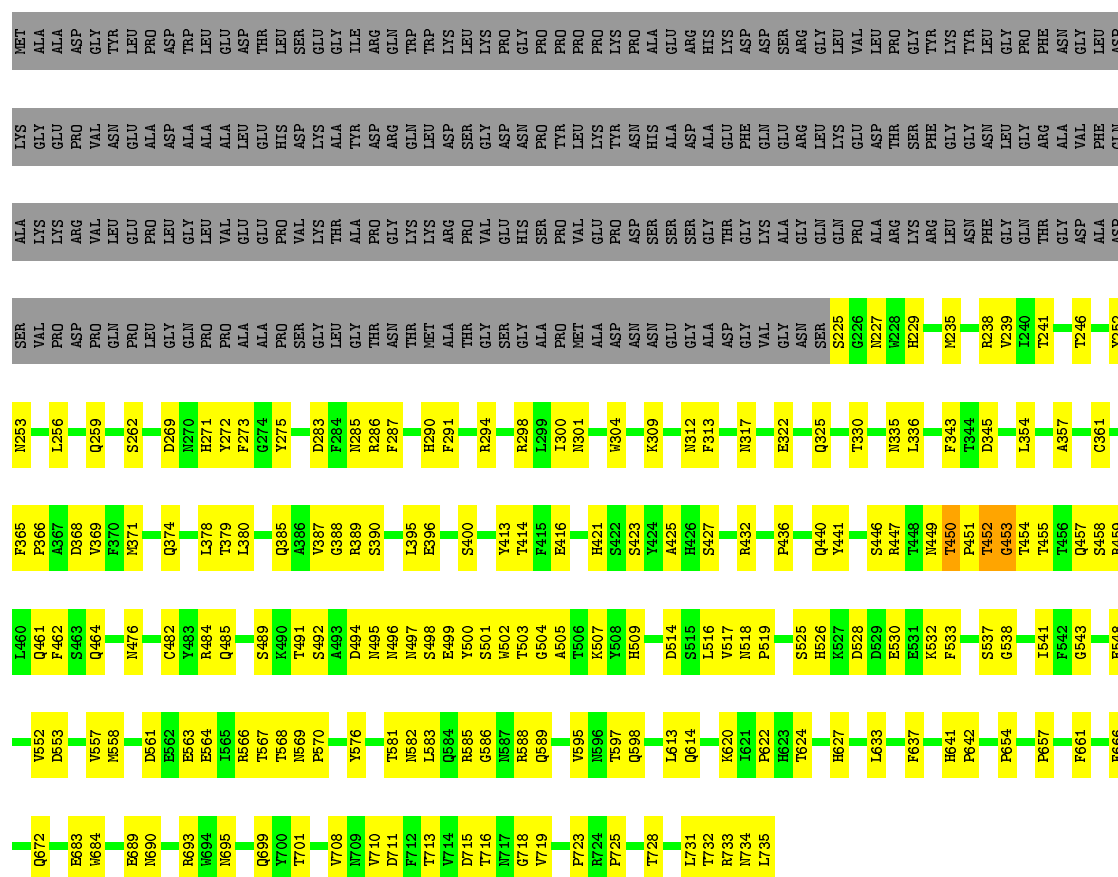
• Molecule 1: Capsid protein VP1





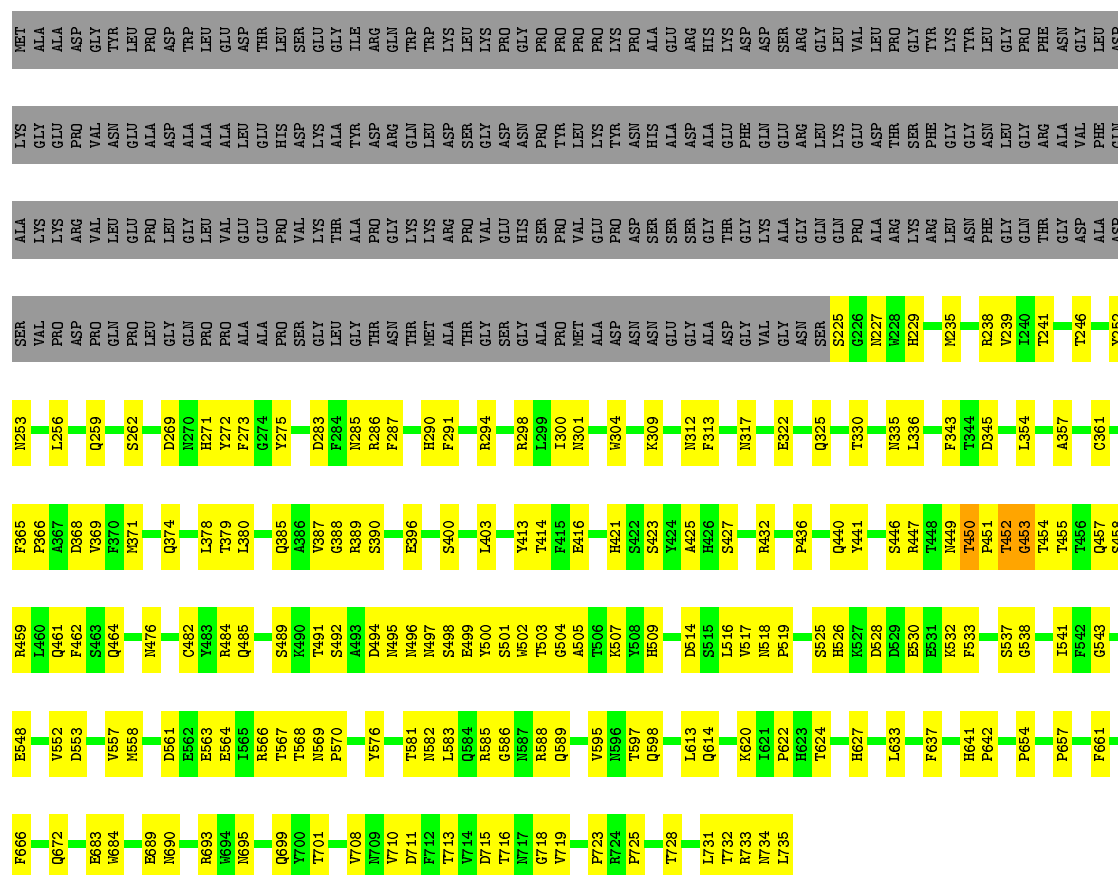
• Molecule 1: Capsid protein VP1

Chain C:



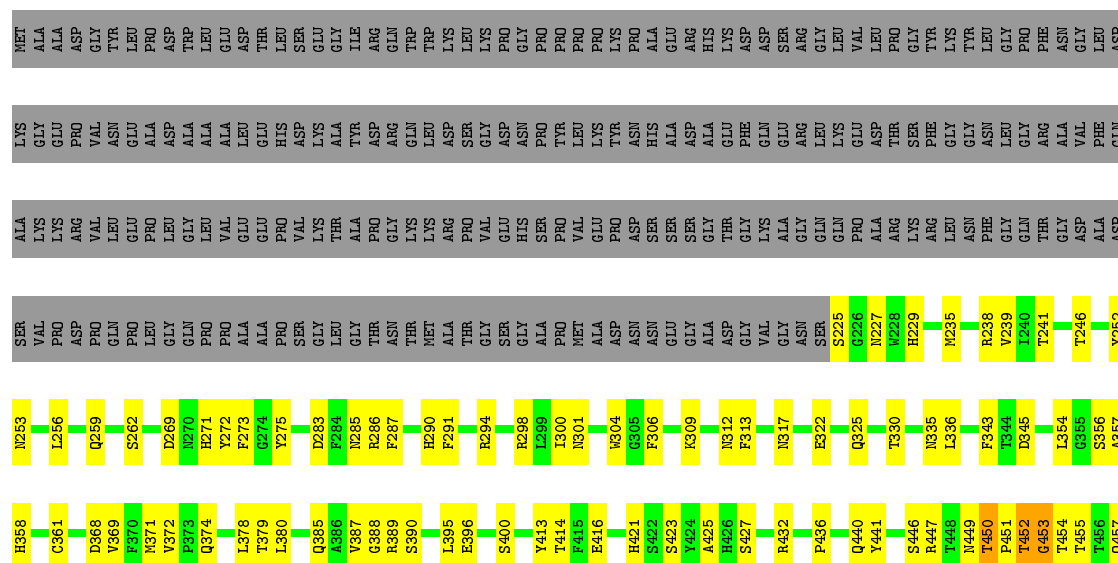
• Molecule 1: Capsid protein VP1

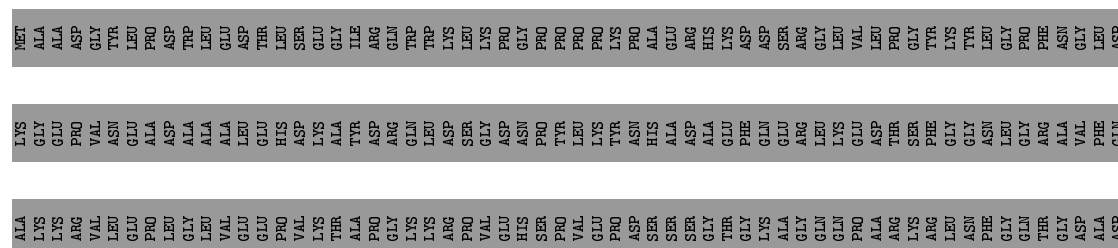
Chain D:  44% 25% 30%



- Molecule 1: Capsid protein VP1

Chain E:  44% 25% 30%





SER	VAL	PRO	ASP	PRO	GLN	PRO	LEU	GLY	GLN	PRO	PRO	ALA	ALA	SER	GLY	LEU	GLY	THR	GLY	THR	MET	ALA	THR	GLY	SER	GLY	ALA	PRO	PRO	MET	ALA	ASP	ASN	ASN	GLU	GLY	ALA	ASP	GLY	VAL	GLY	ASN	SER	S225	G226	N227	H228	H229	N235	R238	V239	I240	T241	S356	A357	H358	Y362																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								

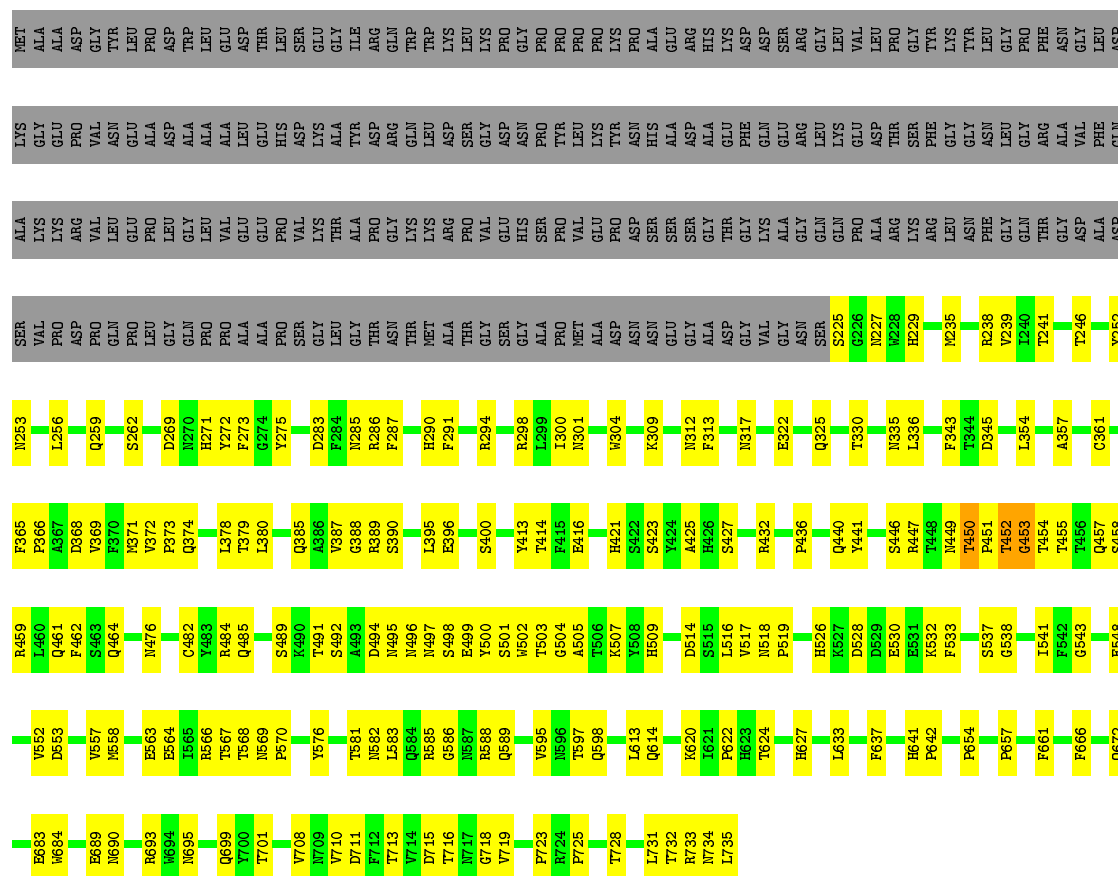
• Molecule 1: Capsid protein VP1

Chain H:  43% 26% 30%

MET	ALA	ALA	ASP	GLY	LEU	TRP	ASP	ASP	GLU	GLU	THR	LEU	SER	GLY	GLY	ILE	ARG	GLN	TRP	TRP	LYS	LEU	LYS	LYS	PRO	GLY	ASP	GLY	ASN	GLY	ASP	GLY	ARG	GLY	LEU	VAL	VAL	LEU	PRO	GLY	GLY	THR	ASN	GLY	LEU	ASP						
LYS	GLY	GLU	PRO	VAL	ASN	GLU	ASP	ALA	ALA	ALA	GLU	GLU	HIS	ASP	LYS	GLY	ASP	GLN	LEU	TRP	ASP	GLY	GLY	GLY	PRO	TYR	TYR	ASN	ALA	ALA	GLY	GLY	ARG	GLY	LEU	LYS	ASP	ASP	GLY	GLY	ASN	GLY	LEU	VAL	PHE	GLN						
ALA	LYS	LYS	ARG	VAL	LEU	GLU	PRO	PRO	GLU	VAL	GLU	GLU	PRO	VAL	LYS	THR	ALA	PRO	LYS	LYS	ARG	ALA	PRO	GLY	GLY	PRO	VAL	GLY	GLY	GLY	GLY	GLY	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP				
SER	VAL	PRO	ASP	GLN	PRO	PRO	LEU	GLY	GLY	GLY	ALA	ALA	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
N253	L256	Q259	S262	D269	N270	H271	Y272	F273	G274	Y275	D283	F284	N285	R286	F287	I300	N301	W304	K309	N312	F313	N317	E322	Q325	T330	N335	L336	F343	T344	D345	L354	N355	T356	S357	G358	H359	T360	N361	S362	D363	N364	S365	A366	H367	Y368							
C361	F365	P366	D367	N368	F369	S370	N371	F372	P373	Q374	L378	T379	L380	Q385	A386	V387	G388	R389	S390	L395	E396	S400	L403	Y413	T414	E415	H421	S422	S423	Y424	A425	S427	R432	P436	Q440	Y441	S446	R447	T448	N449	T450	P451	G452	H453	T454							
Q453	T454	T456	Q457	S458	R459	L460	Q461	F462	S463	Q464	N476	C482	Y483	R484	Q485	S489	K490	T491	S492	A493	D494	N495	N496	N497	S498	E499	Y500	S501	W502	T503	G504	A505	T506	K507	Y508	H509	D514	S515	L516	W517	N518	P519	S525	H526	D527	D528	E529	R530	E531	K532	P533	S537
G538	I541	F542	G543	K544	S547	E548	W552	D553	W557	N558	P561	E562	S563	E564	T565	R566	T567	T568	N569	P570	Y576	T581	N582	L583	Q584	R585	G586	N587	L588	Q589	Y595	H596	T597	Q598	L613	Q614	R620	L621	P622	H623	T624	H627	L633	P637	H641							
P642	V653	P654	P657	F661	F666	Q672	E683	W684	E689	N690	R693	Q699	Y700	T701	V708	N709	V710	D711	F712	L713	T714	D715	T716	N717	G718	V719	P723	R724	P725	T728	L731	T732	R733	N734	L735																	

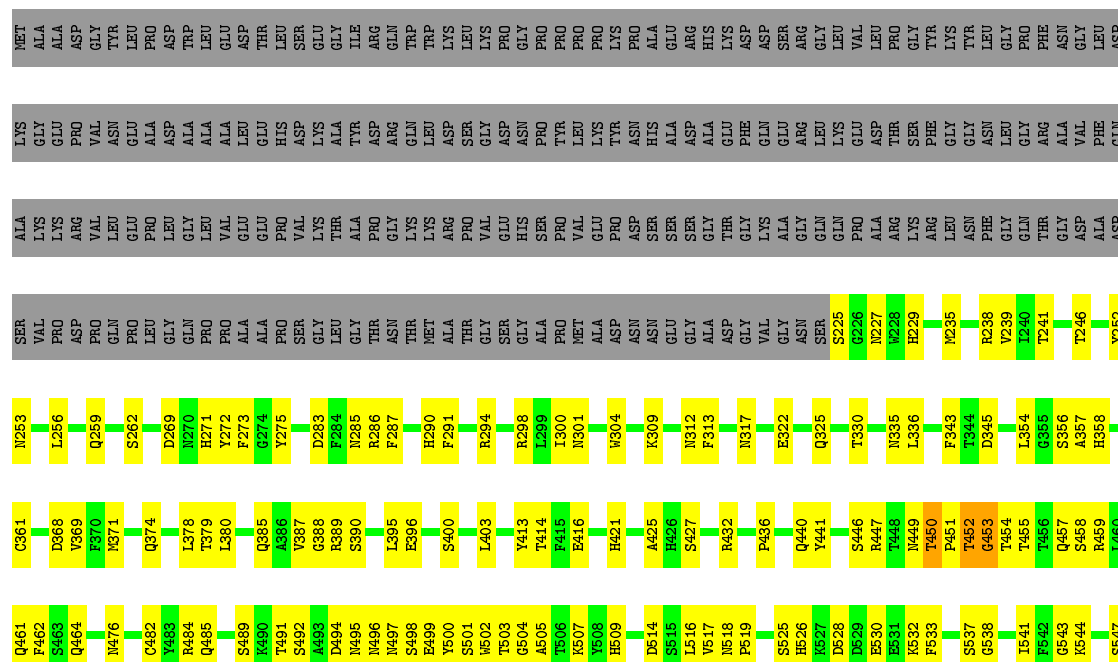
• Molecule 1: Capsid protein VP1

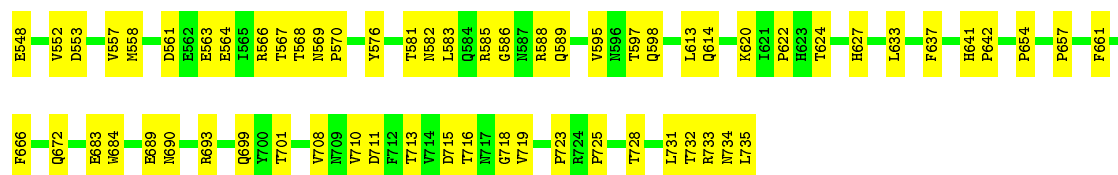
Chain I:  44% 25% 30%



- Molecule 1: Capsid protein VP1

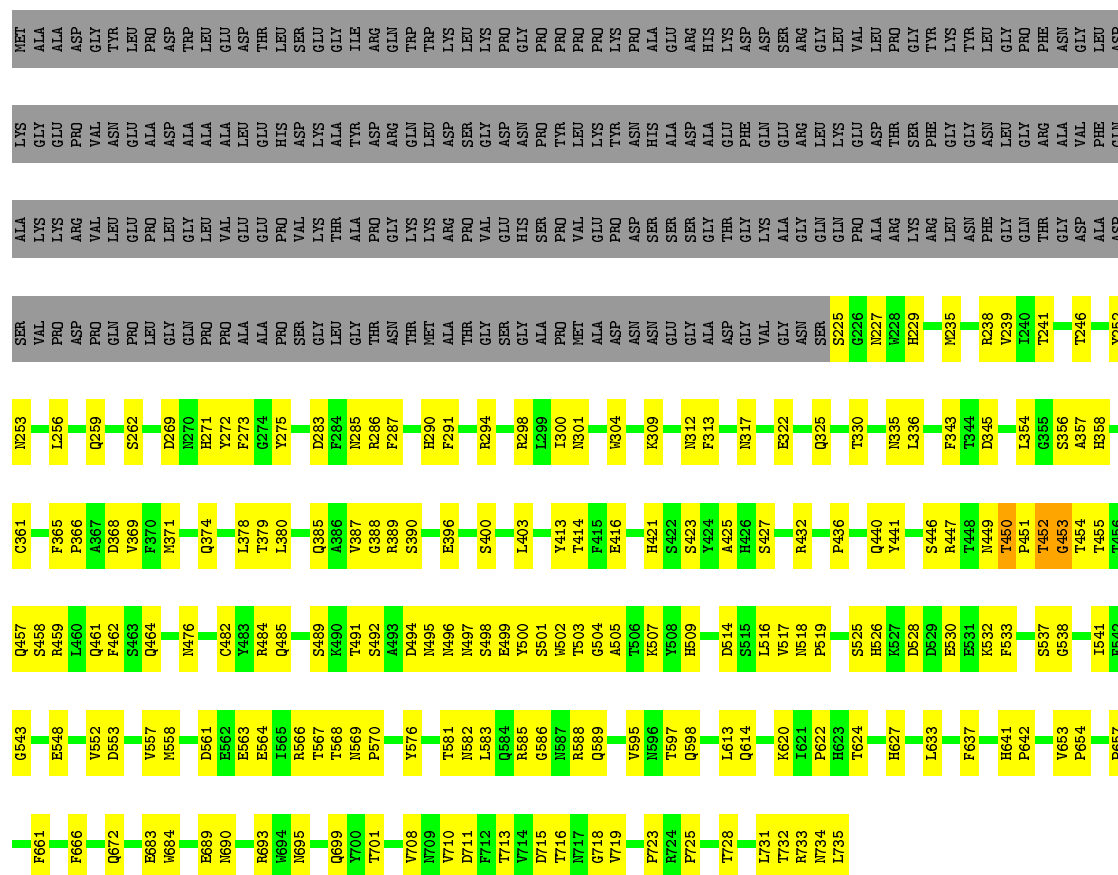
Chain J: 44% 25% 30%





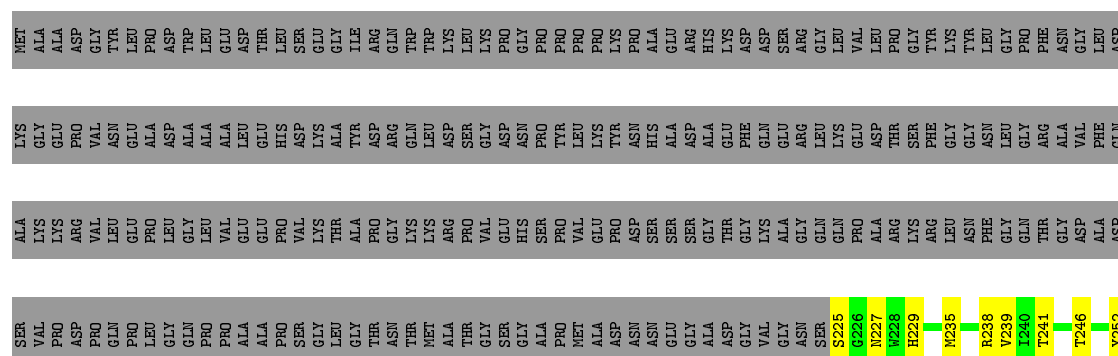
- Molecule 1: Capsid protein VP1

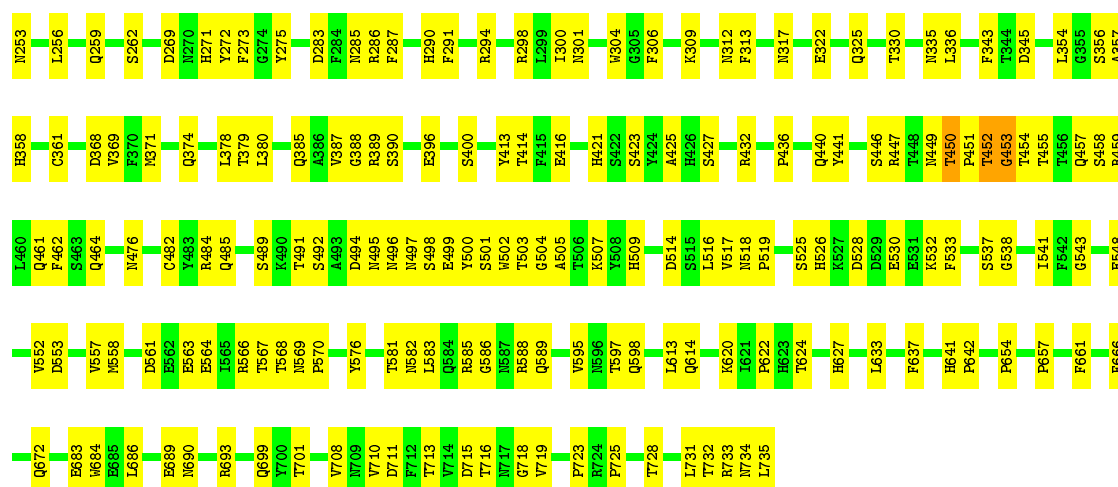
Chain K: 



- Molecule 1: Capsid protein VP1

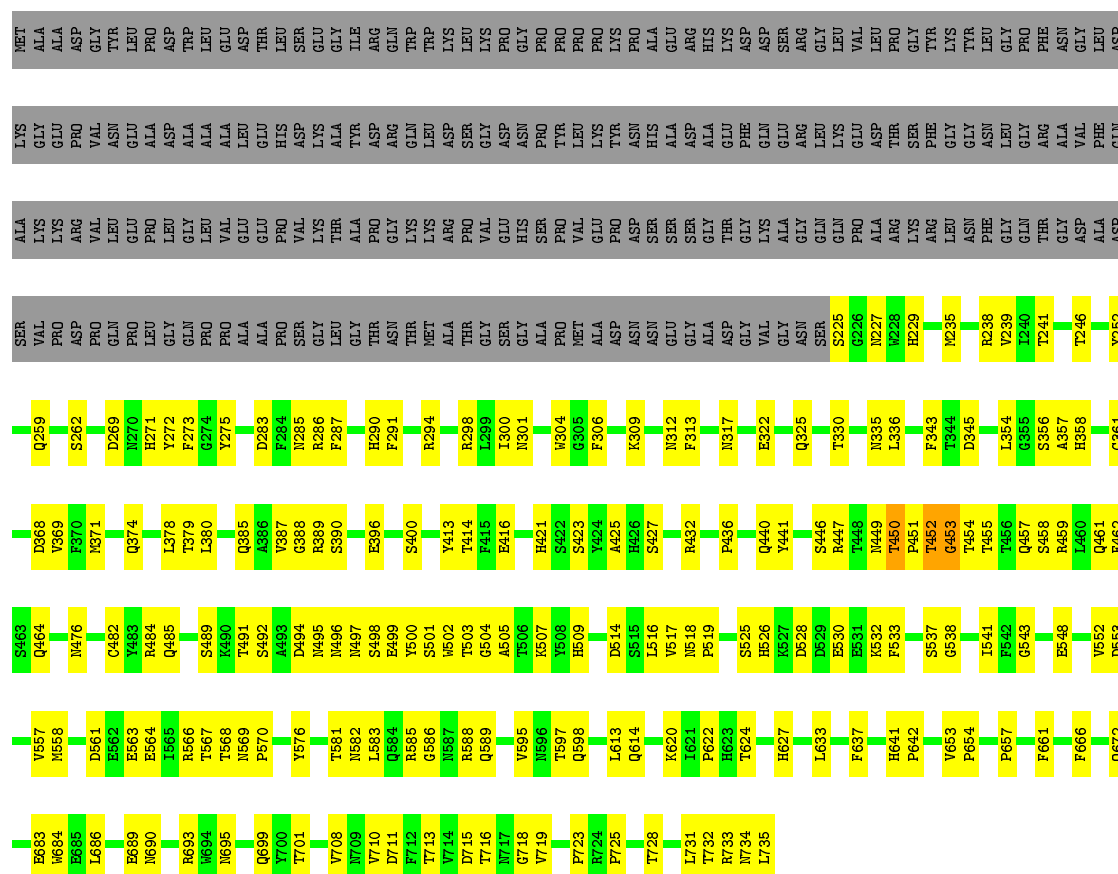
Chain L:  44% 25% 30%





• Molecule 1: Capsid protein VP1

Chain M: 44% 25% 30%



• Molecule 1: Capsid protein VP1

Chain N: 44% 25% 30%



P657	I541	T455	C361	M253	SER	ALA	LYS
F661	F543	T456	F365	L256	VAL	LYS	GLY
F666	E548	S458	P366	Q259	ASP	ARG	PRO
Q672	V552	L460	D368	S262	GLN	VAL	VAL
E683	D553	Q461	F370	F269	PRO	LEU	ASN
W684	V557	S463	N371	D269	GLY	LEU	ALA
E689	W558	Q464	P373	H271	PRO	GLY	ASP
M690	D661	N476	Q374	Y272	PRO	LEU	ALA
R693	E562	C482	L378	F273	ALA	VAL	ALA
Q699	E563	Y483	T379	G274	ALA	GLU	LEU
Y700	E564	R484	L380	Y275	PRO	GLU	GLY
T701	W566	Q485	Q385	D283	SER	VAL	ASP
W708	T567	S489	A386	F284	GLY	LYS	LYS
N709	T568	K490	P387	M285	LEU	THR	ALA
Y710	M569	T491	G388	R286	THR	PRO	TYR
D711	P570	S492	R389	F287	ASN	GLY	ARG
F712	Y576	A493	S390	H290	THR	LYS	GLN
T713	T581	D494	L395	F291	MET	LYS	LEU
D715	N582	N496	E396	R294	ALA	ARG	ASP
T716	L583	N497	S400	Q298	THR	PRO	SER
W717	E584	E499	L403	L299	GLY	HIS	ASN
G718	W585	S501	Y413	I300	ALA	SER	PRO
W719	N587	W502	T414	N301	PRO	PRO	TYR
P723	O588	T503	F415	M304	MET	VAL	LEU
R724	O589	G504	E416	K309	ASP	GLU	LYS
P725	W595	T506	E421	N312	ASN	ASP	TYR
T728	W596	K507	S422	F313	ASN	SER	HIS
L731	T597	W508	S423	N317	GLU	SER	ALA
R732	O598	H509	Y424	E322	ALA	GLY	ALA
R733	L613	D514	A425	N317	THR	GLY	GLU
W734	Q614	S515	H426	E322	VAL	LYS	PHE
L735	W620	W517	S427	Q325	GLY	ALA	GLU
	P621	N518	R432	Q325	ASN	GLY	LEU
	P622	P519	R432	T330	SER	GLN	ARG
	H623		P436	N335	S225	PRO	LYS
	W624	S525	Q440	L336	G226	ALA	ASP
	H627	K527	Y441	F343	N227	ARG	THR
	L633	D528	S446	T344	H228	LYS	SER
	F637	E530	R447	D345	H229	ARG	PHE
	H641	K532	T448	L354	M235	ASN	GLY
P642	P642	F533	M449	G355	R238	ASN	GLY
		S537	T451	A356	V239	GLY	LEU
	P654	G538	W452	F451	T240	THR	ARG
			T452	A357	T241	GLY	ALA
			T453	G453	T246	ASP	VAL
			W454	H558	ALA	ALA	PHE
					ASP	ASP	GLN

- Molecule 1: Capsid protein VP1

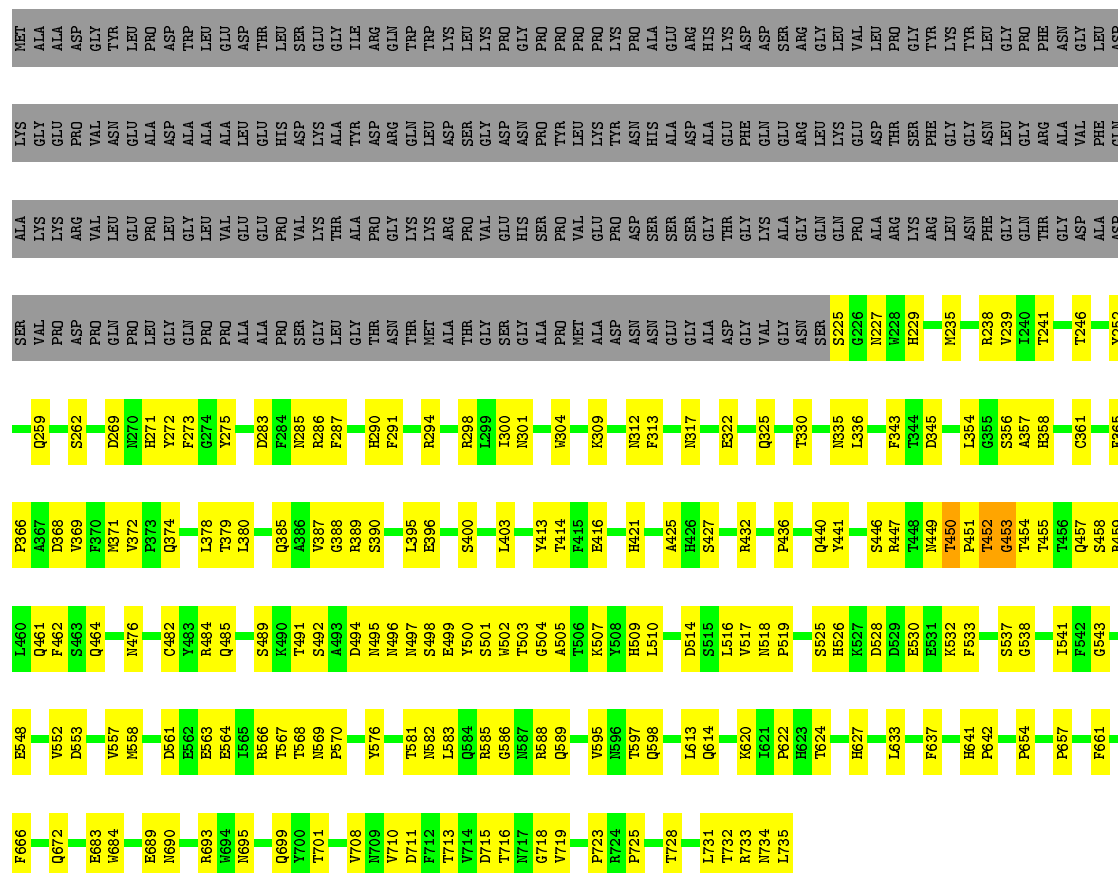
Chain O: 

F542	T546	C361	M253	SER	ALA	LYS	LYS	MET
G543	Q457	F365	L256	VAL	VAL	GLY	GLY	ALA
E548	S458	R366	L256	ASP	ARG	PRO	PRO	ALA
V552	R459	A367	Q259	PRO	VAL	VAL	GLY	TTR
D553	Q461	D368	S262	GLN	LEU	ASN	ASN	
F557	F462	F369	S262	PRO	GLU	GLU	GLU	PRO
M558	A463	F370	F370	GLY	LEU	ASP	ASP	ASP
	Q464	M371	D269	GLN	GLY	ALA	ALA	TRP
			N270	PRO	LEU	ALA	ALA	LEU
D561	M476	Q374	H271	PRO	VAL	ALA	ALA	GLU
E562	C482	L378	Y272	ALA	GLU	LEU	LEU	ASP
E563	Y483	T379	F273	ALA	GLU	GLU	GLU	THR
E564	R484	L380	G274	PRO	PRO	HIS	HIS	LEU
I565	Q485		Y275	SER	VAL	ASP	ASP	SER
R566	S489	Q385	D283	GLY	LYS	LYS	LYS	GLY
T567	F490	A386	F284	LEU	THR	ALA	ALA	GLY
T568	T491	V387	M285	GLY	ALA	TYR	TYR	ILE
M569	T491	G388	R286	THR	PRO	ASP	ASP	ARG
P570	A492	R389	F287	ASN	GLY	ARG	GLN	GLN
	A493	S390		THR	LYS	GLN	GLN	TRP
Y576	D494		H290	MET	LYS	LEU	LEU	TRP
	M495	L385	F291	ALA	ARG	ASP	ASP	LYS
T581	M496	E396		THR	PRO	SER	SER	LEU
M582	M497		R294	GLY	VAL	GLY	GLY	LYS
L583	A498	S400		SER	GLU	ASP	ASP	PRO
Q584	E499	Y413	R298	GLY	HIS	ASN	ASN	GLY
R585	Y500	T414	L299	GLY	SER	PRO	PRO	PRO
G586	S501	T414	I300	PRO	PRO	TYR	TYR	PRO
M587	W502	F415	N301	MET	VAL	LEU	LEU	PRO
R588	T503	E416		ALA	GLU	LYS	LYS	PRO
G589	G504		V304	ASP	PRO	TYR	TYR	LYS
	A505	H421		ASN	ASP	ASN	ASN	PRO
V595	T506	S422	K309	ASN	SER	HIS	HIS	ALA
M596	K507	S423		GLU	SER	ALA	ALA	GLU
T597	Y508	T424	N312	GLY	SER	ASP	ASP	ARG
Q598	H509	A425	F313	ALA	GLY	ALA	ALA	HIS
		H426		ASP	THR	GLU	GLU	LYS
L613	D514	S427	N317	GLY	GLY	PHE	PHE	ASP
Q614	S515			VAL	LYS	GLN	GLN	ASP
	L516	L430	E322	GLY	ALA	GLU	GLU	SER
K620	V517	D431		ASN	GLY	ARG	ARG	ARG
N518	N518	R432	Q325	SER	GLN	LEU	LEU	GLY
P622	P519				GLN	GLU	GLU	LEU
		P436	T330	S225	PRO	GLU	GLU	VAL
H623	S525			G226	ALA	ASP	ASP	LEU
T624	H526	Q440	N335	N227	ALA	THR	THR	PRO
	R527	Y441	L336	H228	ARG	SER	SER	GLY
H627	D528			ARG	LYS	PHE	PHE	TYR
L633	D529	S446	F343		ASN	GLY	GLY	LYS
	E530	R447	T344		ASN	ASN	ASN	LEU
F637	E531	T448	D345		PHE	GLY	GLY	TYR
	K532	M449			GLY	LEU	LEU	GLY
H641	F533	T450	L354		THR	GLY	GLY	PRO
P642		P451	G355	T241	ARG	ARG	ARG	PHE
V653	S537	T452	S356	T241	GLY	ALA	ALA	ASN
	G538	G453	A357	T246	ASP	VAL	VAL	GLY
P654		T454	H358		ALA	PHE	PHE	LEU
	T541	T455		Y352	ASP	GLN	GLN	ASP



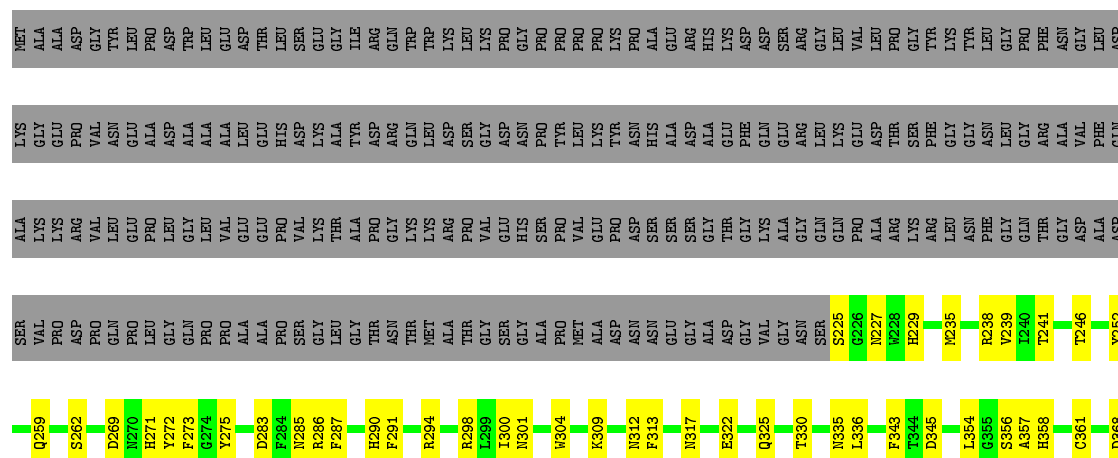
• Molecule 1: Capsid protein VP1

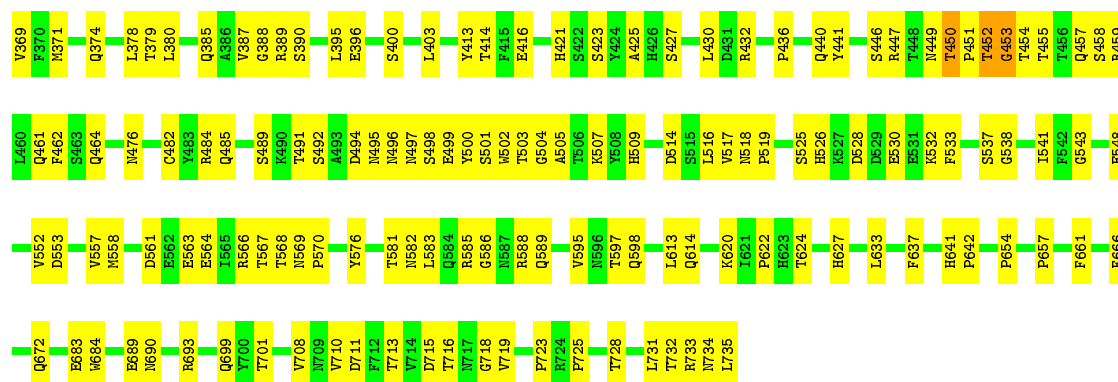
Chain P: 44% 25% 30%



• Molecule 1: Capsid protein VP1

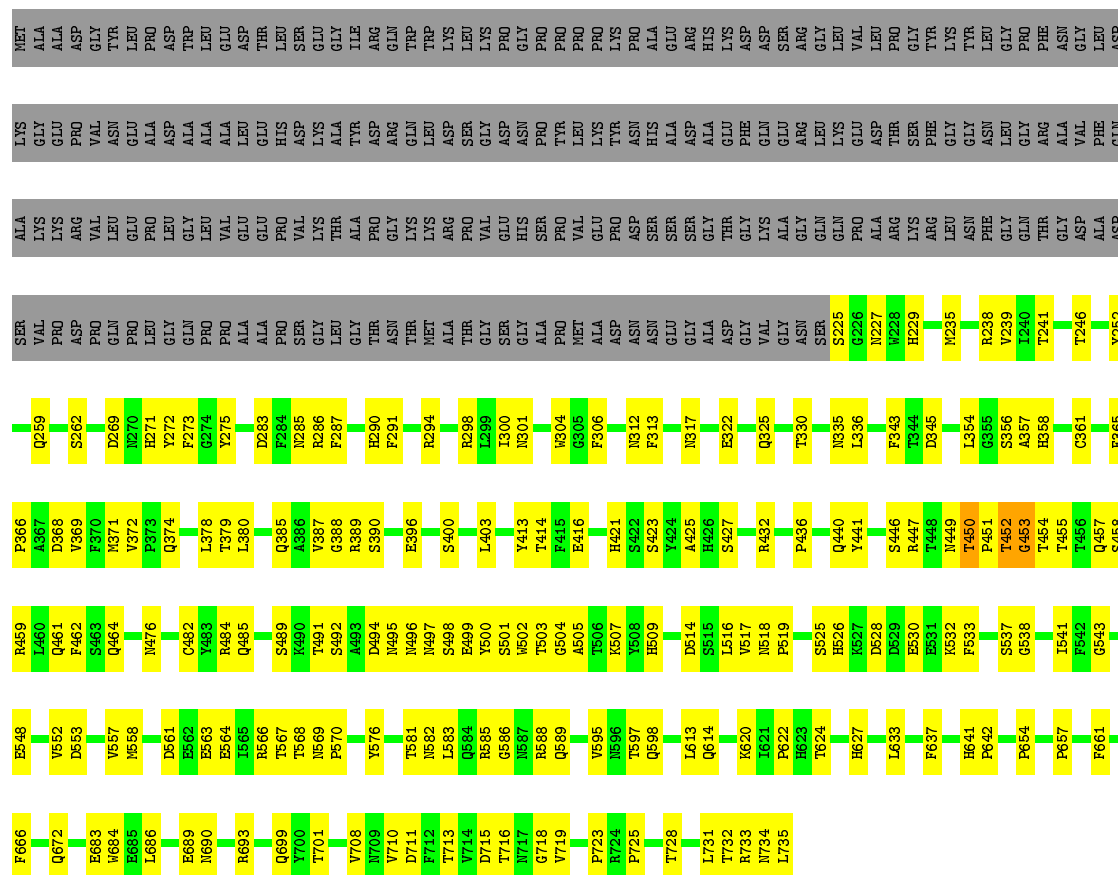
Chain Q: 44% 25% 30%





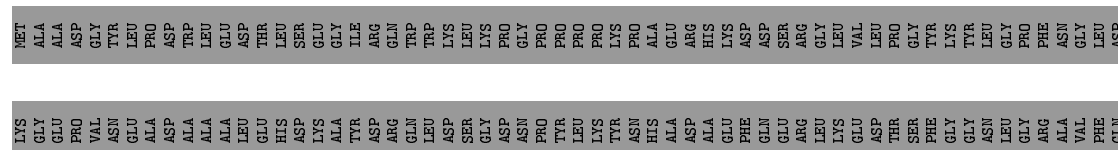
• Molecule 1: Capsid protein VP1

Chain R: 44% 25% 30%



• Molecule 1: Capsid protein VP1

Chain S: 43% 26% 30%



ALA	VAL	N253	H358	Q453	P654	T541	H358	Q453	P654
LYS	PRO	L256	C361	T454	P657	G542	C361	T454	P657
ARG	ASP	Q259	F365	T456	F661	G543	F365	T456	F661
VAL	PRO	S262	P366	S458	F666	K544	P366	S458	F666
LEU	GLN	D269	A367	S459	S647	S647	A367	S459	S647
PRO	LEU	H271	D368	L460	E548	E548	D368	L460	E548
GLY	GLN	H270	V369	Q461	V552	V552	V369	Q461	V552
LEU	PRO	H272	F370	S462	D553	D553	F370	S462	D553
VAL	PRO	Y273	K371	S463	W684	W684	K371	S463	W684
GLU	ALA	F274	P373	Q464	E685	E685	P373	Q464	E685
GLU	ALA	G274	Q374	N476	L686	L686	Q374	N476	L686
PRO	PRO	Y275	L378	C482	E689	E689	L378	C482	E689
VAL	SER	D283	T379	Y483	N690	N690	D283	T379	Y483
LYS	GLY	F284	L380	R484	G693	G693	F284	L380	R484
THR	GLY	N285	Q385	Q485	T697	T697	N285	Q385	Q485
ALA	THR	R286	A386	S489	Q699	Q699	R286	A386	S489
PRO	ASN	F287	V387	K490	Y700	Y700	F287	V387	K490
GLY	THR	H290	G388	T491	T701	T701	H290	G388	T491
LYS	MET	F291	R389	S492	Y708	Y708	F291	R389	S492
ARG	ALA	R294	S390	A493	H709	H709	R294	S390	A493
PRO	VAL	GLY	L395	D494	V710	V710	GLY	L395	D494
VAL	GLU	SER	E396	N495	D711	D711	SER	E396	N495
GLU	HIS	GLY	L299	N496	F712	F712	GLY	L299	N496
HIS	ALA	ALA	S400	N497	Q884	Q884	ALA	S400	N497
SER	PRO	PRO	Y413	S498	G885	G885	PRO	Y413	S498
PRO	PRO	PRO	N301	E499	G886	G886	PRO	N301	E499
VAL	VAL	ALA	W304	Y500	H897	H897	VAL	W304	Y500
GLU	GLU	ASP	F306	S501	T716	T716	GLU	F306	S501
ASP	ASN	ASP	G305	W502	H717	H717	ASP	G305	W502
SER	ASN	ASN	F415	T503	G718	G718	SER	F415	T503
SER	GLY	GLY	K309	G504	V719	V719	SER	K309	G504
GLY	ALA	ALA	H421	A505	P723	P723	GLY	H421	A505
THR	ASP	ASP	S422	T506	R724	R724	THR	S422	T506
GLY	THR	GLY	N312	K507	P725	P725	GLY	N312	K507
LYS	VAL	VAL	F313	Y508	Q598	Q598	LYS	F313	Y508
ALA	GLY	GLY	N317	H509	L613	L613	ALA	N317	H509
GLY	ASN	ASN	E322	D514	Q614	Q614	GLY	E322	D514
GLN	SER	SER	Q325	S515	K620	K620	GLN	Q325	S515
PRO	GLN	GLN	N335	L516	I621	I621	PRO	N335	L516
ALA	ALA	ALA	Q326	V517	R732	R732	ALA	Q326	V517
ARG	ARG	ARG	T330	N518	R733	R733	ARG	T330	N518
LYS	LYS	LYS	N336	P519	N734	N734	LYS	N336	P519
ARG	ARG	ARG	N335	H526	L735	L735	ARG	N335	H526
LEU	ASN	ASN	L336	K527	H627	H627	LEU	L336	K527
ASN	ASN	ASN	F343	D528	L633	L633	ASN	F343	D528
PHE	PHE	PHE	R238	E530	P637	P637	PHE	R238	E530
GLY	GLY	GLY	V239	E531	H641	H641	GLY	V239	E531
GLN	GLN	GLN	I240	E532	P642	P642	GLN	I240	E532
THR	THR	THR	T241	K532	P644	P644	THR	T241	K532
GLY	GLY	GLY	L354	F533	H641	H641	GLY	L354	F533
ASP	ASP	ASP	G355	S537	P642	P642	ASP	G355	S537
ALA	ALA	ALA	T452	P451	P657	P657	ALA	T452	P451
ASP	ASP	ASP	T452	S537	P657	P657	ASP	T452	S537
			Y252	G538	V653	V653		Y252	G538

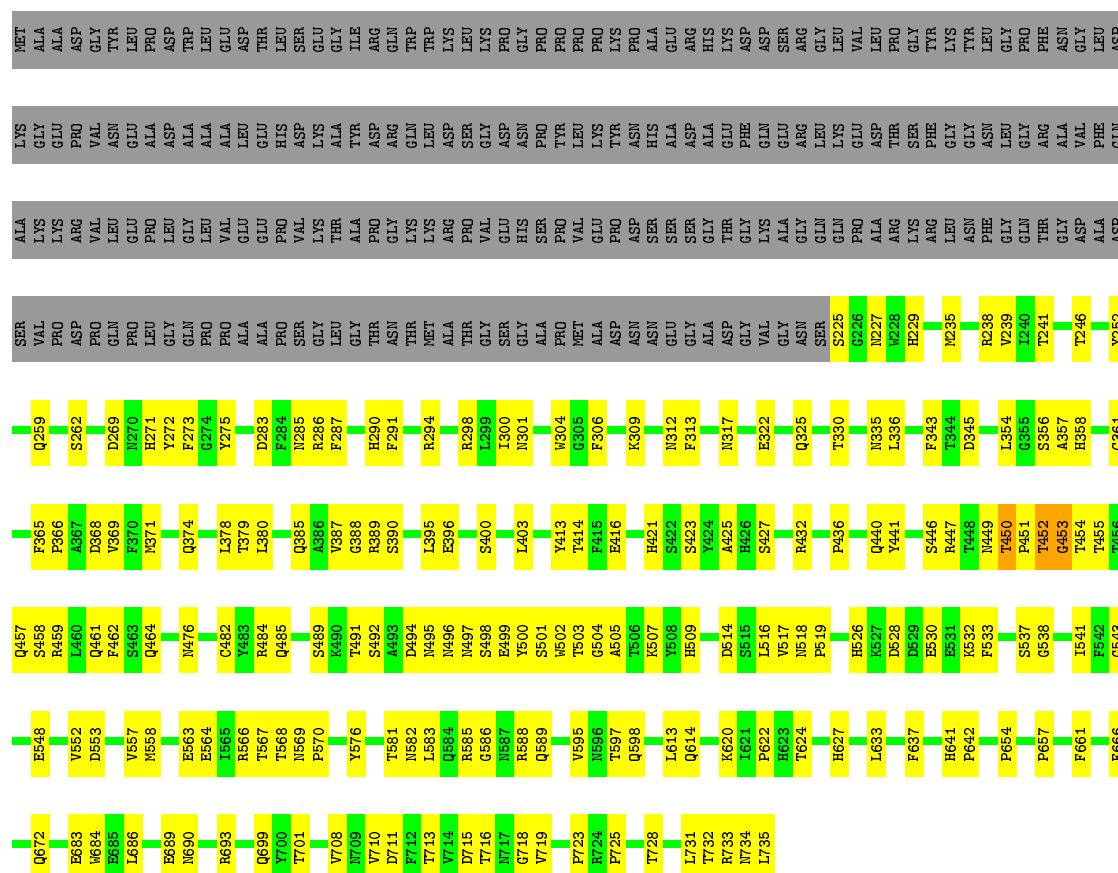
• Molecule 1: Capsid protein VP1

Chain T:  44% 25% 30%

MET	LYS	ALA	VAL	Q259	F365	Q457	G543	F661
ALA	GLY	ALA	PRO	S262	A367	S458	E548	F666
ASP	PRO	ARG	ASP	D269	D368	R459	S531	
GLY	VAL	VAL	ASN	H271	V369	Q461	D553	
TVR	LEU	LEU	PRO	N270	F370	S453	V557	
LEU	ALA	ALA	ALA	H272	K371	Q464	M558	
PRO	ALA	PRO	PRO	F273	Q374	N476	D561	
ASP	ASP	ASP	GLY	G274	L378	C482	E563	
THR	LEU	LEU	ALA	Y275	T379	R484	E584	
THR	GLU	GLU	GLU	D283	L380	Q485	I585	
LEU	HIS	PRO	VAL	F284	Q385	S489	R586	
LEU	ASP	VAL	PRO	R285	A386	T490	T587	
LEU	GLY	THR	LYS	R286	V387	K490	T588	
GLY	ALA	ALA	THR	F287	G388	T491	N589	
THR	TVR	PRO	ALA	H290	R389	S492	P570	
ARG	ASP	GLY	ALA	F291	S390	A493	Y576	
GLN	ANG	GLY	PRO	R294	L395	D494	T581	
TRP	GLN	LYS	LYS	R298	E396	N495	L583	
TRP	TRP	LYS	VAL	L299	S400	N496	G584	
TRP	TRP	LYS	VAL	N301	L403	N497	R585	
LYS	LYS	ARG	PRO	W304	Y413	S498	G586	
LYS	ASP	ASP	VAL	G305	T414	T502	N587	
LEU	LEU	LEU	GLU	F306	F415	T503	R588	
PRO	LYS	PRO	PRO	N309	E416	G504	Q589	
PRO	LYS	PRO	ASP	K309	H421	A505	V596	
LYS	THR	LYS	GLY	N312	S422	T506	N596	
ASP	ALA	ALA	ALA	F313	S423	Y508	T597	
ASP	ASP	GLY	GLY	N317	Y424	H509	Q598	
GLY	HIS	ASP	THR	E322	A425		L613	
ASP	ASP	PHE	GLY	Q325	H426		Q614	
GLY	ASP	GLN	LYS	N326	S427		L516	
GLY	ARG	GLY	ALA	Q326	R432		K620	
ARG	ARG	ARG	GLN	N335	P436		N621	
GLY	GLY	GLY	GLN	T330	N336		P622	
LEU	VAL	VAL	GLN	N335	Q440		H623	
LEU	VAL	VAL	PRO	N336	Y441		T624	
TVR	PRO	THR	ARG	L336	D528		H627	
TVR	GLY	PHE	LYS	F343	K529		L633	
LYS	TVR	GLY	LEU	T344	E530		F637	
LYS	TYR	GLY	ASN	D345	E531		H641	
TYR	TYR	GLY	PHE	R238	F533		P642	
LEU	LEU	LEU	GLY	V239	T451		P644	
LEU	GLY	GLY	GLN	I240	T452			
PRO	PRO	ARG	THR	T241	Q453			
PRO	PHE	ALA	ALA	T246	T454			
ASN	ASN	VAL	GLY	H358	T455			
ASN	GLY	PHE	LEU	C361				
LEU	GLY	GLN	GLN					

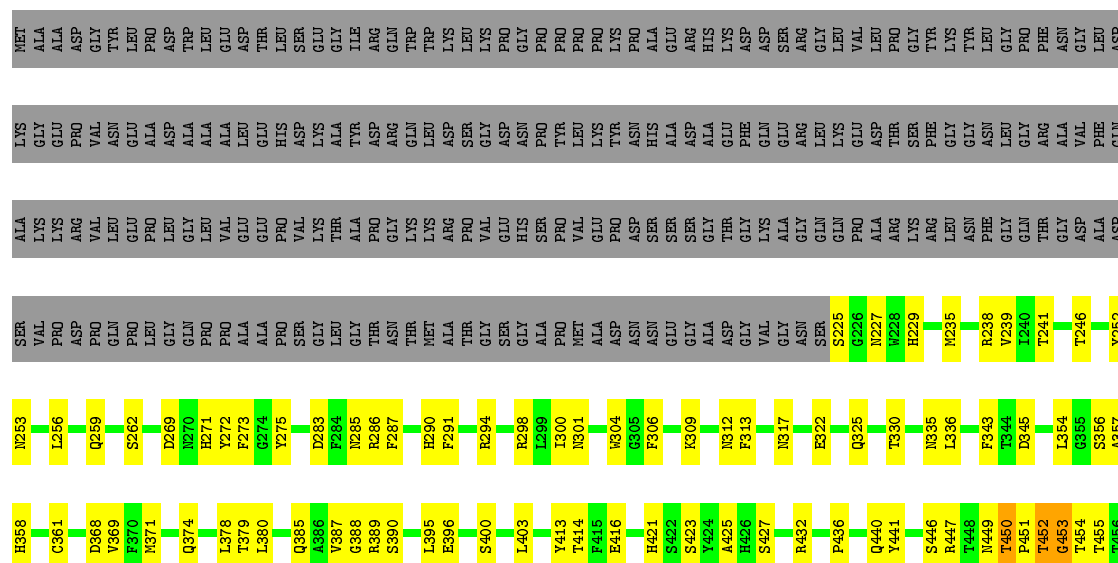
• Molecule 1: Capsid protein VP1

Chain U: 44% 25% 30%



- Molecule 1: Capsid protein VP1

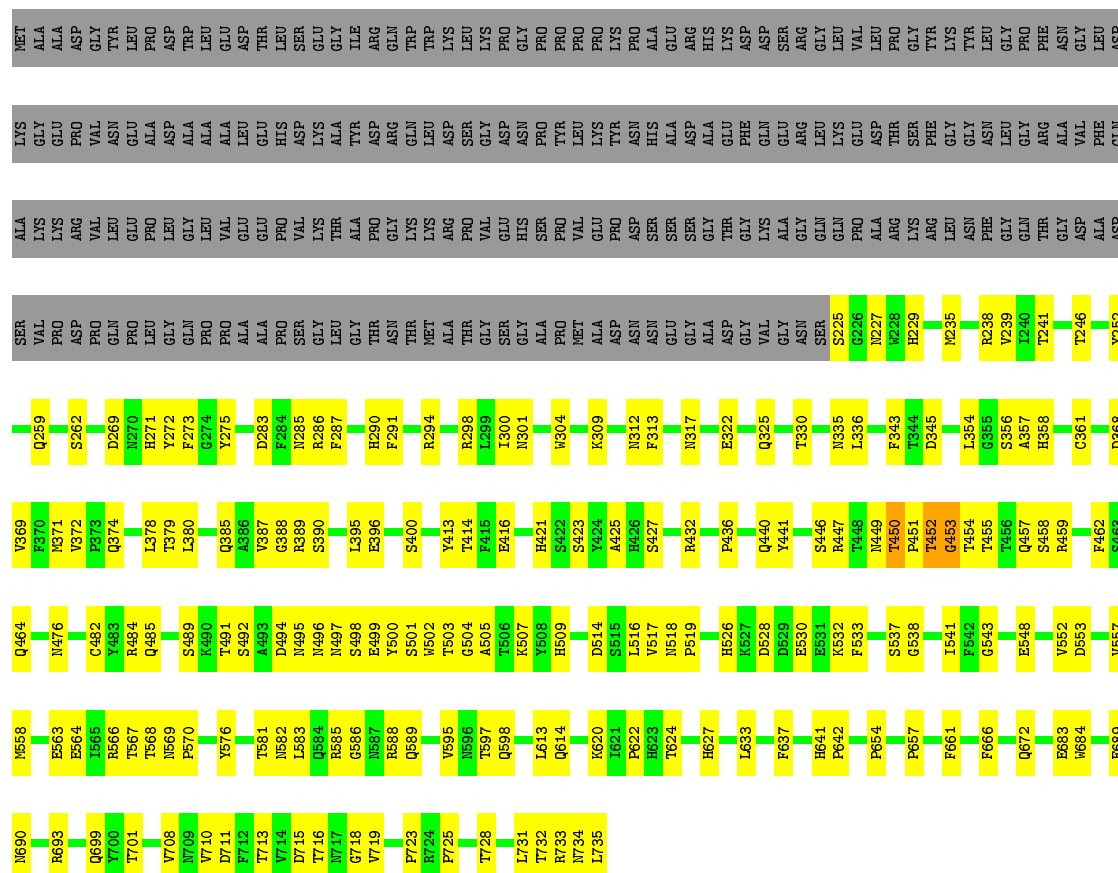
Chain V:  44% 25% 30%





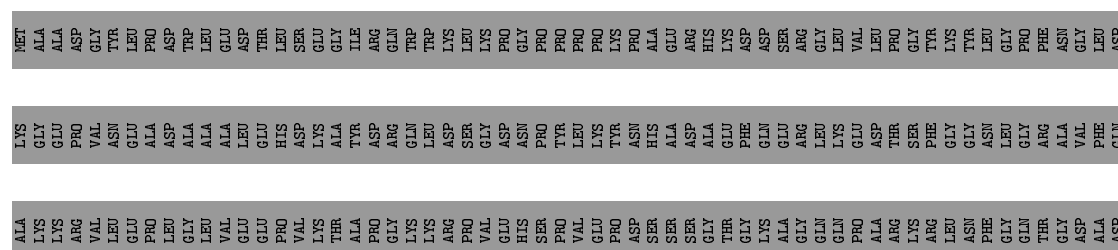
• Molecule 1: Capsid protein VP1

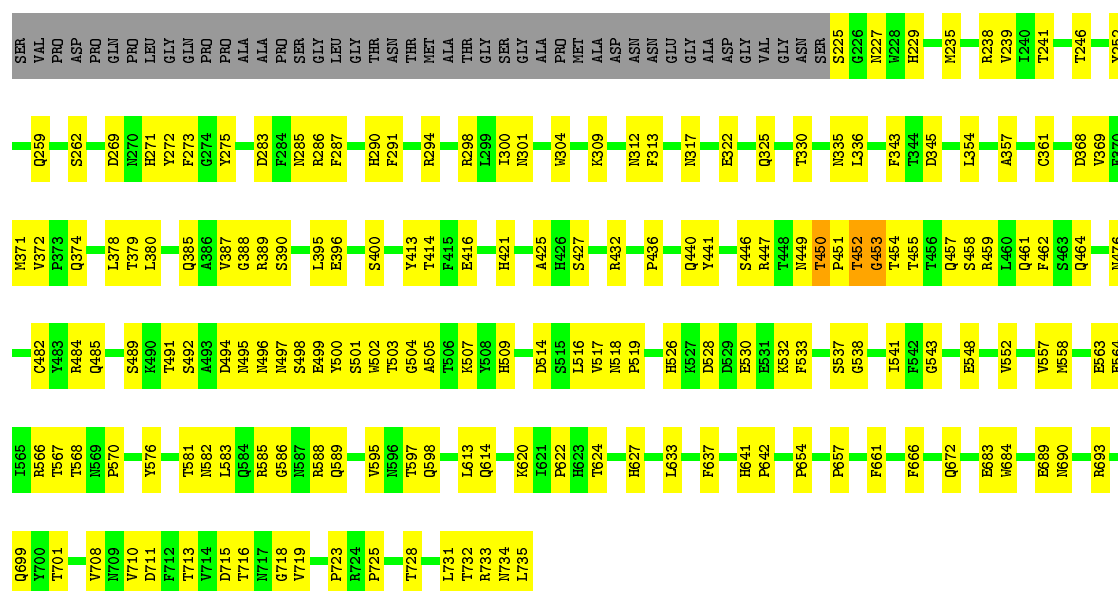
Chain W: 45% 24% 30%



• Molecule 1: Capsid protein VP1

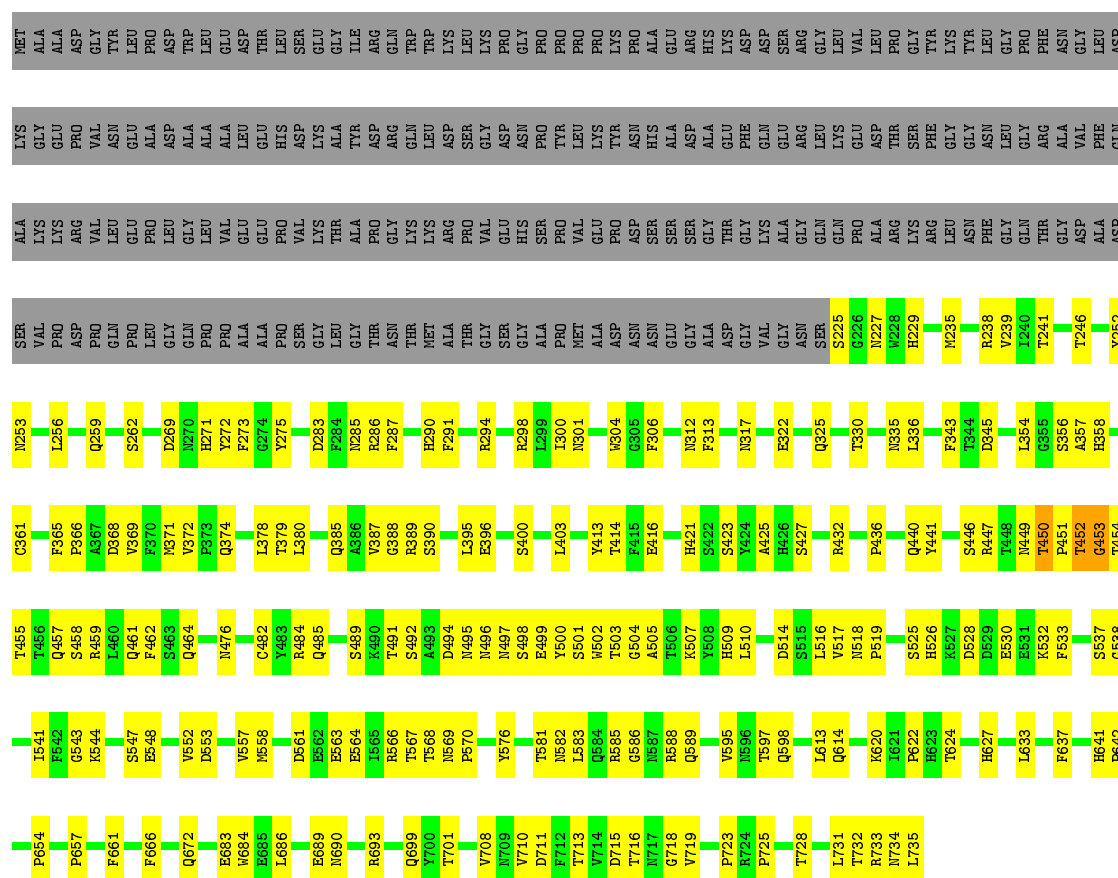
Chain X: 46% 24% 30%





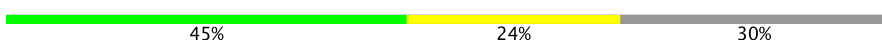
- Molecule 1: Capsid protein VP1

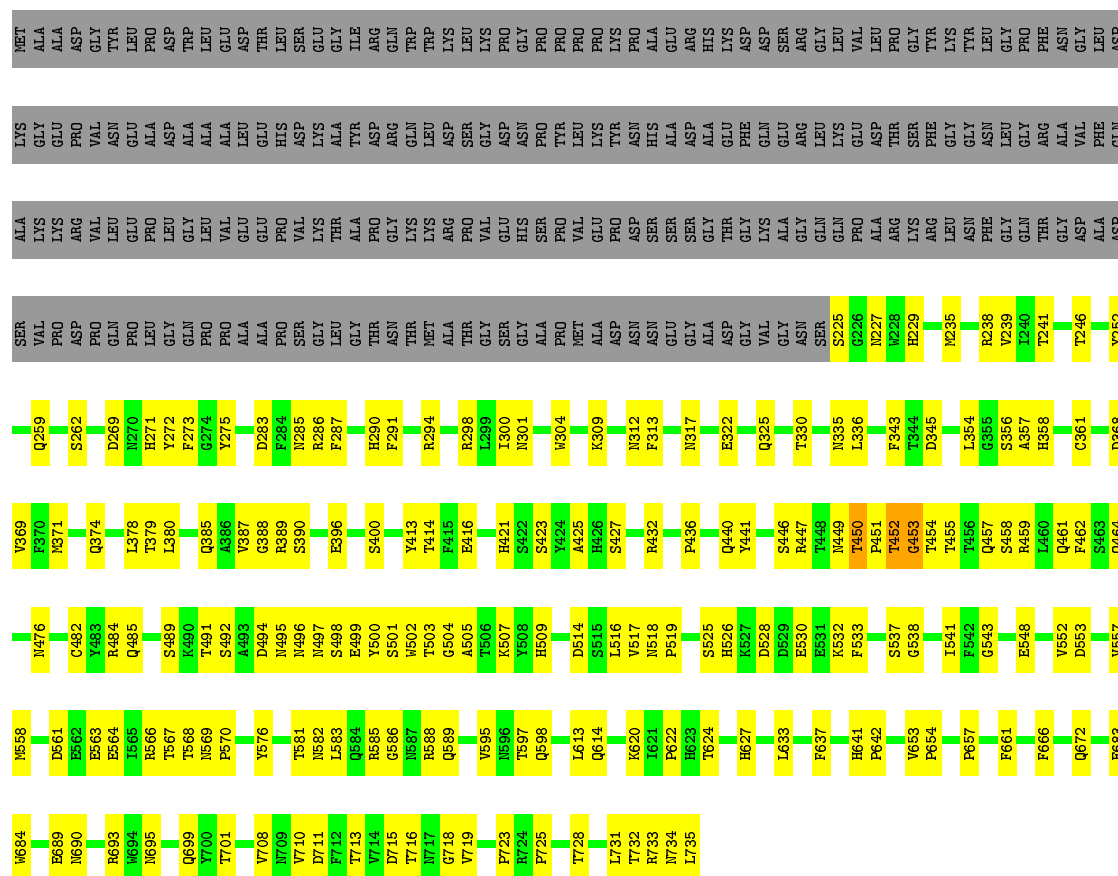
Chain Y:



- Molecule 1: Capsid protein VP1

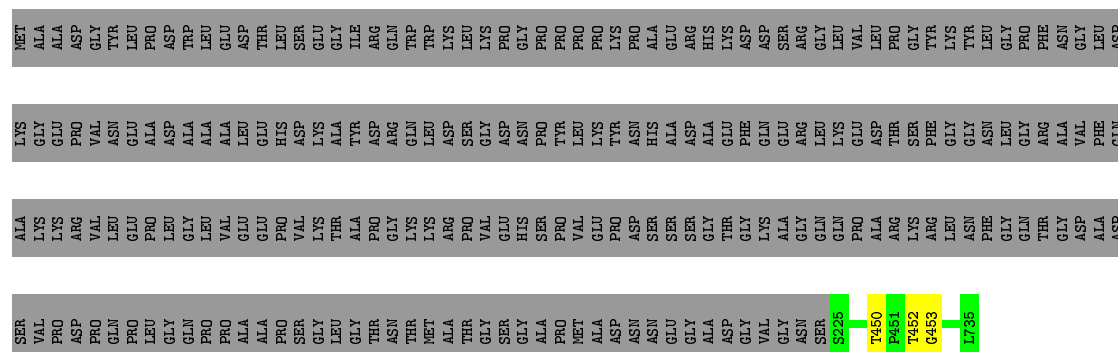
Chain Z:





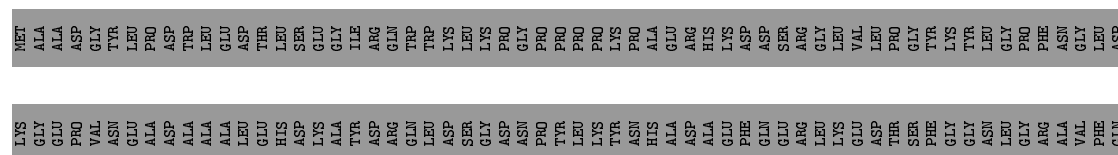
- Molecule 1: Capsid protein VP1

Chain a: 69% 30%



- Molecule 1: Capsid protein VP1

Chain b: 69% 30%



[illegible]

- Molecule 1: Capsid protein VP1

Chain c:  69% 30%

ser	val	ser	ala	lys	met
val	pro	pro	lys	gly	ala
asp	asp	pro	arg	pro	asp
gln	gln	pro	val	asn	tyr
pro	pro	pro	glu	glu	leu
leu	leu	leu	pro	ala	pro
gln	gln	leu	glu	asp	asp
pro	pro	pro	leu	ala	leu
pro	pro	pro	val	ala	glu
ala	ala	ala	glu	leu	asp
ala	ala	pro	pro	his	thr
ser	ser	ser	val	asp	ser
gly	gly	lys	lys	lys	glu
leu	leu	thr	thr	ala	gly
gly	gly	ala	ala	tyr	ile
thr	thr	pro	pro	asp	arg
asn	asn	lys	gly	arg	gln
thr	thr	lys	lys	gln	trp
met	met	lys	lys	leu	trp
ala	ala	arg	arg	asp	lys
thr	thr	pro	pro	ser	leu
ser	ser	val	val	gly	lys
gly	gly	his	glu	asp	pro
ala	ala	ser	his	asn	gly
pro	pro	pro	ser	pro	pro
met	met	val	val	tyr	pro
ala	ala	glu	glu	leu	pro
asp	asp	pro	pro	lys	pro
asn	asn	asp	asn	tyr	lys
asn	asn	ser	ser	his	pro
glu	glu	ser	ser	ala	ala
gly	gly	ser	ser	asp	glu
ala	ala	gly	gly	ala	arg
asp	asp	thr	thr	ala	his
gly	gly	lys	lys	phe	lys
val	val	lys	lys	gln	asp
gly	gly	ala	ala	glu	ser
asn	asn	gly	gly	arg	ser
ser	ser	gln	gln	leu	arg
s225		lys	lys	lys	gly
t450		pro	pro	asp	leu
t461		ala	ala	thr	pro
t462		arg	arg	ser	asn
g463		lys	lys	phe	gly
		arg	arg	tyr	tyr
		leu	leu	lys	lys
		asn	asn	gly	tyr
		phe	phe	asn	leu
		gln	gln	leu	gly
		thr	thr	gly	pro
		gly	gly	ala	asn
		asp	asp	val	gly
		ala	ala	phe	leu

- Molecule 1: Capsid protein VP1

Chain d:  69% 30%

[illegible]

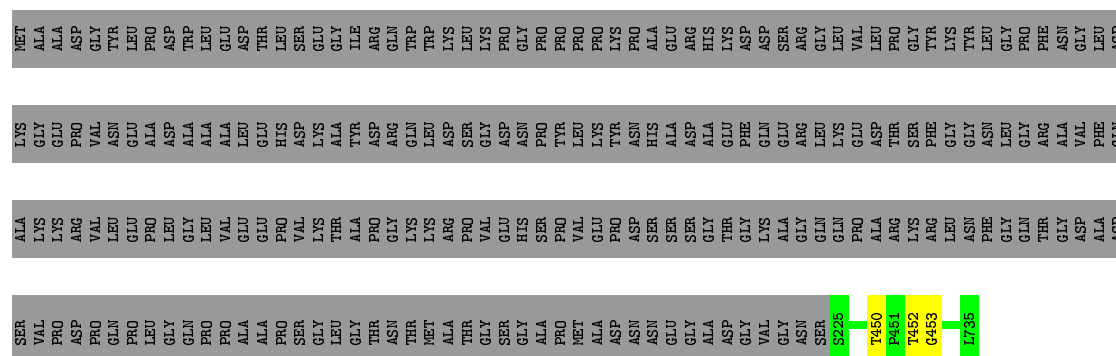
- Molecule 1: Capsid protein VP1

Chain e:  69% 30%

[illegible]

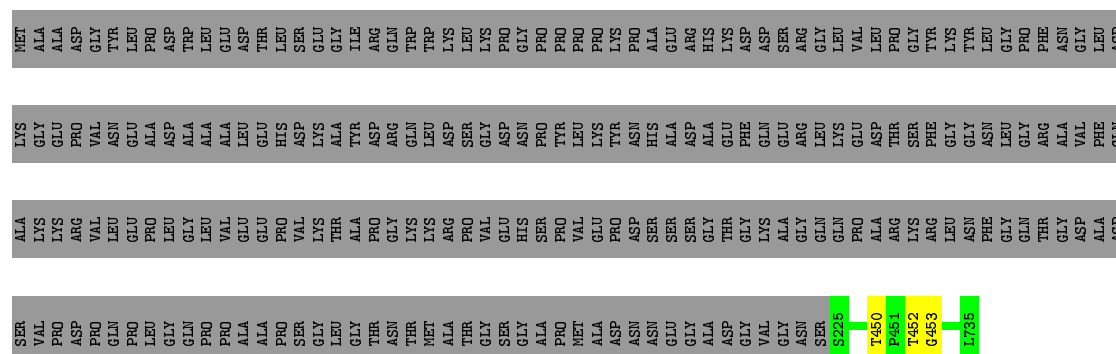
- Molecule 1: Capsid protein VP1

Chain f:  69% 30%



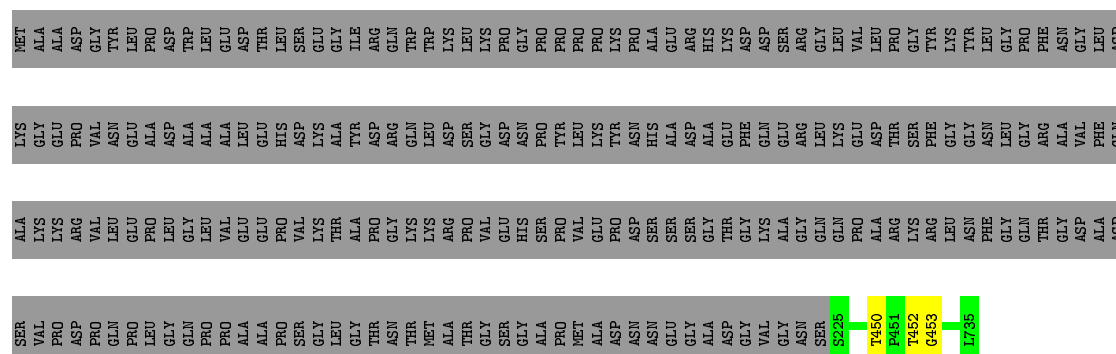
- Molecule 1: Capsid protein VP1

Chain g:  69% 30%



- Molecule 1: Capsid protein VP1

Chain h: 69% 30%



- Molecule 1: Capsid protein VP1

Chain i:  69% 30%

[illegible]

- Molecule 1: Capsid protein VP1

Chain j:  69% 30%

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

- Molecule 1: Capsid protein VP1

Chain k: 69% 30%

[illegible]

- Molecule 1: Capsid protein VP1

Chain 1: 69% 30%

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

[illegible]

- Molecule 1: Capsid protein VP1

Chain m:  69% 30%

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

[illegible]

- Molecule 1: Capsid protein VP1

Chain n: 69% 30%

[illegible][illegible]

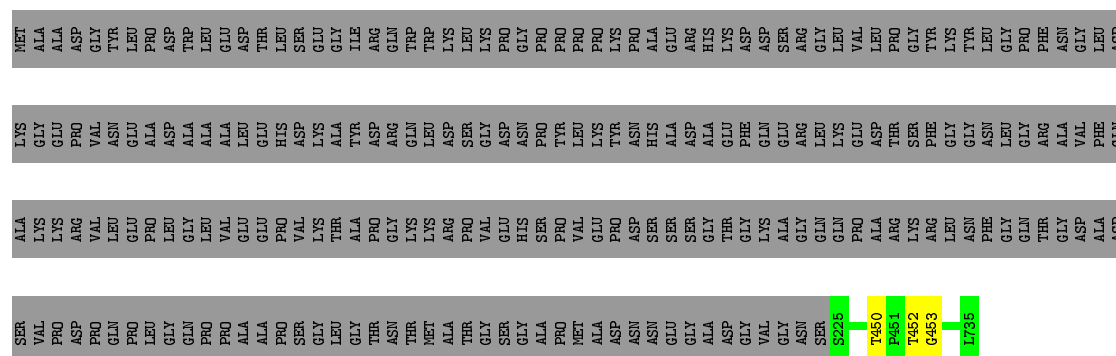
- Molecule 1: Capsid protein VP1

Chain o: 69% 30%

[illegible][illegible]

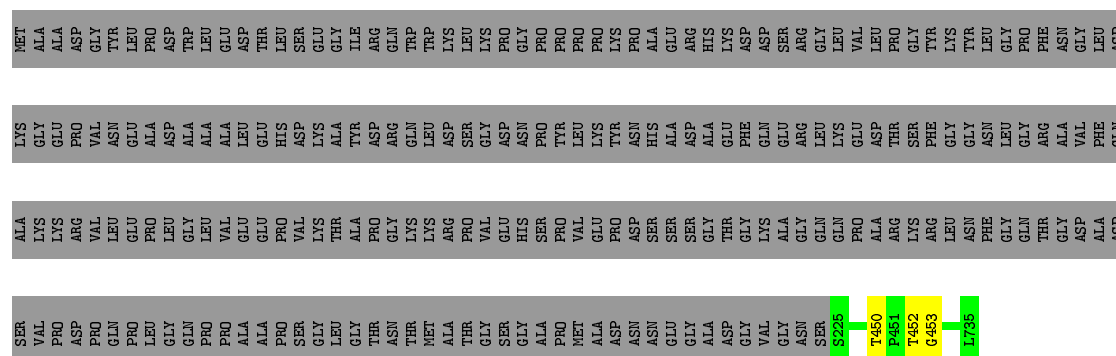
- Molecule 1: Capsid protein VP1

Chain p:  69% 30%



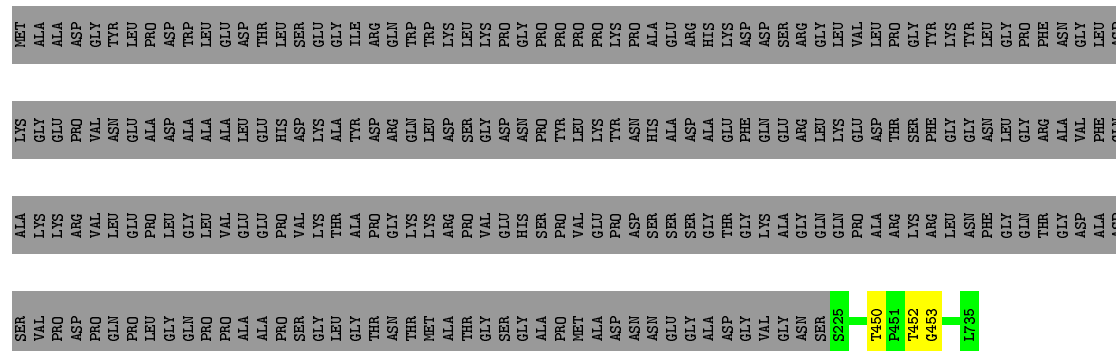
- Molecule 1: Capsid protein VP1

Chain q: 69% 30%



- Molecule 1: Capsid protein VP1

Chain r: 69% 30%



- Molecule 1: Capsid protein VP1

Chain s: 69% 30%

MET	LYS	ALA	LYS	SER
ALA	GLY	LYS	VAL	VAL
ASP	PRO	ARG	ASP	PRO
GLY	VAL	VAL	PRO	GLN
TYR	ASN	LEU	GLN	PRO
LEU	GLU	GLU	PRO	LEU
PRO	ALA	PRO	LEU	ASP
ASP	ASP	LEU	GLY	GLY
TRP	ALA	TRP	GLN	GLN
LEU	ALA	LEU	LEU	LEU
GLU	ALA	VAL	PRO	ASP
ASP	LEU	GLU	ALA	THR
THR	GLU	GLU	PRO	LEU
LEU	HIS	PRO	VAL	GLY
SER	ASP	SER	SER	GLY
GLY	LYS	LYS	GLY	ILE
ILE	TYR	ARG	THR	ARG
ARG	ASP	GLN	ASN	GLN
GLN	ARG	GLY	THR	TRP
TRP	GLN	LYS	LYS	LYS
LYS	LEU	TRP	TRP	LEU
LEU	ASP	ASP	ASP	LYS
LYS	SER	LEU	PRO	LEU
LYS	GLY	LYS	VAL	LYS
PRO	ASP	PRO	GLU	PRO
GLY	ASN	GLY	HIS	PRO
ASN	PRO	ALA	GLY	PRO
PRO	TYR	SER	PRO	PRO
PRO	LEU	VAL	VAL	PRO
PRO	LYS	PRO	ALA	PRO
LYS	TYR	ASP	ASP	LYS
ASN	ASN	ASN	ASN	ASN
ALA	HIS	SER	GLU	ALA
GLU	ASP	SER	SER	GLY
ARG	ALA	GLY	ALA	ALA
HIS	THR	THR	GLY	ASP
LYS	PHE	GLY	GLY	ASP
ASP	GLN	LYS	VAL	VAL
SER	GLU	ALA	GLY	GLY
SER	ARG	GLY	ASN	ASN
GLY	LEU	LEU	SER	SER
LEU	LYS	GLN	SER	SER
VAL	GLU	PRO	T450	T450
LEU	ASP	ALA	P451	P451
PRO	THR	ARG	T452	T452
GLY	SER	LYS	G453	G453
TYR	PHE	TYR	L735	L735
LYS	GLY	LYS		
TYR	GLY	TYR		
LEU	ASN	LEU		
GLY	LEU	GLY		
PRO	GLN	PRO		
PHE	ARG	THR		
ASN	ALA	GLY		
GLY	VAL	ASP		
LEU	PHE	ALA		
ASP	GLN	ASP		

● Molecule 1: Capsid protein VP1

Chain t:

69%

30%

MET	LYS	ALA	LYS	SER
ALA	GLY	LYS	VAL	VAL
ASP	PRO	ARG	ASP	PRO
GLY	VAL	VAL	PRO	GLN
TYR	ASN	LEU	GLN	PRO
LEU	GLU	GLU	PRO	LEU
PRO	ALA	PRO	LEU	ASP
ASP	ASP	LEU	GLY	GLY
TRP	ALA	TRP	GLN	GLN
LEU	ALA	LEU	LEU	LEU
GLU	ALA	VAL	PRO	ASP
ASP	LEU	GLU	ALA	THR
THR	GLU	GLU	PRO	LEU
LEU	HIS	PRO	VAL	GLY
SER	ASP	SER	SER	GLY
GLY	LYS	LYS	GLY	ILE
ILE	TYR	ARG	THR	ARG
ARG	ASP	GLN	ASN	GLN
GLN	ARG	GLY	THR	TRP
TRP	GLN	LYS	LYS	LYS
LYS	LEU	TRP	TRP	LEU
LEU	ASP	ASP	ASP	LYS
LYS	SER	LEU	PRO	LEU
LYS	GLY	LYS	VAL	LYS
PRO	ASP	PRO	GLU	PRO
GLY	ASN	GLY	HIS	PRO
ASN	PRO	ALA	GLY	PRO
PRO	TYR	SER	SER	PRO
PRO	LEU	VAL	VAL	PRO
PRO	LYS	PRO	ALA	PRO
LYS	TYR	ASP	ASP	LYS
ASN	ASN	ASN	ASN	ASN
ALA	HIS	SER	GLU	ALA
GLU	ASP	SER	SER	GLY
ARG	ALA	GLY	ALA	ALA
HIS	THR	THR	GLY	ASP
LYS	PHE	GLY	GLY	ASP
ASP	GLN	LYS	VAL	VAL
SER	GLU	ALA	GLY	GLY
SER	ARG	GLY	ASN	ASN
GLY	LEU	LEU	SER	SER
LEU	LYS	GLN	SER	SER
VAL	GLU	PRO	T450	T450
LEU	ASP	ALA	P451	P451
PRO	THR	ARG	T452	T452
GLY	SER	LYS	G453	G453
TYR	PHE	TYR	L735	L735
LYS	GLY	LYS		
TYR	GLY	TYR		
LEU	ASN	LEU		
GLY	LEU	GLY		
PRO	GLN	PRO		
PHE	ARG	THR		
ASN	ALA	GLY		
GLY	VAL	ASP		
LEU	PHE	ALA		
ASP	GLN	ASP		

● Molecule 1: Capsid protein VP1

Chain u:

69%

30%

MET	LYS	ALA	LYS	SER
ALA	GLY	LYS	VAL	VAL
ASP	PRO	ARG	ASP	PRO
GLY	VAL	VAL	PRO	GLN
TYR	ASN	LEU	GLN	PRO
LEU	GLU	GLU	PRO	LEU
PRO	ALA	PRO	LEU	ASP
ASP	ASP	LEU	GLY	GLY
TRP	ALA	TRP	GLN	GLN
LEU	ALA	LEU	LEU	LEU
GLU	ALA	VAL	PRO	ASP
ASP	LEU	GLU	ALA	THR
THR	GLU	GLU	PRO	LEU
LEU	HIS	PRO	VAL	GLY
SER	ASP	SER	SER	GLY
GLY	LYS	LYS	GLY	ILE
ILE	TYR	ARG	THR	ARG
ARG	ASP	GLN	ASN	GLN
GLN	ARG	GLY	THR	TRP
TRP	GLN	LYS	LYS	LYS
LYS	LEU	TRP	TRP	LEU
LEU	ASP	ASP	ASP	LYS
LYS	SER	LEU	PRO	LEU
LYS	GLY	LYS	VAL	LYS
PRO	ASP	PRO	GLU	PRO
GLY	ASN	GLY	HIS	PRO
ASN	PRO	ALA	GLY	PRO
PRO	TYR	SER	SER	PRO
PRO	LEU	VAL	VAL	PRO
PRO	LYS	PRO	ALA	PRO
LYS	TYR	ASP	ASP	LYS
ASN	ASN	ASN	ASN	ASN
ALA	HIS	SER	GLU	ALA
GLU	ASP	SER	SER	GLY
ARG	ALA	GLY	ALA	ALA
HIS	THR	THR	GLY	ASP
LYS	PHE	GLY	GLY	ASP
ASP	GLN	LYS	VAL	VAL
SER	GLU	ALA	GLY	GLY
SER	ARG	GLY	ASN	ASN
GLY	LEU	LEU	SER	SER
LEU	LYS	GLN	SER	SER
VAL	GLU	PRO	T450	T450
LEU	ASP	ALA	P451	P451
PRO	THR	ARG	T452	T452
GLY	SER	LYS	G453	G453
TYR	PHE	TYR	L735	L735
LYS	GLY	LYS		
TYR	GLY	TYR		
LEU	ASN	LEU		
GLY	LEU	GLY		
PRO	GLN	PRO		
PHE	ARG	THR		
ASN	ALA	GLY		
GLY	VAL	ASP		
LEU	PHE	ALA		
ASP	GLN	ASP		

● Molecule 1: Capsid protein VP1

Chain v:

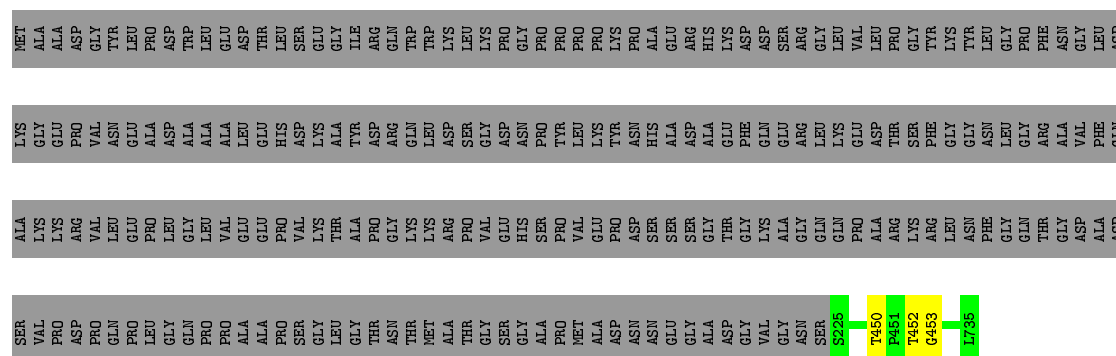
69%

30%

MET	LYS	ALA	LYS	SER
ALA	GLY	LYS	VAL	VAL
ASP	PRO	ARG	ASP	PRO
GLY	VAL	VAL	PRO	GLN
TYR	ASN	LEU	GLN	PRO
LEU	GLU	GLU	PRO	LEU
PRO	ALA	PRO	LEU	ASP
ASP	ASP	LEU	GLY	GLY
TRP	ALA	TRP	GLN	GLN
LEU	ALA	LEU	LEU	LEU
GLU	ALA	VAL	PRO	ASP
ASP	LEU	GLU	ALA	THR
THR	GLU	GLU	PRO	LEU
LEU	HIS	PRO	VAL	GLY
SER	ASP	SER	SER	GLY
GLY	LYS	LYS	GLY	ILE
ILE	TYR	ARG	THR	ARG
ARG	ASP	GLN	ASN	GLN
GLN	ARG	GLY	THR	TRP
TRP	GLN	LYS	LYS	LYS
LYS	LEU	TRP	TRP	LEU
LEU	ASP	ASP	ASP	LYS
LYS	SER	LEU	PRO	LEU
LYS	GLY	LYS	VAL	LYS
PRO	ASP	PRO	GLU	PRO
GLY	ASN	GLY	HIS	PRO
ASN	PRO	ALA	GLY	PRO
PRO	TYR	SER	SER	PRO
PRO	LEU	VAL	VAL	PRO
PRO	LYS	PRO	ALA	PRO
LYS	TYR	ASP	ASP	LYS
ASN	ASN	ASN	ASN	ASN
ALA	HIS	SER	GLU	ALA
GLU	ASP	SER	SER	GLY
ARG	ALA	GLY	ALA	ALA
HIS	THR	THR	GLY	ASP
LYS	PHE	GLY	GLY	ASP
ASP	GLN	LYS	VAL	VAL
SER	GLU	ALA	GLY	GLY
SER	ARG	GLY	ASN	ASN
GLY	LEU	LEU	SER	SER
LEU	LYS	GLN	SER	SER
VAL	GLU	PRO	T450	T450
LEU	ASP	ALA	P451	P451
PRO	THR	ARG	T452	T452
GLY	SER	LYS	G453	G453
TYR	PHE	TYR	L735	L735
LYS	GLY	LYS		
TYR	GLY	TYR		
LEU	ASN	LEU		
GLY	LEU	GLY		
PRO	GLN	PRO		
PHE	ARG	THR		
ASN	ALA	GLY		
GLY	VAL	ASP		
LEU	PHE	ALA		
ASP	GLN	ASP		

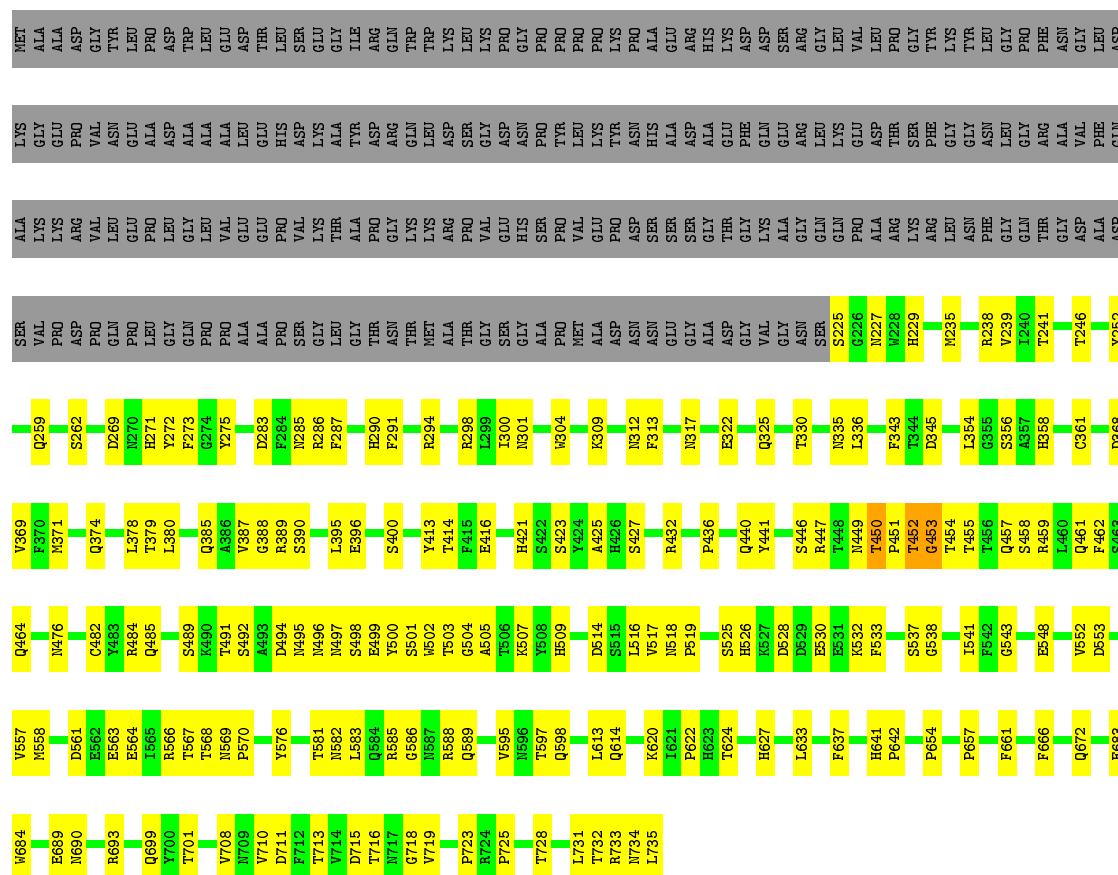
- Molecule 1: Capsid protein VP1

Chain z:  69% 30%



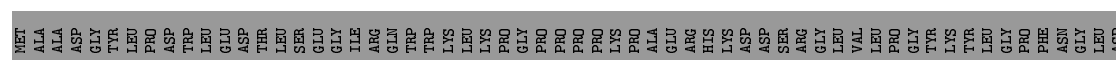
- Molecule 1: Capsid protein VP1

Chain 1:  45% 24% 30%



- Molecule 1: Capsid protein VP1

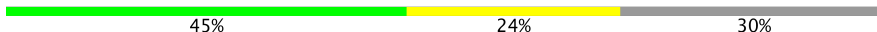
Chain 2:  45% 24% 30%



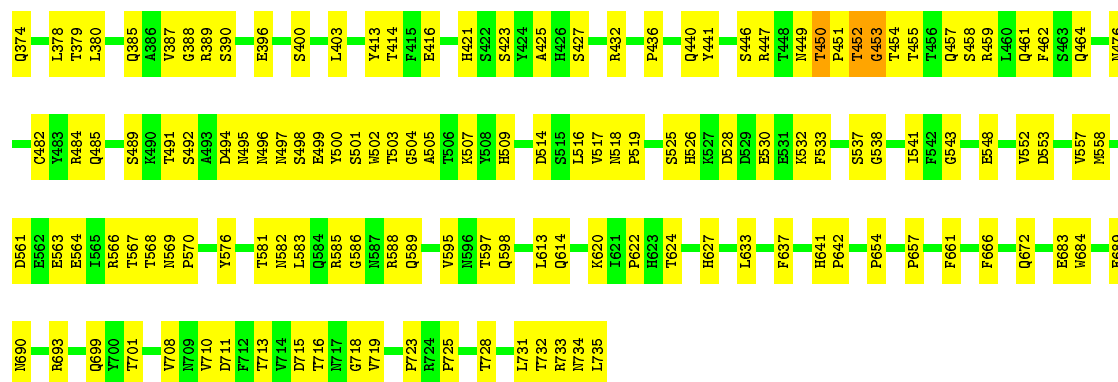
E689 N690	D561 E562	N476 C482	M371 Q374	Q259	SER VAL	ALA LYS	LYS
							GLY
R693	E563	Y483	L378 T379	S262	ASP	ARG	PRO
	E564	Q485		GLN	VAL		
Q699 T700	E565	S489 K490	L380	D269	PRO	LEU	ASN
	E566			H270	GLY	GLU	
T701	T567	A491	Q386 V387	F272	GLY	LEU	ASP
T708	T568	T492		G274	PRO	ALA	
T709	E570	S492	Q388 G389	Y275	PRO	VAL	ALA
T710	E576	A493		Y275	VAL	ALA	
T711	T581	D494	R389	D283	ALA	GLU	LEU
T712		N495	S390	F284	GLU	GLU	
T713	N582	N496	E396	N285	PRO	VAL	HIS
T714	L583	N497		R286	GLY	LYS	
T715	L584	S498	S400	F287	LYS	THR	ALA
T716	E584	E499		GLY	ALA	TYR	
T717	R585	Y500	Y413 T414	E290	THR	PRO	ASP
T718	E586	S501		F291	GLY	ASN	ARG
T719	E587	W502	T414	F291	THR	LYS	GLN
T720	L588	T503	F415	R294	MET	LYS	LEU
T721	Q589	G504	E416	R298	ALA	ARG	ASP
T722	E595	A505	R421		THR	PRO	SER
T723	E596	T506	S422	L299	GLY	VAL	GLY
T725	N596	K507	S423	I300	SER	GLU	ASP
T728	T597	Y508	Y424	N301	GLY	HIS	ASN
L731	L613	D514	A425	A304	ALA	SER	PRO
					E598	ALA	TYR
T732	Q614	S515	S427	K309	VAL	VAL	LEU
T733	L516	N517	L430	N312 F313	ASP	GLU	LYS
T734	R620	N518	D431		ASN	PRO	TYR
L735	P621	P519	R432	N317	ASN	ASP	ASN
	P622	E623	P436		ASN	SER	HIS
T736	E624	S525	E526	GLY	SER	SER	ALA
L737	L633	E627	D528	Y441	GLY	GLY	ALA
					E629	VAL	LYS
T738	P637	E530	S446	T330	GLY	ALA	GLU
T739	H641	K532	T448	N335	ASN	GLY	LEU
T740	P642	F633	N449	L336	GLN	GLN	LYS
L741	P654	E637	G538	P451	G226	PRO	GLY
					T227	ALA	ASP
T742	P657	I541	T452	K228	ARG	LYS	SER
T743	F661	F542	G453	T344	THR	ARG	PHE
T744	F662	G543	T454	D345	LYS	LEU	GLY
T745	P666	E548	T455	M235	ASN	ASN	GLY
T746					PHE	ASN	GLY
T747	Q672	V552	F462	R238	GLY	LEU	LEU
T748	E683	D553	S458	V239	GLY	GLY	GLY
T749	H684	V557	R459	T241	THR	THR	ARG
T750	E684	N559	S463	T246	GLY	ALA	VAL
T751	E685	V560	Q464	E252	ASP	GLY	PHE

- Molecule 1: Capsid protein VP1

Chain 3:

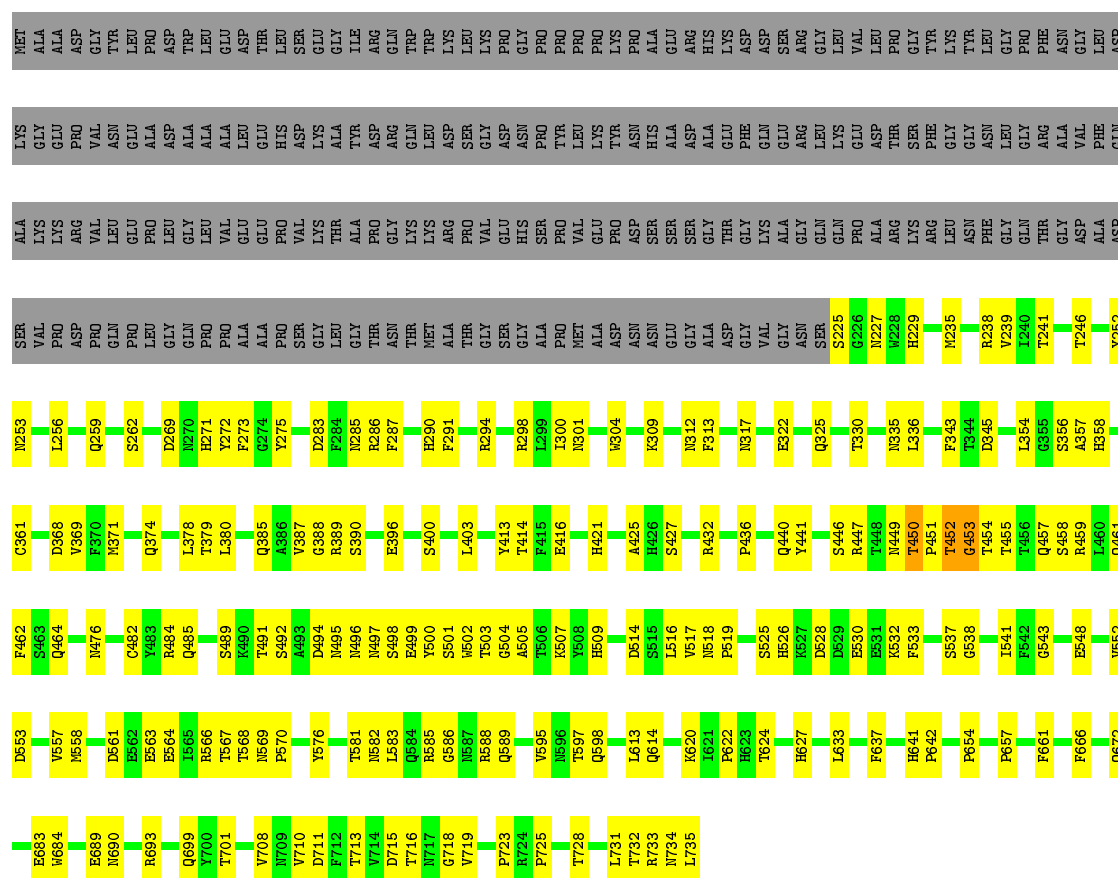


Metabolite	D561	D668	Q259	SER	ALA	LYS	LYS	GLY	ALA
	E562	V369	Q259	VAL	VAL	LYS	LYS	GLY	ALA
	E563	F370	S262	ASP	ARG	ARG	ARG	PRO	ASP
	E564	K371	S262	PRO	VAL	VAL	VAL	ASN	GLY
	I565	Q374	D269	GLN	LEU	LEU	LEU	ASN	TTR
	R566	L378	H271	PRO	GLU	GLU	GLU	GLU	LEU
	T567	T379	Z272	LEU	PRO	PRO	PRO	ALA	PRO
	T568	F273	F273	GLY	GLY	LEU	LEU	ASP	ASP
	N569	L380	F273	GLN	GLY	GLY	GLY	ALA	TSP
	P570	S492	G274	PRO	LEU	LEU	ALA	ALA	LEU
Metabolite	A493	Q385	Z275	PRO	VAL	VAL	VAL	ALA	GLU
	D494	A386	Z275	ALA	ALA	GLU	GLU	LEU	ASP
	N495	R387	D283	ALA	ALA	GLU	GLU	LEU	THR
	N496	G388	F284	PRO	PRO	PRO	HIS	HIS	THR
	N497	R389	N285	SER	VAL	VAL	ASP	ASP	SER
	L583	S390	R286	GLY	LYS	LYS	LYS	LYS	GLY
	G584	E396	F287	LEU	THR	THR	ALA	ALA	GLY
	R585	Y500	H290	GLY	ALA	ALA	TYR	TYR	ILE
	G586	S501	H290	THR	PRO	PRO	ASP	ASP	ARG
	N587	Y502	F291	ASN	GLY	GLY	ARG	ARG	GLN
Metabolite	R588	Y503	THR	THR	LYS	LYS	GLN	LEU	TRP
	Q589	G504	R294	MET	LYS	LYS	LEU	LEU	TRP
	A505	Y413	R294	ALA	ARG	ARG	ASP	ASP	LYS
	V506	T414	R298	ALA	PRO	PRO	SER	SER	LEU
	N596	F415	L299	THR	VAL	VAL	GLY	GLY	LYS
	T597	E416	L300	SER	GLU	GLU	ASP	ASP	PRO
	Y508	N301	N301	GLY	HIS	HIS	ASN	ASN	GLY
	H509	H421	N301	ALA	GLY	GLY	ASN	PRO	PRO
	D514	A425	N304	PRO	PRO	PRO	TYR	TYR	PRO
	S515	H426	N304	MET	VAL	VAL	LEU	LEU	PRO
Metabolite	L516	S427	K309	ALA	ALA	GLU	LYS	LYS	PRO
	V517	S427	K309	ASP	PRO	PRO	TYR	TYR	PRO
	N518	R432	N312	ASN	ASP	ASP	ASN	ASN	PRO
	P519	F313	F313	ASN	SER	SER	HIS	HIS	ALA
	H623	P436	N317	GLU	SER	SER	ALA	ALA	GLU
	S525	Q440	N317	GLY	SER	SER	ASP	ASP	ARG
	H526	Y441	E322	ALA	GLY	GLY	ALA	ALA	HIS
	K527	Y441	E322	ASP	THR	THR	GLU	GLU	LYS
	D528	S446	Q325	VAL	GLY	GLY	PHE	PHE	ASP
	N529	R447	Q325	VAL	LYS	LYS	GLN	GLN	ASP
Metabolite	E530	R447	Q325	GLY	ALA	ALA	GLU	GLU	SER
	E531	T448	T330	ASN	GLY	GLY	ARG	ARG	ARG
	K532	N449	T330	SER	GLN	GLN	LEU	LEU	GLY
	F533	P450	N335	SER	S225	S225	LYS	LYS	LEU
	H641	T452	L336	G226	PRO	PRO	GLU	GLU	VAL
	P642	G453	N227	N227	ALA	ALA	ASP	ASP	LEU
	V653	F454	F343	H228	ARG	ARG	THR	THR	PRO
	P654	T456	T344	L229	LYS	LYS	SER	SER	GLY
	F661	T456	D345	M235	ARG	ARG	PHE	PHE	TYR
	G543	T456	D345	M235	ASN	ASN	GLY	GLY	LYS
Metabolite	F666	Q457	L354	ASN	ASN	ASN	GLY	GLY	LEU
	Q672	R459	A357	PHE	PHE	PHE	LEU	LEU	GLY
	E683	L460	C361	V239	GLY	GLY	LEU	LEU	PHE
	N684	Q462	T241	T241	THR	THR	ARG	ARG	ASN
	H684	F462	T241	T241	GLY	GLY	ALA	ALA	GLY
	V657	F463	T246	T246	ASP	ASP	VAL	VAL	LEU
	N680	Q464	P366	P366	ALA	ALA	PHE	PHE	GLN
	S680	P366	Y362	Y362	ASP	ASP	THR	THR	ALA
	L613	L613	S615	S615	ALA	ALA	LYS	LYS	GLY
	Q614	L613	S615	S615	ALA	ALA	LYS	LYS	GLY



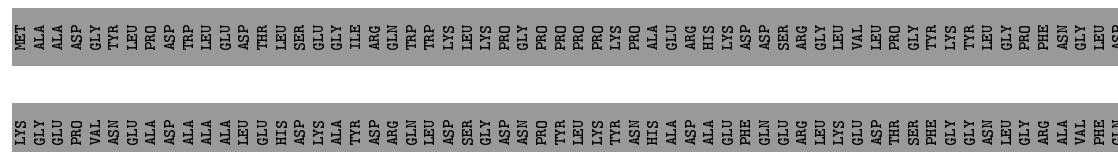
- Molecule 1: Capsid protein VP1

Chain 6: 45% 24% 30%



- Molecule 1: Capsid protein VP1

Chain 7: 44% 25% 30%



Q672	V552	Q461	H388	M253	SER VAL	ALA LYS
E683	D563	S462	C361	L256	PRO	ARG
W694	V557	Q464			ASP	
E685	W558		D368	Q259	PRO	VAL
L686		W476	V369		GLN	LEU
	D561		F370	S262	PRO	GLU
E689	E562	C482	M371		LEU	PRO
M690	E563	Y483		D269	GLY	LEU
	E564	R484	Q374	D270	GLN	LEU
R693	W566	Q485		E271	PRO	
Q699	W567	S489	L378	Y272	PRO	VAL
T700	W568	K490	T379	F273	ALA	GLU
T701	W569	T491	L380	G274	ALA	GLU
	P570	S492		Y275	PRO	PRO
V708		A493	Q385		SER	VAL
W709	Y576	D494	A386	D283	GLY	LYS
V710		N495	V387	F284	LEU	THR
D711	T581	N496	G388	M285	GLY	ALA
F712	W582	N497	R389	R286	THR	PRO
T713	L583	S498	S390	F287	ASN	GLY
V714	W584	E499			THR	LYS
D715	W585	Y500	L395	E290	MET	LYS
T716	G586	S501	E396	F291	ALA	ARG
W717	W587	W502	S400		THR	PRO
G718	S588	T503		R294	GLY	VAL
V719	Q589	G504	Y413	R298	GLY	HIS
		A505	T414	T299	ALA	SER
P723	W595	T506	F415	I300	PRO	PRO
R724	W596	K507	E416	M301	MET	VAL
P725	T597	Y508			ALA	GLU
	Q598	W509	H421	K304	ASP	PRO
T728				G305	ASN	ASP
	L613	D514	A425	F306	ASN	SER
L731	Q614	S515	H426		GLU	SER
T732	L616	W516	S427	K309	GLY	SER
R733	W620	N517			ALA	GLY
N734	L621	N518	R432	N312	ASP	THR
L735	P622	P519		F313	GLY	GLY
	H623		P436		VAL	LYS
	T624	S525		N317	GLY	ALA
		H526	Q440		ASN	GLN
	H627	K527	Y441	E322	SER	GLN
		D528			S225	GLN
L633		D529	S446	Q325	G226	PRO
		E530	R447		N227	ALA
	P637	E531	T448	T330	H228	ARG
		K532	M449			LYS
H641		F533	T450	N335	ARG	ARG
P642			P451	L336		LEU
		S537	T452		M235	ASN
P654		G538	O453	F343		PHE
			R454	T344	V239	GLY
P657	T541	F542	T455	D345	L240	GLN
	F661	G543	T456		T241	THR
				L354		GLY
			S458	G355	T246	ASP
	P666	E548	R459	S356		ALA
			T460	A357	Y252	ALA

- Molecule 1: Capsid protein VP1

Chain 8: 45% 24% 30%

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	23039	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)	1100	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	56924	Depositor
Image detector	KODAK SO-163 FILM	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 >2	RMSZ	# Z >2
1	1	0.54	0/4229	0.59	3/5767 (0.1%)
1	2	0.54	0/4229	0.59	3/5767 (0.1%)
1	3	0.54	0/4229	0.59	3/5767 (0.1%)
1	4	0.54	0/4229	0.59	3/5767 (0.1%)
1	5	0.54	0/4229	0.59	3/5767 (0.1%)
1	6	0.54	0/4229	0.59	3/5767 (0.1%)
1	7	0.54	0/4229	0.59	3/5767 (0.1%)
1	8	0.54	0/4229	0.59	3/5767 (0.1%)
1	A	0.54	0/4229	0.59	3/5767 (0.1%)
1	B	0.54	0/4229	0.59	3/5767 (0.1%)
1	C	0.54	0/4229	0.59	3/5767 (0.1%)
1	D	0.54	0/4229	0.59	3/5767 (0.1%)
1	E	0.54	0/4229	0.59	3/5767 (0.1%)
1	F	0.54	0/4229	0.59	3/5767 (0.1%)
1	G	0.54	0/4229	0.59	3/5767 (0.1%)
1	H	0.54	0/4229	0.59	3/5767 (0.1%)
1	I	0.54	0/4229	0.59	3/5767 (0.1%)
1	J	0.54	0/4229	0.59	3/5767 (0.1%)
1	K	0.54	0/4229	0.59	3/5767 (0.1%)
1	L	0.54	0/4229	0.59	3/5767 (0.1%)
1	M	0.54	0/4229	0.59	3/5767 (0.1%)
1	N	0.54	0/4229	0.59	3/5767 (0.1%)
1	O	0.54	0/4229	0.59	3/5767 (0.1%)
1	P	0.54	0/4229	0.59	3/5767 (0.1%)
1	Q	0.54	0/4229	0.59	3/5767 (0.1%)
1	R	0.54	0/4229	0.59	3/5767 (0.1%)
1	S	0.54	0/4229	0.59	3/5767 (0.1%)
1	T	0.54	0/4229	0.59	3/5767 (0.1%)
1	U	0.54	0/4229	0.59	3/5767 (0.1%)
1	V	0.54	0/4229	0.59	3/5767 (0.1%)
1	W	0.54	0/4229	0.59	3/5767 (0.1%)
1	X	0.54	0/4229	0.59	3/5767 (0.1%)
1	Y	0.54	0/4229	0.59	3/5767 (0.1%)
1	Z	0.54	0/4229	0.59	3/5767 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.54	0/4229	0.59	3/5767 (0.1%)
1	b	0.54	0/4229	0.59	3/5767 (0.1%)
1	c	0.54	0/4229	0.59	3/5767 (0.1%)
1	d	0.54	0/4229	0.59	3/5767 (0.1%)
1	e	0.54	0/4229	0.59	3/5767 (0.1%)
1	f	0.54	0/4229	0.59	3/5767 (0.1%)
1	g	0.54	0/4229	0.59	3/5767 (0.1%)
1	h	0.54	0/4229	0.59	3/5767 (0.1%)
1	i	0.54	0/4229	0.59	3/5767 (0.1%)
1	j	0.54	0/4229	0.59	3/5767 (0.1%)
1	k	0.54	0/4229	0.59	3/5767 (0.1%)
1	l	0.54	0/4229	0.59	3/5767 (0.1%)
1	m	0.54	0/4229	0.59	3/5767 (0.1%)
1	n	0.54	0/4229	0.59	3/5767 (0.1%)
1	o	0.54	0/4229	0.59	3/5767 (0.1%)
1	p	0.54	0/4229	0.59	3/5767 (0.1%)
1	q	0.54	0/4229	0.59	3/5767 (0.1%)
1	r	0.54	0/4229	0.59	3/5767 (0.1%)
1	s	0.54	0/4229	0.59	3/5767 (0.1%)
1	t	0.54	0/4229	0.59	3/5767 (0.1%)
1	u	0.54	0/4229	0.59	3/5767 (0.1%)
1	v	0.54	0/4229	0.59	3/5767 (0.1%)
1	w	0.54	0/4229	0.59	3/5767 (0.1%)
1	x	0.54	0/4229	0.59	3/5767 (0.1%)
1	y	0.54	0/4229	0.59	3/5767 (0.1%)
1	z	0.54	0/4229	0.59	3/5767 (0.1%)
All	All	0.54	0/253740	0.59	180/346020 (0.1%)

There are no bond length outliers.

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	450	THR	C-N-CD	-8.07	102.84	120.60
1	w	450	THR	C-N-CD	-8.07	102.84	120.60
1	I	450	THR	C-N-CD	-8.07	102.85	120.60
1	l	450	THR	C-N-CD	-8.07	102.85	120.60
1	L	450	THR	C-N-CD	-8.07	102.85	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4106	0	3868	159	0
1	2	4106	0	3868	160	0
1	3	4106	0	3868	160	0
1	4	4106	0	3868	160	0
1	5	4106	0	3868	158	0
1	6	4106	0	3868	164	0
1	7	4106	0	3868	163	0
1	8	4106	0	3868	164	0
1	A	4106	0	3868	223	0
1	B	4106	0	3868	216	0
1	C	4106	0	3868	214	0
1	D	4106	0	3868	213	0
1	E	4106	0	3868	217	0
1	F	4106	0	3868	219	0
1	G	4106	0	3868	222	0
1	H	4106	0	3868	220	0
1	I	4106	0	3868	215	0
1	J	4106	0	3868	220	0
1	K	4106	0	3868	220	0
1	L	4106	0	3868	211	0
1	M	4106	0	3868	217	0
1	N	4106	0	3868	220	0
1	O	4106	0	3868	218	0
1	P	4106	0	3868	215	0
1	Q	4106	0	3868	209	0
1	R	4106	0	3868	198	0
1	S	4106	0	3868	205	0
1	T	4106	0	3868	216	0
1	U	4106	0	3868	216	0
1	V	4106	0	3868	218	0
1	W	4106	0	3868	213	0
1	X	4106	0	3868	205	0
1	Y	4106	0	3868	220	0
1	Z	4106	0	3868	210	0
1	a	4106	0	3868	0	0
1	b	4106	0	3868	0	0
1	c	4106	0	3868	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	4106	0	3868	0	0
1	e	4106	0	3868	0	0
1	f	4106	0	3868	0	0
1	g	4106	0	3868	0	0
1	h	4106	0	3868	0	0
1	i	4106	0	3868	0	0
1	j	4106	0	3868	0	0
1	k	4106	0	3868	0	0
1	l	4106	0	3868	0	0
1	m	4106	0	3868	0	0
1	n	4106	0	3868	0	0
1	o	4106	0	3868	0	0
1	p	4106	0	3868	0	0
1	q	4106	0	3868	0	0
1	r	4106	0	3868	0	0
1	s	4106	0	3868	0	0
1	t	4106	0	3868	0	0
1	u	4106	0	3868	0	0
1	v	4106	0	3868	0	0
1	w	4106	0	3868	0	0
1	x	4106	0	3868	0	0
1	y	4106	0	3868	0	0
1	z	4106	0	3868	0	0
All	All	246360	0	232080	5437	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 11.

The worst 5 of 5437 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)
1:6:507:LYS:HG2	1:6:516:LEU:HA	1.59	0.85
1:R:507:LYS:HG2	1:R:516:LEU:HA	1.59	0.85
1:F:507:LYS:HG2	1:F:516:LEU:HA	1.59	0.85
1:Y:507:LYS:HG2	1:Y:516:LEU:HA	1.59	0.85
1:J:507:LYS:HG2	1:J:516:LEU:HA	1.59	0.84

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	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	2	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	3	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	4	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	5	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	6	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	7	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	8	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	A	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	B	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	C	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	D	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	E	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	F	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	G	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	H	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	I	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	J	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	K	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	L	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	M	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	N	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	O	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	P	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	Q	509/735 (69%)	469 (92%)	40 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	S	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	T	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	U	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	V	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	W	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	X	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	Y	509/735 (69%)	468 (92%)	41 (8%)	0	100	100
1	Z	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	a	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	b	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	c	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	d	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	e	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	f	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	g	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	h	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	i	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	j	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	k	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	l	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	m	509/735 (69%)	468 (92%)	41 (8%)	0	100	100
1	n	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	o	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	p	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	q	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	r	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	s	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	t	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	u	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	v	509/735 (69%)	469 (92%)	40 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	x	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	y	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	z	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
All	All	30540/44100 (69%)	28138 (92%)	2402 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	2	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	3	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	4	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	5	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	6	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	7	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	8	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	A	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	B	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	C	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	D	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	E	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	F	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	G	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	H	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	I	455/630 (72%)	454 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	K	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	L	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	M	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	N	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	O	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	P	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	Q	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	R	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	S	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	T	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	U	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	V	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	W	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	X	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	Y	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	Z	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	a	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	b	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	c	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	d	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	e	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	f	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	g	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	h	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	i	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	j	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	k	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	l	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	m	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	n	455/630 (72%)	454 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	p	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	q	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	r	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	s	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	t	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	u	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	v	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	w	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	x	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	y	455/630 (72%)	454 (100%)	1 (0%)	94	98
1	z	455/630 (72%)	454 (100%)	1 (0%)	94	98
All	All	27300/37800 (72%)	27240 (100%)	60 (0%)	95	98

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	452	THR
1	h	452	THR
1	4	452	THR
1	e	452	THR
1	j	452	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 424 such sidechains are listed below:

Mol	Chain	Res	Type
1	b	457	GLN
1	h	518	ASN
1	4	485	GLN
1	c	325	GLN
1	e	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.