



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 06:51 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 : unknown
Resolution : 3.70 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

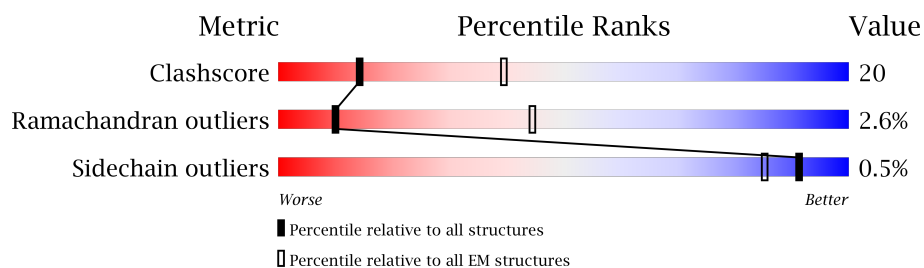
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



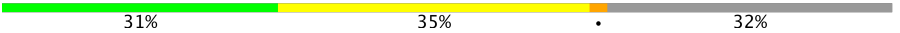
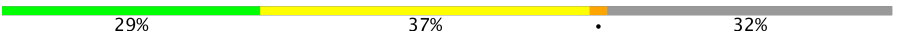
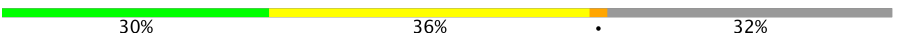
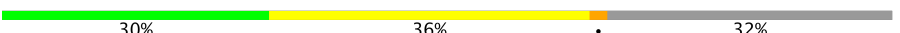
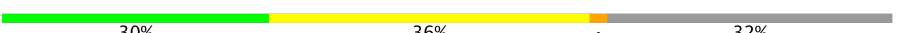
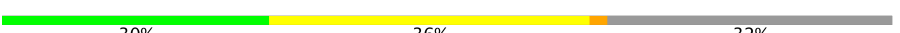
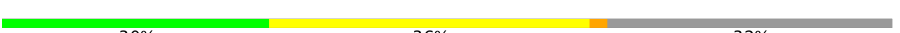




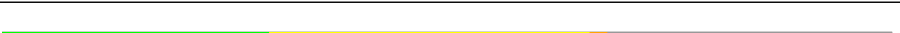



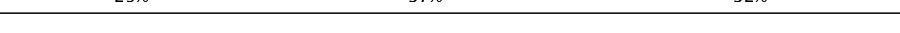
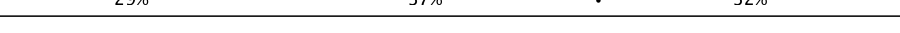
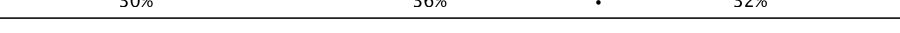
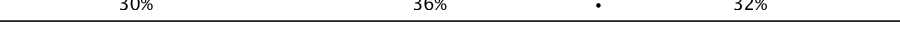
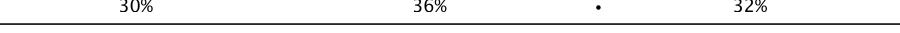
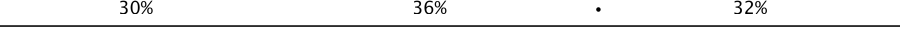
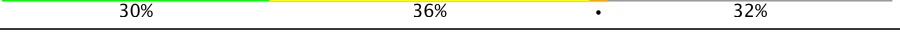
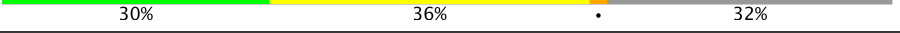
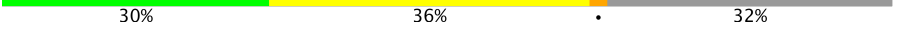
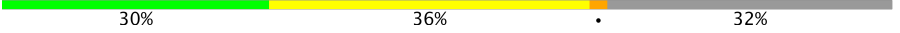
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	30% 36% • 32%
1	2	735	31% 35% • 32%
1	3	735	31% 35% • 32%
1	4	735	30% 36% • 32%
1	5	735	30% 36% • 32%
1	6	735	30% 36% • 32%
1	7	735	30% 36% • 32%
1	8	735	31% 35% • 32%
1	A	735	30% 36% • 32%


























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Mol	Chain	Length	Quality of chain			
1	B	735		31%	35%	32%
1	C	735		29%	37%	32%
1	D	735		30%	36%	32%
1	E	735		30%	36%	32%
1	F	735		30%	36%	32%
1	G	735		30%	36%	32%
1	H	735		30%	36%	32%
1	I	735		30%	36%	32%
1	J	735		30%	36%	32%
1	K	735		30%	36%	32%
1	L	735		30%	36%	32%
1	M	735		30%	36%	32%
1	N	735		29%	37%	32%
1	O	735		30%	36%	32%
1	P	735		29%	37%	32%
1	Q	735		29%	37%	32%
1	R	735		30%	36%	32%
1	S	735		30%	36%	32%
1	T	735		30%	36%	32%
1	U	735		30%	36%	32%
1	V	735		30%	36%	32%
1	W	735		30%	36%	32%
1	X	735		30%	36%	32%
1	Y	735		30%	36%	32%
1	Z	735		30%	36%	32%

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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>65%</div><div></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	C	N	O	S	0	0
			4009	2528	697	773	11		
1	S	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	T	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	U	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	V	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	W	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	X	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	Y	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
1	Z	500	Total	C	N	O	S	0	0
			4009	2528	697	773	11		
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		

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

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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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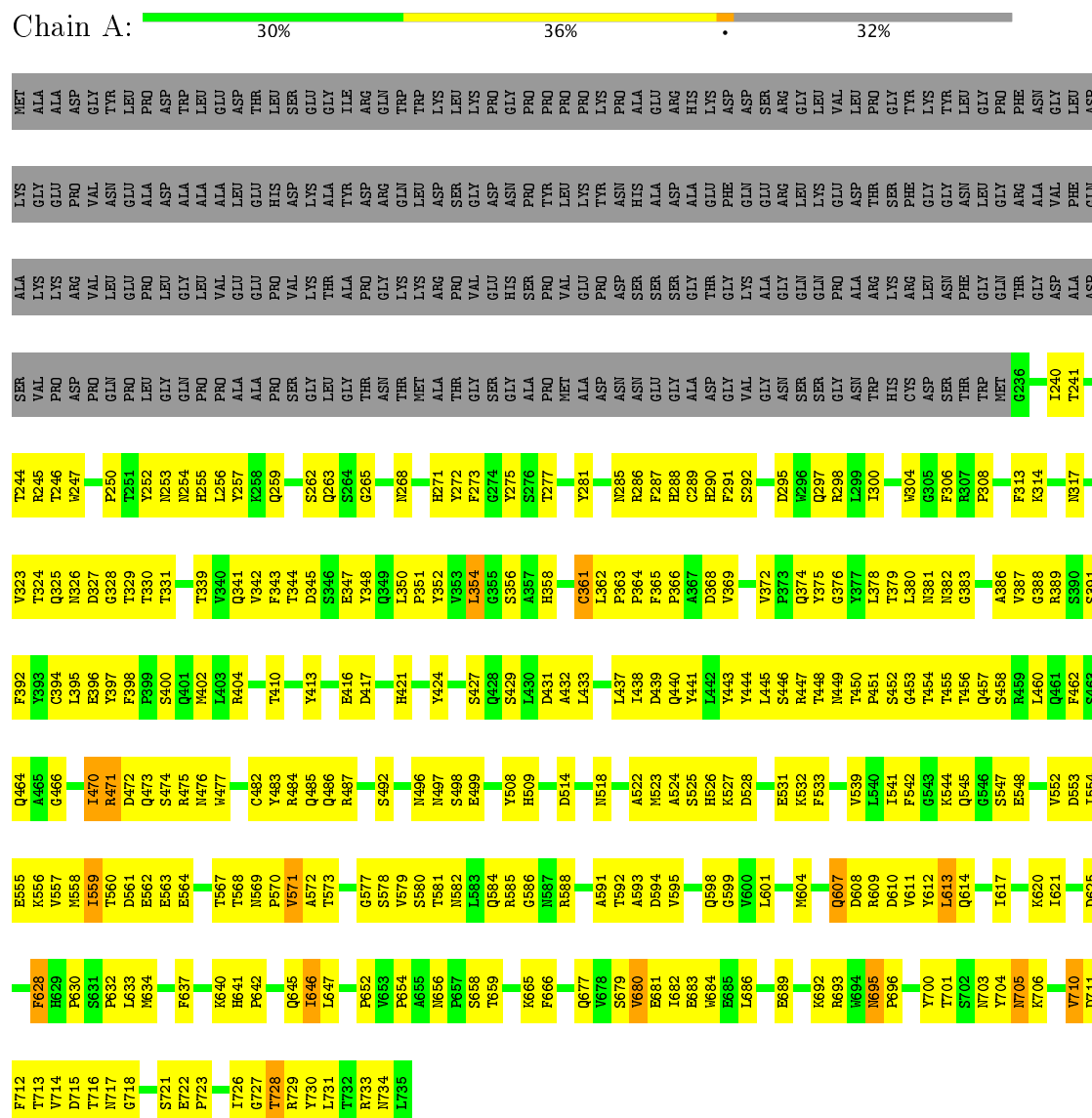
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Chain	Residue	Modelled	Actual	Comment	Reference
k	432	ALA	ARG	engineered mutation	UNP P03135
l	432	ALA	ARG	engineered mutation	UNP P03135
m	432	ALA	ARG	engineered mutation	UNP P03135
n	432	ALA	ARG	engineered mutation	UNP P03135
o	432	ALA	ARG	engineered 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 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

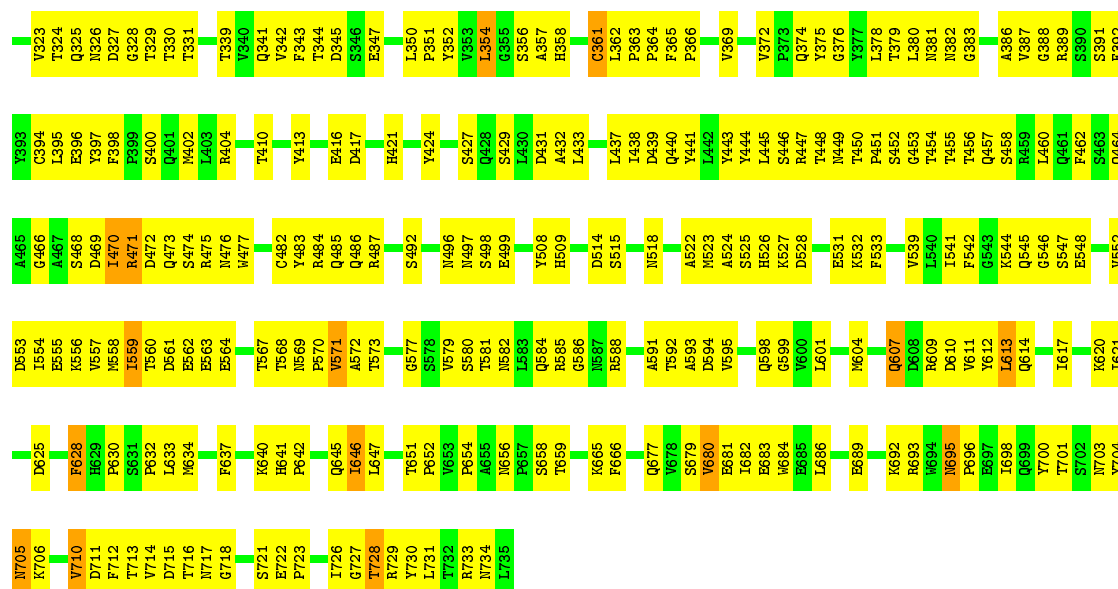


G718	S631	I569	E396	T324	R245	SER	ALA	LVS	LYS	MET
P632	P632	T560	F397	Q325	T246	VAL	LYS	GLY	ALA	ALA
L633	L633	D561	F398	N326	W247	PRO	LYS	GLY	ALA	GLY
E722	M634	E562	P399	D327		ASP	ARG	PRO	GLY	ASP
F723	P637	E563	S400	G328	P250	PRO	VAL	VAL	ASN	GLY
		E564	Q401	T329	T251	GLN	LEU	LEU		TTR
T726			M402	T330	Y252	PRO	GLU	GLU	GLU	LEU
G727	K640	T567	L403	T331	N253	LEU	PRO	ALA	ALA	LEU
T728	H641	N568	R404		N254	GLY	LEU	ASP	ASP	ASP
R729	P642	T569	T410	T339	H255	GLN	GLY	ALA	ALA	TRP
Y730	P570	P570	Y483	Q341	L256	PRO	LEU	LEU	ALA	LEU
L731	Q645	A571	Y413	Q342	T257	PRO	VAL	VAL	ALA	GLU
T732	L646	A572	Y416	F343	A258	ALA	GLU	LEU	LEU	ASP
R733	L647	T573	E416	Q344	Q259	ALA	THR	GLU	GLU	THR
N734			D417	T344		PRO	PRO	HIS	HIS	LEU
L735	T651	G577	D417		S262	SER	VAL	ASP	ASP	GLU
	P652	S578		E347	Q263	GLY	LYS	LYS	LYS	SER
		V579	H421		S264	LEU	THR	ALA	ALA	GLY
S580	N656	S580	Y424	L350	G285	THR	GLY	TTR	TTR	ILE
P657	T581	M496	Y424	P351		ASN	PRO	ASP	ASP	GLY
S658	N582	S498		Y352	N268	THR	LYS	GLN	GLN	TRP
T659	L583	E499	S427	V353		THR	LYS	LYS	LYS	TRP
	Q584		Q428	L354	H271	MET	LYS	LEU	ASP	TRP
Q677	R585	Y508	S429	G355	Y272	ALA	ARG	ASP	ASP	LYS
F678	G586	H509	L430	S356	T273	THR	PRO	SER	LEU	LYS
S679	N587		A431	A357	G274	GLY	VAL	GLY	GLY	PRO
F680	R588	D514	A432	H358	Y275	SER	GLU	ASP	ASP	LYS
E681			L433		S276	GLY	HIS	ASN	ASN	GLY
L682	A591	M518		G361	T277	ALA	SER	PRO	PRO	PRO
S683	T592		L437	L362		PRO	PRO	TTR	TTR	PRO
M684	A593	A522	L438	P363	Y281	MET	VAL	LEU	LEU	PRO
L685	D594	M523	D439	P364		ALA	GLU	LYS	LYS	PRO
L686	V595	A524	Q440	F365	N285	ASP	PRO	TTR	TTR	LYS
		S525	Y441	P366	R286	ASN	ASP	ASN	ASN	PRO
	Q598	H526	L442		F287	ASN	SER	HIS	ALA	PRO
S599	G599	K527	Y443	V369	H288	GLU	SER	ALA	GLU	GLU
V600	L601	D528	Y444		C289	GLY	SER	ASP	ARG	ARG
M604		E531	L445	V372	H290	ALA	THR	GLU	GLY	LYS
		K532	S446	P373	F291	ASP	ALA	THR	GLY	LYS
	M604	F533	T448	Q374	S292	GLY	LYS	PHE	GLN	ASP
Q607			M449	Y375		VAL	LYS	GLN	GLN	ASP
D608	D608	V539	T450	G376	D295	GLY	ALA	GLU	GLU	SER
R609	R609	L540	P451	T377	F296	ASN	GLY	ARG	ARG	ARG
D610	D610	I541	S452	L378	Q297	SER	GLN	LEU	GLY	GLY
V611	V611	F542	G453	T379	R298	SER	GLN	LYS	LYS	TTR
S702	S702	G543	T454	L380	L299	GLY	PRO	GLU	GLU	VAL
N703	N703	K544	T455	N381	I300	ASN	ALA	ASP	LEU	LEU
Y704	Q614	Q545	T456	N382		THR	ARG	THR	PRO	PRO
N705		S547	G457	G383	W304	HIS	LYS	SER	GLY	GLY
K706	I617	E548	S458	A386	G305	CYS	ARG	PHE	TTR	TTR
			R459	V387	R307	THR	ASN	GLY	GLY	LYS
			L460	G388	P308	THR	PHE	ASN	ASN	TTR
			Q461	R389		TRP	GLY	LEU	LEU	GLY
			F462	S390	F313	MET	GLN	GLY	GLY	PRO
			S463	S391	K314	THR	THR	ARG	ARG	PHE
			Q464	F392			GLY	ALA	ALA	GLY
			A465	Y393	N317	ASP	ASP	VAL	VAL	GLY
	F628	H529	G466	C394	T241	ALA	ALA	PHE	PHE	ASP
	D620	M558		L305		LEU	ASP	GLN	GLN	LEU

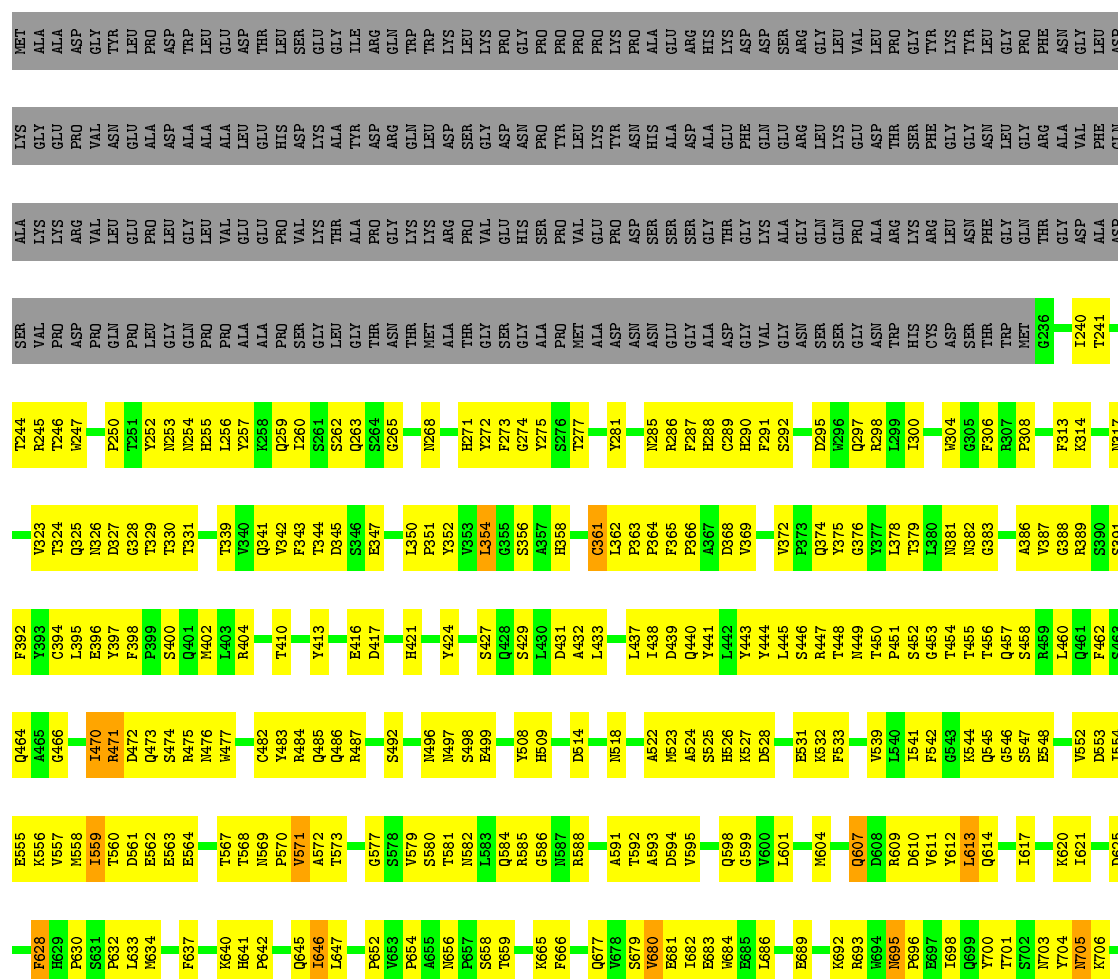
- Molecule 1: Capsid protein VP1

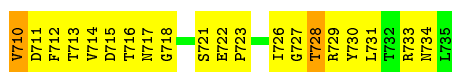
Chain C:  29% 37% . 32%

T244	SER	ALA	LYS	GLY	MET
R245	VAL	LYS	LYS	GLU	ALA
T246	PRO	ARG	VAL	PRO	ASP
W247	ASP	VAL	LEU	VAL	GLY
P250	GLN	LEU	GLU	ASN	TTR
T251	PRO	GLU	PRO	GLU	LEU
Y252	LEU	PRO	ALA	ALA	PRO
N253	GLN	LEU	GLY	ALA	ASP
N254	GLN	LEU	LEU	ALA	TRP
H255	PRO	VAL	VAL	ALA	LEU
L256	PRO	VAL	GLU	ALA	GLU
K258	ALA	GLU	GLU	LEU	ASP
Q259	PRO	PRO	PRO	LEU	LEU
S262	SER	VAL	LYS	GLY	SER
Q263	GLY	THR	THR	ALA	GLY
S264	GLY	ALA	ALA	ILE	GLY
G265	THR	PRO	PRO	TTR	ILE
N268	ASN	GLY	ARG	ASP	ARG
T269	THR	LYS	GLN	GLN	GLN
N270	MET	LYS	LEU	LEU	TRP
H271	ALA	ARG	ASP	ASP	TRP
Y272	THR	PRO	SER	LEU	LYS
F273	GLY	VAL	GLY	GLY	LYS
G274	SER	GLU	ASP	ASP	PRO
Y275	GLY	HIS	HIS	ASN	GLY
Y276	ALA	SER	PRO	PRO	PRO
T277	PRO	PRO	TTR	TTR	PRO
Y281	MET	VAL	LEU	LEU	PRO
N285	ALA	GLU	LYS	LYS	PRO
R286	ASN	ASP	ASN	ASN	PRO
T287	GLU	SER	SER	HIS	ALA
H288	GLY	SER	ASP	ALA	GLU
C289	ALA	GLY	GLY	ASP	ARG
H290	ASP	THR	GLU	HIS	LYS
F291	GLY	GLY	PHE	LYS	LYS
S292	VAL	LYS	GLN	ASP	ASP
D295	GLY	ALA	GLU	SER	SER
T296	ASN	GLN	ARG	GLY	GLY
T297	SER	GLN	LEU	ARG	GLY
Q297	SER	GLN	LYS	LEU	LEU
R298	GLY	PRO	GLU	VAL	LEU
L299	ASN	ALA	ASP	LEU	LEU
I300	TRP	ARG	THR	PRO	PRO
W304	HIS	LYS	SER	GLY	GLY
G305	CYS	ARG	PHE	LYS	TTR
F306	ASP	LEU	GLY	GLY	TTR
E307	SER	ASN	ASN	GLY	TTR
E307	THR	PHE	PHE	ASN	TTR
P308	TRP	GLY	LEU	LEU	GLY
F313	MET	GLN	GLY	GLY	PRO
K314	Q236	THR	ARG	ARG	PHE
T240	ASP	GLY	ALA	ALA	GLY
T241	ASP	ALA	ALA	PHE	GLY
T242	ASP	ALA	GLN	GLN	LEU



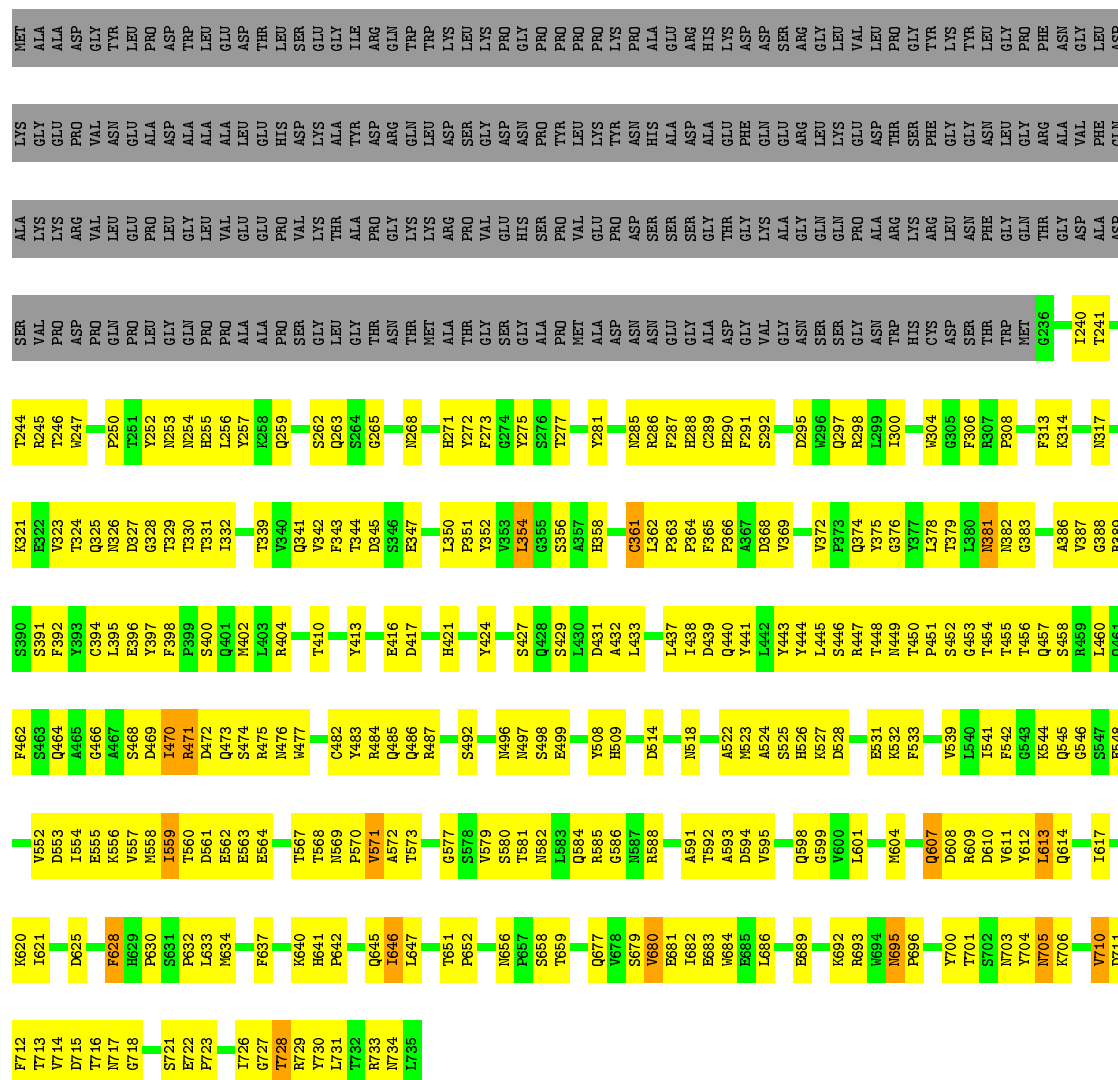
• Molecule 1: Capsid protein VP1





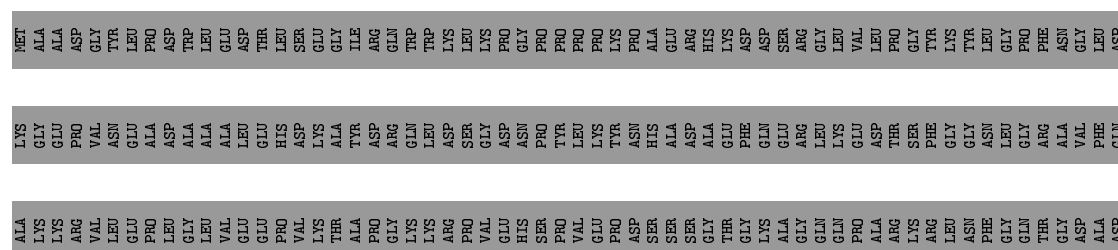
- Molecule 1: Capsid protein VP1

Chain E:  30% 36% . 32%

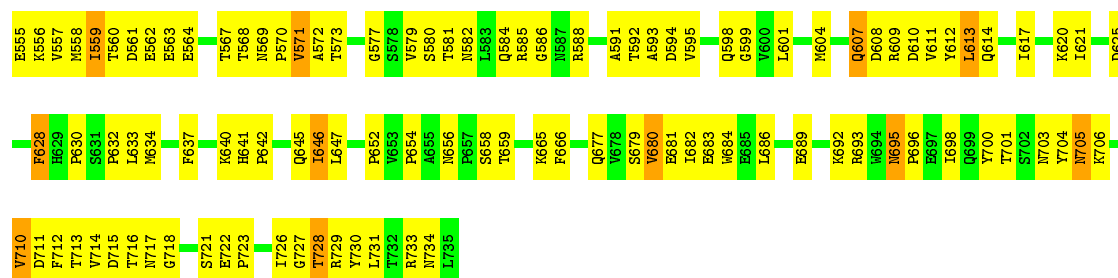


- Molecule 1: Capsid protein VP1

Chain F: 30% 36% 1% 32%

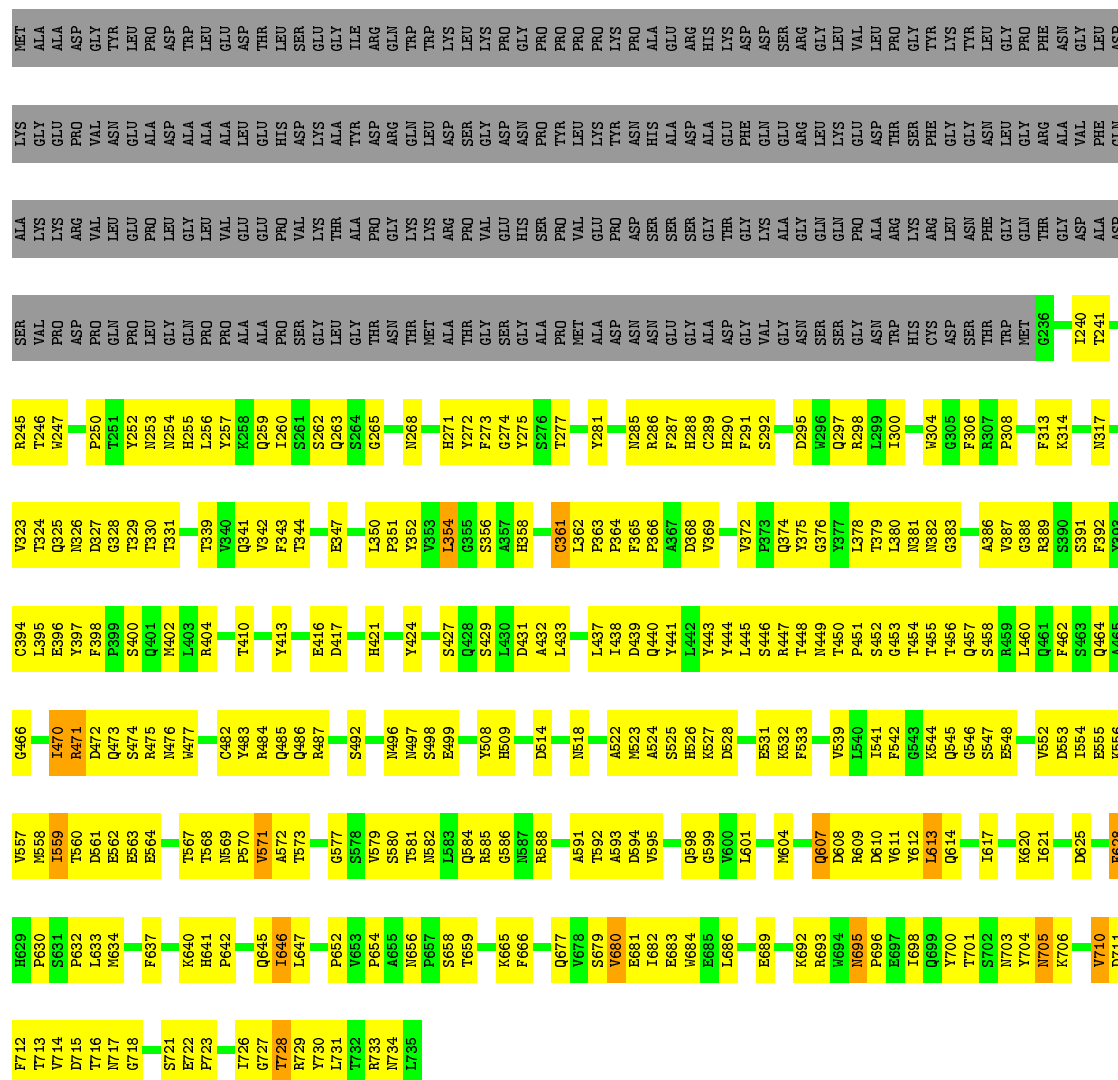


SER	T244	R321	S390	F462	V552	I621	N705	VAL	S391	F463	V553	I625	N706	PRO	S392	F464	V554	D625	K706	ASP	F393	L465	E555	V710	GLN	F712	T713	T714	D715	L716	N717	G718	LEU	T250	R325	S396	F470	V557	I628	N711	F713	T715	L717	G719	GLY	T252	R327	S397	F472	V558	I630	N712	T716	L718	D717	L466	E556	V714	D718	L467	V559	I632	N713	T717	L719	THR	T253	R328	F398	F473	V560	I633	N714	T718	L720	ALA	T254	R329	F399	S474	V561	I634	N715	T719	L721	GLY	T255	R330	F400	S475	V562	I635	N716	T720	L722	GLY	T256	R331	F401	S476	V563	I636	N717	T721	L723	THR	T257	R332	F402	S477	V564	I637	N718	T722	L724	ALA	T258	R333	F403	S478	V565	I638	N719	T723	L725	GLY	T259	R334	F404	S479	V566	I639	N720	T724	L726	GLY	T260	R335	F405	S480	V567	I640	N721	T725	L727	THR	T261	R336	F406	S481	V568	I641	N722	T726	L728	ALA	T262	R337	F407	S482	V569	I642	N723	T727	L729	GLY	T263	R338	F408	S483	V570	I643	N724	T728	L730	THR	T264	R339	F409	S484	V571	I644	N725	T729	L731	GLY	T265	R340	F410	S485	V572	I645	N726	T730	L732	THR	T266	R341	F411	S486	V573	I646	N727	T731	L733	ALA	T267	R342	F412	S487	V574	I647	N728	T732	L734	GLY	T268	R343	F413	S488	V575	I648	N729	T733	L735	THR	T269	R344	F414	S489	V576	I649	N730	T734	L736	ALA	T270	R345	F415	S490	V577	I650	N731	T735	L737	GLY	T271	R346	F416	S491	V578	I651	N732	T736	L738	THR	T272	R347	F417	S492	V579	I652	N733	T737	L739	ALA	T273	R348	F418	S493	V580	I653	N734	T738	L740	GLY	T274	R349	F419	S494	V581	I654	N735	T739	L741	THR	T275	R350	F420	S495	V582	I655	N736	T740	L742	ALA	T276	R351	F421	S496	V583	I656	N737	T741	L743	GLY	T277	R352	F422	S497	V584	I657	N738	T742	L744	THR	T278	R353	F423	S498	V585	I658	N739	T743	L745	ALA	T279	R354	F424	S499	V586	I659	N740	T744	L746	GLY	T280	R355	F425	S500	V587	I660	N741	T745	L747	THR	T281	R356	F426	S501	V588	I661	N742	T746	L748	ALA	T282	R357	F427	S502	V589	I662	N743	T747	L749	GLY	T283	R358	F428	S503	V590	I663	N744	T748	L750	THR	T284	R359	F429	S504	V591	I664	N745	T749	L751	ALA	T285	R360	F430	S505	V592	I665	N746	T750	L752	GLY	T286	R361	F431	S506	V593	I666	N747	T751	L753	THR	T287	R362	F432	S507	V594	I667	N748	T752	L754	ALA	T288	R363	F433	S508	V595	I668	N749	T753	L755	GLY	T289	R364	F434	S509	V596	I669	N750	T754	L756	THR	T290	R365	F435	S510	V597	I670	N751	T755	L757	ALA	T291	R366	F436	S511	V598	I671	N752	T756	L758	GLY	T292	R367	F437	S512	V599	I672	N753	T757	L759	THR	T293	R368	F438	S513	V600	I673	N754	T758	L760	ALA	T294	R369	F439	S514	V601	I674	N755	T759	L761	GLY	T295	R370	F440	S515	V602	I675	N756	T760	L762	THR	T296	R371	F441	S516	V603	I676	N757	T761	L763	ALA	T297	R372	F442	S517	V604	I677	N758	T762	L764	GLY	T298	R373	F443	S518	V605	I678	N759	T763	L765	THR	T299	R374	F444	S519	V606	I679	N760	T764	L766	ALA	T300	R375	F445	S520	V607	I680	N761	T765	L767	GLY	T301	R376	F446	S521	V608	I681	N762	T766	L768	THR	T302	R377	F447	S522	V609	I682	N763	T767	L769	ALA	T303	R378	F448	S523	V610	I683	N764	T768	L770	GLY	T304	R379	F449	S524	V611	I684	N765	T769	L771	THR	T305	R380	F450	S525	V612	I685	N766	T770	L772	ALA	T306	R381	F451	S526	V613	I686	N767	T771	L773	GLY	T307	R382	F452	S527	V614	I687	N768	T772	L774	THR	T308	R383	F453	S528	V615	I688	N769	T773	L775	ALA	T309	R384	F454	S529	V616	I689	N770	T774	L776	GLY	T310	R385	F455	S530	V617	I690	N771	T775	L777	THR	T311	R386	F456	S531	V618	I691	N772	T776	L778	ALA	T312	R387	F457	S532	V619	I692	N773	T777	L779	GLY	T313	R388	F458	S533	V620	I693	N774	T778	L780	THR	T314	R389	F459	S534	V621	I694	N775	T779	L781	ALA	T315	R390	F460	S535	V622	I695	N776	T780	L782	GLY	T316	R391	F461	S536	V623	I696	N777	T781	L783	THR	T317	R392	F462	S537	V624	I697	N778	T782	L784	ALA	T318	R393	F463	S538	V625	I698	N779	T783	L785	GLY	T319	R394	F464	S539	V626	I699	N780	T784	L786	THR	T320	R395	F465	S540	V627	I700	N781	T785	L787	ALA	T321	R396	F466	S541	V628	I701	N782	T786	L788	GLY	T322	R397	F467	S542	V629	I702	N783	T787	L789	THR	T323	R398	F468	S543	V630	I703	N784	T788	L790	ALA	T324	R399	F469	S544	V631	I704	N785	T789	L791	GLY	T325	R400	F470	S545	V632	I705	N786	T790	L792	THR	T326	R401	F471	S546	V633	I706	N787	T791	L793	ALA	T327	R402	F472	S547	V634	I707	N788	T792	L794	GLY	T328	R403	F473	S548	V635	I708	N789	T793	L795	THR	T329	R404	F474	S549	V636	I709	N790	T794	L796	ALA	T330	R405	F475	S550	V637	I710	N791	T795	L797	GLY	T331	R406	F476	S551	V638	I711	N792	T796	L798	THR	T332	R407	F477	S552	V639	I712	N793	T797	L799	ALA	T333	R408	F478	S553	V640	I713	N794	T798	L800	GLY	T334	R409	F479	S554	V641	I714	N795	T799	L801	THR	T335	R410	F480	S555	V642	I715	N796	T800	L802	ALA	T336	R411	F481	S556	V643	I716	N797	T801	L803	GLY	T337	R412	F482	S557	V644	I717	N798	T802	L804	THR	T338	R413	F483	S558	V645	I718	N799	T803	L805	ALA	T339	R414	F484	S559	V646	I719	N800	T804	L806	GLY	T340	R415	F485	S560	V647	I720	N801	T805	L807	THR	T341	R416	F486	S561	V648	I721	N802	T806	L808	ALA	T342	R417	F487	S562	V649	I722	N803	T807	L809	GLY	T343	R418	F488	S563	V650	I723	N804	T808	L810	THR	T344	R419	F489	S564	V651	I724	N805	T809	L811	ALA	T345	R420	F490	S565	V652	I725	N806	T810	L812	GLY	T346	R421	F491	S566	V653	I726	N807	T811	L813	THR	T347	R422	F492	S567	V654	I727	N808	T812	L814	ALA	T348	R423	F493	S568	V655	I728	N809	T813	L815	GLY	T349	R424	F494	S569	V656	I729	N810	T814	L816	THR	T350	R425	F495	S570	V657	I730	N811	T815	L817	ALA	T351	R426	F496	S571	V658	I731	N812	T816	L818	GLY	T352	R427	F497	S572	V659	I732	N813	T817	L819	THR	T353	R428	F498	S573	V660	I733	N814	T818	L820	ALA	T354	R429	F499	S574	V661	I734	N815	T819	L821	GLY	T355	R430	F500	S575	V662	I735	N816	T820	L822	THR	T356	R431	F501	S576	V663	I736	N817	T821	L823	ALA	T357	R432	F502	S577	V664	I737	N818	T822	L824	GLY	T358	R433	F503	S578	V665	I738	N819	T823	L825	THR	T359	R434	F504	S579	V666	I739	N820	T824	L826	ALA	T360	R435	F505	S580	V667	I740	N821	T825	L827	GLY	T361	R436	F506	S581	V668	I741	N822	T826	L828	THR	T362	R437	F507	S582	V669	I742	N823	T827	L829	ALA	T363	R438	F508	S583	V670	I743	N824	T828	L830	GLY	T364	R439	F509	S584	V671	I744	N825	T829	L831	THR	T365	R440	F510	S585	V672	I745	N826	T830	L832	ALA	T366	R441	F511	S586	V673	I746	N827	T831	L833	GLY	T367	R442	F512	S587	V674	I747	N828	T832	L834	THR	T368	R443	F513	S588	V675	I748	N829	T833	L835	ALA	T369	R444	F514	S589	V676	I749	N830	T834	L836	GLY	T370	R445	F515	S590	V677	I750	N831	T835	L837	THR	T371	R446	F516	S591	V678	I751	N832	T836	L838	ALA	T372	R447	F517	S592	V679	I752	N833	T837	L839	GLY	T373	R448	F518	S593	V680	I753	N834	T838	L840	THR	T374	R449	F519	S594	V681	I754	N835	T839	L841	ALA	T375	R450	F520	S595	V682	I755	N836	T840	L842	GLY	T376	R451	F521	S596	V683	I756	N837	T841	L843	THR	T377	R452	F522	S597	V684	I757	N838	T842	L844	ALA	T378	R453	F523	S598	V685	I758	N839	T843	L845	GLY	T379	R454	F524	S599	V686	I759	N840	T844	L846	THR	T380	R455	F525	S600	V687	I760	N841	T845	L847	ALA	T381	R456	F526	S601	V688	I761	N842	T846	L848	GLY	T382	R457	F527	S602	V689	I762	N843	T847	L849	THR	T383	R458	F528	S603	V690	I763	N844	T848	L850	ALA	T384	R459	F529	S604	V691	I764	N845	T849	L851	GLY	T385	R460	F530	S605	V692	I765	N846	T850	L852	THR	T386	R461	F531	S606	V693	I766	N847	T851	L853	ALA	T387	R462	F532	S607	V694	I767	N848	T852	L854	GLY	T388	R463	F533	S608	V695	I768	N849	T853	L855	THR	T389	R464	F534	S609	V696	I769	N850	T854	L856	ALA	T390	R465	F535	S610	V697	I770	N851	T855	L857	GLY	T391	R466	F536	S611	V698	I771	N852	T856	L858	THR	T392	R467	F537	S612	V699	I772	N853	T857	L859	ALA	T393	R468	F538	S613	V700	I773	N854	T858	L860	GLY	T394	R469	F539	S614	V701	I774	N855	T859	L861	THR	T395	R470	F540	S615	V702	I775	N856	T860	L862	ALA	T396	R471	F541	S616	V703	I776	N857	T861	L863	GLY	T397	R472	F542	S617	V704	I777	N858	T862	L864	THR	T398	R473	F543	S618	V705	I778	N859	T863	L865	ALA	T399	R474	F544	S619	V706	I779	N860	T864	L866	GLY	T400	R475	F545	S620	V707	I780	N861	T865	L867	THR	T401	R476	F546	S621	V708	I781	N862	T866	L868	ALA	T402	R477	F547	S622	V709	I782
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• Molecule 1: Capsid protein VP1

Chain H: 30% 36% 32%



• Molecule 1: Capsid protein VP1

Chain I: 30% 36% 32%

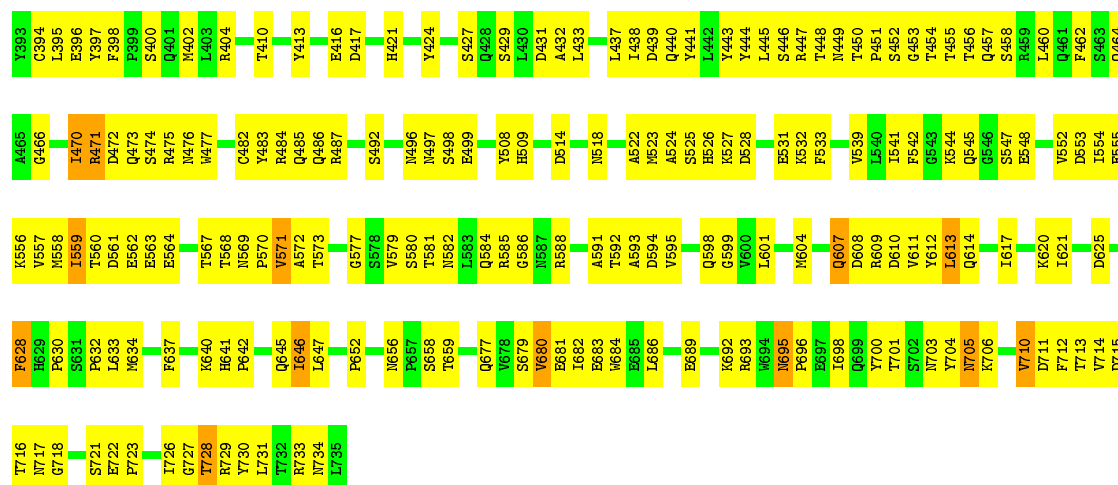


LYS	ALA	SER	T244	V323	C394	G466	V557	H529	V710
GLY	LYS	VAL	R245	T324	L395	T470	M558	P630	D711
GLU	LYS	PRO	R246	Q325	E396	T470	T559	S631	F712
PRO	ARG	ASP	W247	N326	Y397	R471	D661	P632	T713
VAL	VAL	PRO	P250	D327	F398	D472	E562	L633	V714
ASN	LEU	GLN	T251	G328	P399	Q473	E563	M634	D715
GLU	GLU	PRO	Y252	T329	S400	S474	E564	F637	T716
ALA	PRO	LEU	T253	T330	Q401	R475	E564		T717
ASP	LEU	GLY	N254	T331	M402	M476			T718
ALA	GLY	PRO	N255	T339	R404	N477	T567	K640	S721
ALA	LEU	PRO	N256	V340	C482		T568	H641	E722
ALA	VAL	ALA	N257	Q341	Y483		M569	P642	F723
LEU	GLU	ALA	K258	N342	R484		P570	Q645	
GLU	GLU	ALA	Q259	F343	Q485		V571	I646	
HIS	PRO	SER		T344	Q486		A572	L647	
ASP	VAL	THR		D345	R487		T573	I648	
LYS	LYS	GLY	S262	G346	D417		G577		
ALA	THR	LEU	Q263	S347	H421		S578	T651	
ALA	ALA	GLY	S264	E347			V579	P652	
TYR	PRO	THR	Q265	L350	M496		S580	P653	
ASP	GLY	THR	N268	P351	Y424		T581	G654	
ARG	LYS	LYS		Y352	S498		M582	A655	
LEU	LYS	MET			E499		L583	N656	
ASP	ARG	ALA	H271	L354	S427		Q584	P657	
SER	ASP	PRO	Y272	G355	Q428		R585	S658	
GLY	VAL	GLY	F273	G356	S429		S586	T659	
ASP	GLU	SER	G274	S357	D431		M587		
ASN	HIS	GLY	Y275	H358	A432		R588	K665	
GLY	ASP	ALA	S276		L433			P666	
PRO	SER	PRO	T277					F665	
TYR	PRO	PRO						K666	
LEU	VAL	MET							
LEU	VAL	ALA	Y281	G361	L437		A591	Q677	
LYS	GLU	ALA		L362	I438		T592	V678	
TYR	PRO	ASP		P363	D439		A593		
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ALA	SER	GLY	H288		L442			I682	
ASP	GLY	ALA	C289	V369	Y443		Q598	E683	
ALA	THR	ASP	H290		Y444		C599	E684	
GLU	GLY	ASP	F291		L445		P600	E685	
PHE	GLY	GLY	S292	V372	L446		L601	L686	
GLU	LYS	VAL		P373	S446		M604		
GLN	GLY	GLY	D295	Q374	R447			E689	
LEU	ARG	ASN	P296	Y375	T448		Q607		
LEU	GLN	SER	Q297	G376	M449		D608	K692	
LYS	GLN	SER	R298	T377	T450		R609	R693	
GLU	PRO	GLY	L299	T379	P451		D610	M694	
ALA	ALA	ASN	I300	L380	I541		V611	N695	
THR	ARG	TRP		N381	F542		Y612	P696	
SER	LYS	HIS	W304	N382	G543		L613	E697	
PHE	ARG	CYS	G305	G383	T455		Q614	I698	
GLY	LEU	ASP	F306	A386	Q457		T617	Q699	
ASN	PHE	THR	R307	V387	S458			T701	
GLY	GLY	TRP	P308	G388	E548		K620	S702	
LEU	THR	MET		R389	V552		I621	N703	
ARG	THR		F313	S390	D553			Y704	
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PHE	ALA								
GLN	ASP								

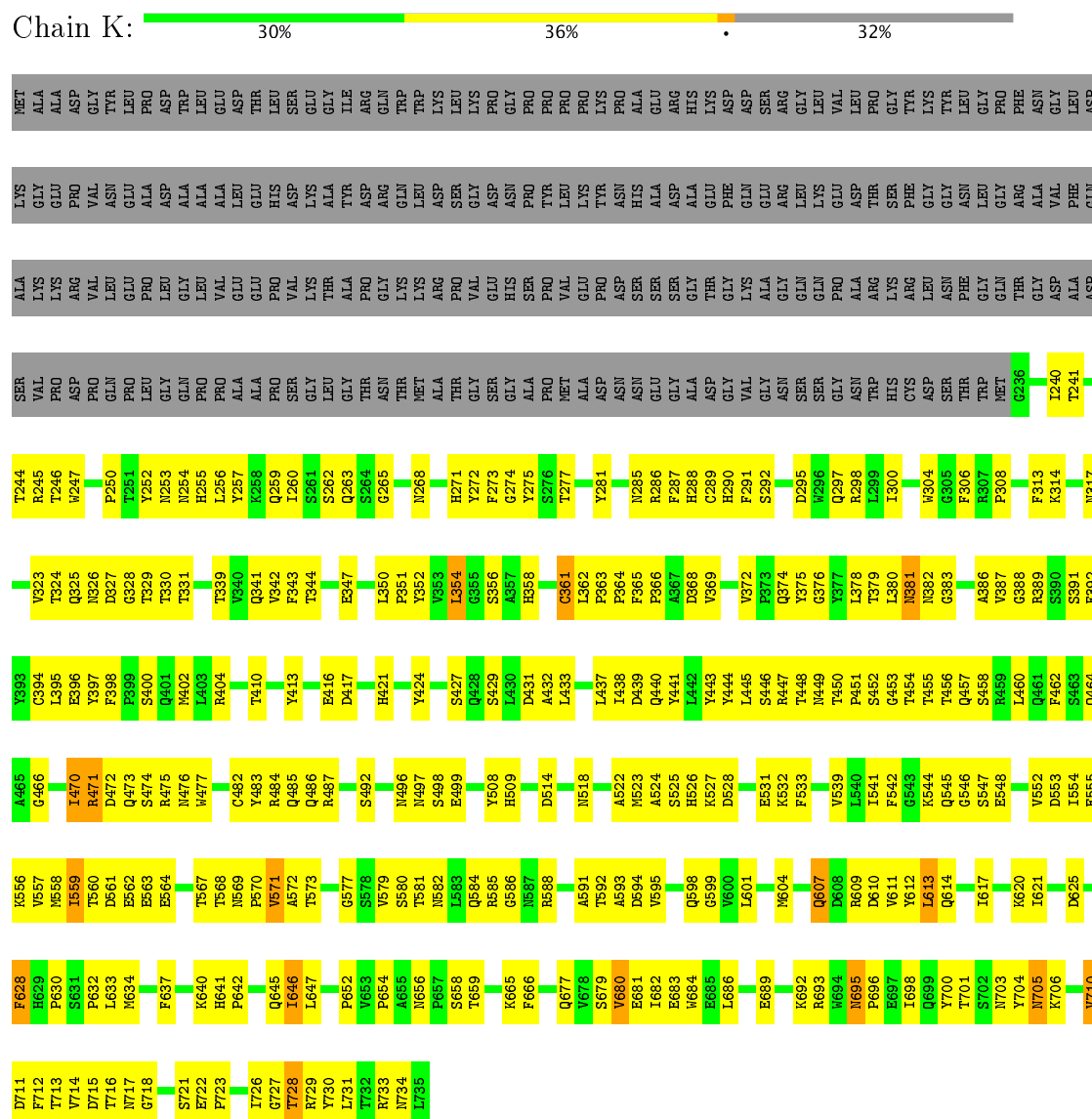
• Molecule 1: Capsid protein VP1

Chain J:  30% 36% 32%

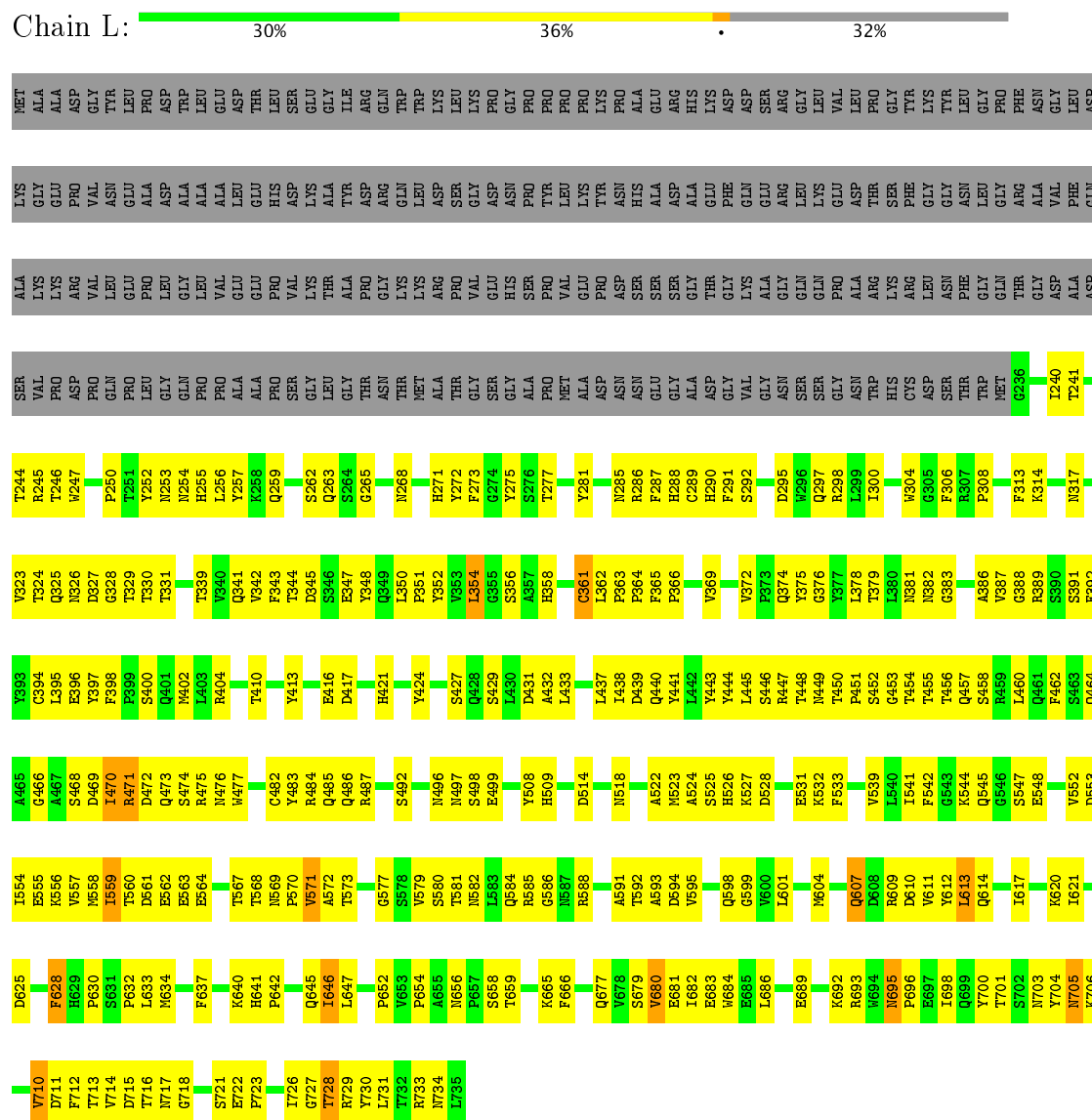
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ALA	GLY	LYS	R245	T324		VAL	R245	T324
ALA	GLU	LYS	T246	Q325		PRO	T246	Q325
ASP	PRO	ARG	W247	N326		ASP	W247	N326
GLY	VAL	VAL		D327		PRO		D327
TYR	ASN	LEU	P250	G328		GLN	P250	G328
LEU	GLU	GLU	T251	T329		LEU	T251	T329
PRO	ALA	PRO	Y252	T330		LEU	Y252	T330
ASP	LEU	ASP	N253	T331		GLY	N253	T331
ALA	GLY	GLN	N254	T339		GLN	N254	T339
LEU	ALA	PRO	N255	T340		PRO	N255	T340
GLU	VAL	VAL	N256	Q341		PRO	N256	Q341
ASP	LEU	GLU	Y257	F342		ALA	Y257	F342
THR	GLU	THR	K258	N342		ALA	K258	N342
	HIS	PRO	Q259	F343		PRO	Q259	F343
	ASP	SER		T344		SER		T344
	LYS	GLY	S262	D345		GLY	S262	D345
	ALA	LEU	Q263	S346		LEU	Q263	S346
	TYR	ALA	S264	E347		ALA	S264	E347
	ASP	THR	G265	L350		THR	G265	L350
	ARG	ASN	N268	P351		ASN	N268	P351
	GLY	THR		Y352		THR		Y352
	LYS	MET				LYS		
	LYS	LYS	H271	L354		LYS	H271	L354
	ASP	ALA	Y272	G355		ALA	Y272	G355
	SER	PRO	F273	S356		PRO	F273	S356
	GLY	GLY	G274	A357		GLY	G274	A357
	ASN	ALA	Y275	H358		ASN	Y275	H358
	GLY	PRO	S276			GLY	S276	
	PRO	PRO	T277			PRO	T277	
	TYR	PRO				TYR		
	LEU	VAL				LEU		
	VAL	MET	Y281	G361		MET	Y281	G361
	GLU	ALA		L362		GLU		L362
	LYS	LYS		P363		LYS		P363
	TYR	TYR	N285	F364		TYR	N285	F364
	ASN	ASN	R286	F365		ASN	R286	F365
	HIS	SER	F287	P366		HIS	F287	P366
	ALA	GLU	H288	A367		ALA	H288	A367
	ASP	ARG	C289	D368		ASP	C289	D368
	HIS	ALA	H290	V369		HIS	H290	V369
	LYS	GLY	F291			LYS	F291	
	ASP	GLY	S292	V372		ASP	S292	V372
	VAL	VAL		P373		VAL		P373
	GLY	GLY	D295	Q374		GLY	D295	Q374
	ARG	ASN	W296	Y375		ARG	W296	Y375
	GLY	SER	Q297	G376		GLY	Q297	G376
	LEU	SER	R298	T377		LEU	R298	T377
	LYS	GLY	L299	T379		LYS	L299	T379
	PRO	THR	I300	T379		PRO	I300	T379
	ARG	HIS		N381		ARG		N381
	LYS	LYS	W304	L380		LYS	W304	L380
	ARG	PHE	G305	N382		PHE	G305	N382
	LEU	ASP	F306	G383		LEU	F306	G383
	ASN	SER	R307	A386		ASN	R307	A386
	GLY	THR	P308	V387		GLY	P308	V387
	LYS	TRP		G388		LYS		G388
	GLY	MET	F313	R389		GLY	F313	R389
	ARG	PHE	K314	S390		ARG	K314	S390
	ALA	ASN	N317	S391		ALA	N317	S391
	GLY	GLY		F392		GLY		F392
	VAL	LEU				VAL		
	PHE	ALA				PHE		
	GLN	ASP				GLN		



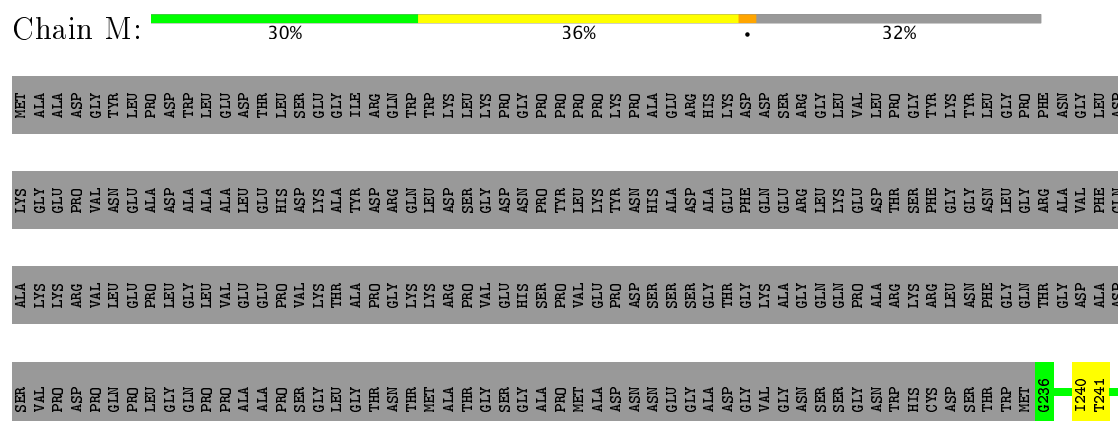
• Molecule 1: Capsid protein VP1



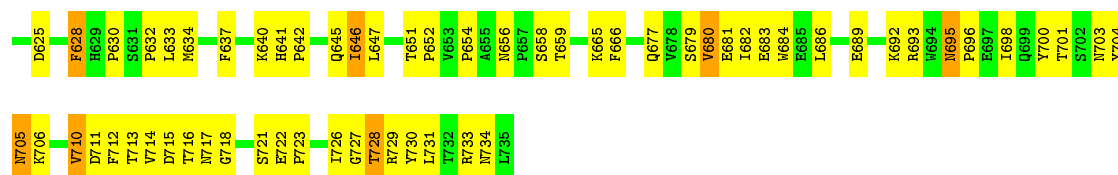
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

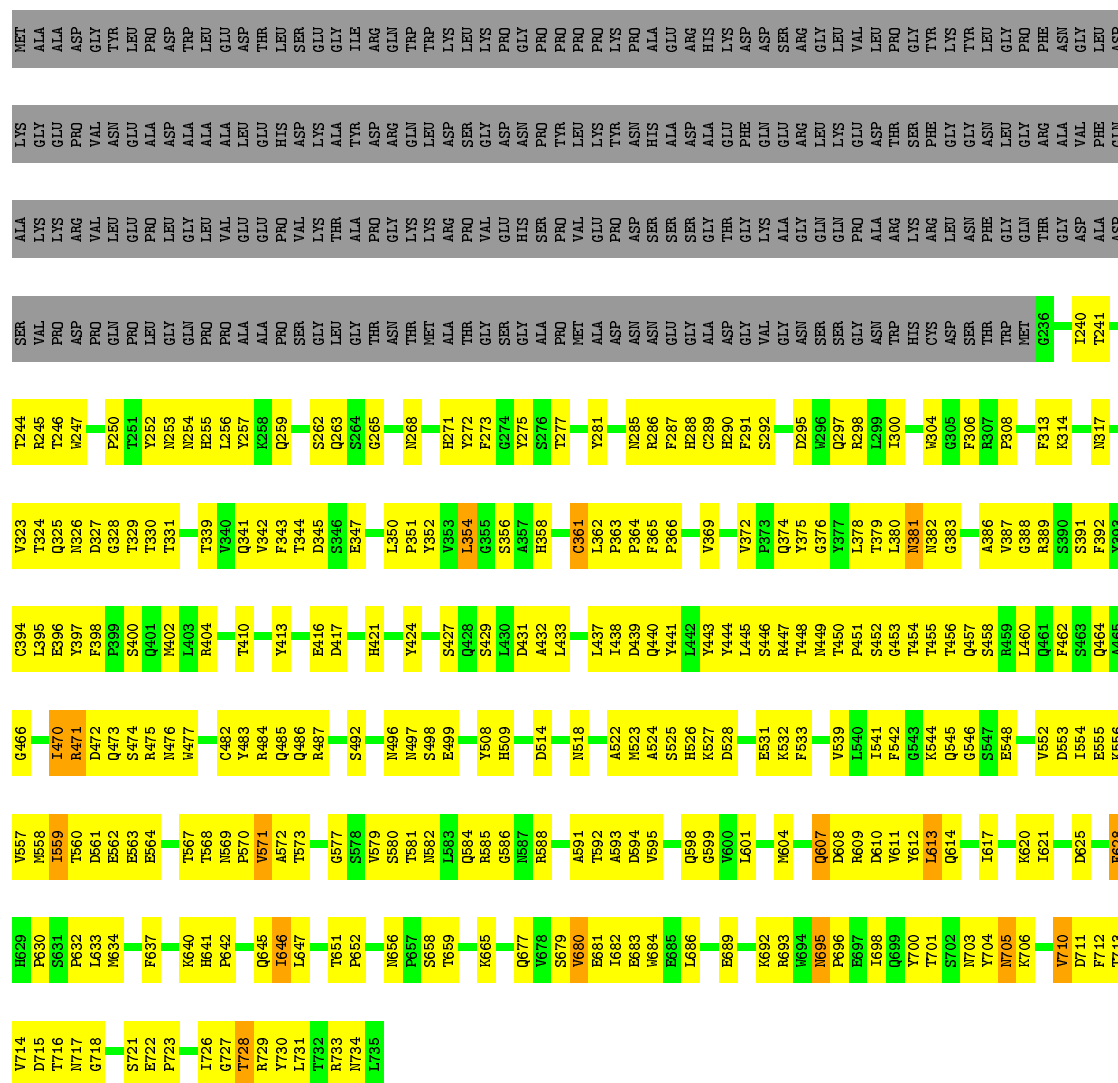






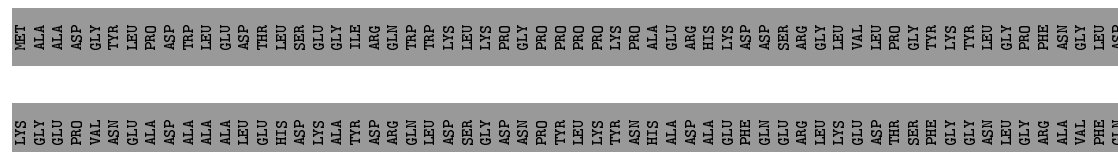
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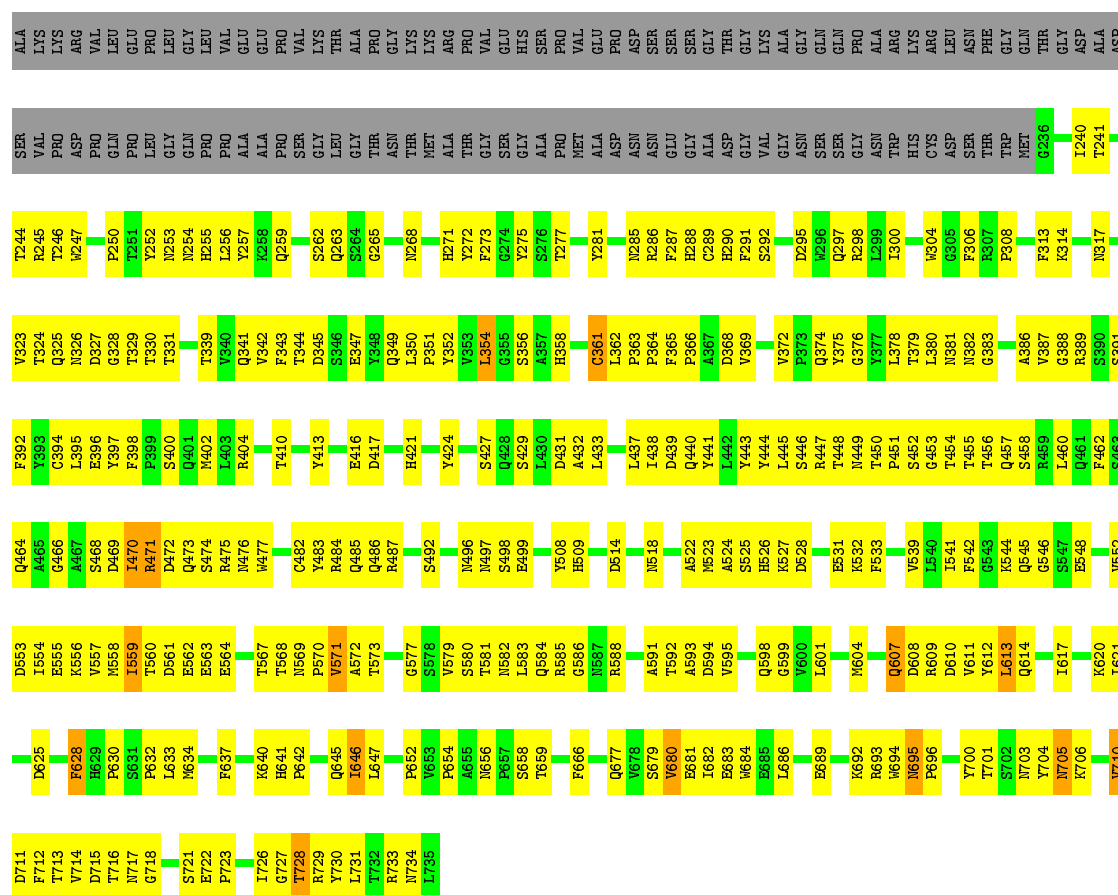
Chain O: 30% 36% 32%



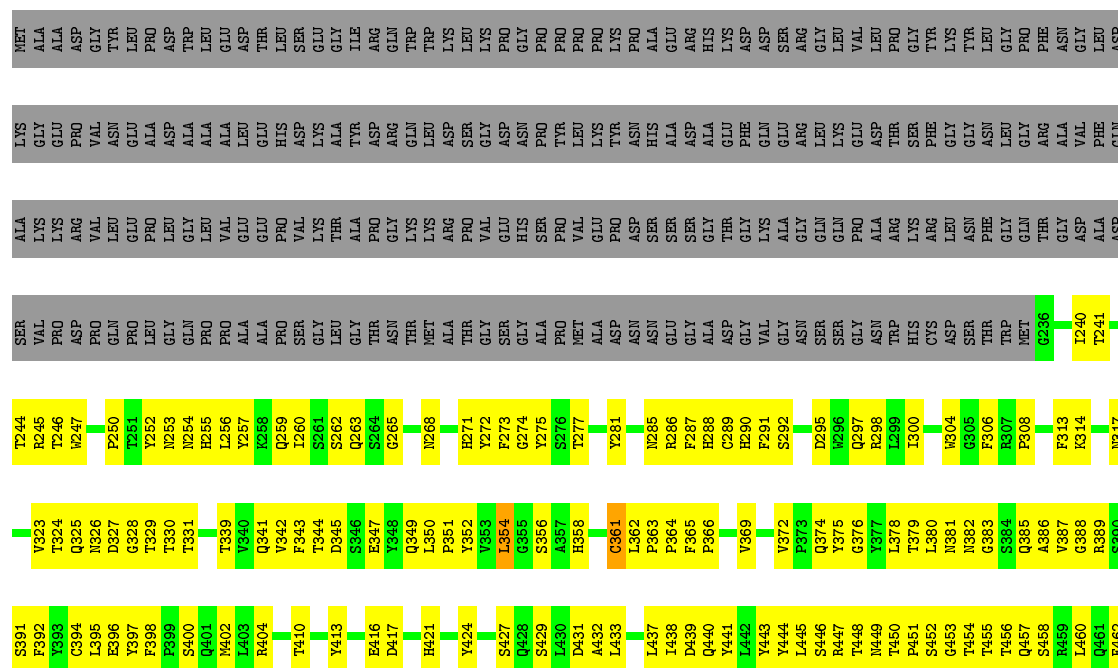
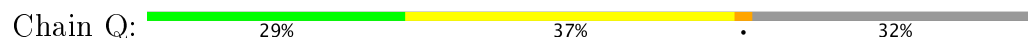
• Molecule 1: Capsid protein VP1

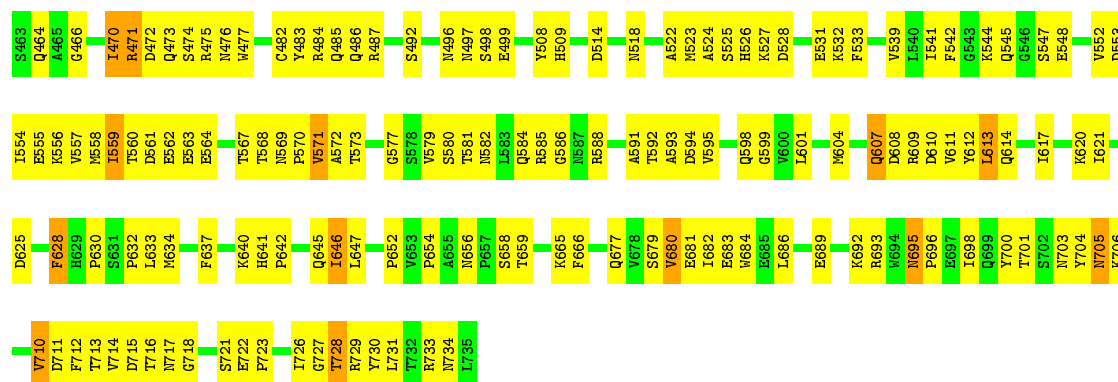
Chain P: 29% 37% 32%





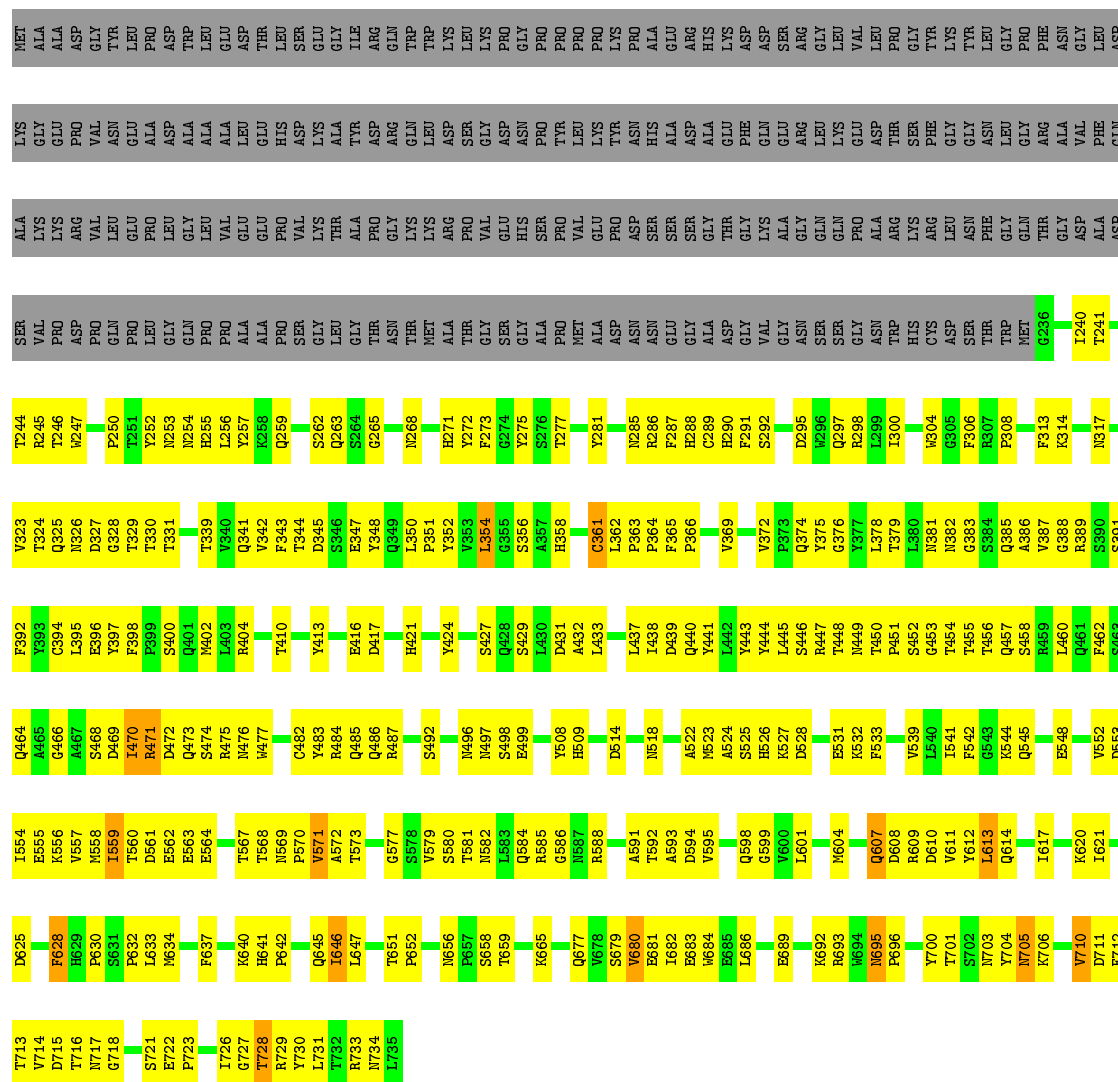
- Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

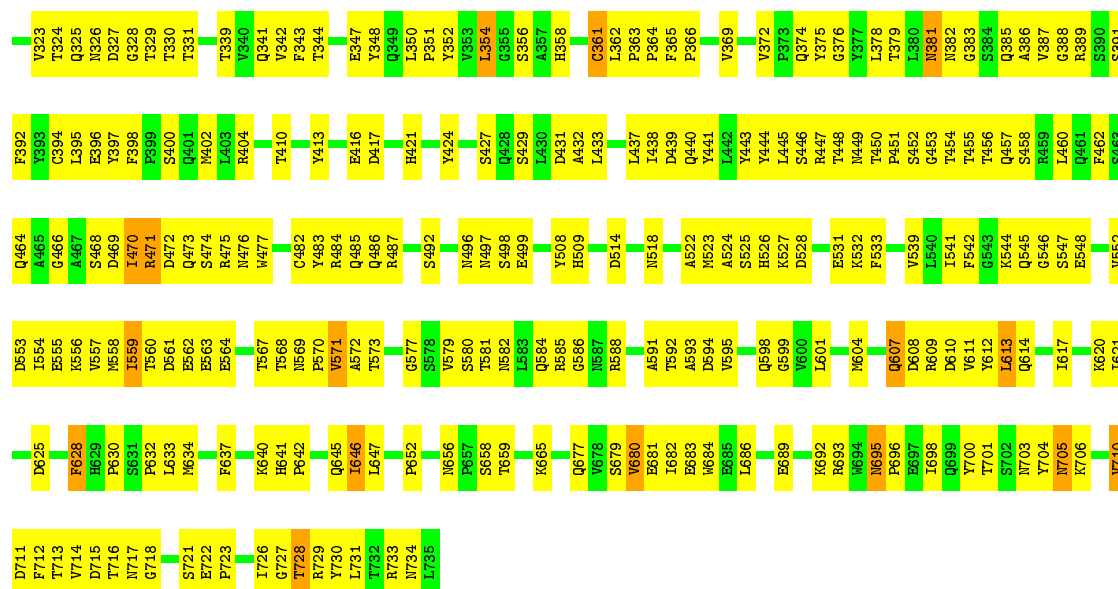
Chain R: 30% 36% 32%



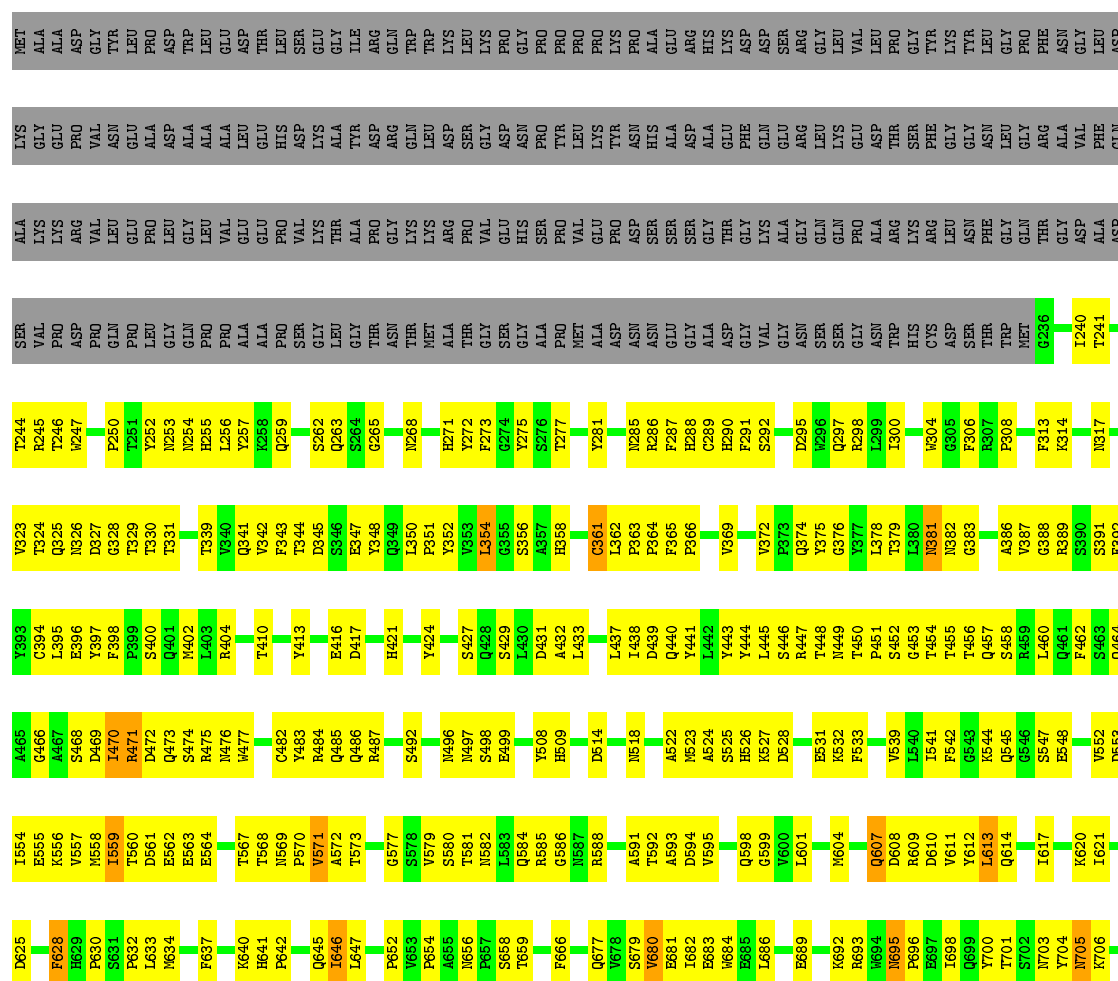
• Molecule 1: Capsid protein VP1

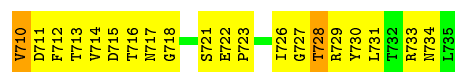
Chain S: 30% 36% 32%

T244	T245	T246	T247	P250	T251	T252	T253	T254	T255	T256	T257	T258	T259	T260	T261	T262	T263	T264	T265	T266	T267	T268	T269	T270	T271	T272	T273	T274	T275	T276	T277	T278	T279	T280	T281	T282	T283	T284	T285	T286	T287	T288	T289	T290	T291	T292	T293	T294	T295	T296	T297	T298	T299	I300	I301	I302	I303	I304	I305	I306	I307	I308	I309	I310	I311	I312	I313	I314	I315	I316	I317	I318	I319	I320	I321	I322	I323	I324	I325	I326	I327	I328	I329	I330	I331	I332	I333	I334	I335	I336	I337	I338	I339	I340	I341	I342	I343	I344	I345	I346	I347	I348	I349	I350	I351	I352	I353	I354	I355	I356	I357	I358	I359	I360	I361	I362	I363	I364	I365	I366	I367	I368	I369	I370	I371	I372	I373	I374	I375	I376	I377	I378	I379	I380	I381	I382	I383	I384	I385	I386	I387	I388	I389	I390	I391	I392	I393	I394	I395	I396	I397	I398	I399	I400	I401	I402	I403	I404	I405	I406	I407	I408	I409	I410	I411	I412	I413	I414	I415	I416	I417	I418	I419	I420	I421	I422	I423	I424	I425	I426	I427	I428	I429	I430	I431	I432	I433	I434	I435	I436	I437	I438	I439	I440	I441	I442	I443	I444	I445	I446	I447	I448	I449	I450	I451	I452	I453	I454	I455	I456	I457	I458	I459	I460	I461	I462	I463	I464	I465	I466	I467	I468	I469	I470	I471	I472	I473	I474	I475	I476	I477	I478	I479	I480	I481	I482	I483	I484	I485	I486	I487	I488	I489	I490	I491	I492	I493	I494	I495	I496	I497	I498	I499	I500	I501	I502	I503	I504	I505	I506	I507	I508	I509	I510	I511	I512	I513	I514	I515	I516	I517	I518	I519	I520	I521	I522	I523	I524	I525	I526	I527	I528	I529	I530	I531	I532	I533	I534	I535	I536	I537	I538	I539	I540	I541	I542	I543	I544	I545	I546	I547	I548	I549	I550	I551	I552	I553	I554	I555	I556	I557	I558	I559	I560	I561	I562	I563	I564	I565	I566	I567	I568	I569	I570	I571	I572	I573	I574	I575	I576	I577	I578	I579	I580	I581	I582	I583	I584	I585	I586	I587	I588	I589	I590	I591	I592	I593	I594	I595	I596	I597	I598	I599	I600	I601	I602	I603	I604	I605	I606	I607	I608	I609	I610	I611	I612	I613	I614	I615	I616	I617	I618	I619	I620	I621	I622	I623	I624	I625	I626	I627	I628	I629	I630	I631	I632	I633	I634	I635	I636	I637	I638	I639	I640	I641	I642	I643	I644	I645	I646	I647	I648	I649	I650	I651	I652	I653	I654	I655	I656	I657	I658	I659	I660	I661	I662	I663	I664	I665	I666	I667	I668	I669	I670	I671	I672	I673	I674	I675	I676	I677	I678	I679	I680	I681	I682	I683	I684	I685	I686	I687	I688	I689	I690	I691	I692	I693	I694	I695	I696	I697	I698	I699	I700	I701	I702	I703	I704	I705	I706	I707	I708	I709	I710	I711	I712	I713	I714	I715	I716	I717	I718	I719	I720	I721	I722	I723	I724	I725	I726	I727	I728	I729	I730	I731	I732	I733	I734	I735	I736	I737	I738	I739	I740	I741	I742	I743	I744	I745	I746	I747	I748	I749	I750	I751	I752	I753	I754	I755	I756	I757	I758	I759	I760	I761	I762	I763	I764	I765	I766	I767	I768	I769	I770	I771	I772	I773	I774	I775	I776	I777	I778	I779	I780	I781	I782	I783	I784	I785	I786	I787	I788	I789	I790	I791	I792	I793	I794	I795	I796	I797	I798	I799	I800	I801	I802	I803	I804	I805	I806	I807	I808	I809	I810	I811	I812	I813	I814	I815	I816	I817	I818	I819	I820	I821	I822	I823	I824	I825	I826	I827	I828	I829	I830	I831	I832	I833	I834	I835	I836	I837	I838	I839	I840	I841	I842	I843	I844	I845	I846	I847	I848	I849	I850	I851	I852	I853	I854	I855	I856	I857	I858	I859	I860	I861	I862	I863	I864	I865	I866	I867	I868	I869	I870	I871	I872	I873	I874	I875	I876	I877	I878	I879	I880	I881	I882	I883	I884	I885	I886	I887	I888	I889	I890	I891	I892	I893	I894	I895	I896	I897	I898	I899	I900	I901	I902	I903	I904	I905	I906	I907	I908	I909	I910	I911	I912	I913	I914	I915	I916	I917	I918	I919	I920	I921	I922	I923	I924	I925	I926	I927	I928	I929	I930	I931	I932	I933	I934	I935	I936	I937	I938	I939	I940	I941	I942	I943	I944	I945	I946	I947	I948	I949	I950	I951	I952	I953	I954	I955	I956	I957	I958	I959	I960	I961	I962	I963	I964	I965	I966	I967	I968	I969	I970	I971	I972	I973	I974	I975	I976	I977	I978	I979	I980	I981	I982	I983	I984	I985	I986	I987	I988	I989	I990	I991	I992	I993	I994	I995	I996	I997	I998	I999	I1000	I1001	I1002	I1003	I1004	I1005	I1006	I1007	I1008	I1009	I1010	I1011	I1012	I1013	I1014	I1015	I1016	I1017	I1018	I1019	I1020	I1021	I1022	I1023	I1024	I1025	I1026	I1027	I1028	I1029	I1030	I1031	I1032	I1033	I1034	I1035	I1036	I1037	I1038	I1039	I1040	I1041	I1042	I1043	I1044	I1045	I1046	I1047	I1048	I1049	I1050	I1051	I1052	I1053	I1054	I1055	I1056	I1057	I1058	I1059	I1060	I1061	I1062	I1063	I1064	I1065	I1066	I1067	I1068	I1069	I1070	I1071	I1072	I1073	I1074	I1075	I1076	I1077	I1078	I1079	I1080	I1081	I1082	I1083	I1084	I1085	I1086	I1087	I1088	I1089	I1090	I1091	I1092	I1093	I1094	I1095	I1096	I1097	I1098	I1099	I1100	I1101	I1102	I1103	I1104	I1105	I1106	I1107	I1108	I1109	I1110	I1111	I1112	I1113	I1114	I1115	I1116	I1117	I1118	I1119	I1120	I1121	I1122	I1123	I1124	I1125	I1126	I1127	I1128	I1129	I1130	I1131	I1132	I1133	I1134	I1135	I1136	I1137	I1138	I1139	I1140	I1141	I1142	I1143	I1144	I1145	I1146	I1147	I1148	I1149	I1150	I1151	I1152	I1153	I1154	I1155	I1156	I1157	I1158	I1159	I1160	I1161	I1162	I1163	I1164	I1165	I1166	I1167	I1168	I1169	I1170	I1171	I1172	I1173	I1174	I1175	I1176	I1177	I1178	I1179	I1180	I1181	I1182	I1183	I1184	I1185	I1186	I1187	I1188	I1189	I1190	I1191	I1192	I1193	I1194	I1195	I1196	I1197	I1198	I1199	I1200	I1201	I1202	I1203	I1204	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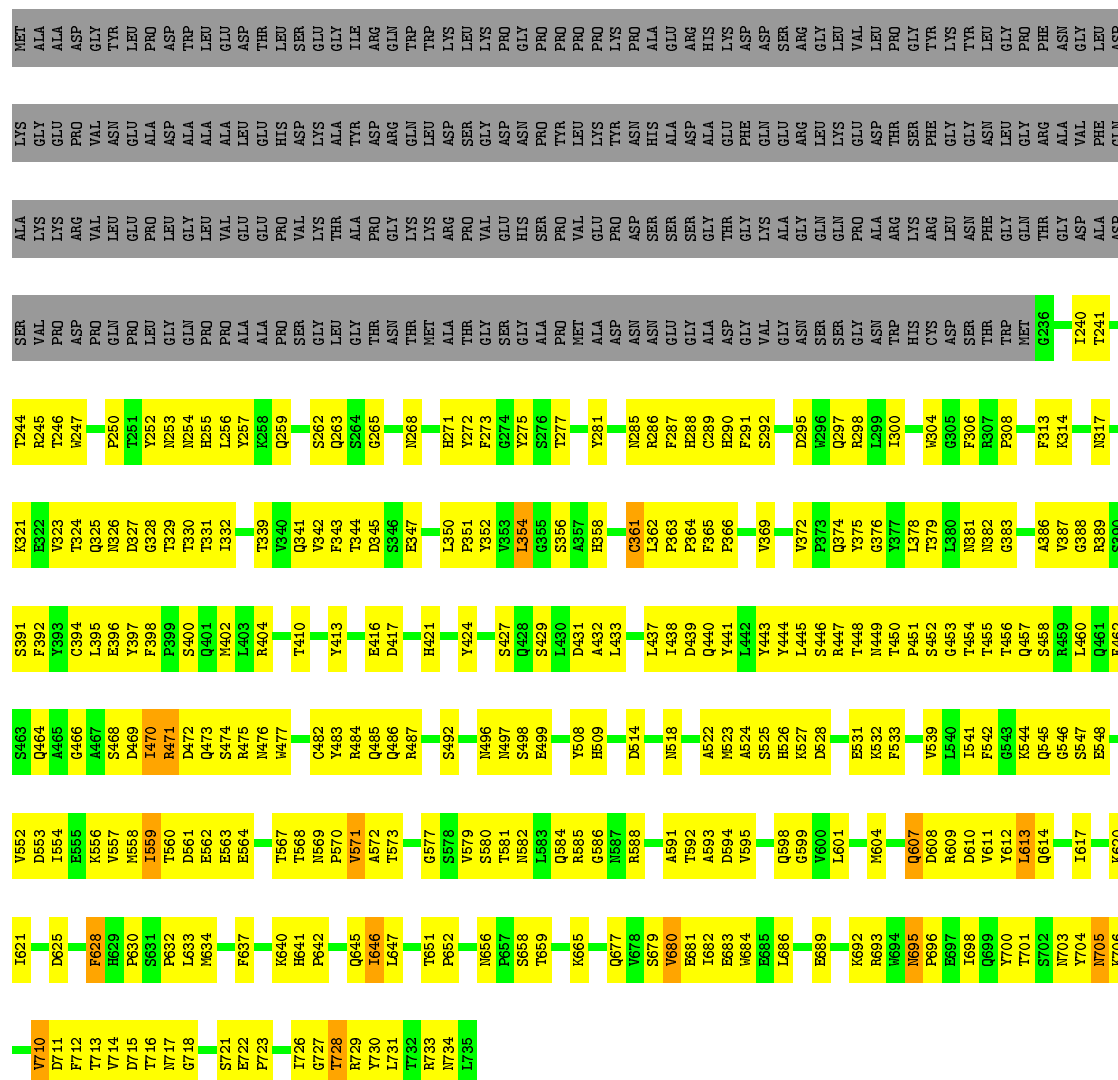
• Molecule 1: Capsid protein VP1





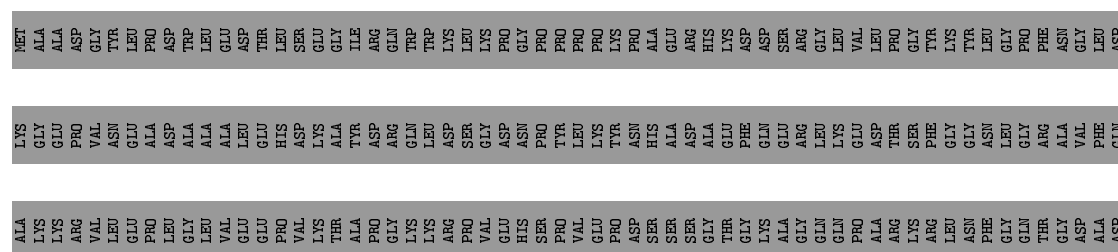
• Molecule 1: Capsid protein VP1

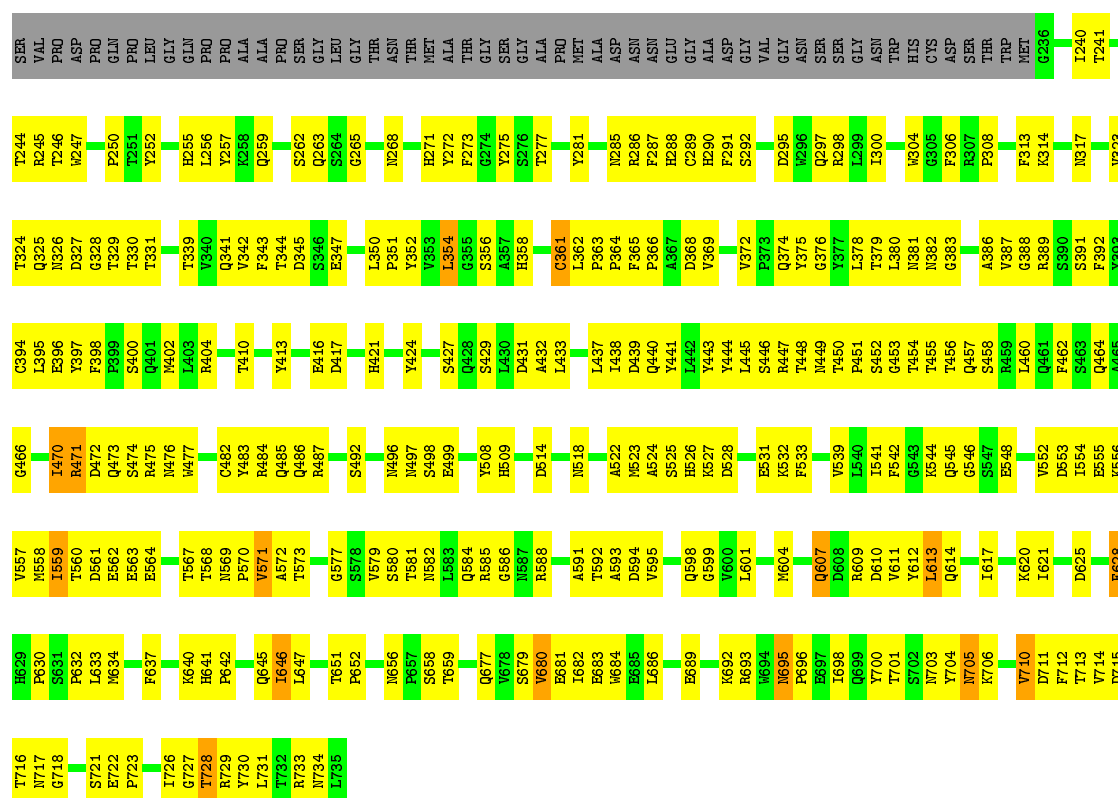
Chain V: 30% 36% 32%



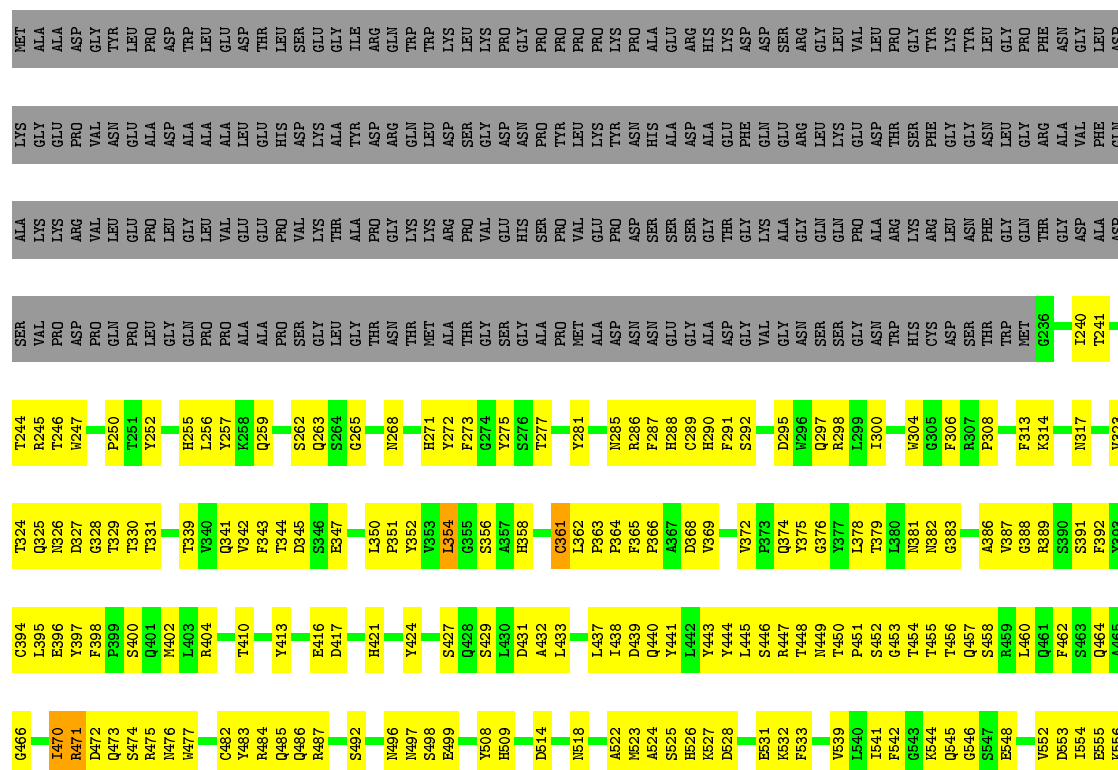
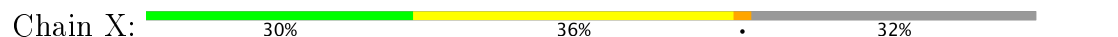
• Molecule 1: Capsid protein VP1

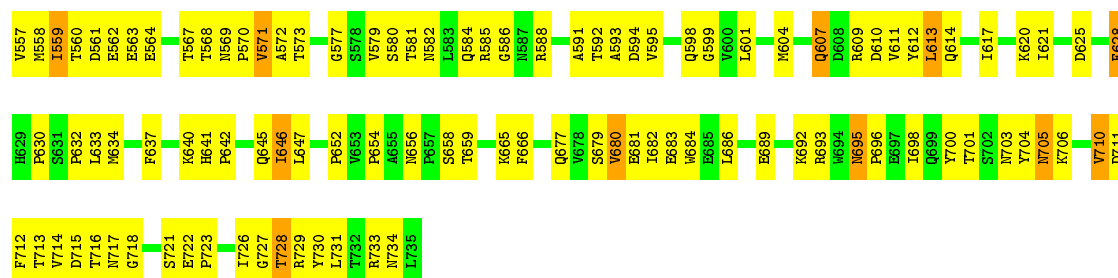
Chain W: 30% 36% 32%





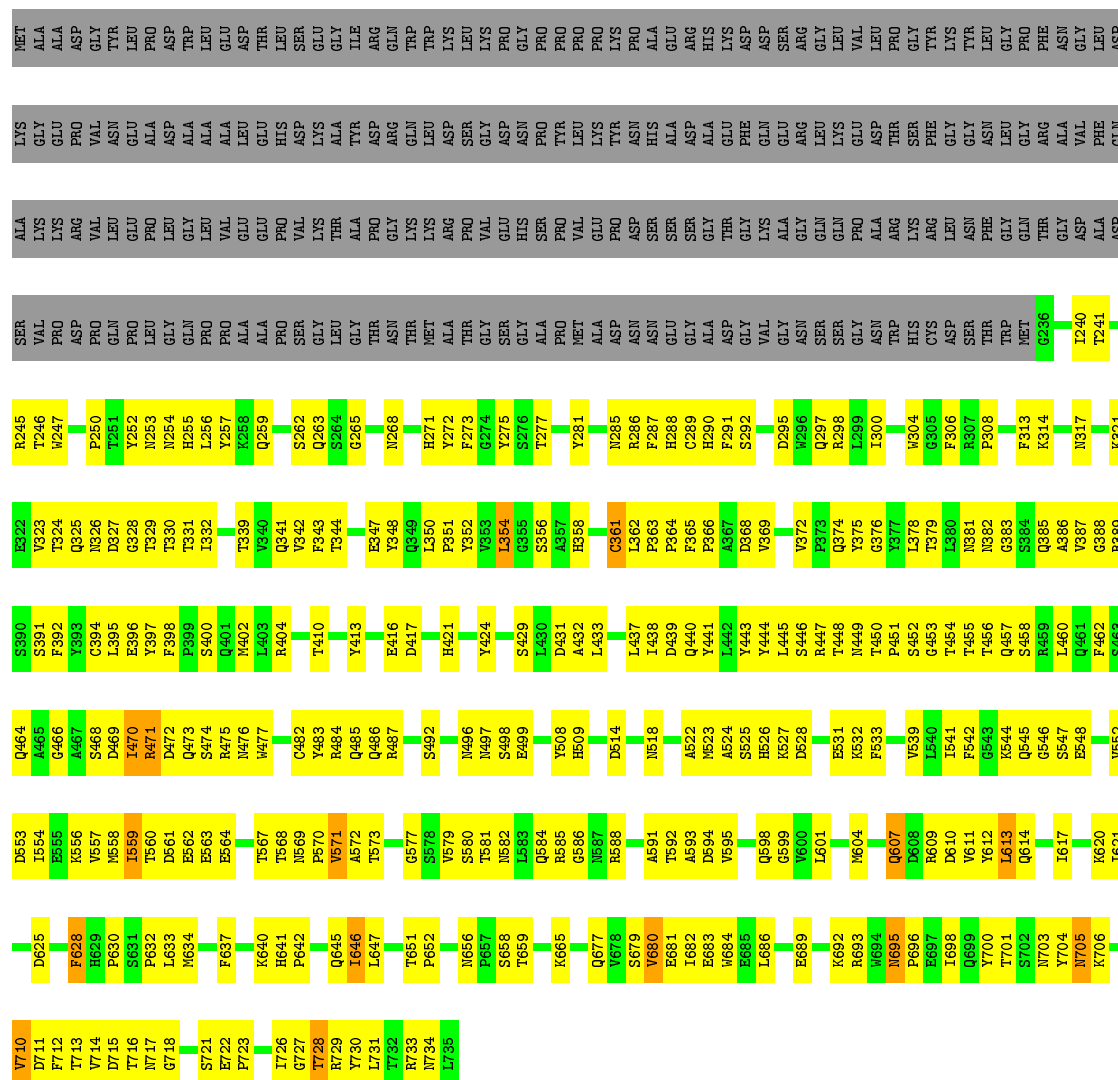
- Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

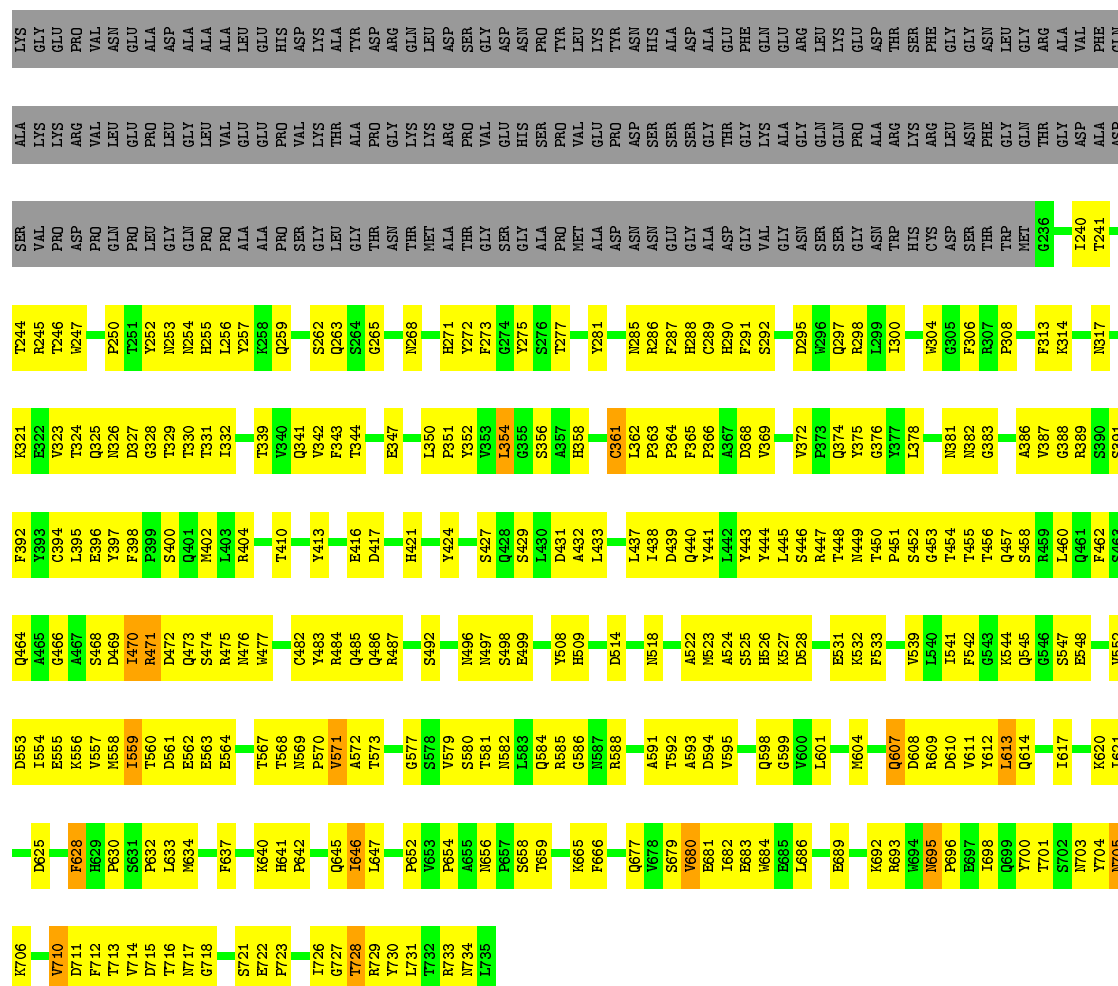
Chain Y: 30% 36% 32%



• Molecule 1: Capsid protein VP1

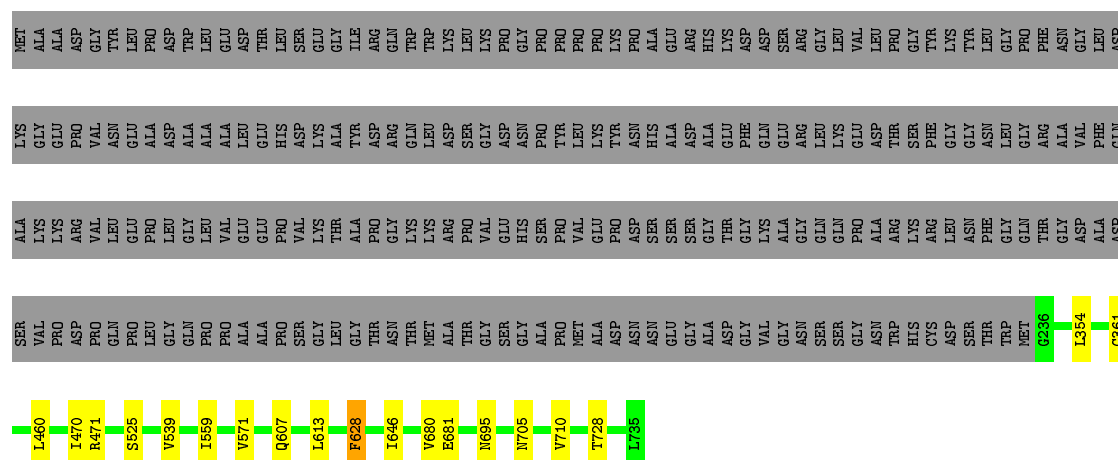
Chain Z: 30% 36% 32%





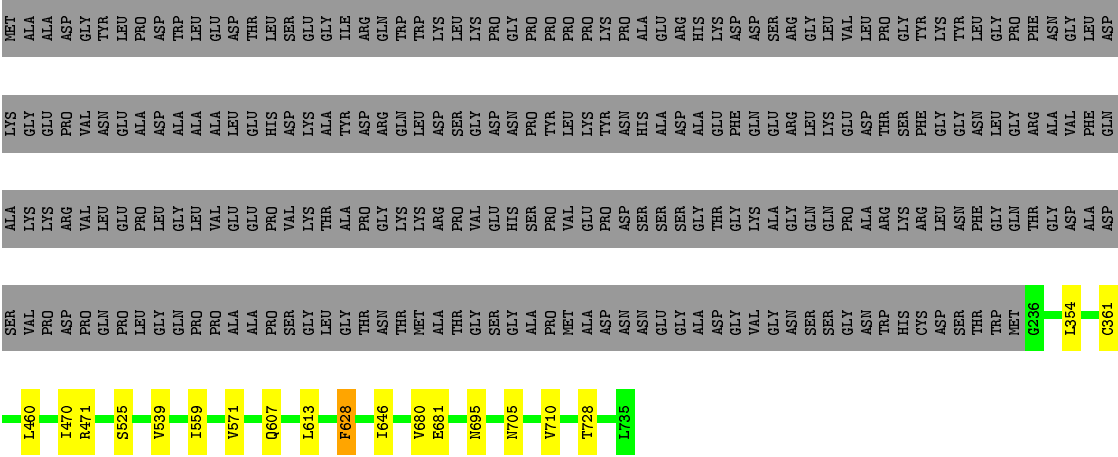
- Molecule 1: Capsid protein VP1

Chain a: 65% 32%



- Molecule 1: Capsid protein VP1

Chain b: 65% 32%

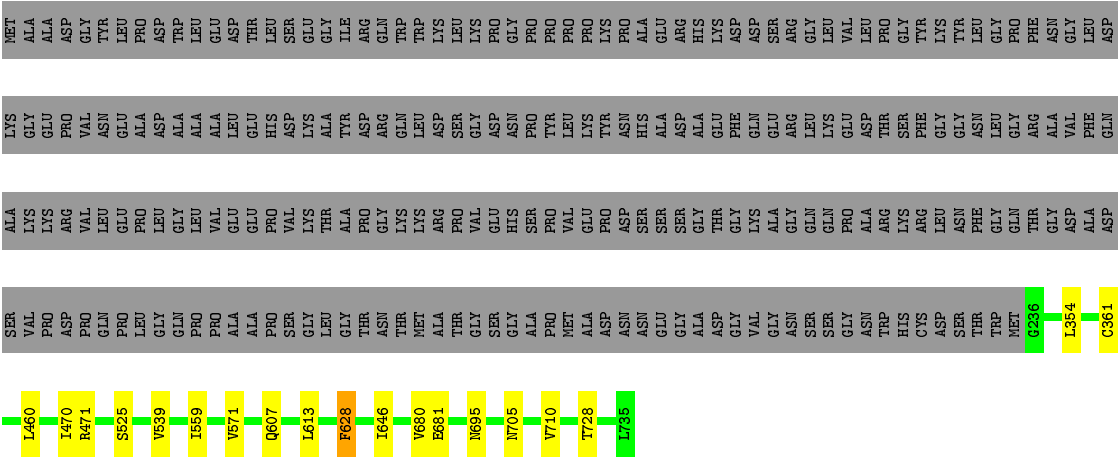


● Molecule 1: Capsid protein VP1

Chain c:

65%

32%

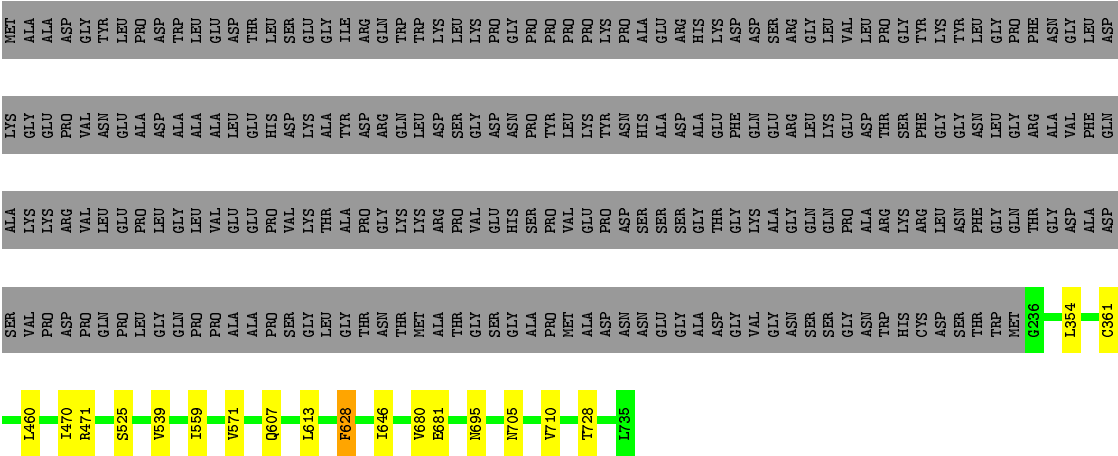


● Molecule 1: Capsid protein VP1

Chain d:

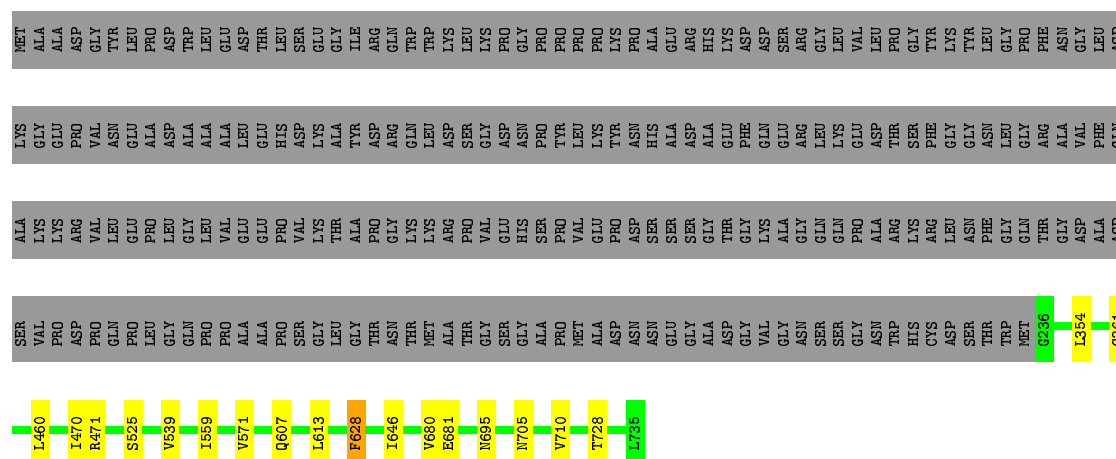
65%

32%



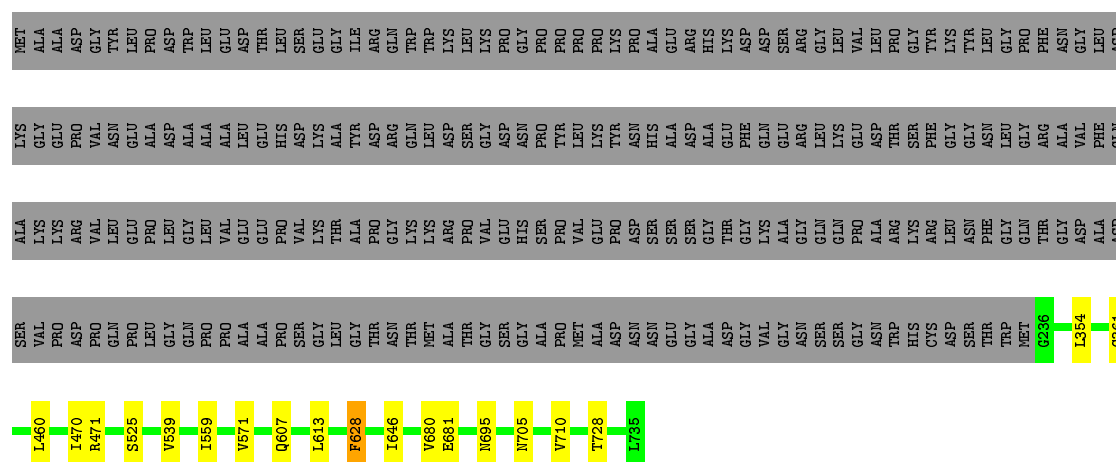
● Molecule 1: Capsid protein VP1

Chain e:



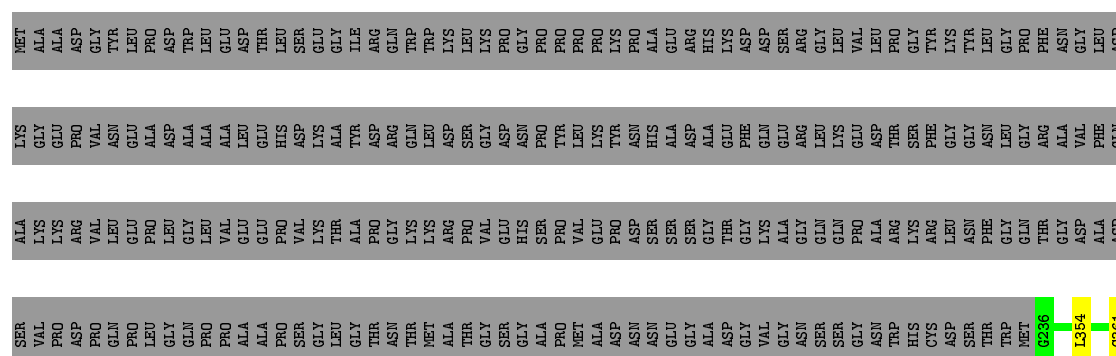
- Molecule 1: Capsid protein VP1

Chain f:



- Molecule 1: Capsid protein VP1

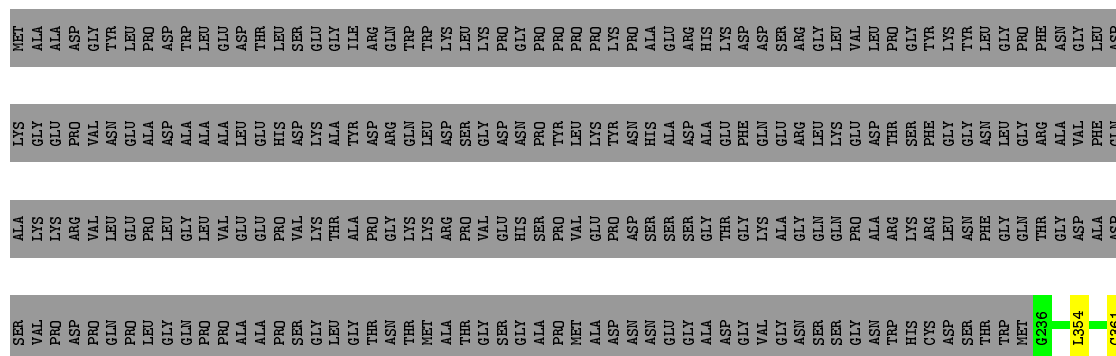
Chain g:





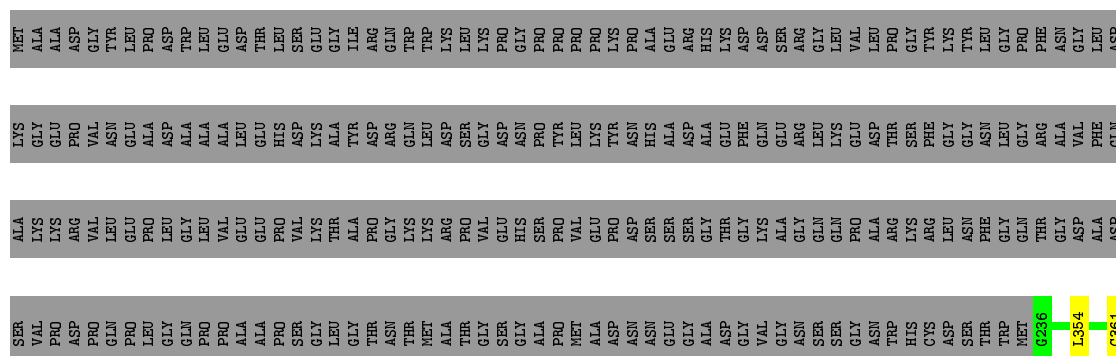
- Molecule 1: Capsid protein VP1

Chain h: 65% . 32%



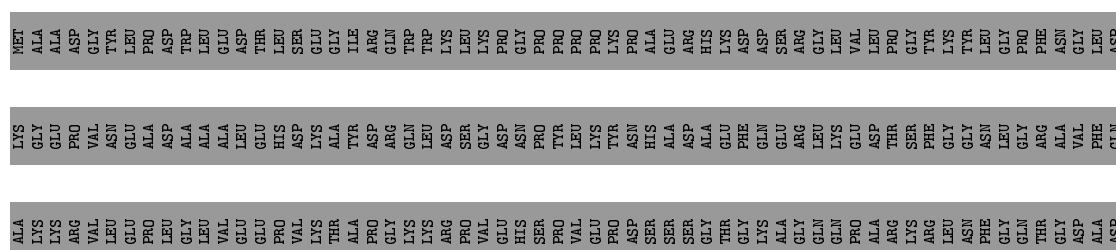
- Molecule 1: Capsid protein VP1

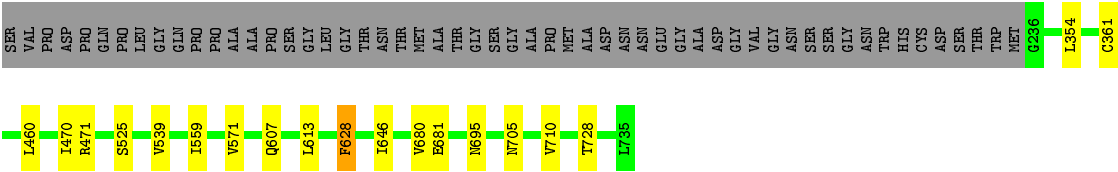
Chain i:  65% • 32%



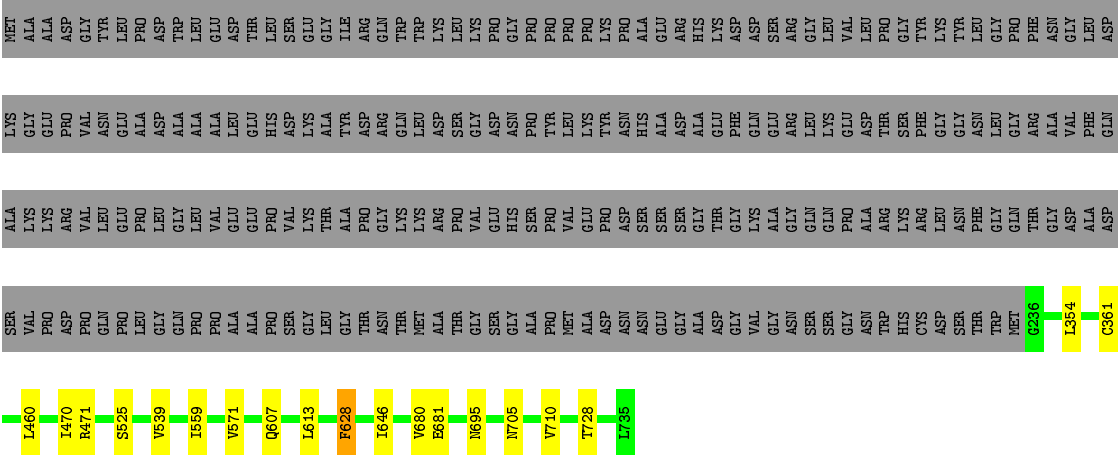
- Molecule 1: Capsid protein VP1

Chain j:  65% . 32%

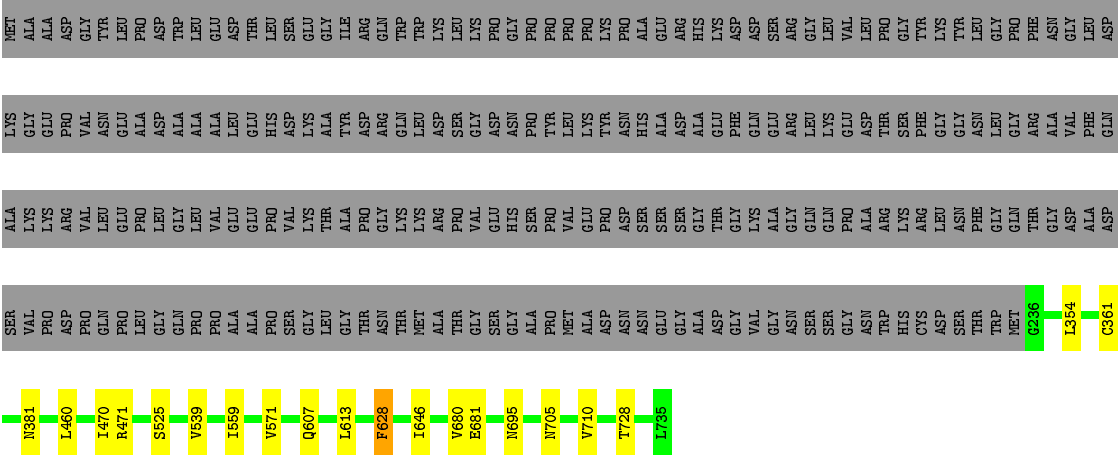




• Molecule 1: Capsid protein VP1

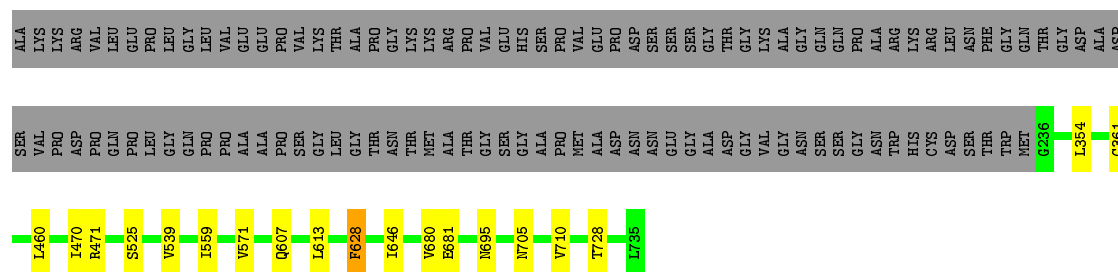


• Molecule 1: Capsid protein VP1

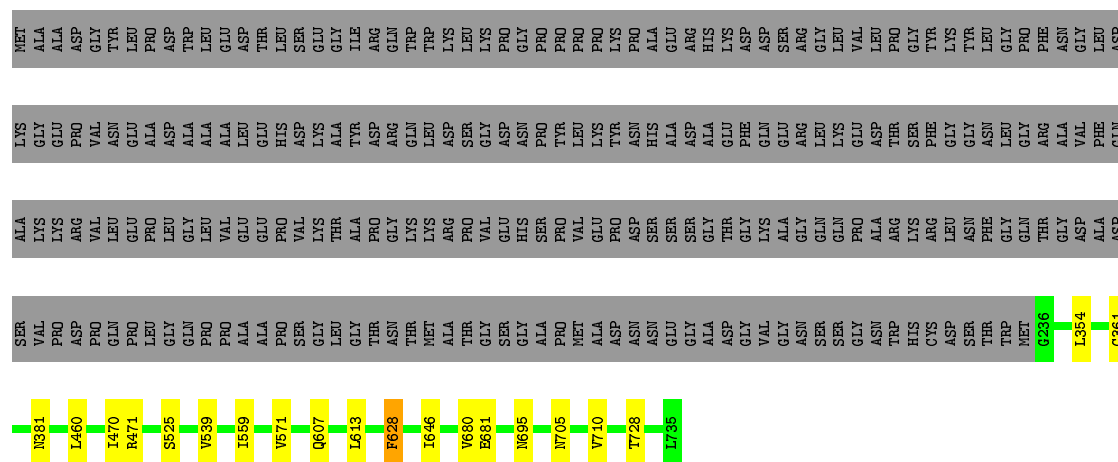


• Molecule 1: Capsid protein VP1

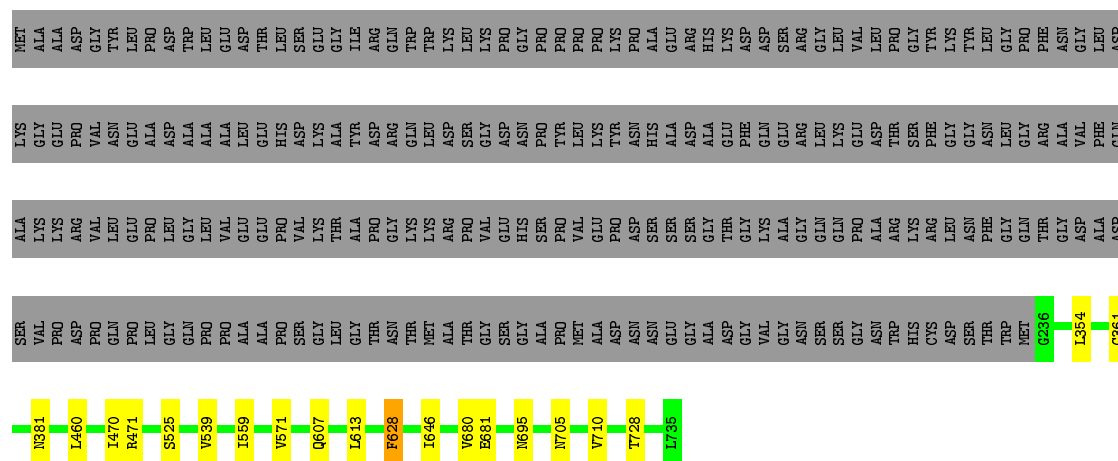




- Molecule 1: Capsid protein VP1

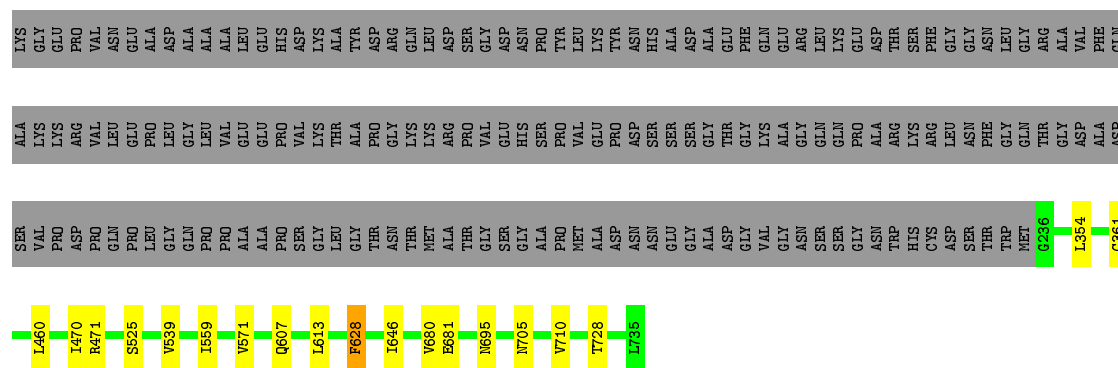


- Molecule 1: Capsid protein VP1

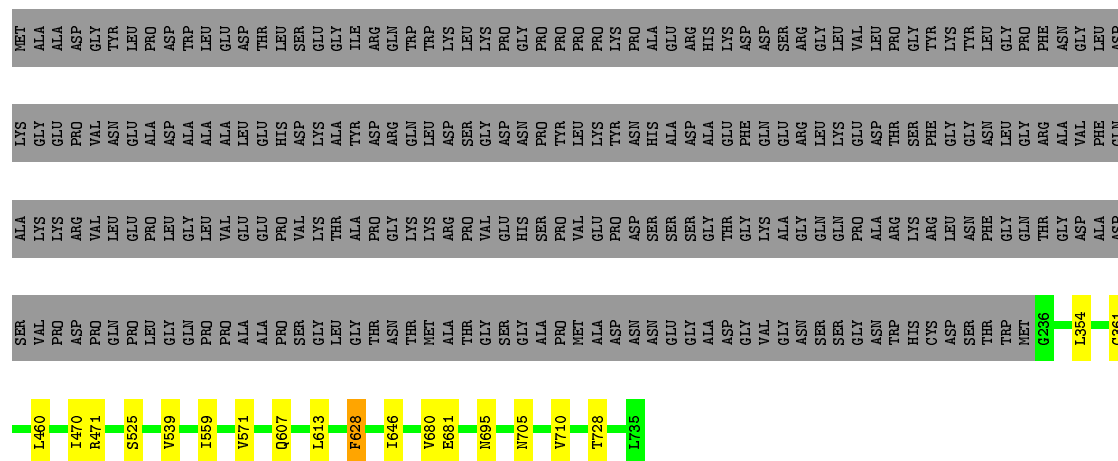


- Molecule 1: Capsid protein VP1

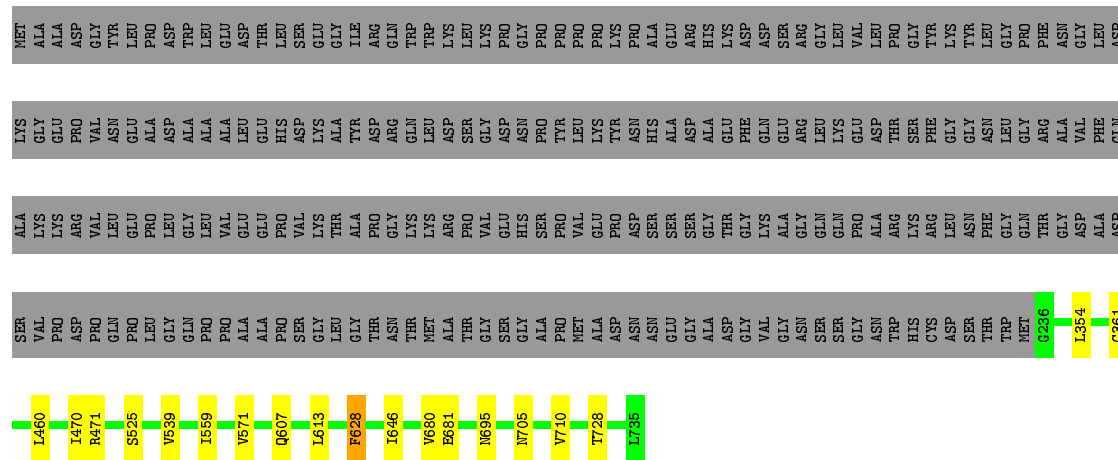




- Molecule 1: Capsid protein VP1

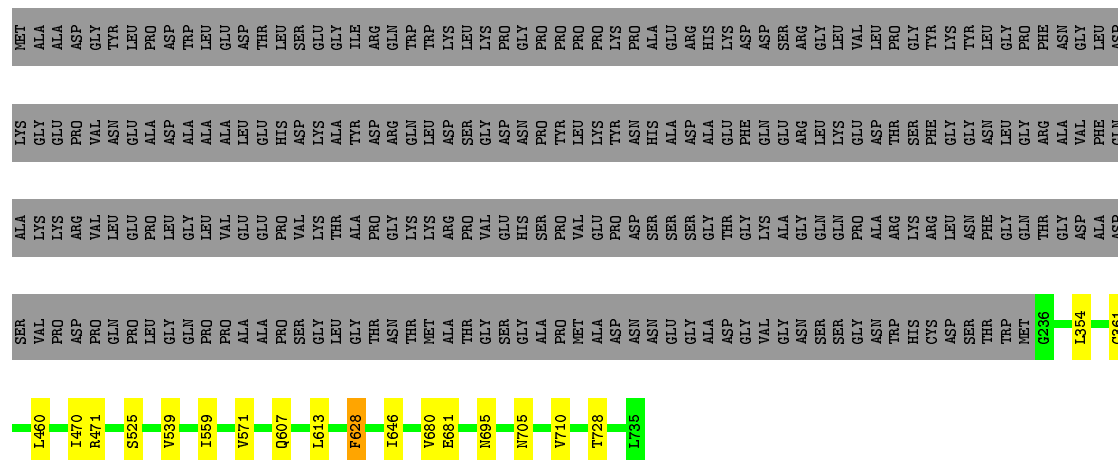


- Molecule 1: Capsid protein VP1



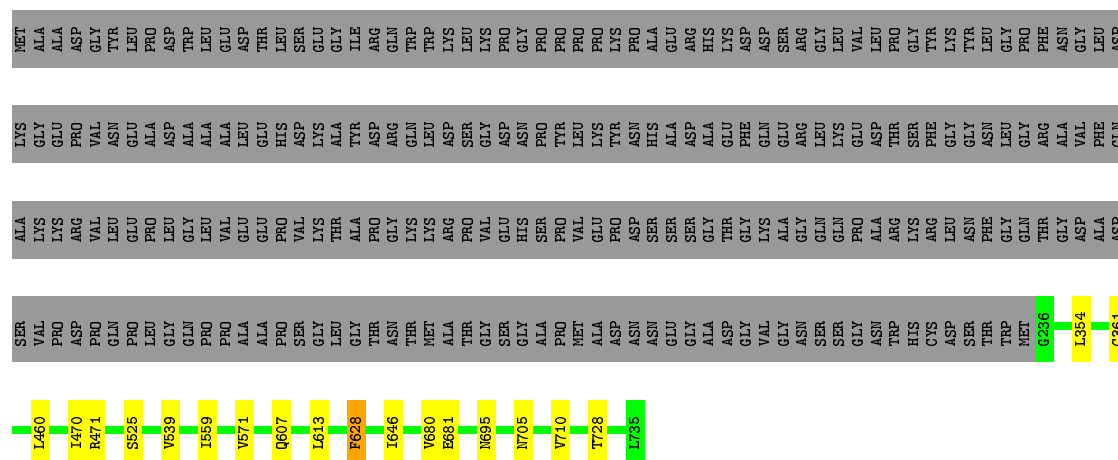
- Molecule 1: Capsid protein VP1





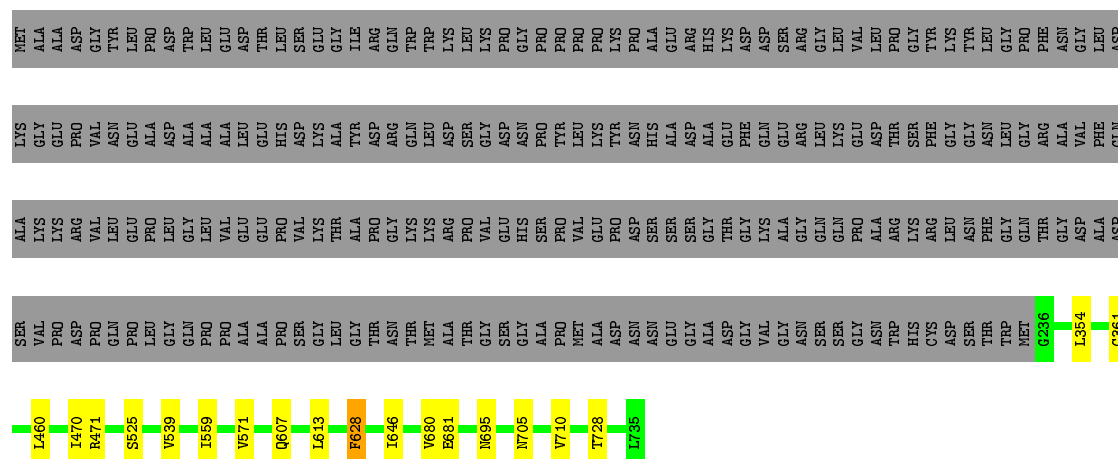
• Molecule 1: Capsid protein VP1

Chain t: 65% 32%



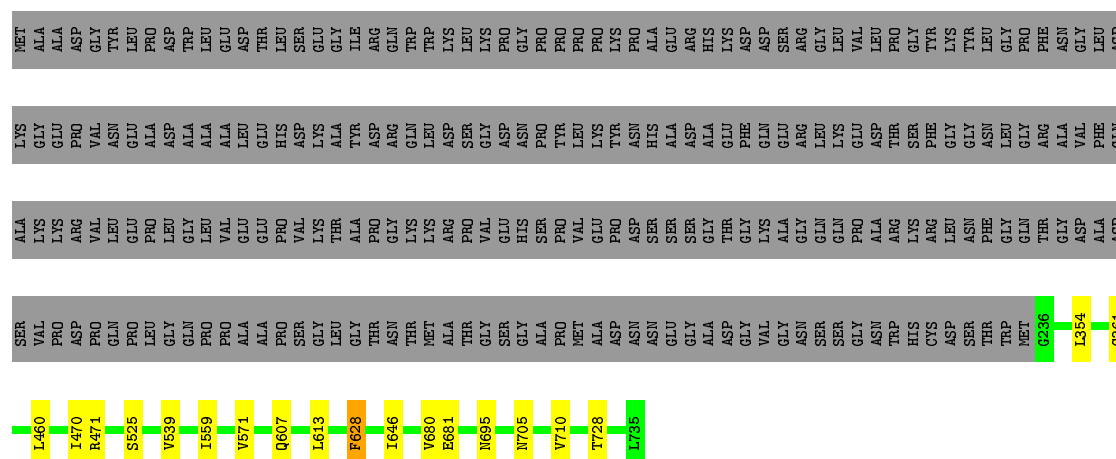
• Molecule 1: Capsid protein VP1

Chain u: 65% 32%



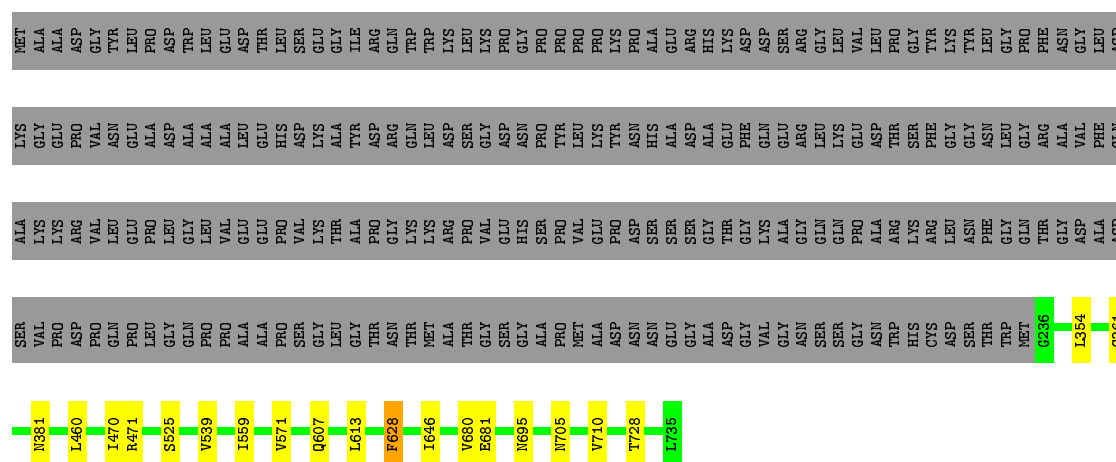
• Molecule 1: Capsid protein VP1

Chain v:



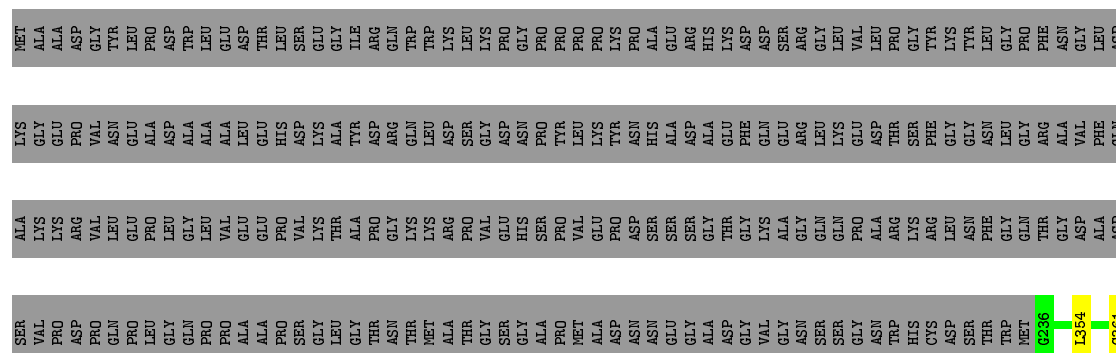
- Molecule 1: Capsid protein VP1

Chain w:



- Molecule 1: Capsid protein VP1

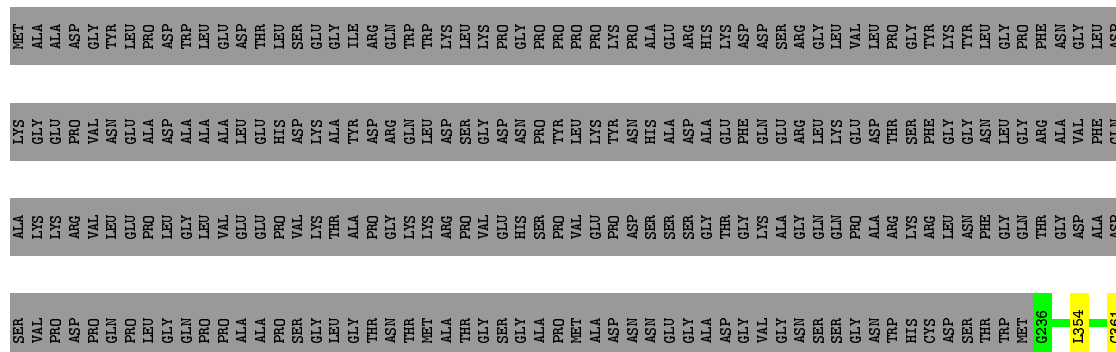
Chain x:





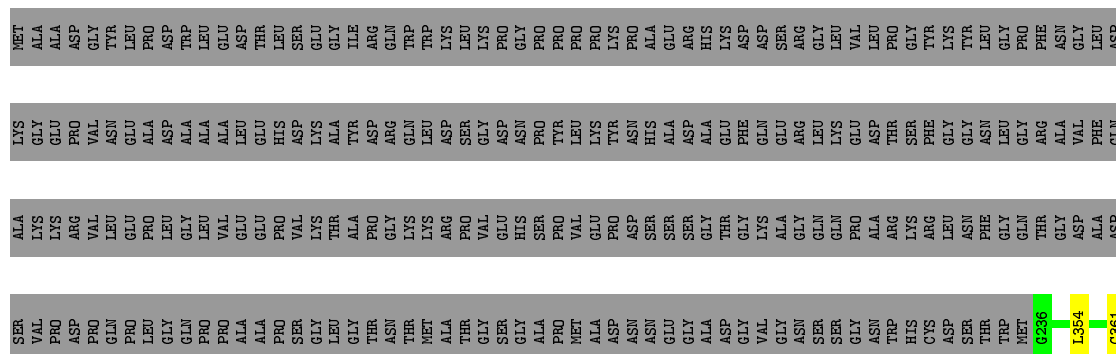
- Molecule 1: Capsid protein VP1

Chain y:  65% . 32%



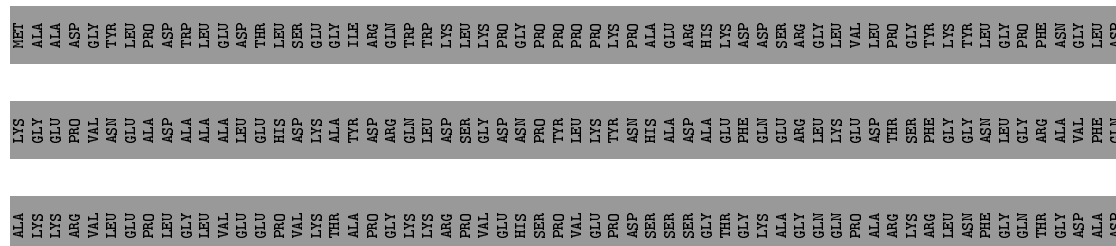
- Molecule 1: Capsid protein VP1

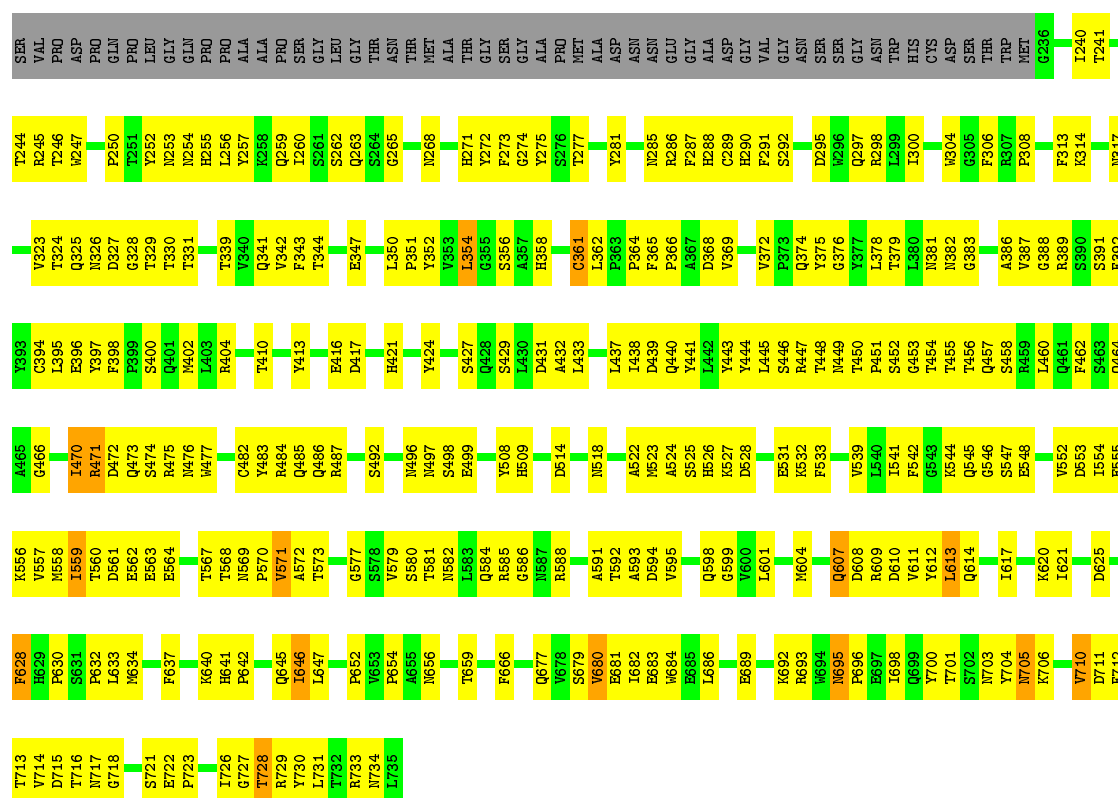
Chain z: 65% . 32%



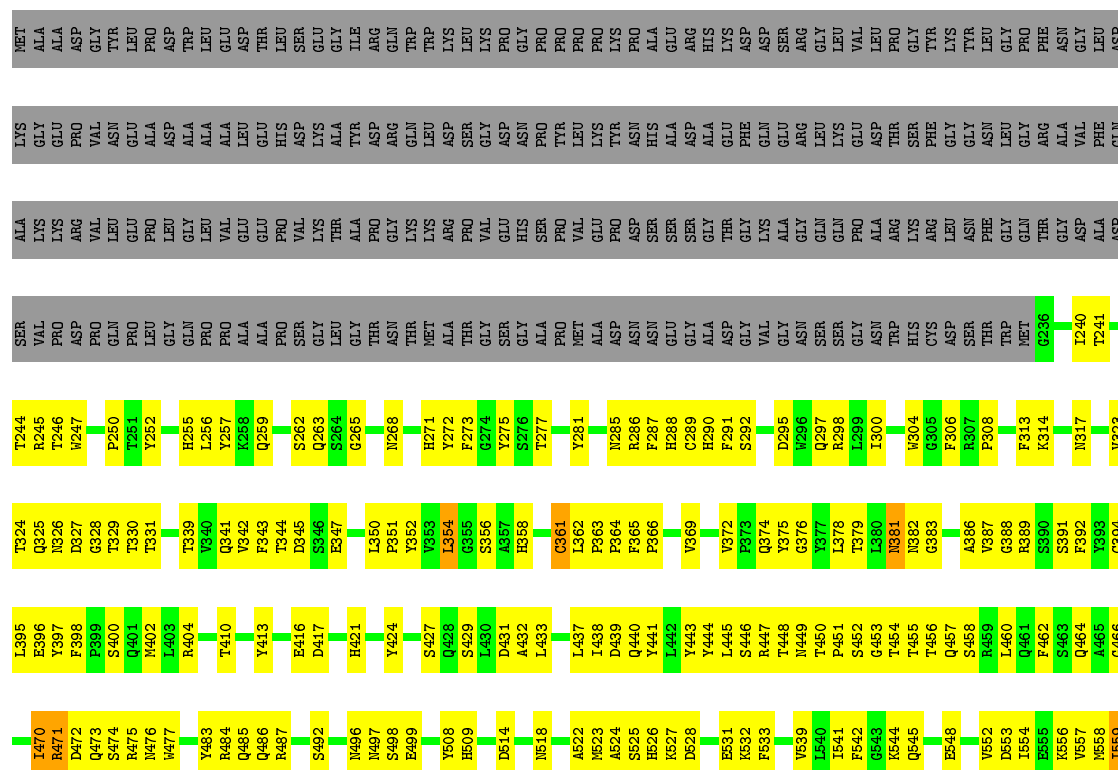
- Molecule 1: Capsid protein VP1

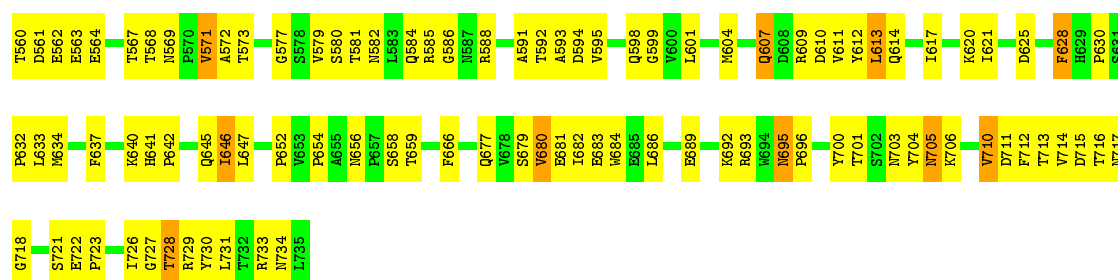
Chain 1: 30% 36% . 32%



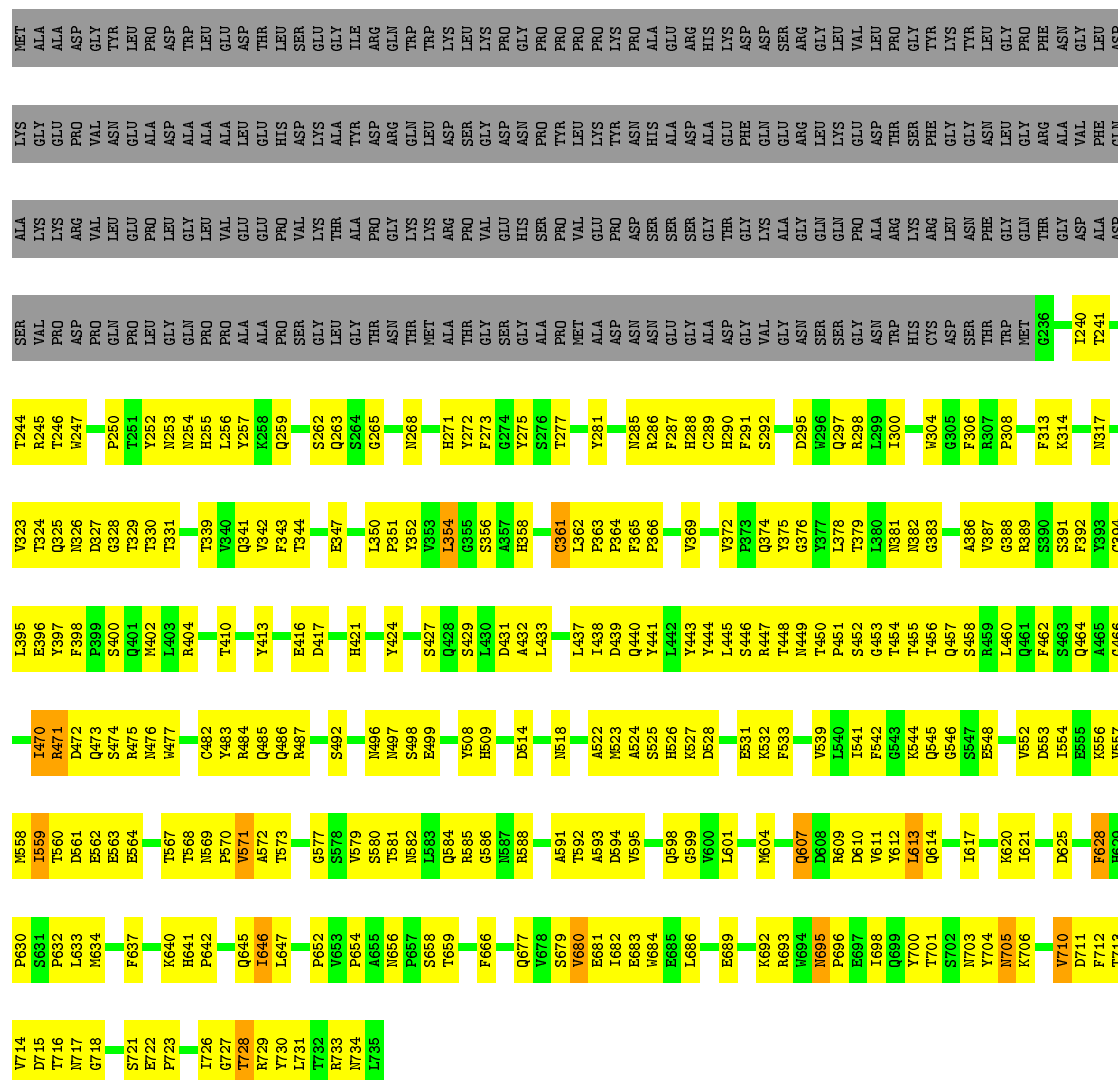


- Molecule 1: Capsid protein VP1



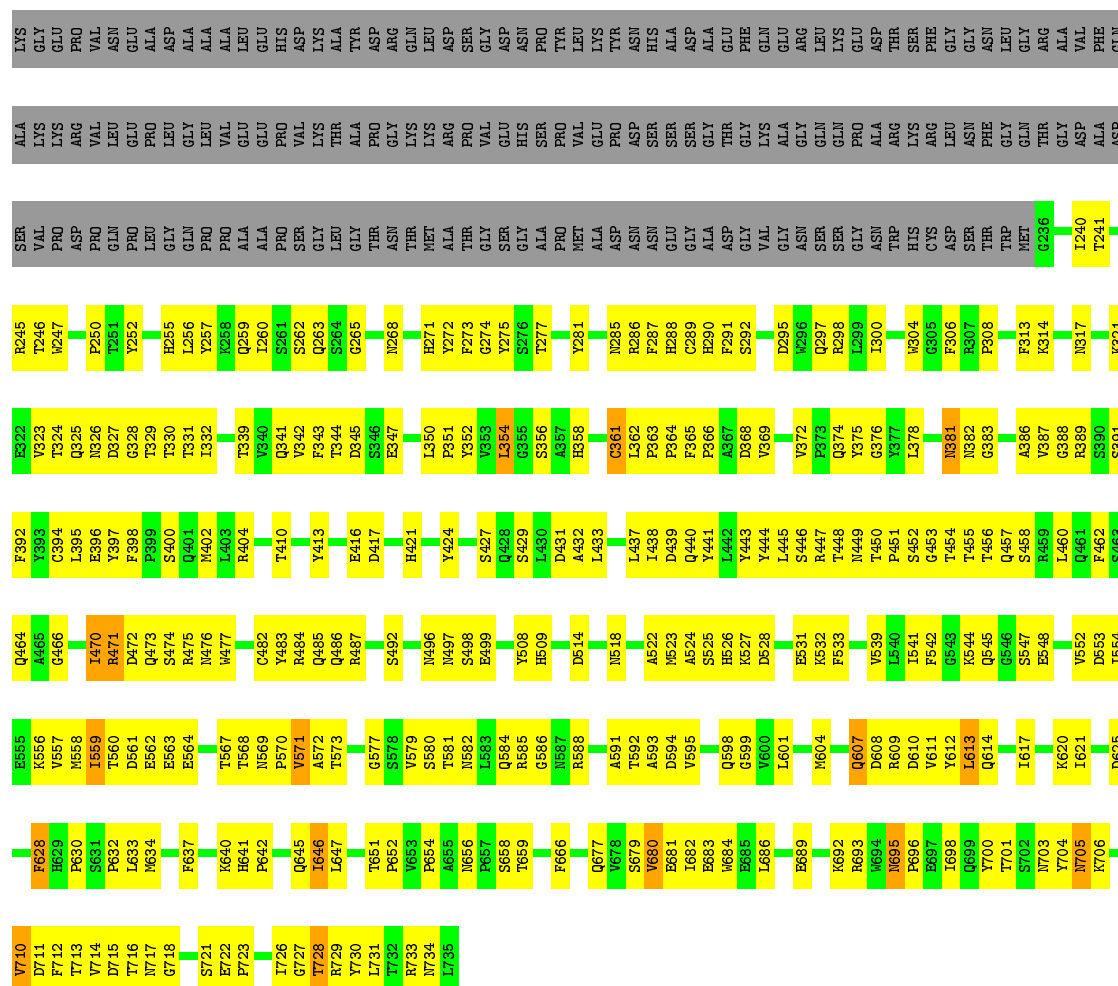


- Molecule 1: Capsid protein VP1



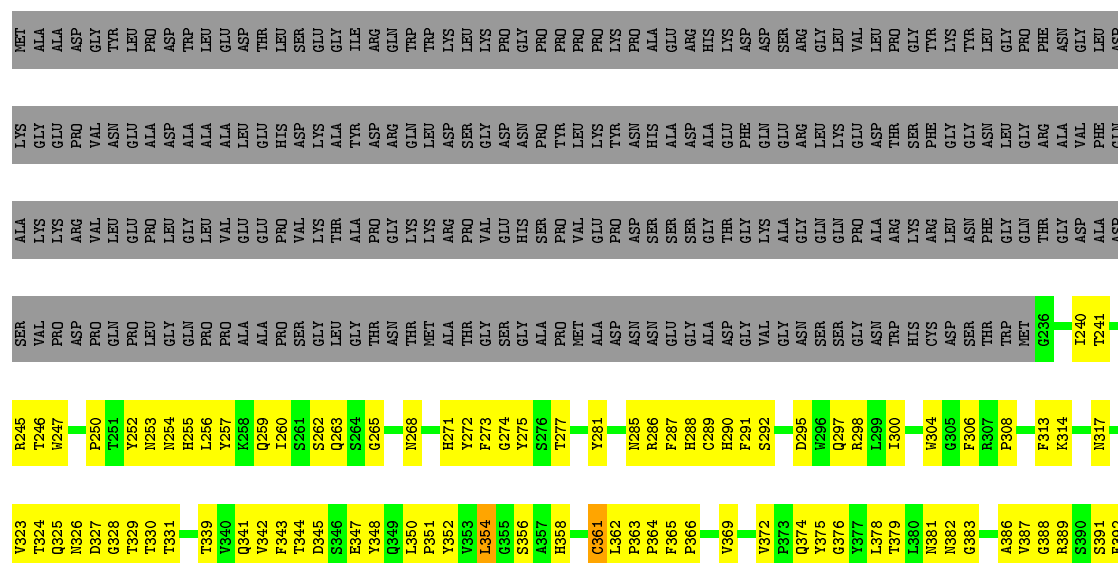
- Molecule 1: Capsid protein VP1



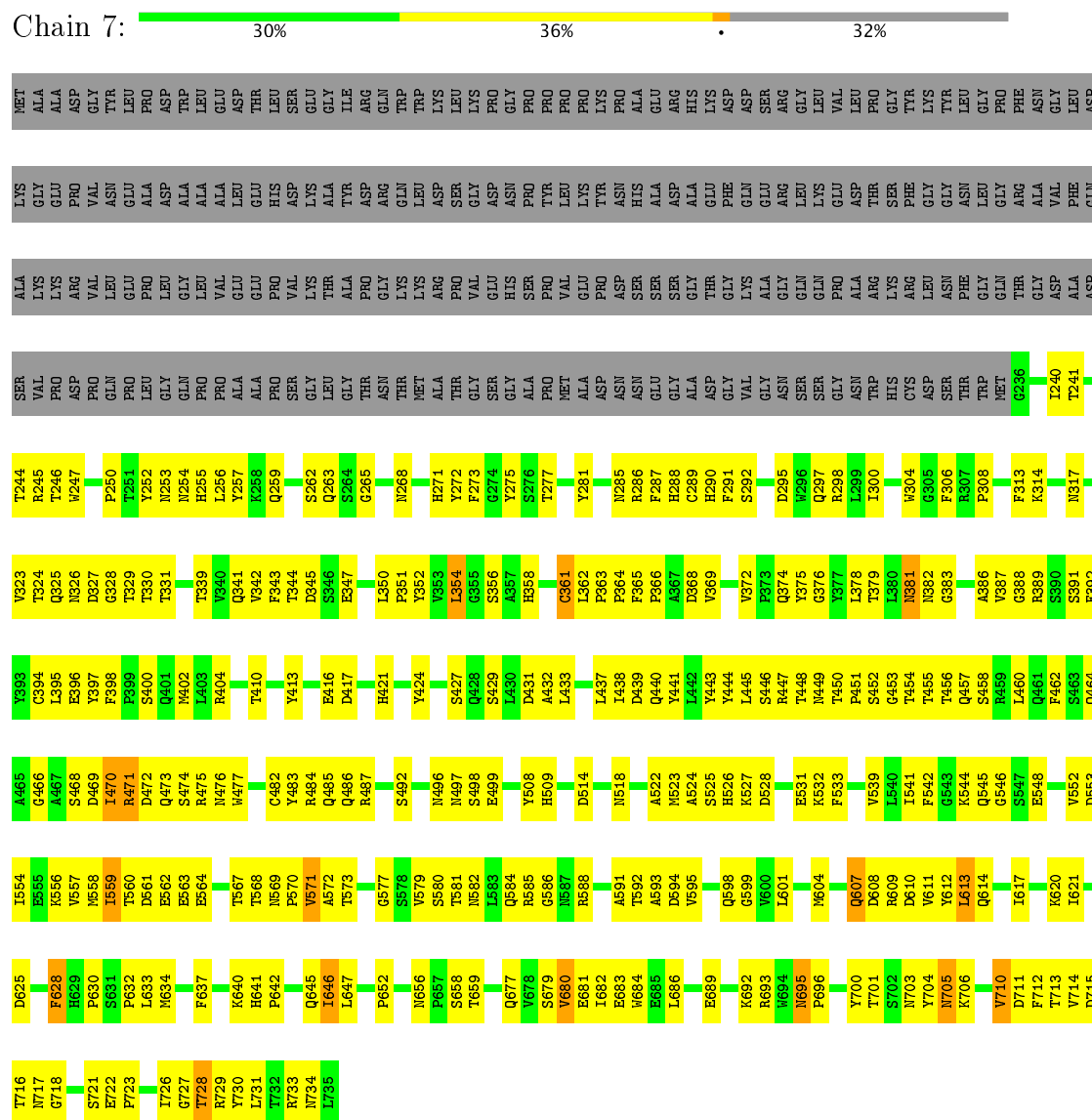


- Molecule 1: Capsid protein VP1

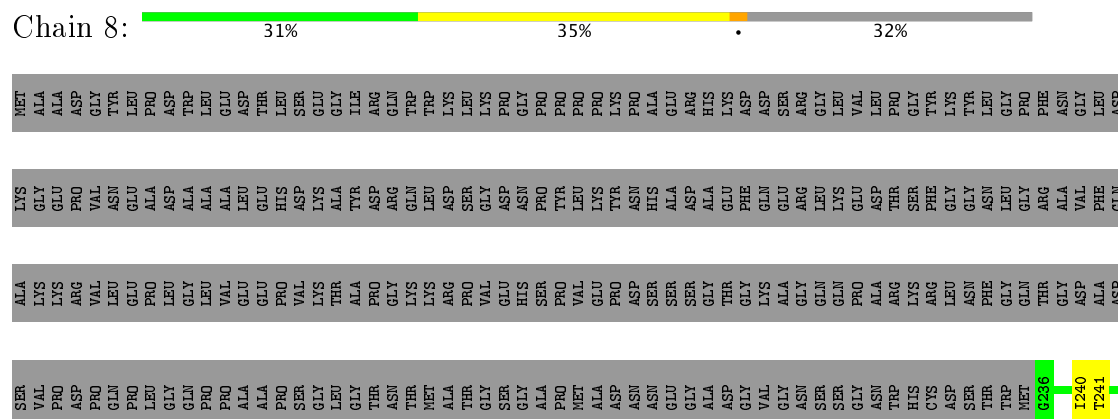
Chain 5:  30% 36% . 32%



• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



N717	G718	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S631	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625	P628	H629	P630	S632	L633	M634	F637	K640	H641	P642	Q645	I646	L647	P652	V653	P654	A655	M656	P657	S658	T659	F666	Q677	V678	S679	V680	L601	M604	Q607	D608	R609	D610	W611	W612	L613	Q614	T617	K620	I621	D625
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
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

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	0.57	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 >2	RMSZ	# Z >2
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

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

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

There are no bond length outliers.

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](#)

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	4009	0	3787	272	0
1	2	4009	0	3787	266	0
1	3	4009	0	3787	267	0
1	4	4009	0	3787	270	0
1	5	4009	0	3787	272	0
1	6	4009	0	3787	268	0
1	7	4009	0	3787	267	0
1	8	4009	0	3787	270	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4009	0	3787	340	0
1	B	4009	0	3787	338	0
1	C	4009	0	3787	343	0
1	D	4009	0	3787	345	0
1	E	4009	0	3787	336	0
1	F	4009	0	3787	340	0
1	G	4009	0	3787	343	0
1	H	4009	0	3787	334	0
1	I	4009	0	3787	337	0
1	J	4009	0	3787	341	0
1	K	4009	0	3787	345	0
1	L	4009	0	3787	338	0
1	M	4009	0	3787	342	0
1	N	4009	0	3787	340	0
1	O	4009	0	3787	340	0
1	P	4009	0	3787	340	0
1	Q	4009	0	3787	336	0
1	R	4009	0	3787	311	0
1	S	4009	0	3787	317	0
1	T	4009	0	3787	341	0
1	U	4009	0	3787	341	0
1	V	4009	0	3787	344	0
1	W	4009	0	3787	335	0
1	X	4009	0	3787	334	0
1	Y	4009	0	3787	341	0
1	Z	4009	0	3787	344	0
1	a	4009	0	3787	0	0
1	b	4009	0	3787	0	0
1	c	4009	0	3787	0	0
1	d	4009	0	3787	0	0
1	e	4009	0	3787	0	0
1	f	4009	0	3787	0	0
1	g	4009	0	3787	0	0
1	h	4009	0	3787	0	0
1	i	4009	0	3787	0	0
1	j	4009	0	3787	0	0
1	k	4009	0	3787	0	0
1	l	4009	0	3787	0	0
1	m	4009	0	3787	0	0
1	n	4009	0	3787	0	0
1	o	4009	0	3787	0	0
1	p	4009	0	3787	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	q	4009	0	3787	0	0
1	r	4009	0	3787	0	0
1	s	4009	0	3787	0	0
1	t	4009	0	3787	0	0
1	u	4009	0	3787	0	0
1	v	4009	0	3787	0	0
1	w	4009	0	3787	0	0
1	x	4009	0	3787	0	0
1	y	4009	0	3787	0	0
1	z	4009	0	3787	0	0
All	All	240540	0	227220	9132	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 20.

The worst 5 of 9132 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:Q:585:ARG:H	1:Q:588:ARG:HB3	1.37	0.90
1:W:585:ARG:H	1:W:588:ARG:HB3	1.37	0.90
1:J:585:ARG:H	1:J:588:ARG:HB3	1.37	0.90
1:C:585:ARG:H	1:C:588:ARG:HB3	1.37	0.90
1:D:585:ARG:H	1:D:588:ARG:HB3	1.36	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	2	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	4	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	5	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	6	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	7	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	8	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	A	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	B	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	C	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	D	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	E	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	F	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	G	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	H	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	I	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	J	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	K	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	L	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	M	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	N	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	O	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	P	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	Q	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	R	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	S	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	T	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	U	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	V	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	W	498 / 735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	X	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	Y	498 / 735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	a	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	b	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	c	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	d	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	e	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	f	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	g	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	h	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	i	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	j	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	k	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	l	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	m	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	n	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	o	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	p	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	q	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	r	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	s	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	t	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
1	u	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	v	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	w	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	x	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	y	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	6	44
1	z	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	6	44
All	All	29880/44100 (68%)	22656 (76%)	6444 (22%)	780 (3%)	10	44

5 of 780 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	680	VAL

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Mol	Chain	Res	Type
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%)	91	96
1	2	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	3	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	4	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	5	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	6	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	7	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	8	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	A	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	B	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	C	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	D	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	E	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	F	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	G	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	H	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	I	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	J	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	K	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	L	444/629 (71%)	442 (100%)	2 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	N	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	O	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	P	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	Q	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	R	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	S	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	T	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	U	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	V	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	W	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	X	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	Y	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	Z	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	a	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	b	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	c	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	d	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	e	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	f	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	g	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	h	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	i	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	j	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	k	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	l	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	m	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	n	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	o	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	p	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	q	444/629 (71%)	442 (100%)	2 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	s	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	t	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	u	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	v	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	w	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	x	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	y	444/629 (71%)	442 (100%)	2 (0%)	91	96
1	z	444/629 (71%)	442 (100%)	2 (0%)	91	96
All	All	26640/37740 (71%)	26520 (100%)	120 (0%)	91	96

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

Mol	Chain	Res	Type
1	b	460	LEU
1	h	613	LEU
1	4	460	LEU
1	b	613	LEU
1	e	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 558 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	656	ASN
1	h	461	GLN
1	4	440	GLN
1	b	598	GLN
1	e	440	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 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.