



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 11:38 PM UTC

PDB ID : 4V86 / pdb_00004v86
Title : Structure-function Analysis of Receptor-binding in Adeno-Associated Virus Serotype 6 (AAV-6)
Authors : Xie, Q.
Deposited on : 2011-09-13
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

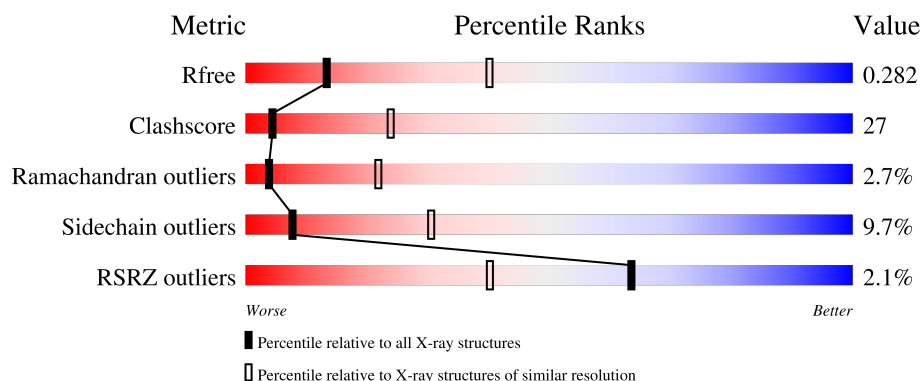
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	0	520	2% 56% 38% 7%
1	1	520	3% 51% 41% 8%
1	2	520	% 52% 41% 7%
1	3	520	3% 55% 38% 7%
1	4	520	% 54% 40% 6%

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Mol	Chain	Length	Quality of chain
1	5	520	
1	6	520	
1	7	520	
1	A	520	
1	B	520	
1	C	520	
1	D	520	
1	E	520	
1	F	520	
1	G	520	
1	H	520	
1	I	520	
1	J	520	
1	K	520	
1	L	520	
1	M	520	
1	N	520	
1	O	520	
1	P	520	
1	Q	520	
1	R	520	
1	S	520	
1	T	520	
1	U	520	
1	V	520	

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Mol	Chain	Length	Quality of chain
1	W	520	
1	X	520	
1	Y	520	
1	Z	520	
1	a	520	
1	b	520	
1	c	520	
1	d	520	
1	e	520	
1	f	520	
1	g	520	
1	h	520	
1	i	520	
1	j	520	
1	k	520	
1	l	520	
1	m	520	
1	n	520	
1	o	520	
1	p	520	
1	q	520	
1	r	520	
1	s	520	
1	t	520	
1	u	520	

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Mol	Chain	Length	Quality of chain
1	v	520	% 55% 37% 8%
1	w	520	2% 54% 38% 7%
1	x	520	% 54% 38% 7%
1	y	520	% 54% 38% 8%
1	z	520	2% 54% 38% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 247260 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	B	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	C	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	D	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	E	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	F	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	G	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	H	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	I	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	J	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	K	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	L	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	M	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	N	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	O	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	P	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	R	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	S	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	T	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	U	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	V	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	W	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	X	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	Y	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	Z	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	a	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	b	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	c	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	d	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	e	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	f	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	g	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	h	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	i	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	j	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	k	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0

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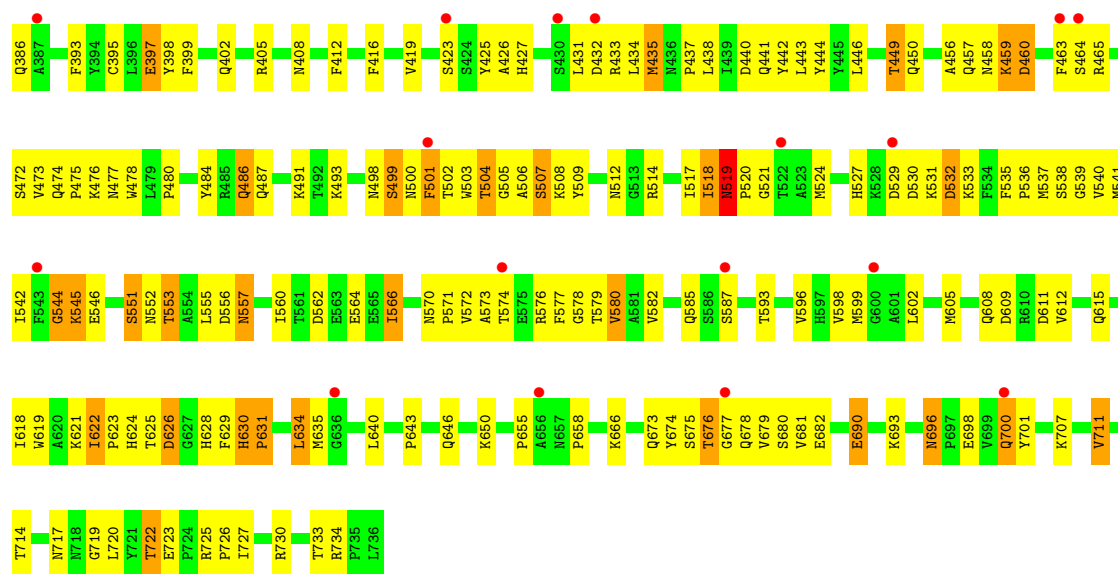
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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1	m	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	n	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	o	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	p	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	q	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	r	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	s	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	t	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	u	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	v	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	w	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	x	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	y	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	z	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	0	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	1	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	2	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	3	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	4	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0
1	5	520	Total 4121	C 2607	N 712	O 786	S 16	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	7	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

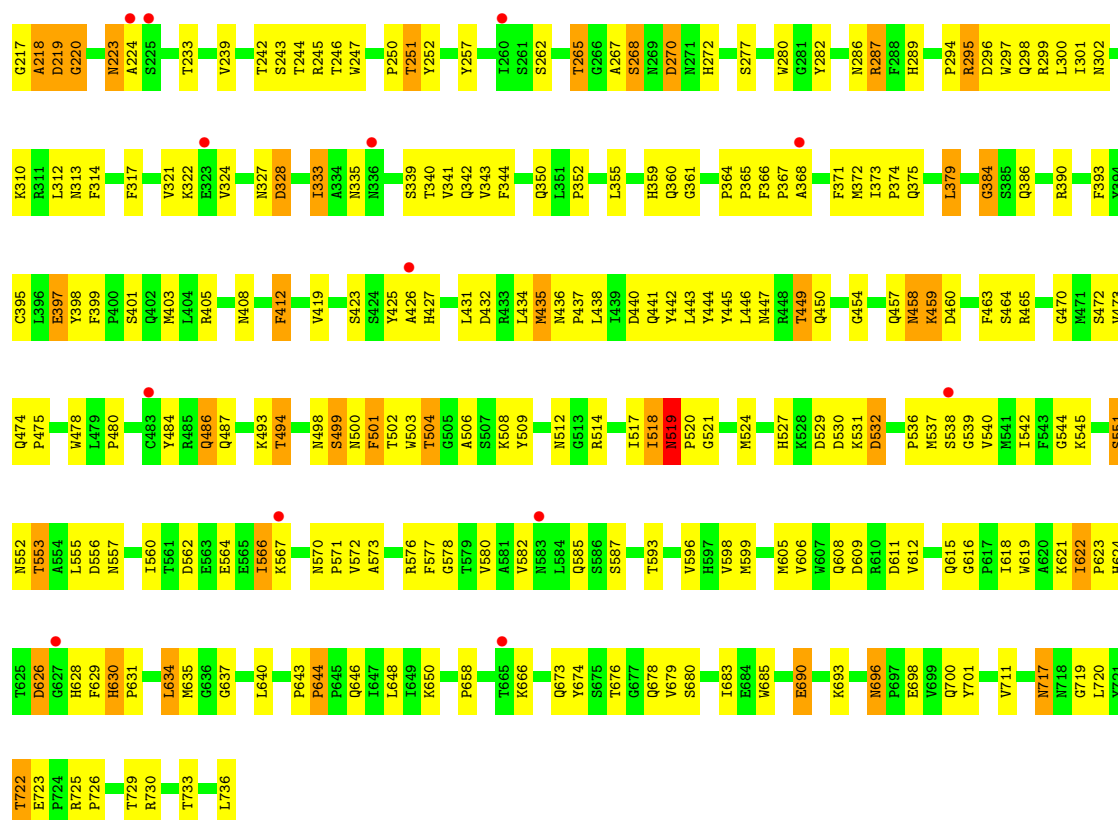


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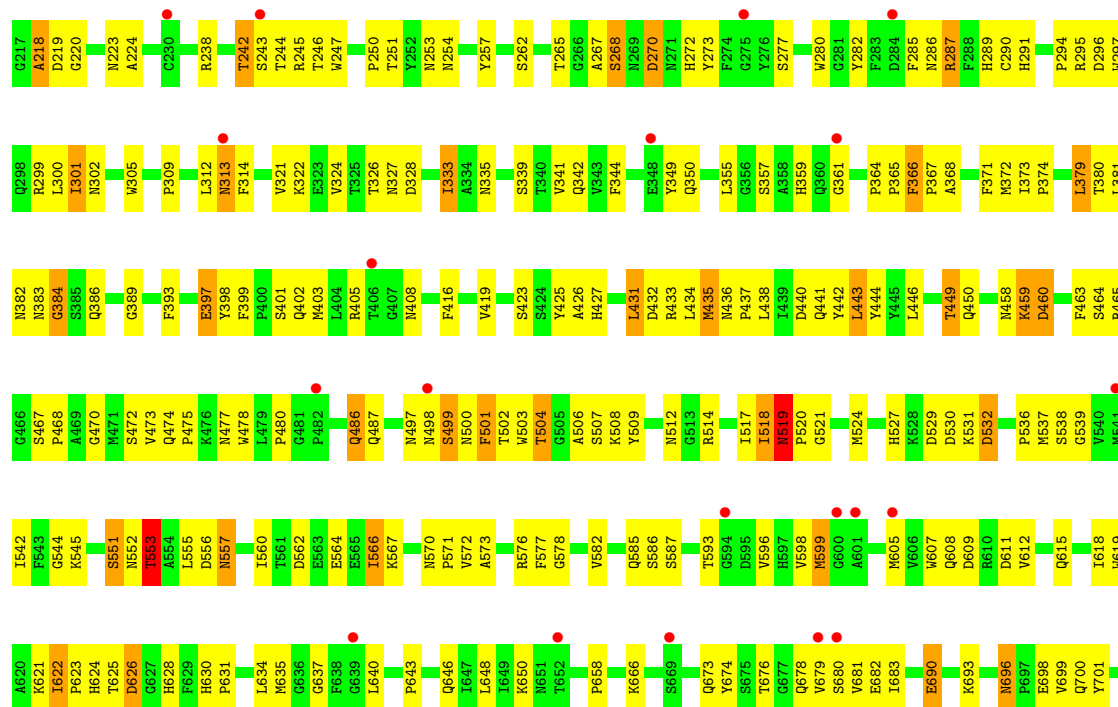


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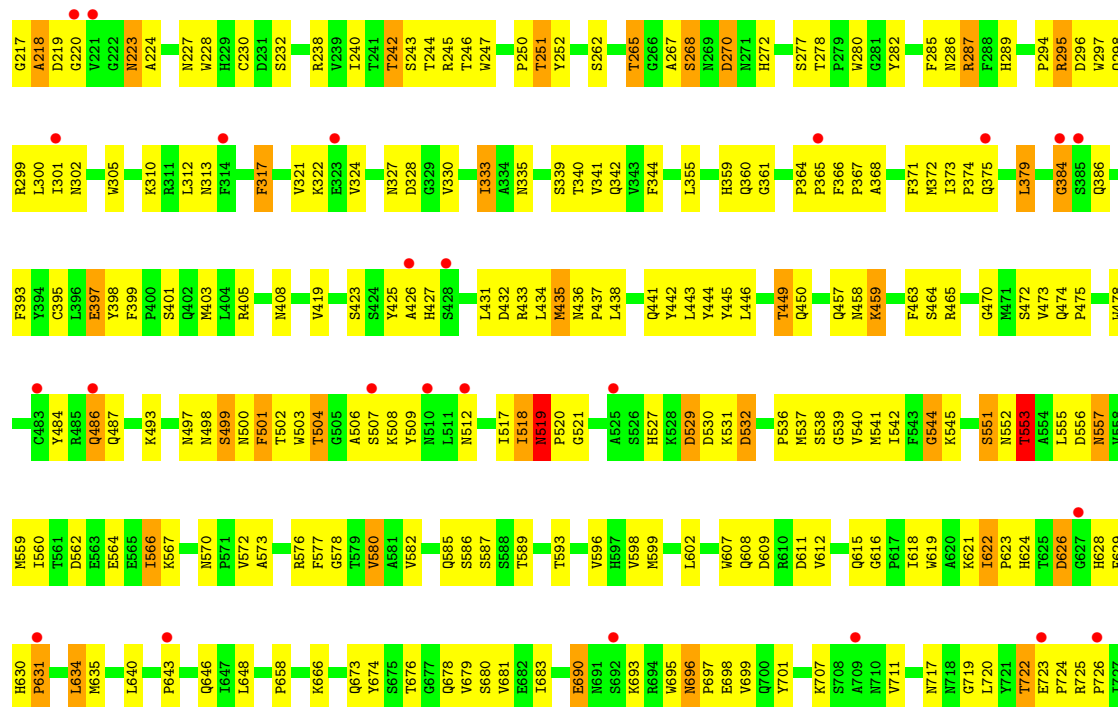


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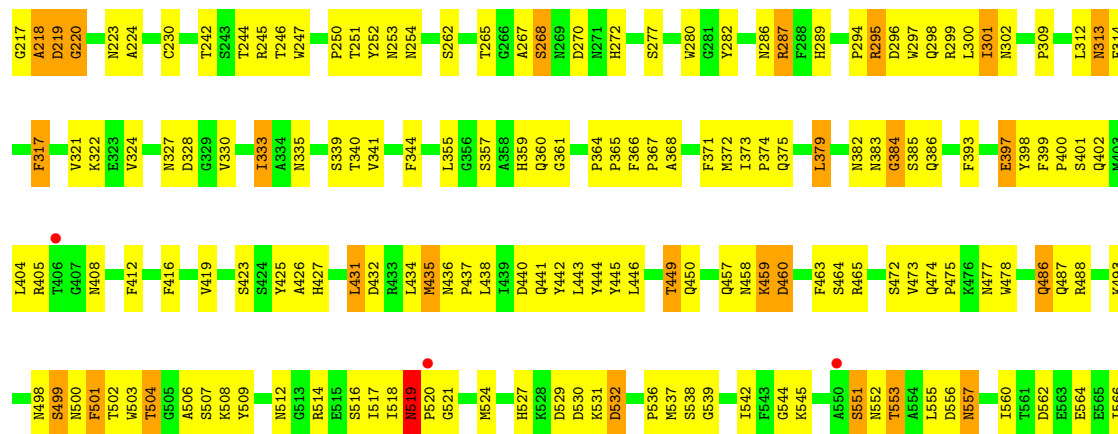


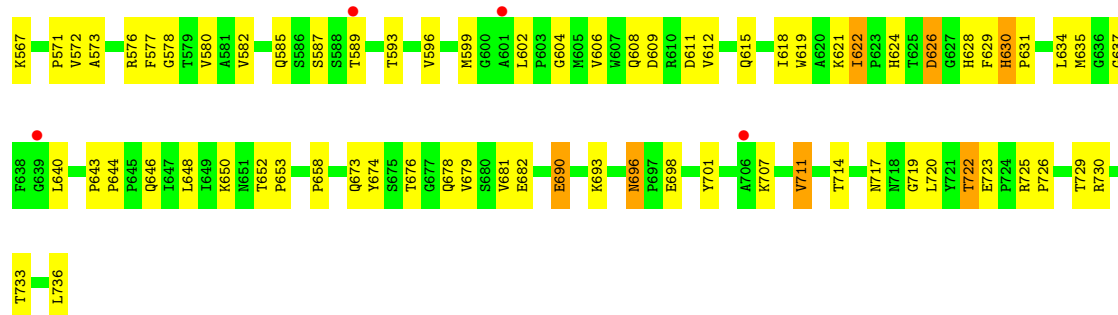


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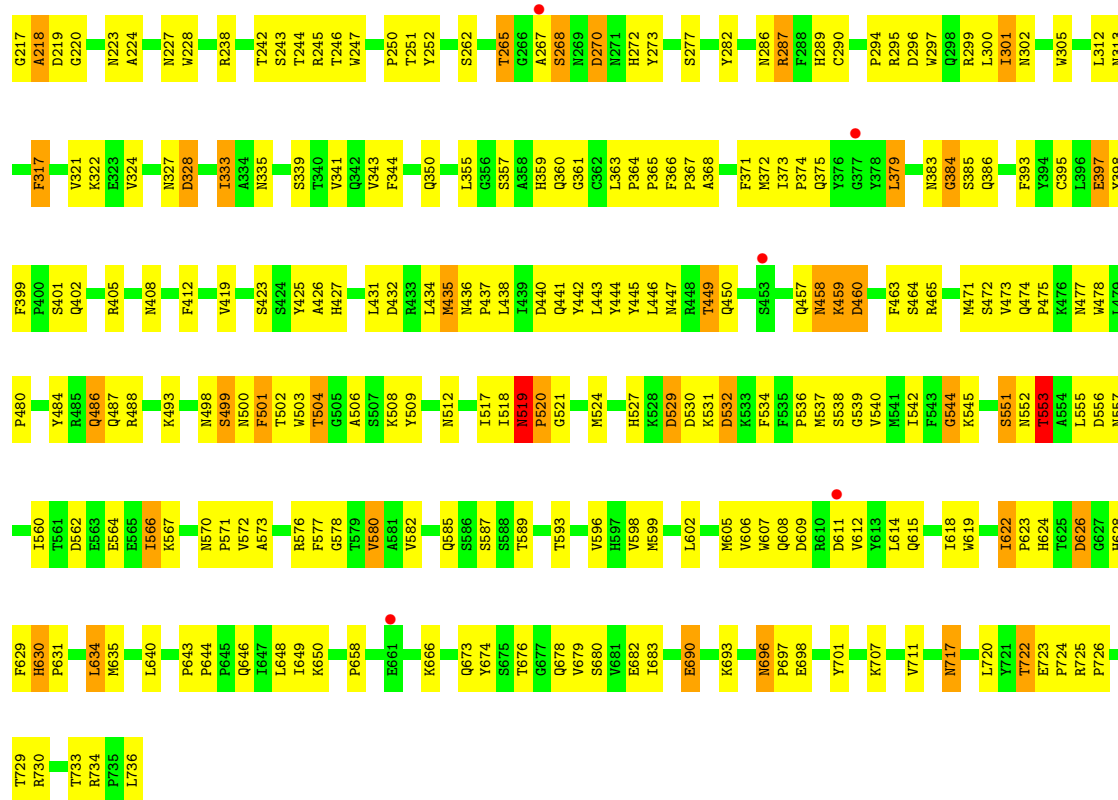


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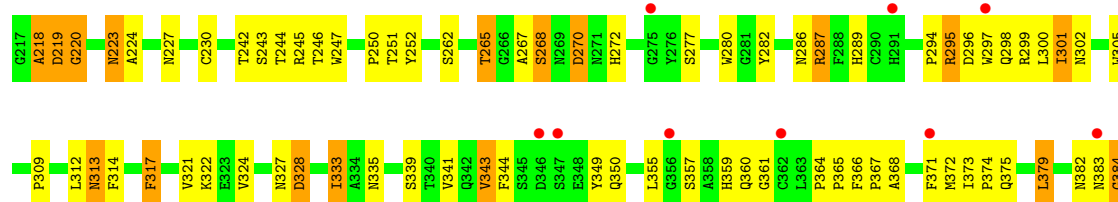


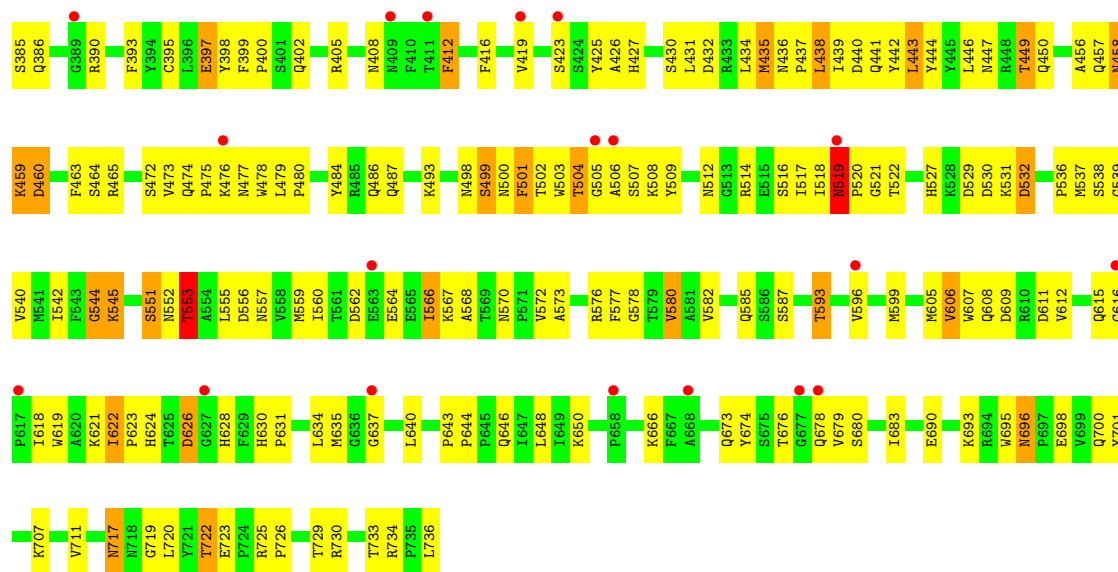


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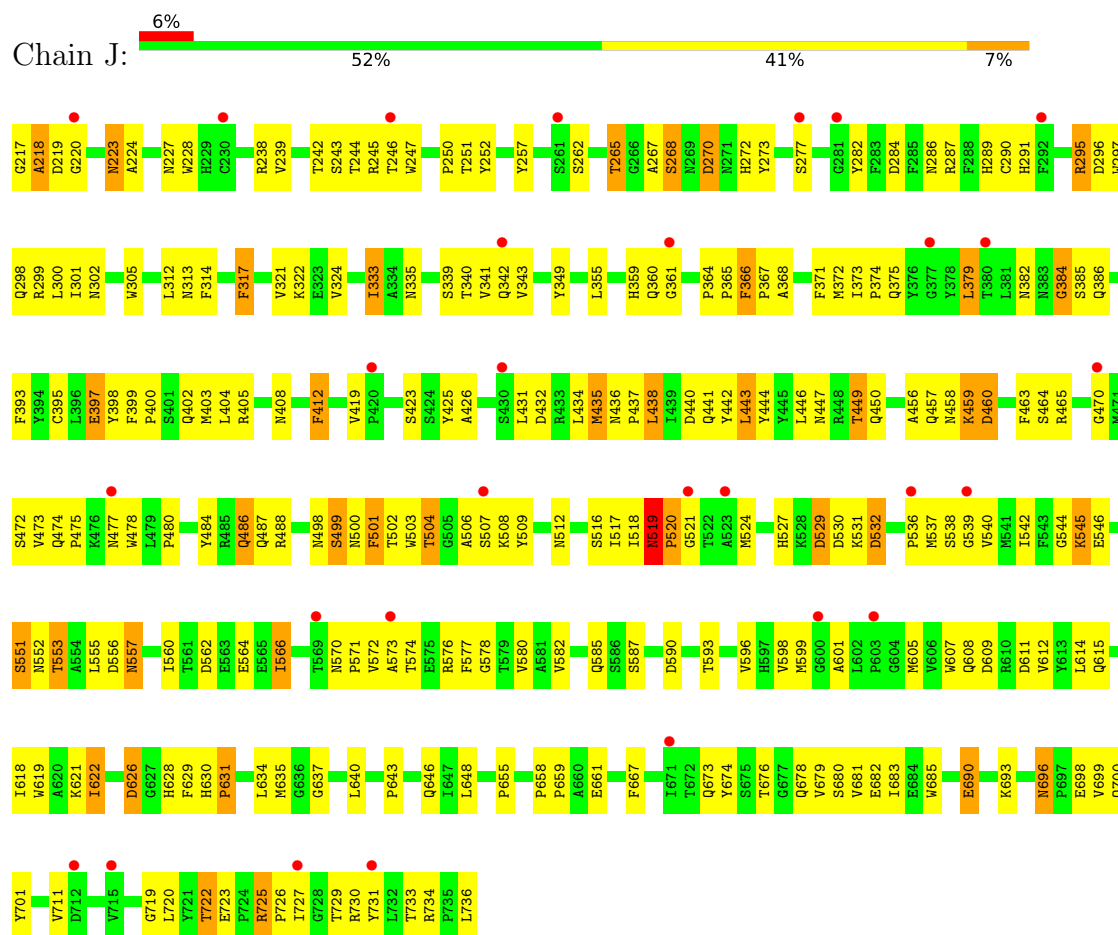


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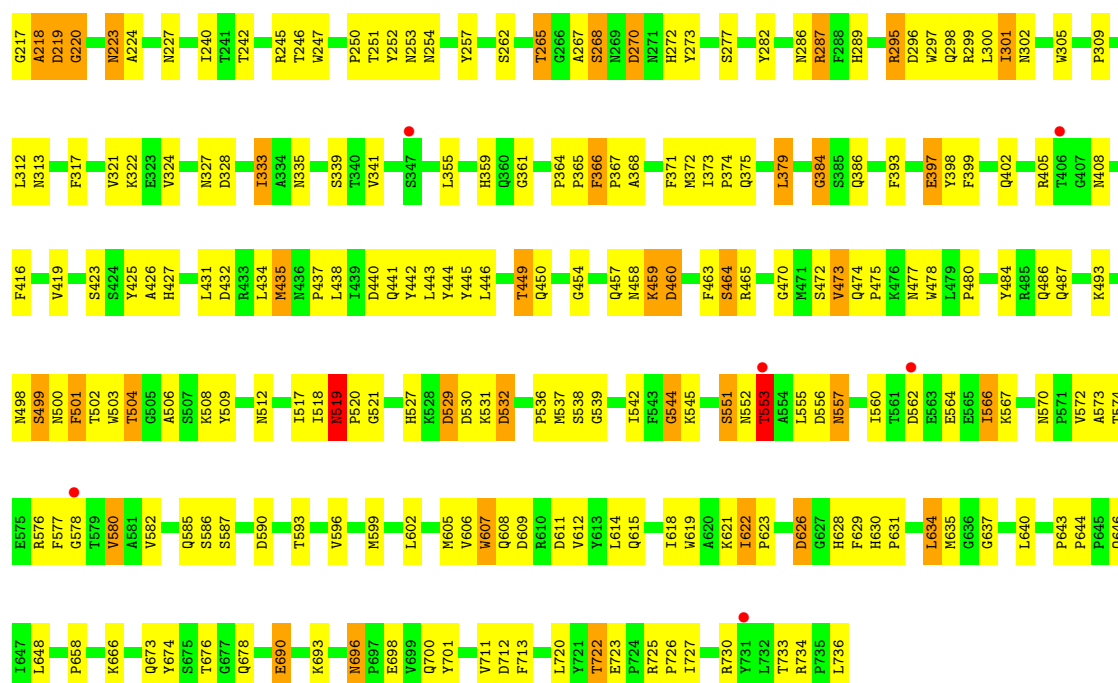


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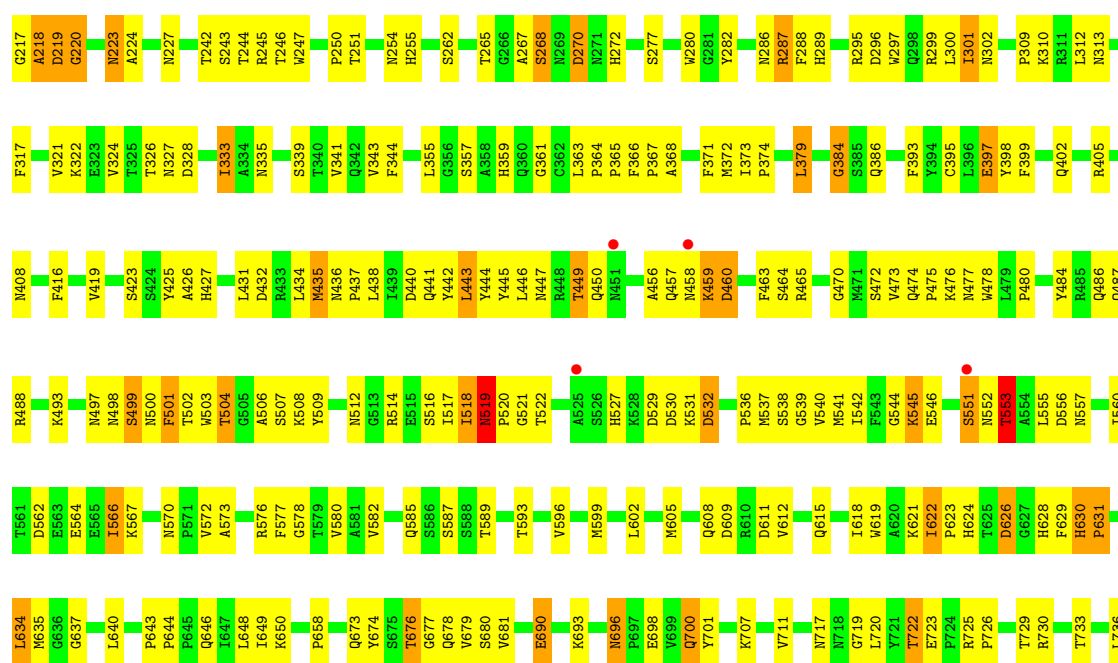


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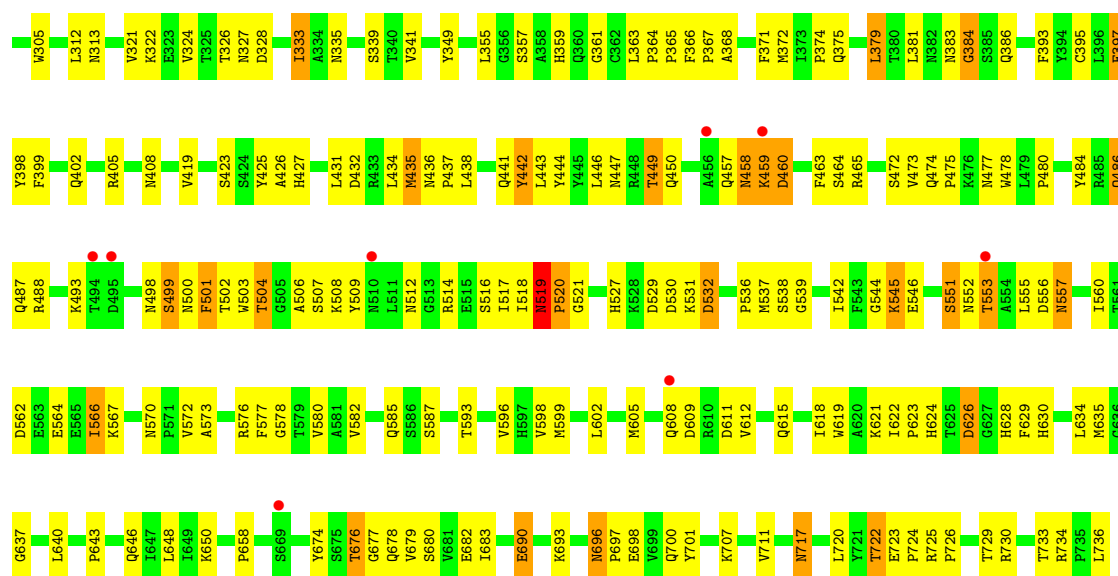


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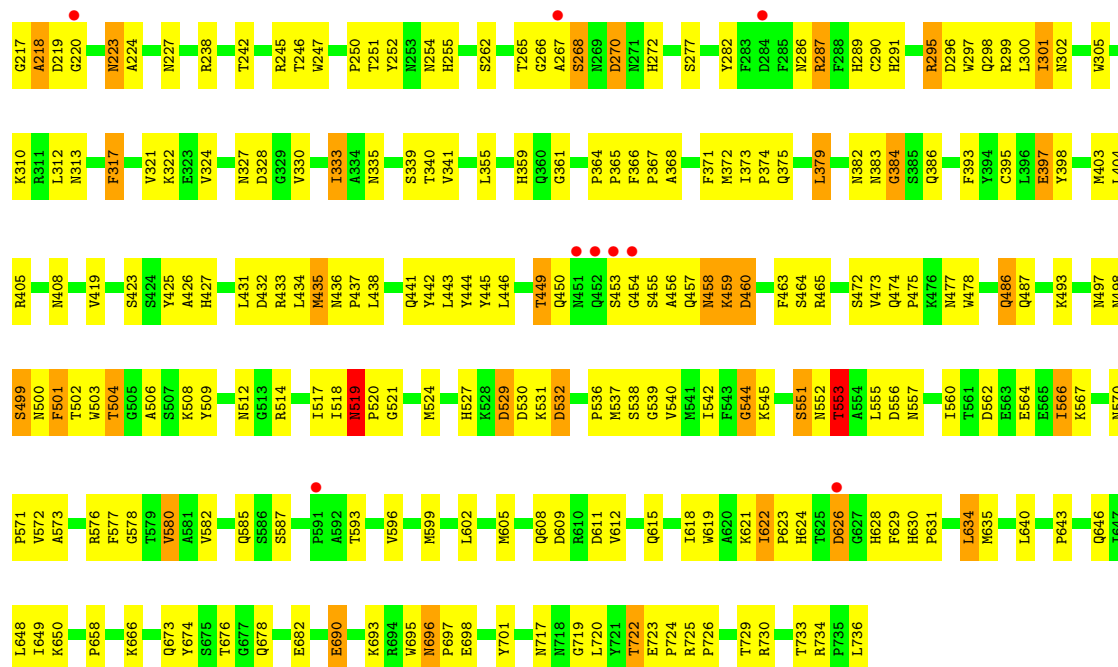


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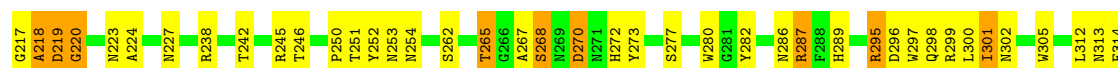


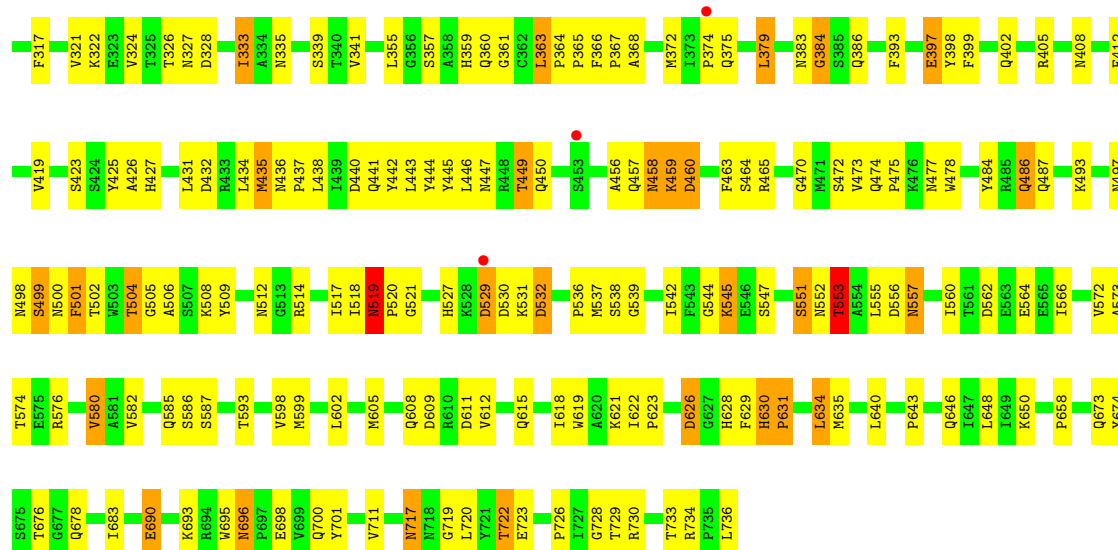


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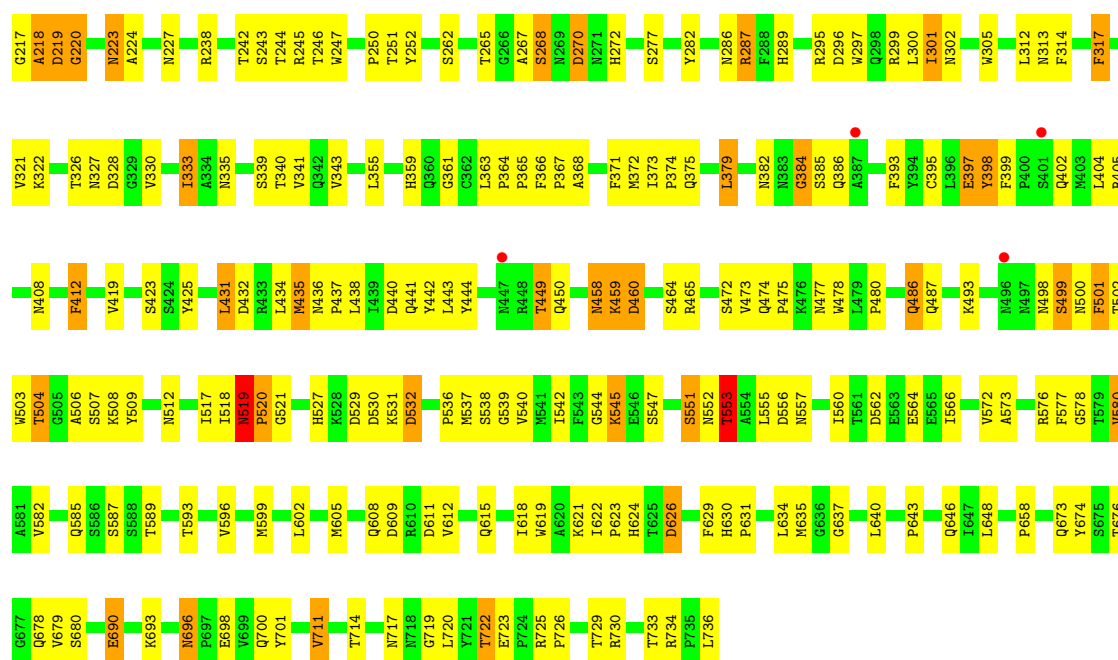


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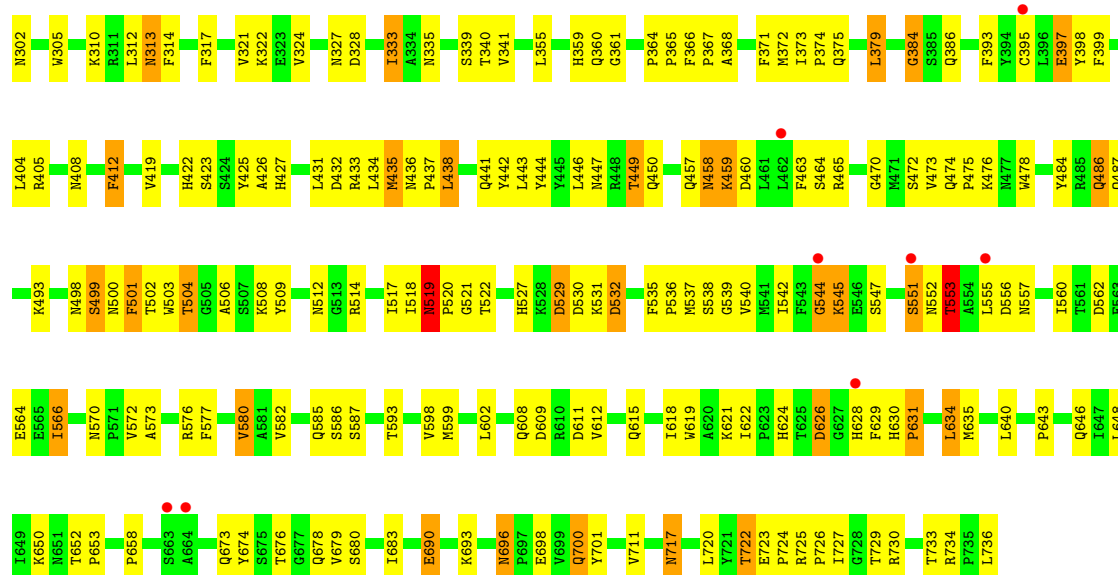


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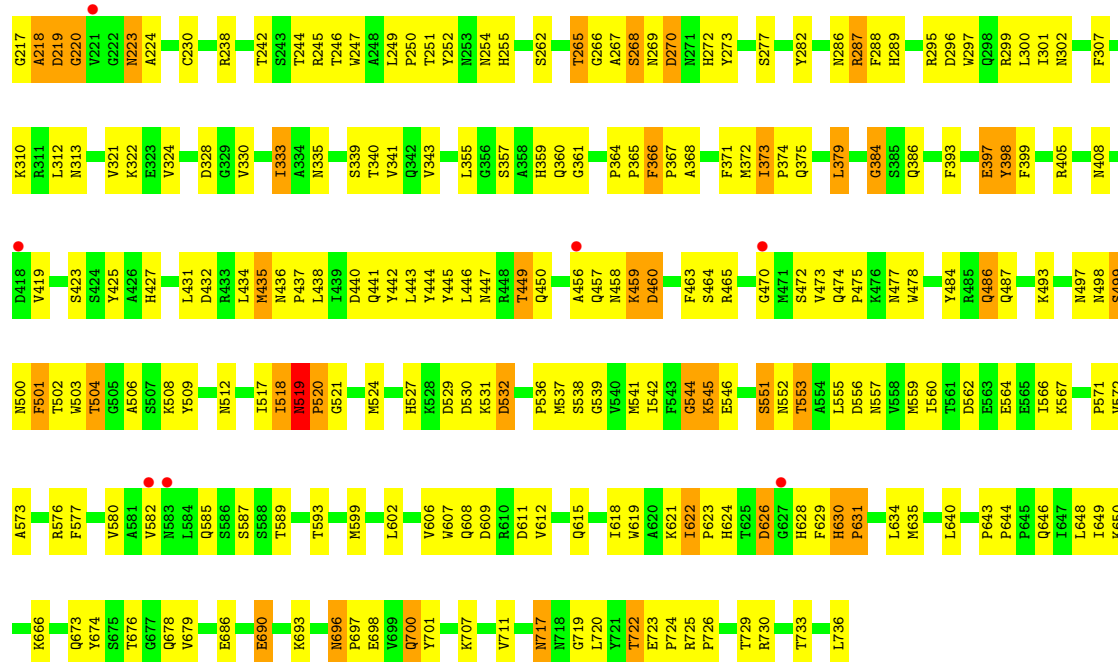


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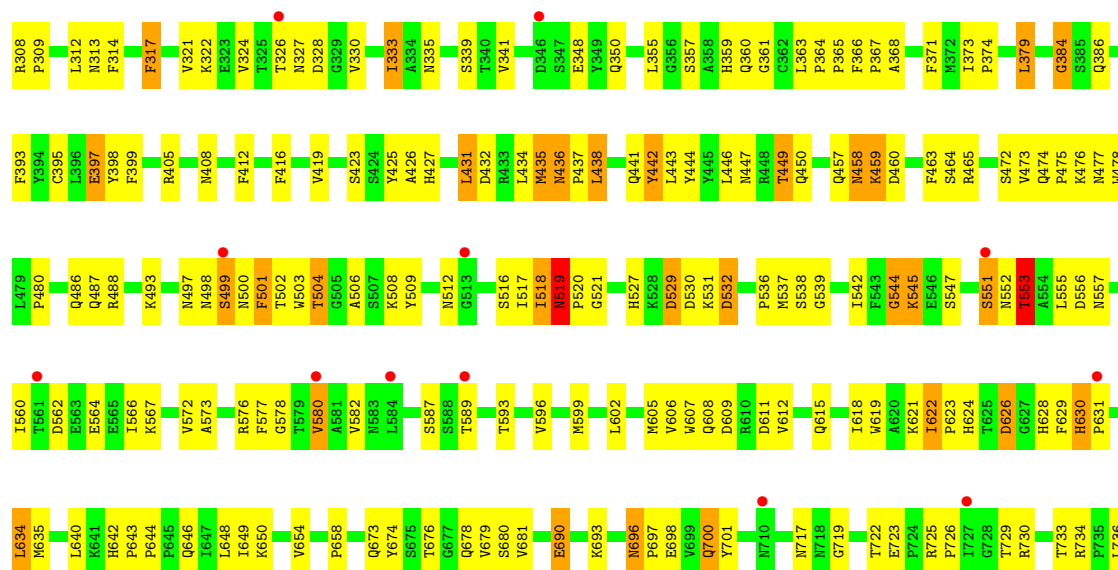


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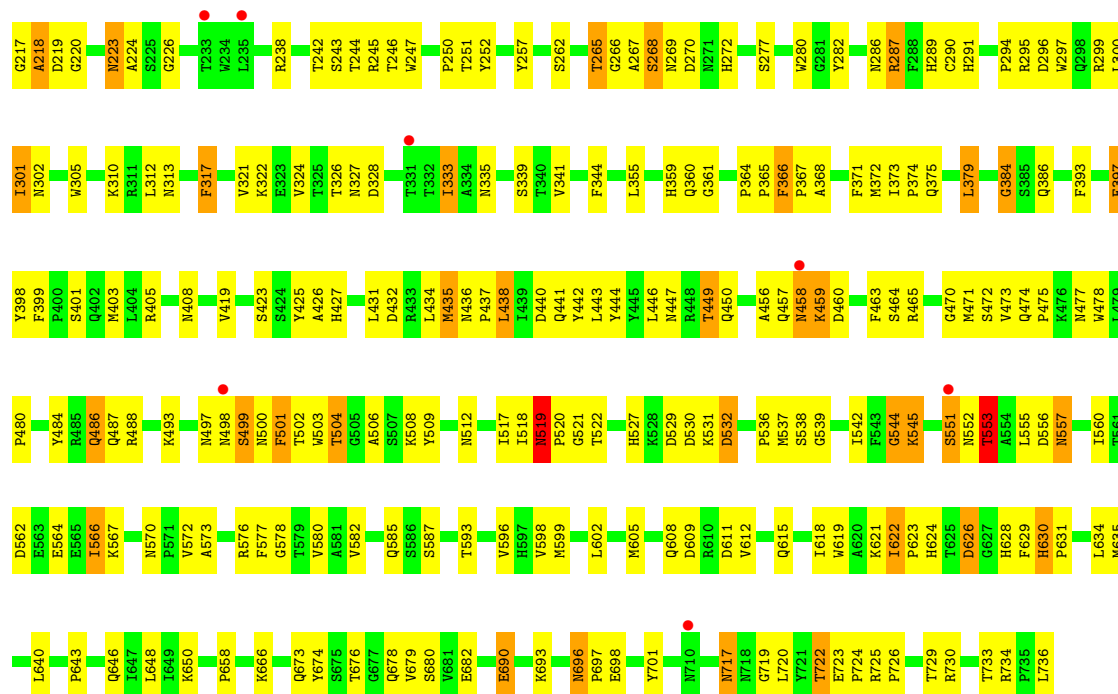


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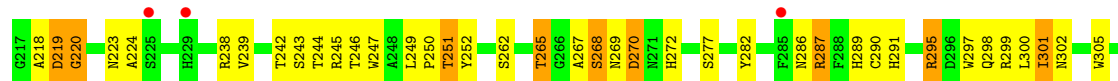


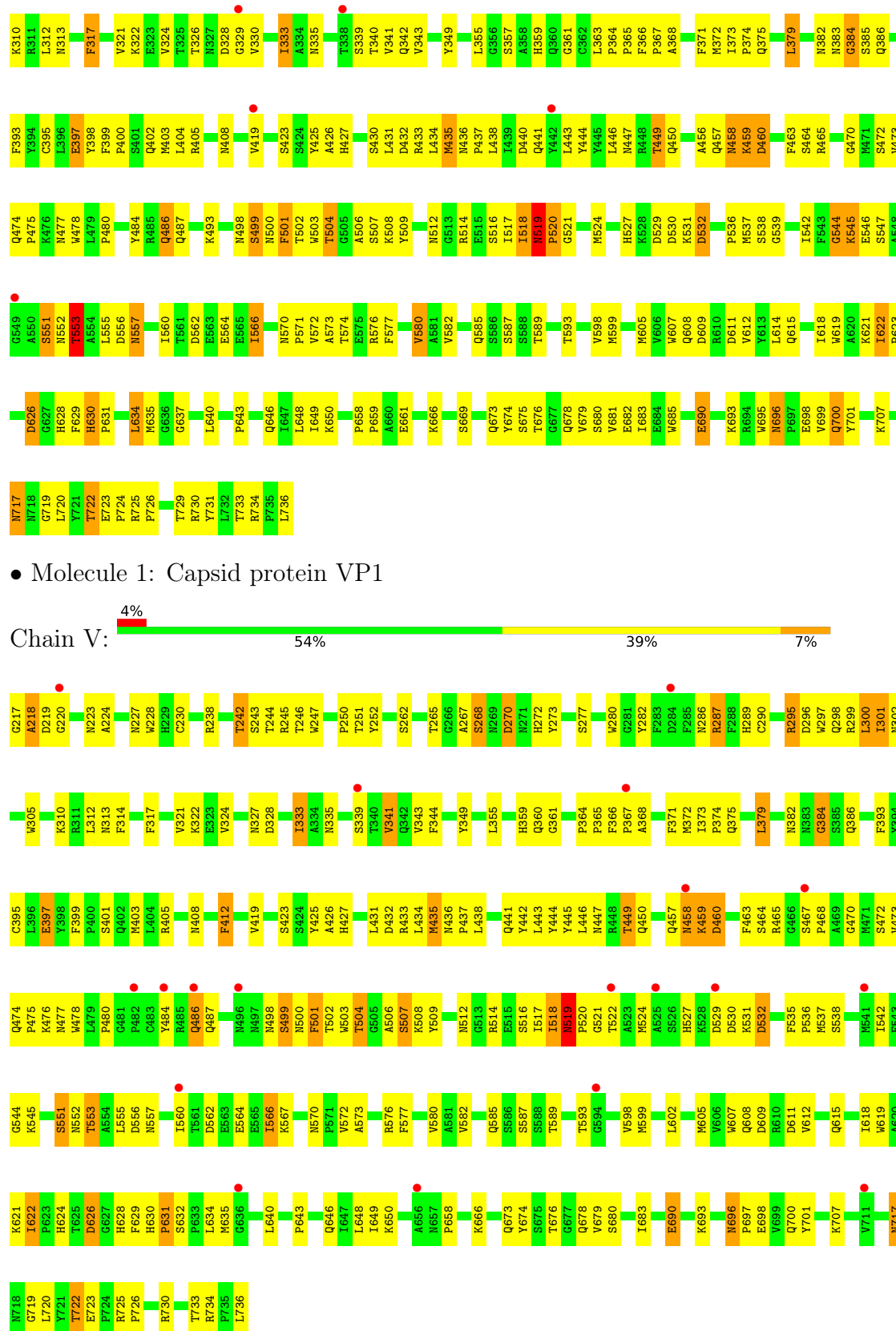


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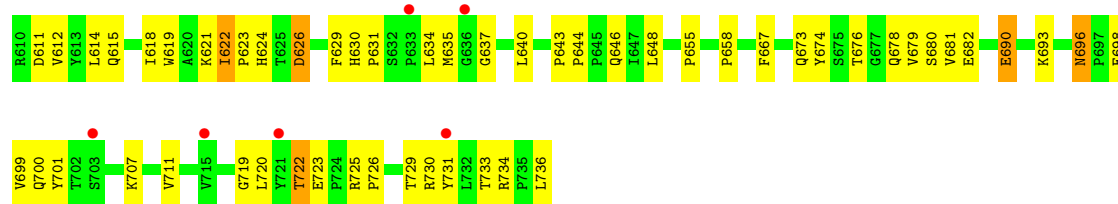


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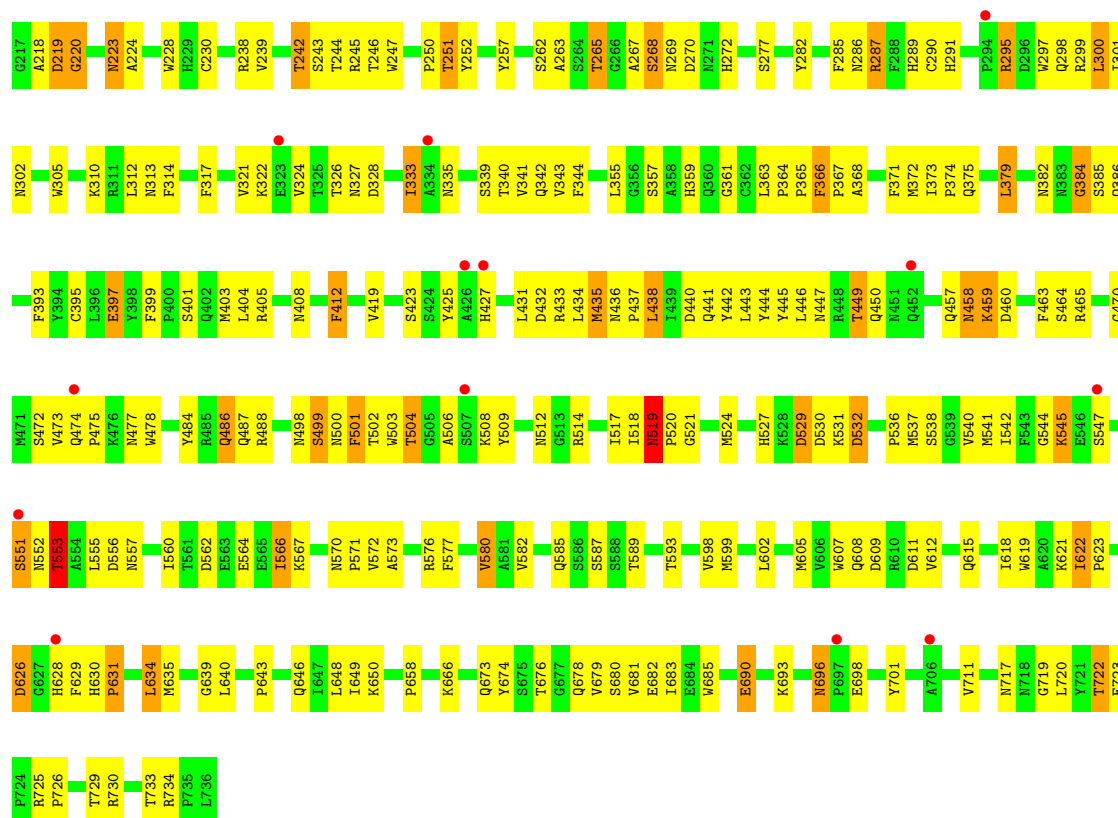




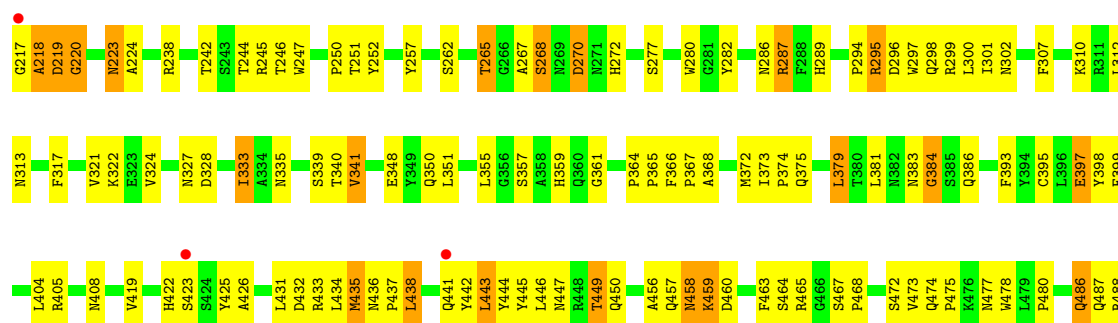


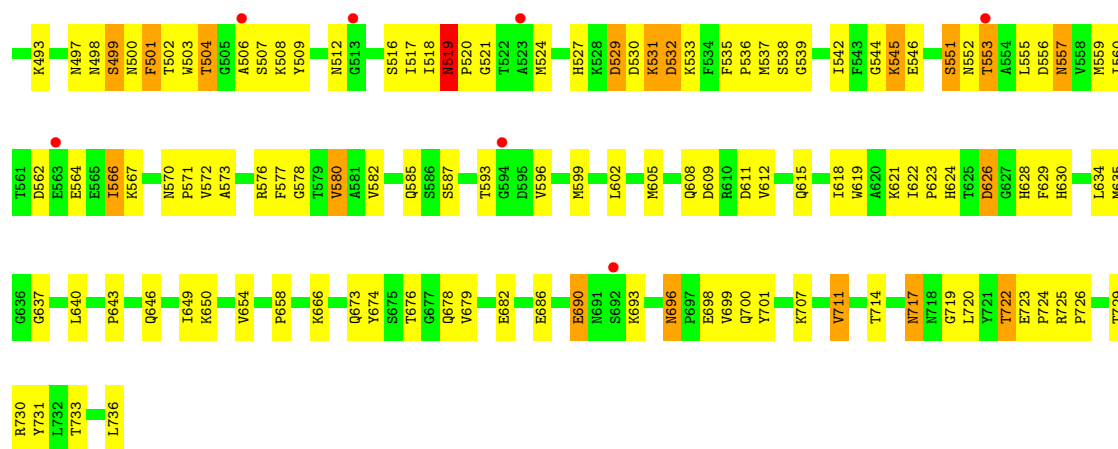


● Molecule 1: Capsid protein VP1



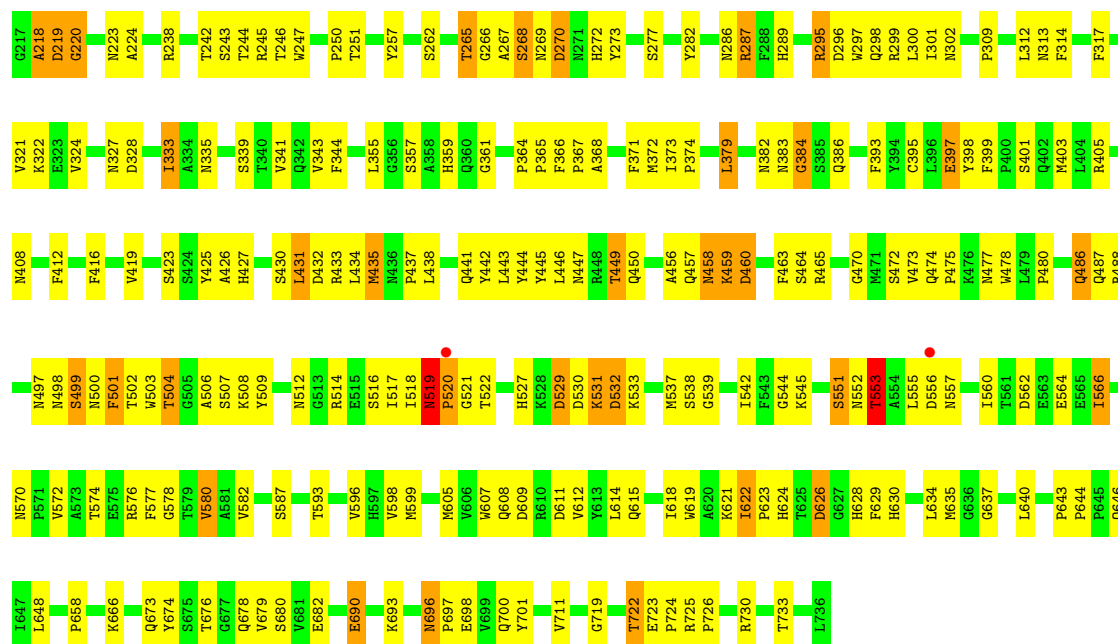
● Molecule 1: Capsid protein VP1





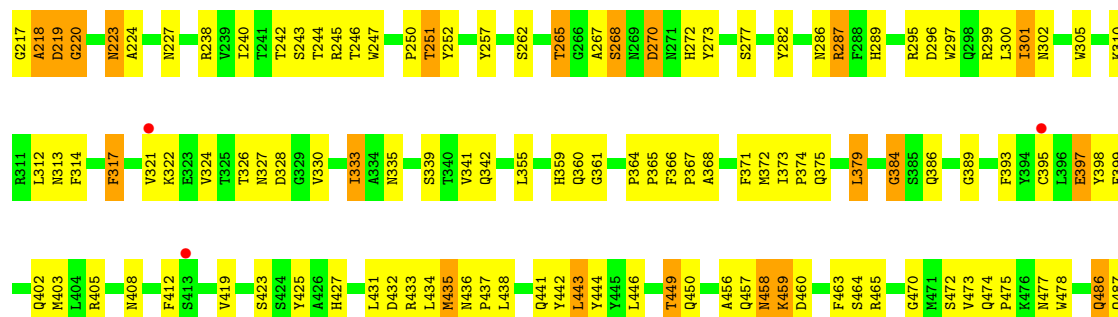
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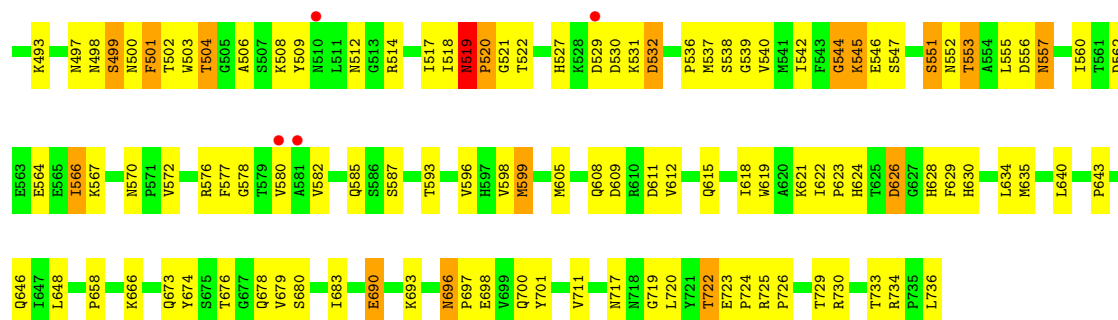
Chain a: 56% 37% 7%



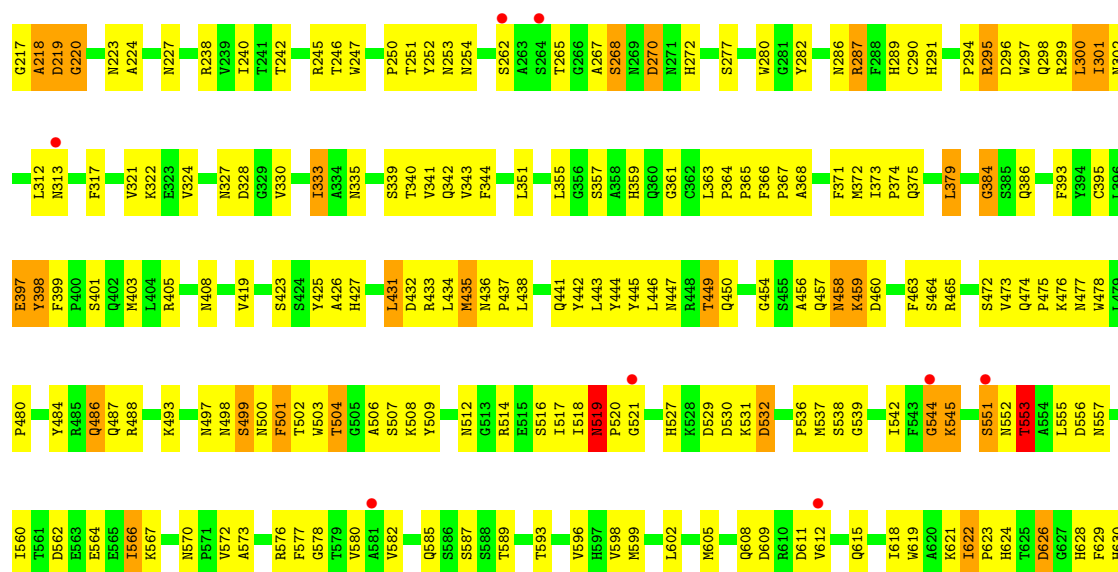
● Molecule 1: Capsid protein VP1

Chain b: 56% 37% 7%

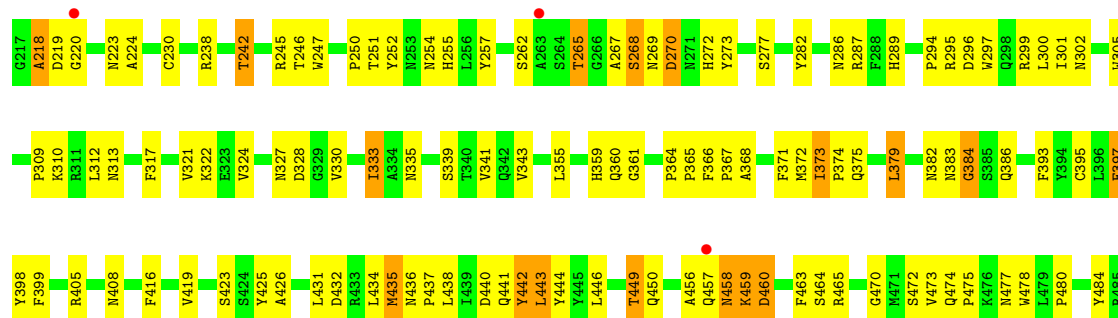


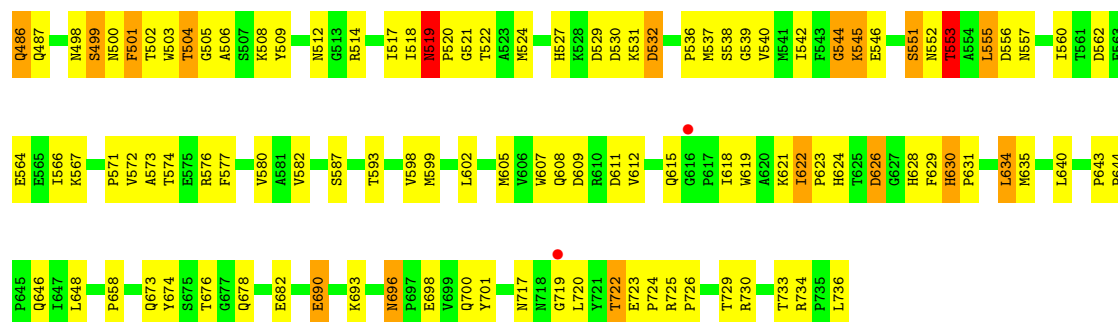


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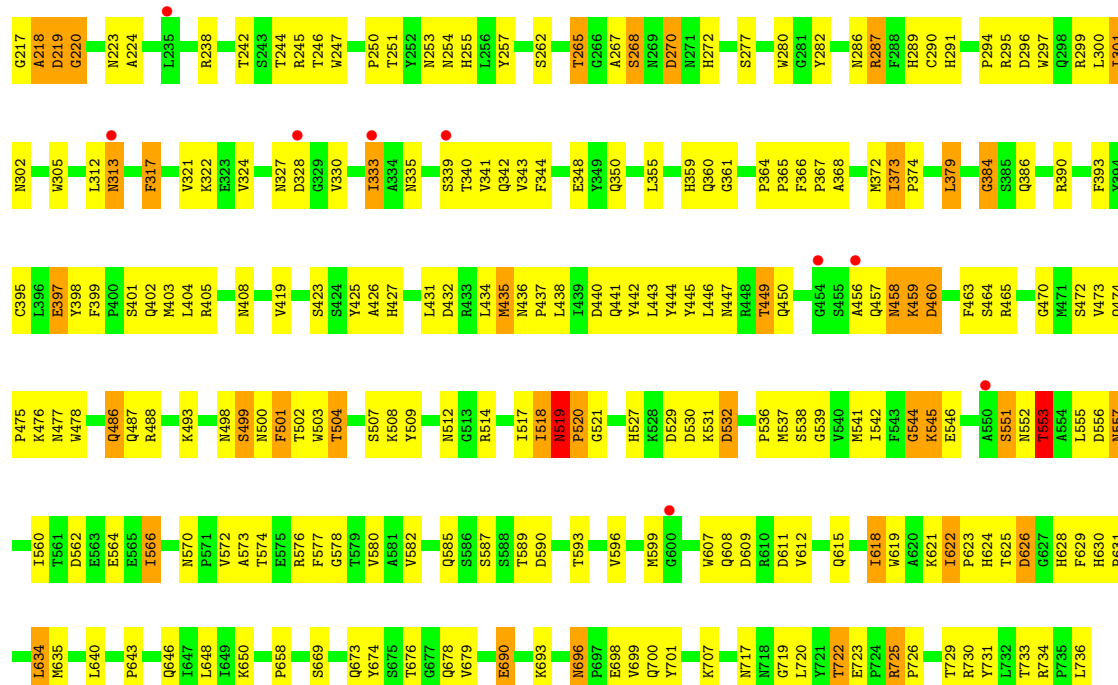


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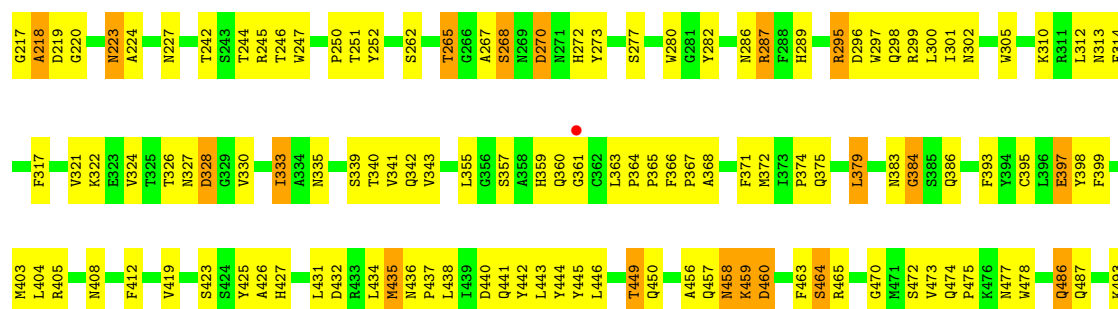


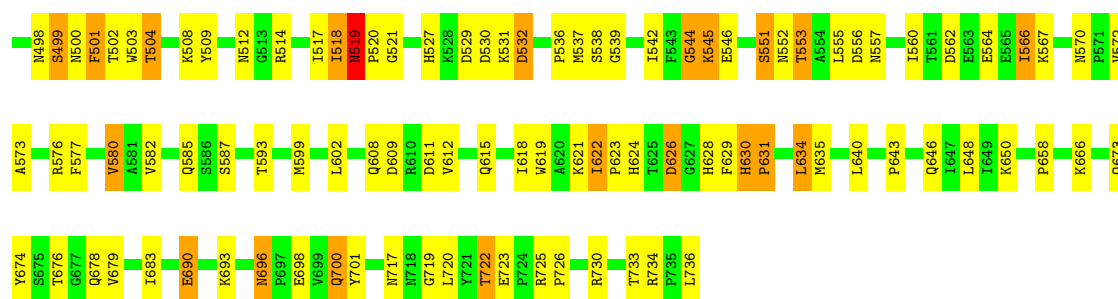


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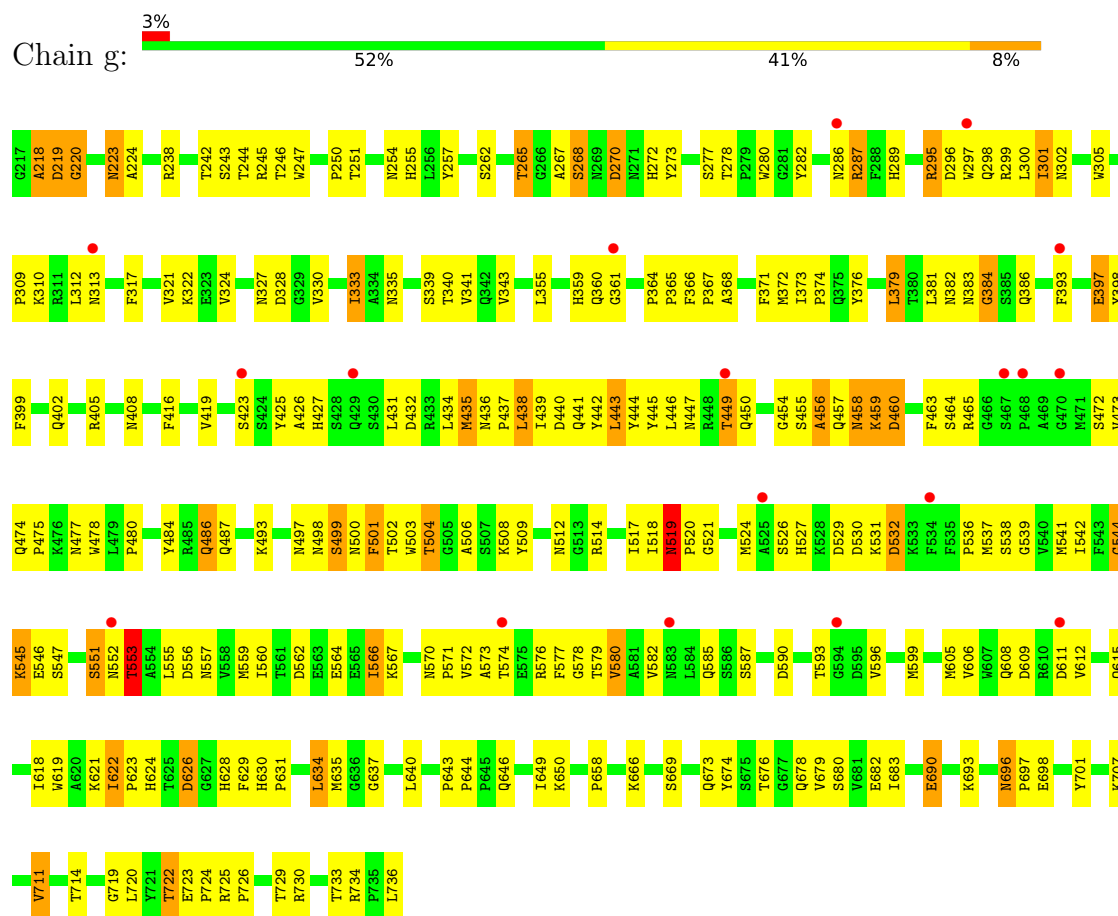


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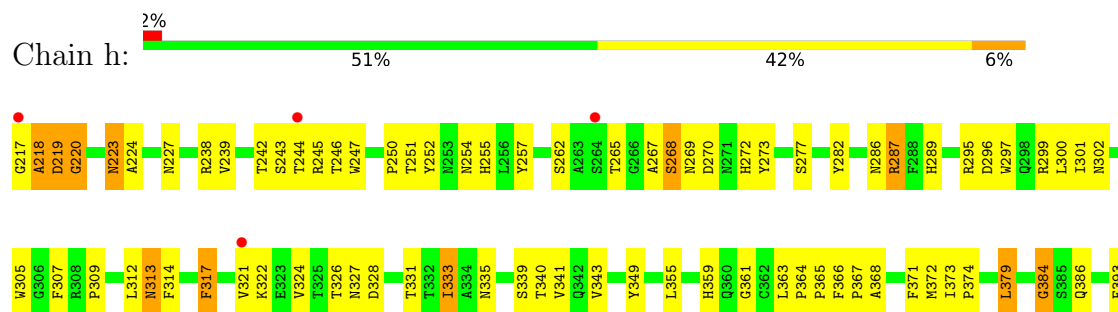


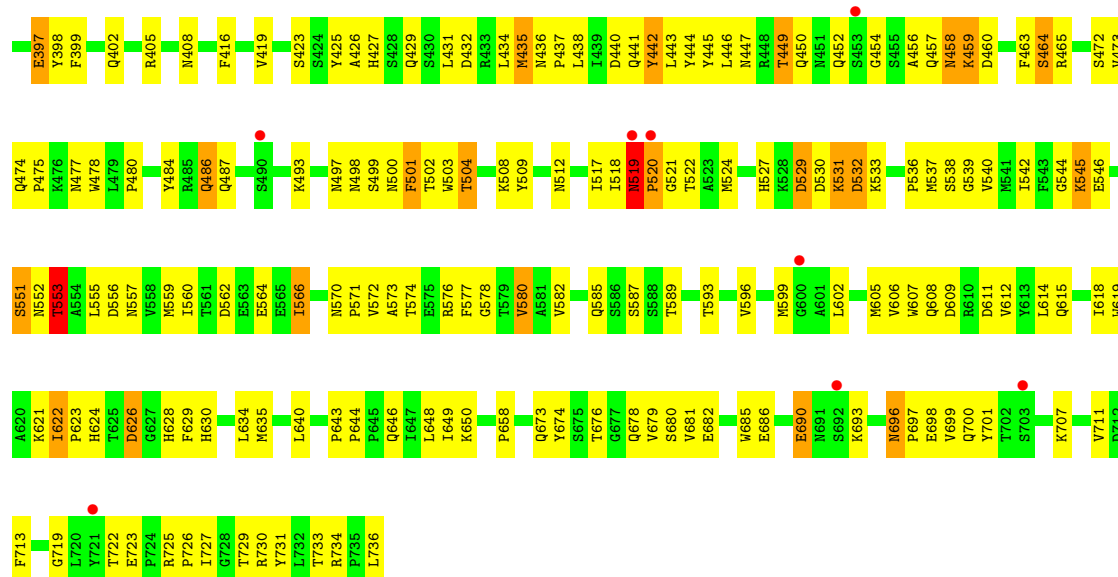


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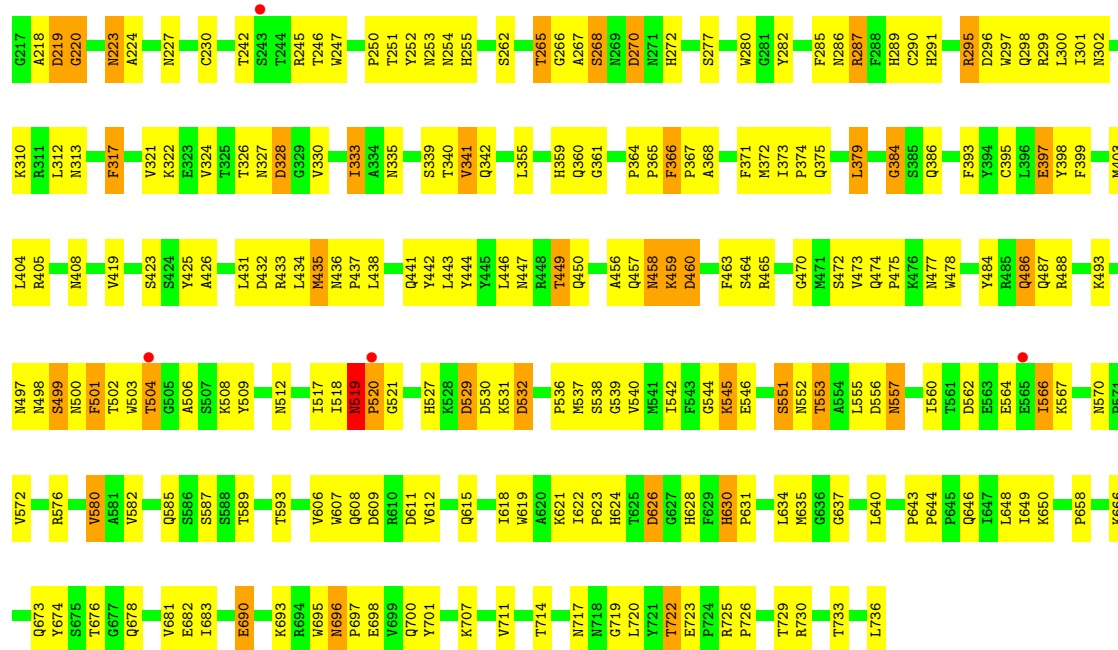


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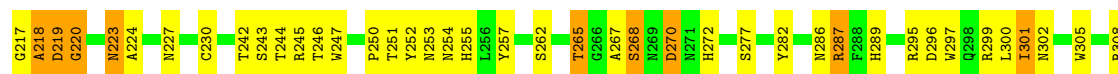


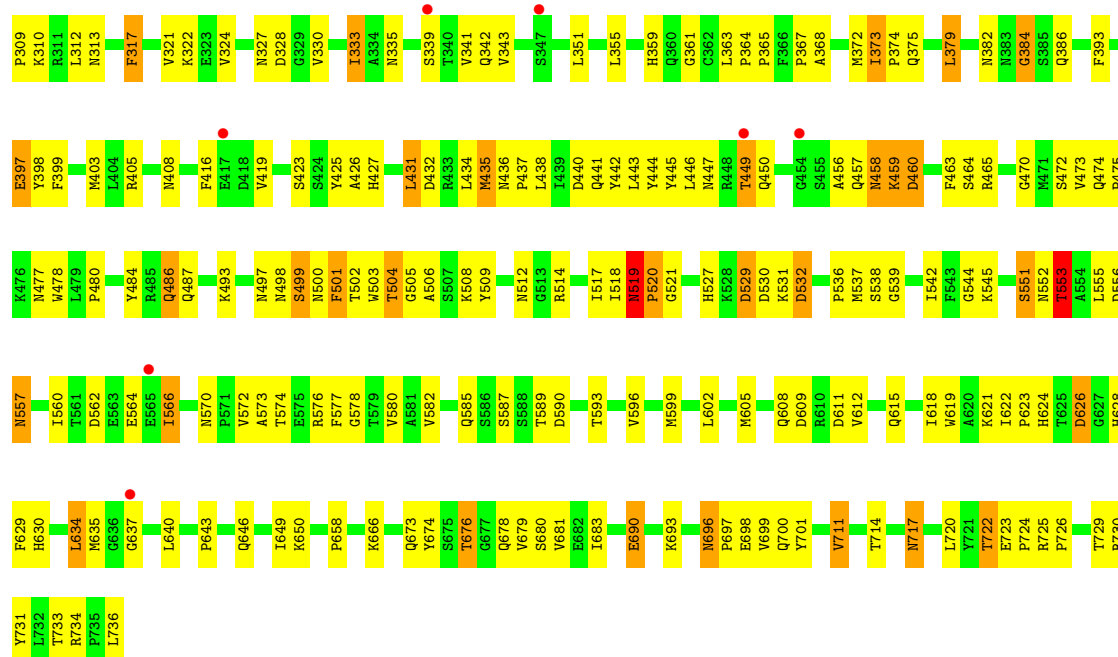


• Molecule 1: Capsid protein VP1

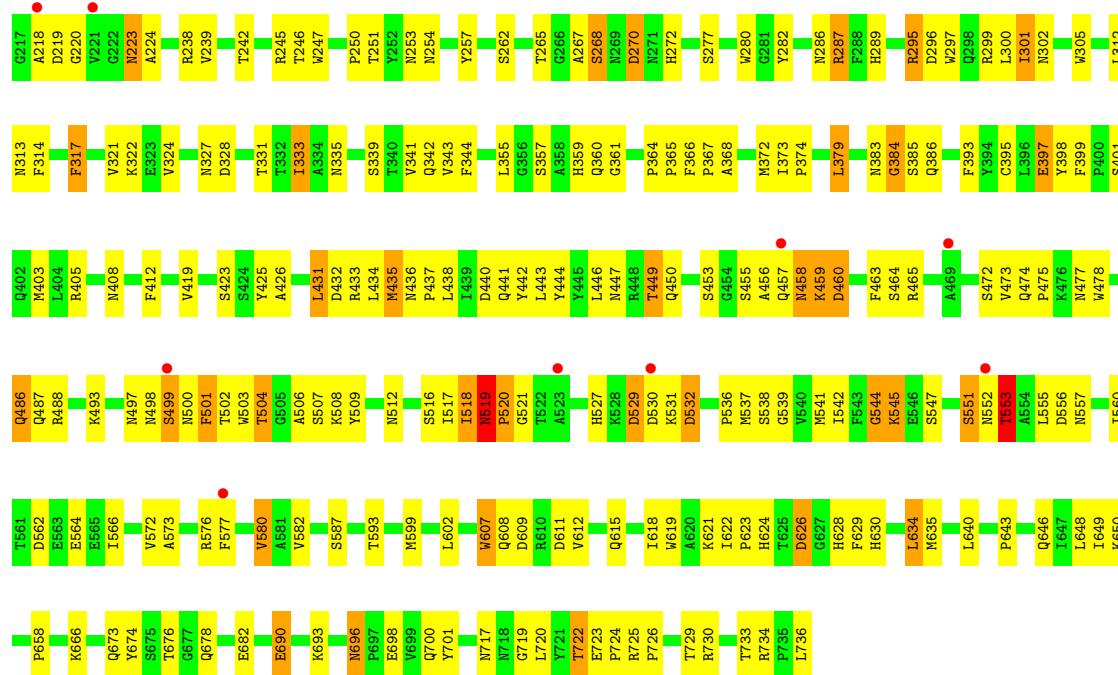


• Molecule 1: Capsid protein VP1



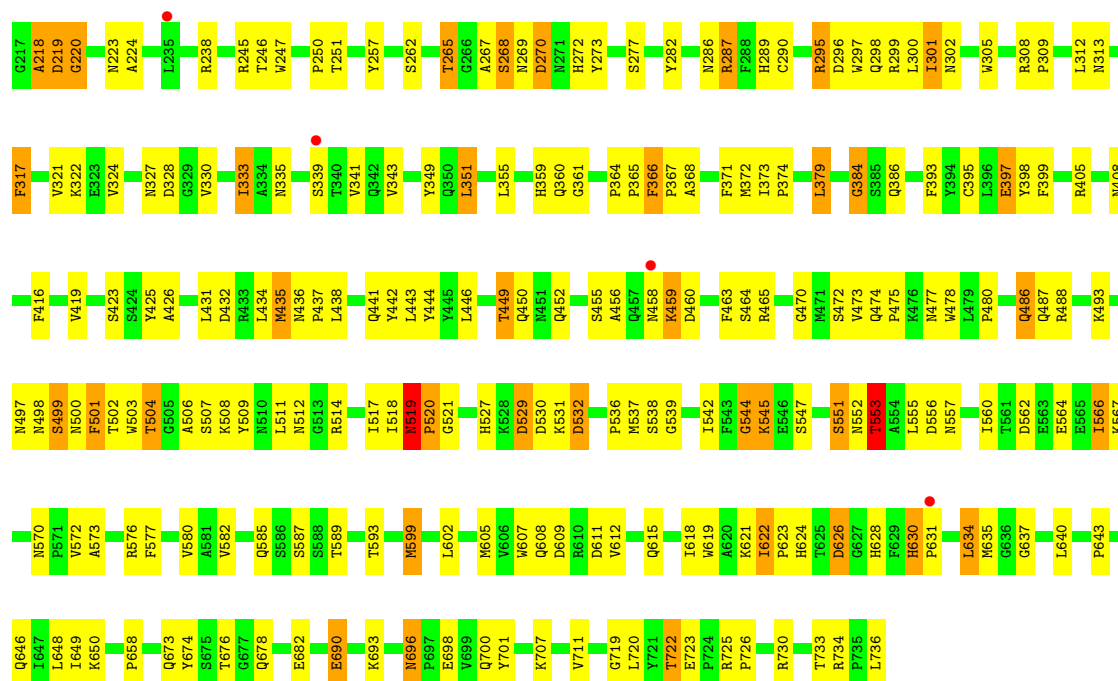


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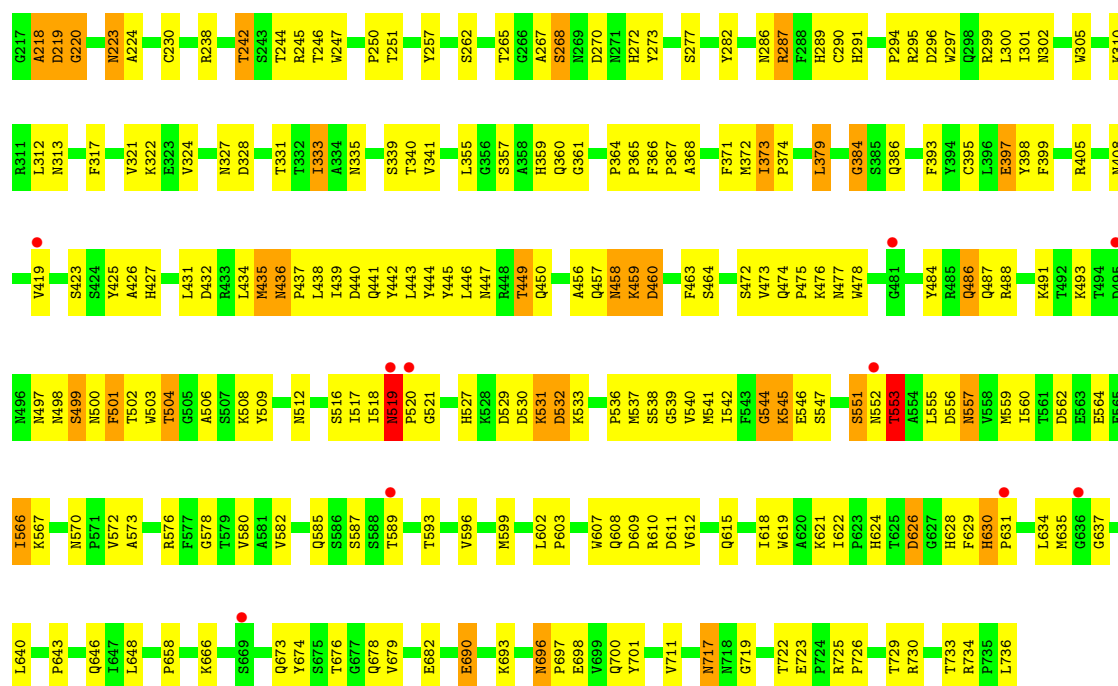


• Molecule 1: Capsid protein VP1



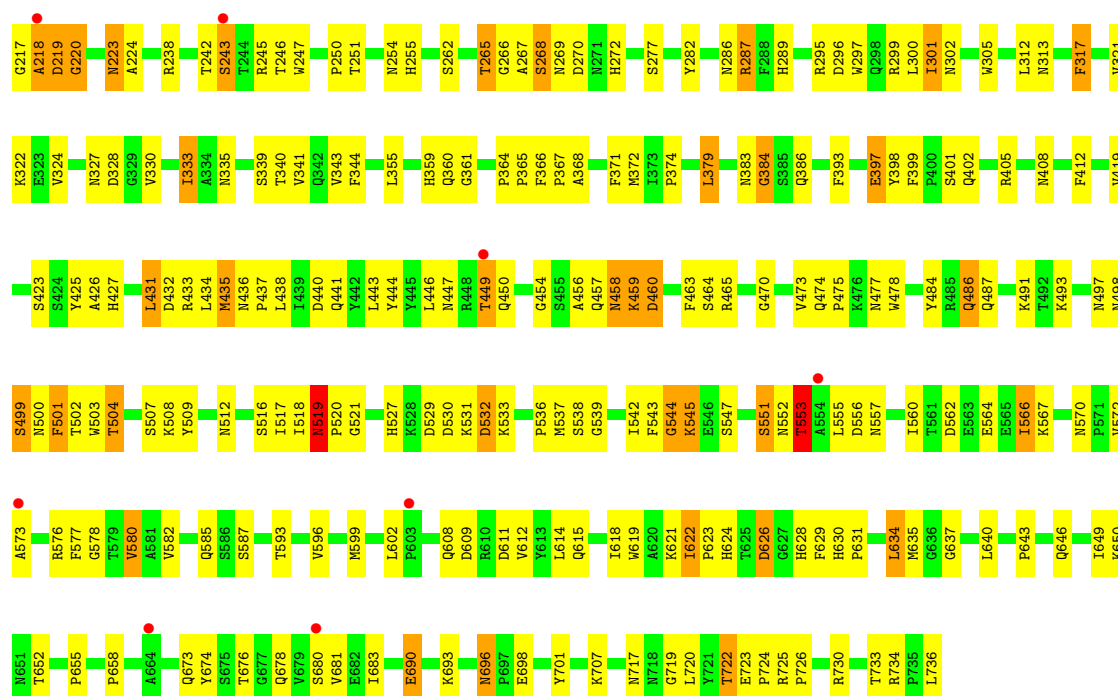


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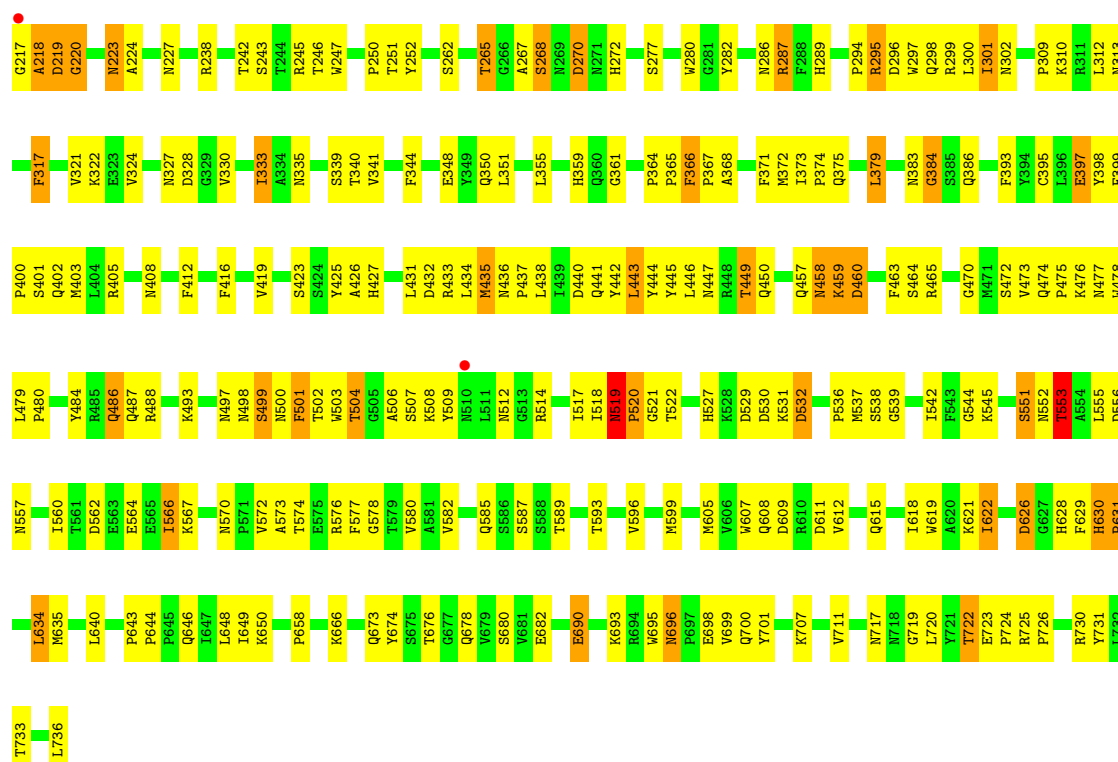
• Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

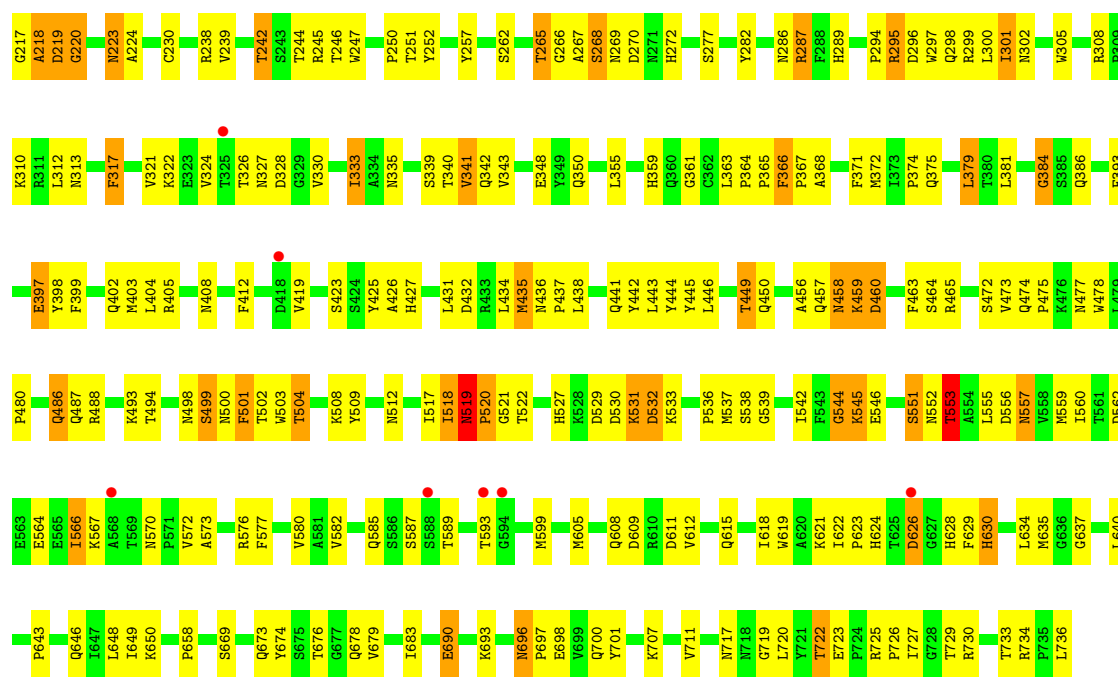
Chain o: 53% 39% 7%



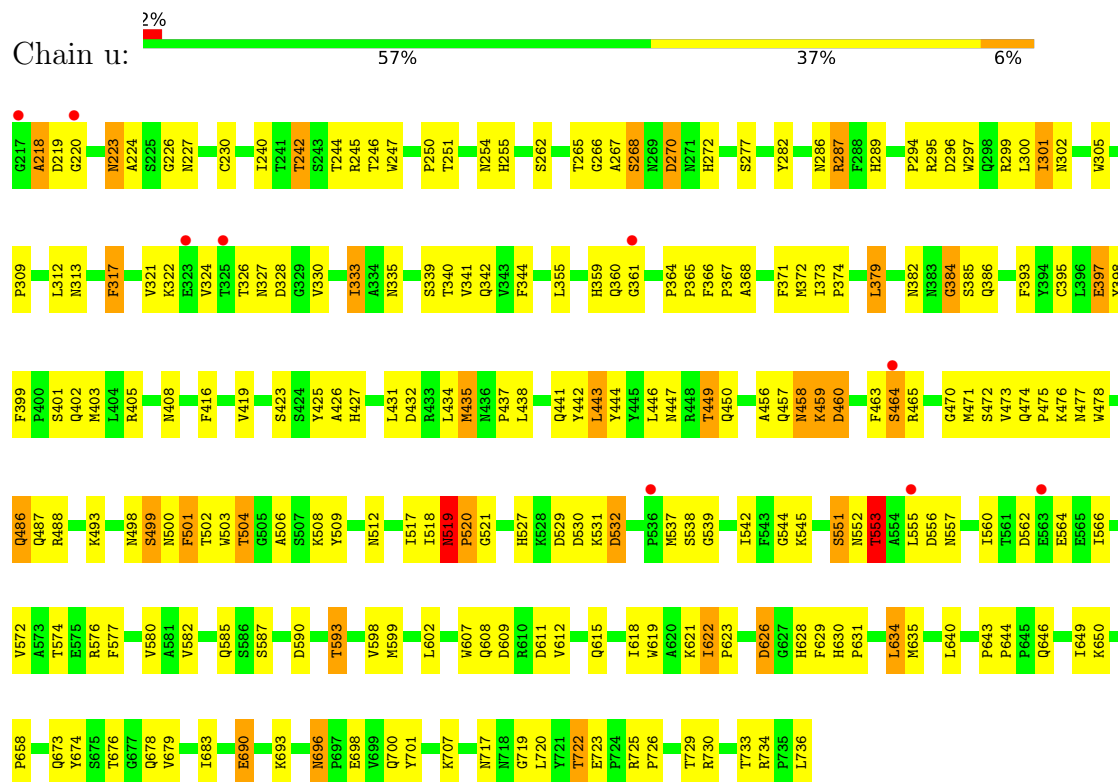
• Molecule 1: Capsid protein VP1

Chain p: 52% 39% 8%

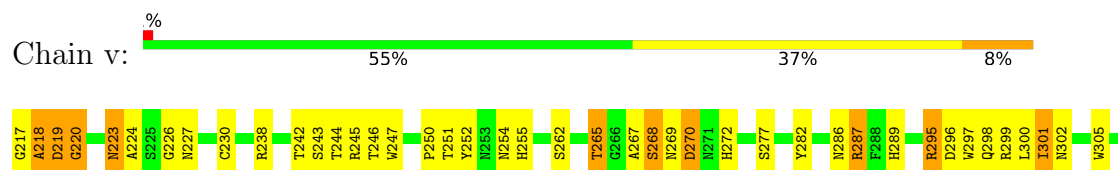


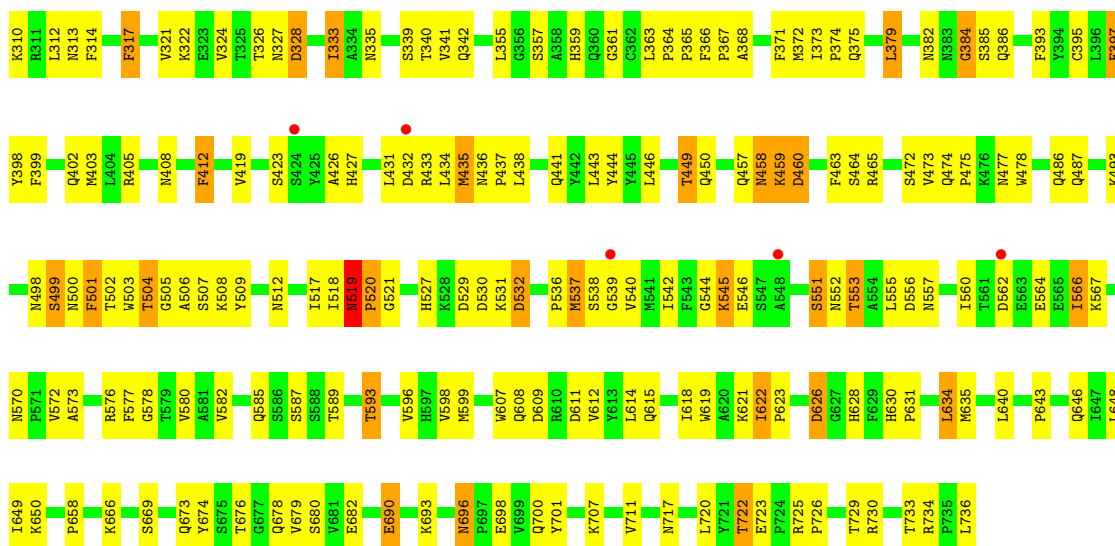


• Molecule 1: Capsid protein VP1

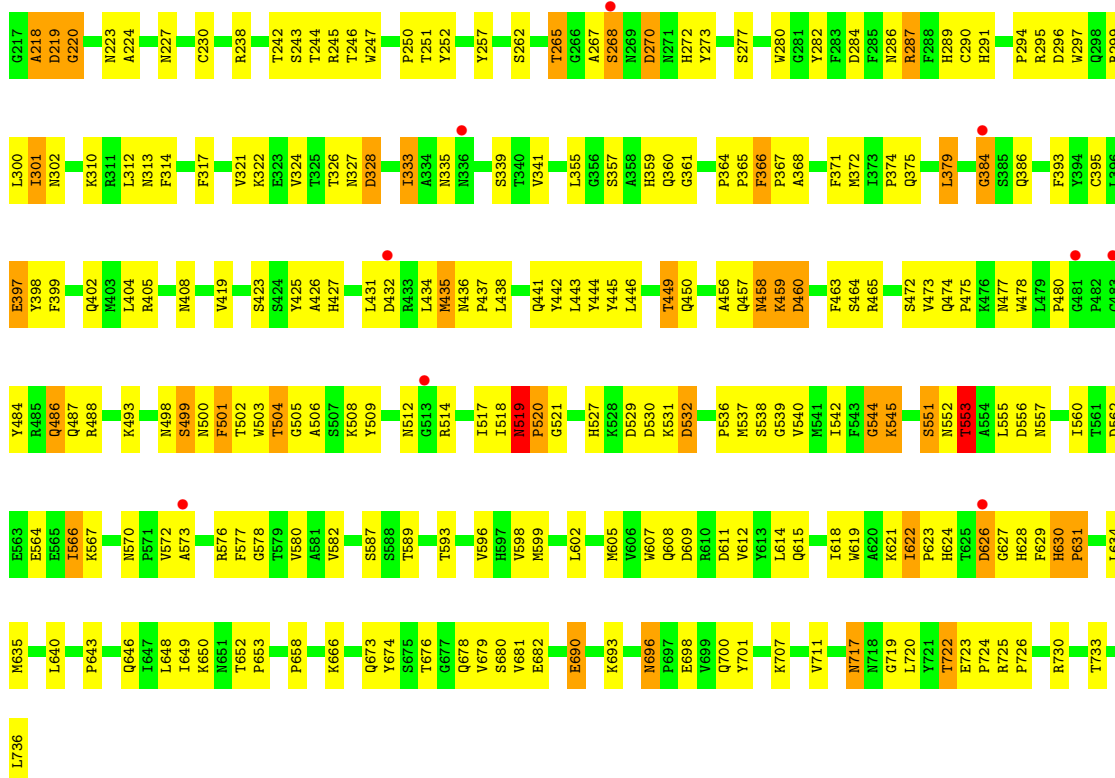


• Molecule 1: Capsid protein VP1



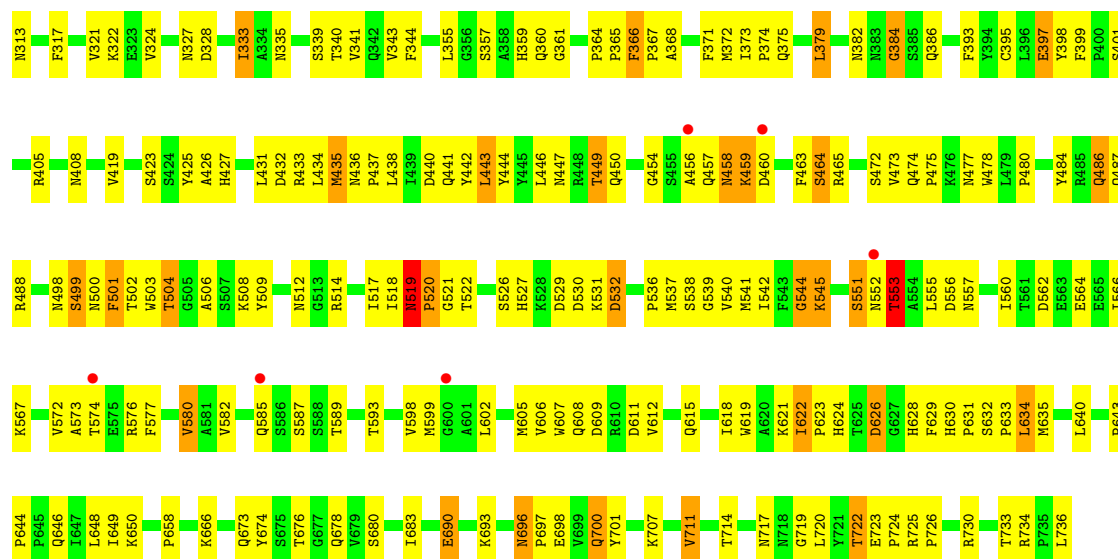


• Molecule 1: Capsid protein VP1

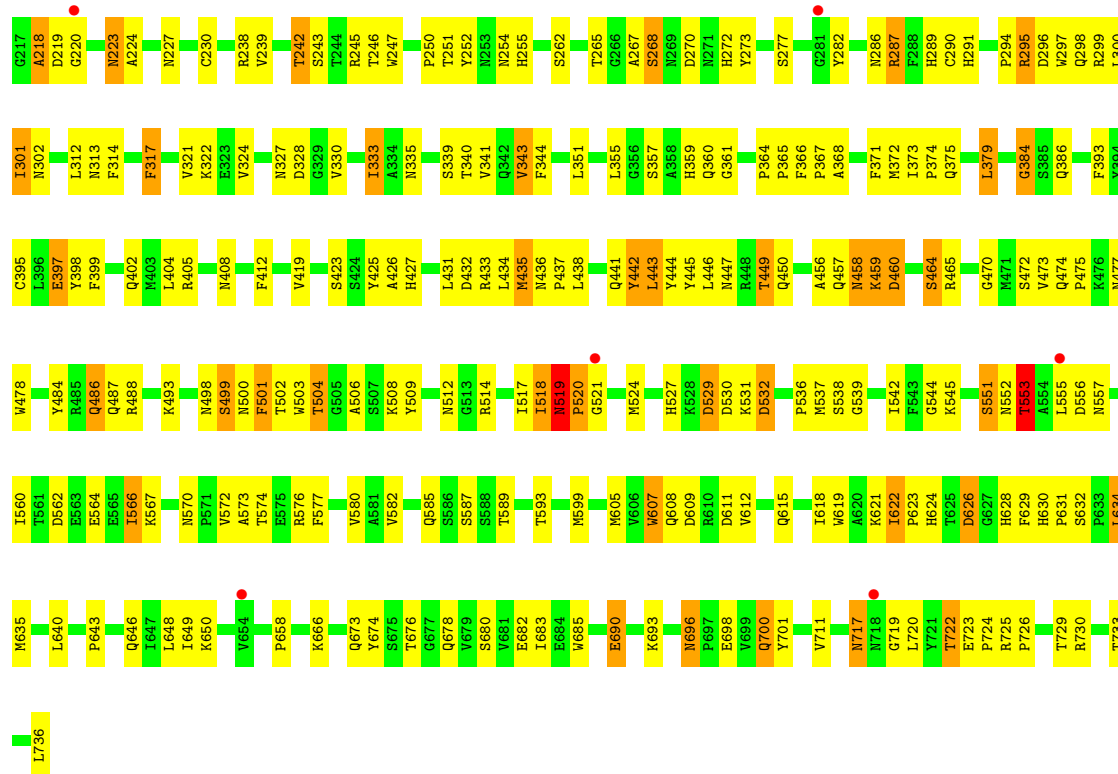


• Molecule 1: Capsid protein VP1



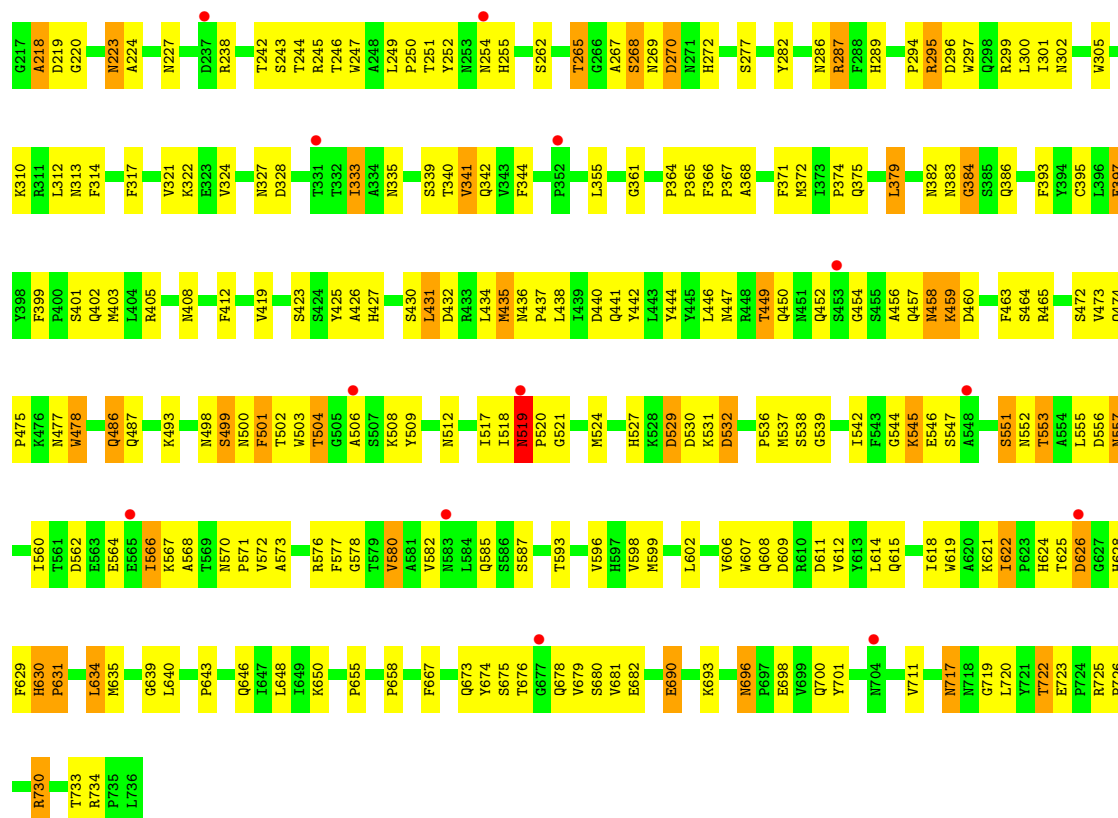


• Molecule 1: Capsid protein VP1

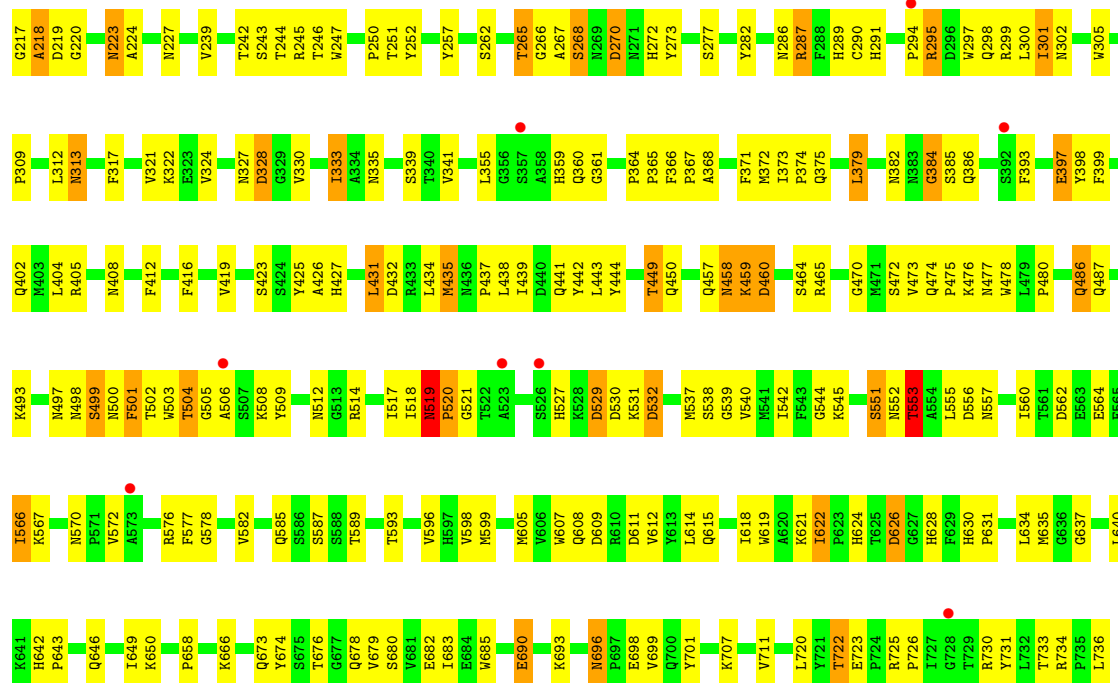


• Molecule 1: Capsid protein VP1

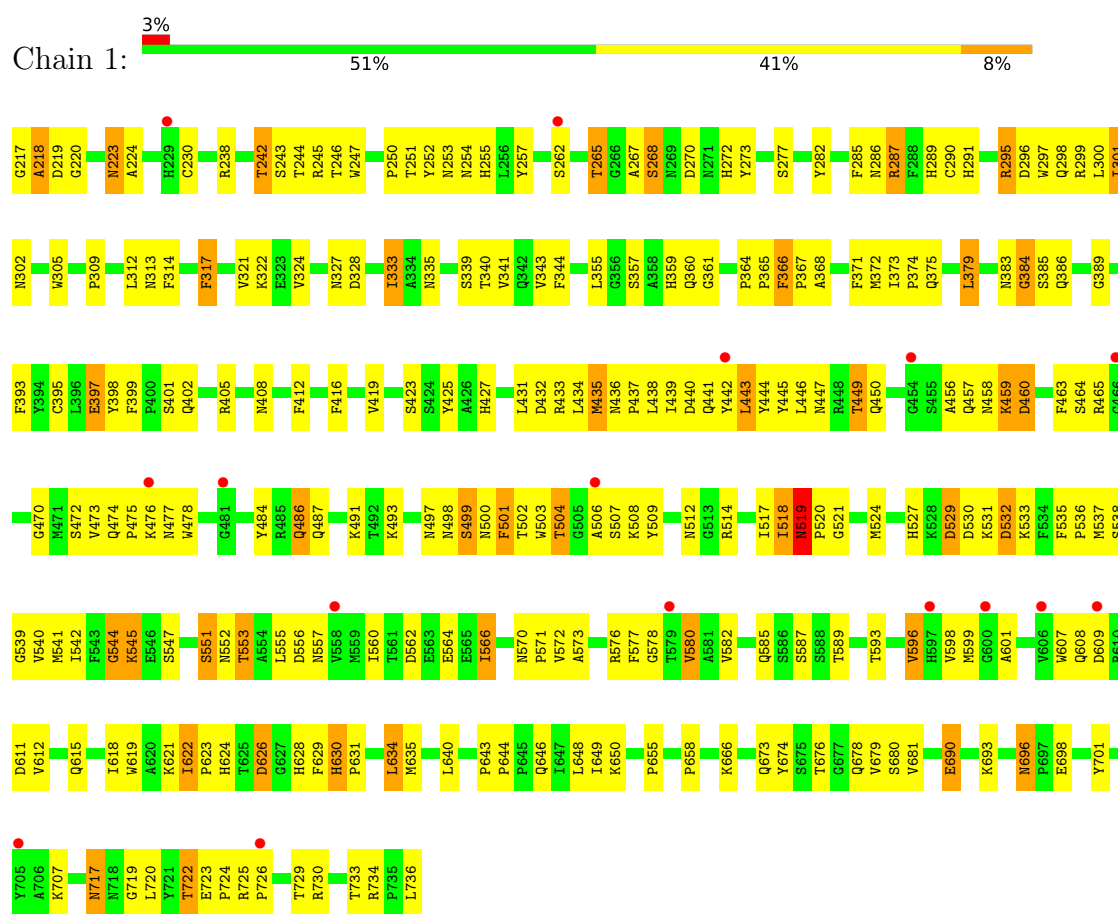




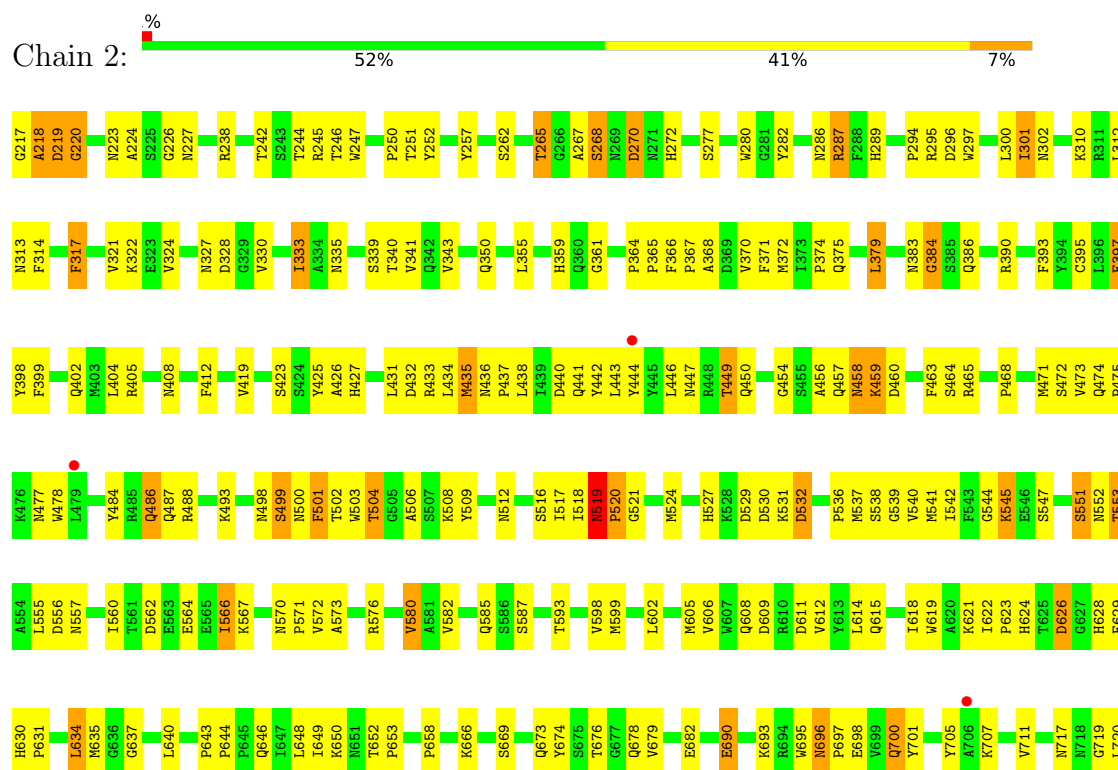
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

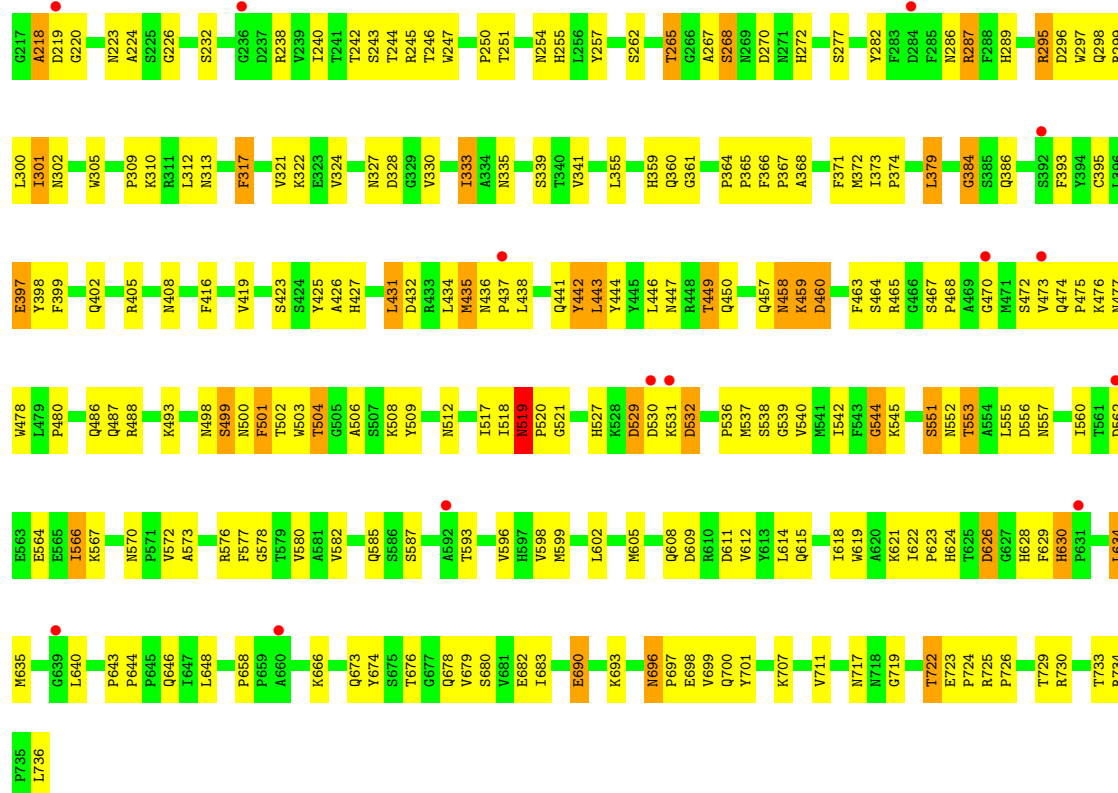


- Molecule 1: Capsid protein VP1

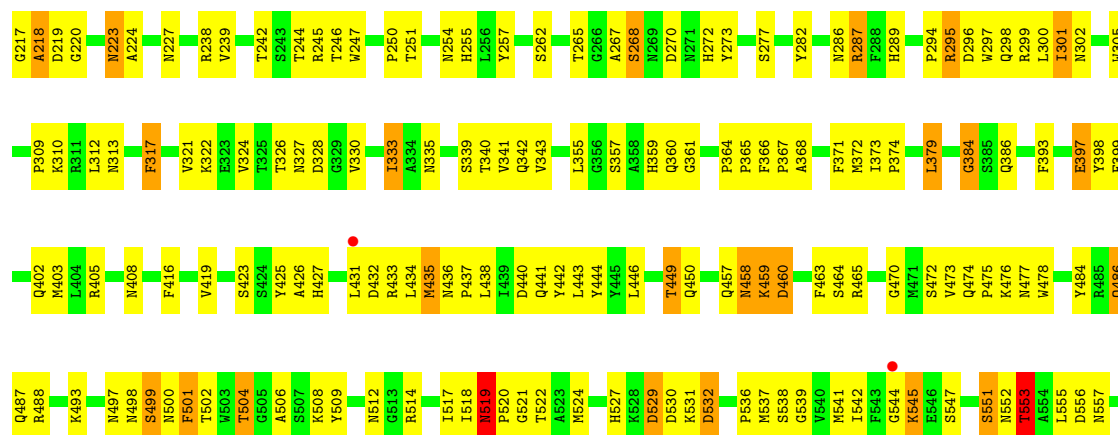


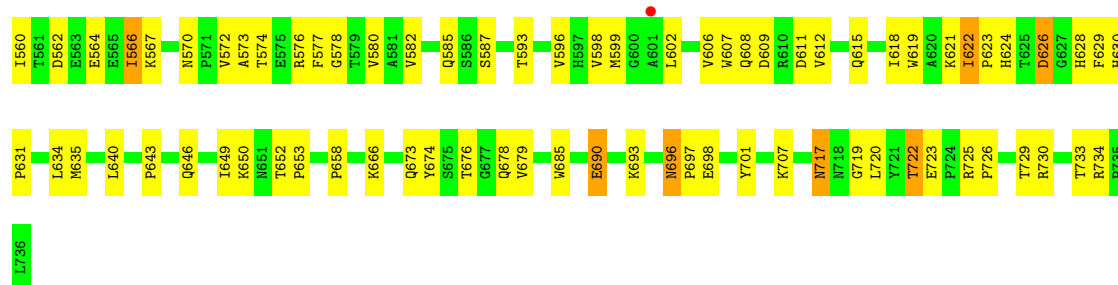


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

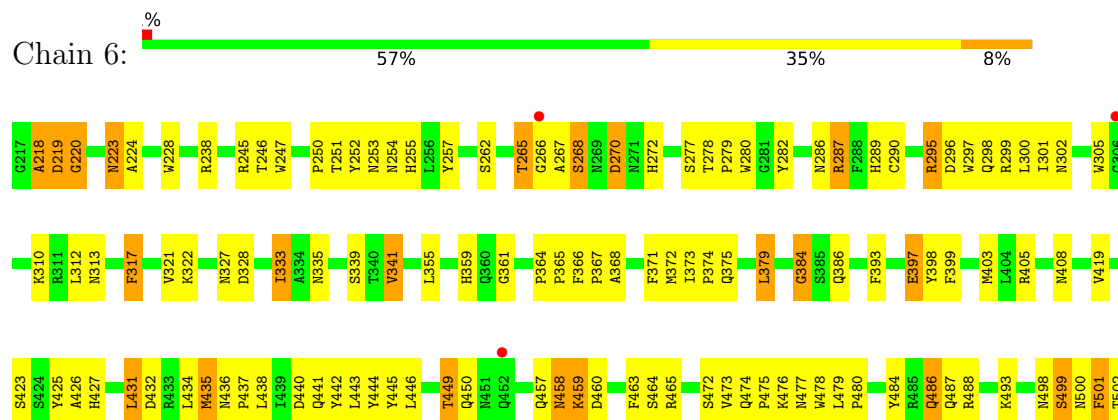


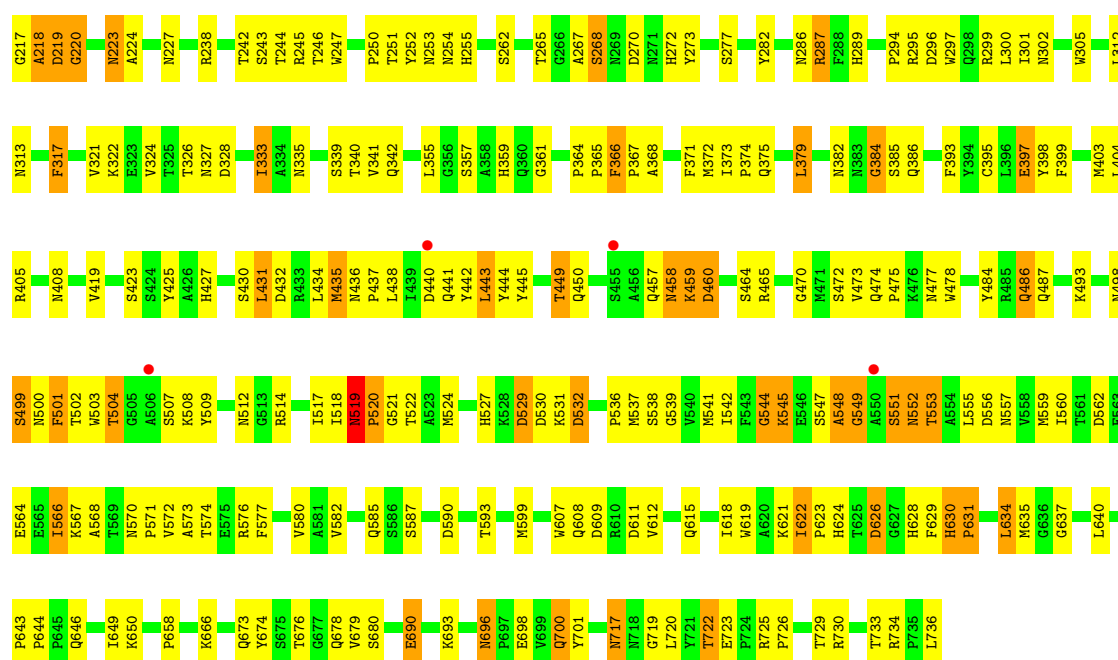


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	354.79Å 363.90Å 371.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.00 49.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	35.1 (49.21-3.00) 35.1 (49.21-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.251 , 0.286 0.248 , 0.282	Depositor DCC
R_{free} test set	3268 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k 0.009 for -l,-k,-h 0.023 for k,h,-l 0.008 for k,l,h 0.008 for l,h,k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	247260	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.70	0/4247	0.98	11/5790 (0.2%)
1	1	0.73	0/4247	0.96	11/5790 (0.2%)
1	2	0.67	0/4247	0.96	9/5790 (0.2%)
1	3	0.67	0/4247	0.95	10/5790 (0.2%)
1	4	0.65	0/4247	0.95	7/5790 (0.1%)
1	5	0.74	0/4247	0.97	10/5790 (0.2%)
1	6	0.79	1/4247 (0.0%)	0.97	9/5790 (0.2%)
1	7	0.69	0/4247	0.97	15/5790 (0.3%)
1	A	0.79	1/4247 (0.0%)	0.97	11/5790 (0.2%)
1	B	0.76	0/4247	0.97	8/5790 (0.1%)
1	C	0.69	0/4247	0.95	11/5790 (0.2%)
1	D	0.71	2/4247 (0.0%)	0.97	13/5790 (0.2%)
1	E	0.74	0/4247	0.96	8/5790 (0.1%)
1	F	0.73	0/4247	0.97	6/5790 (0.1%)
1	G	0.68	0/4247	0.94	9/5790 (0.2%)
1	H	0.66	0/4247	0.96	10/5790 (0.2%)
1	I	0.76	0/4247	0.98	7/5790 (0.1%)
1	J	0.81	0/4247	0.99	10/5790 (0.2%)
1	K	0.75	1/4247 (0.0%)	0.98	12/5790 (0.2%)
1	L	0.70	0/4247	0.96	9/5790 (0.2%)
1	M	0.68	0/4247	0.93	8/5790 (0.1%)
1	N	0.70	0/4247	0.95	8/5790 (0.1%)
1	O	0.71	0/4247	0.96	11/5790 (0.2%)
1	P	0.71	0/4247	0.97	9/5790 (0.2%)
1	Q	0.71	0/4247	0.98	8/5790 (0.1%)
1	R	0.72	0/4247	0.97	11/5790 (0.2%)
1	S	0.79	1/4247 (0.0%)	0.99	17/5790 (0.3%)
1	T	0.76	0/4247	0.98	10/5790 (0.2%)
1	U	0.71	1/4247 (0.0%)	0.98	13/5790 (0.2%)
1	V	0.71	0/4247	0.94	6/5790 (0.1%)
1	W	0.80	1/4247 (0.0%)	1.00	12/5790 (0.2%)
1	X	0.80	0/4247	1.01	11/5790 (0.2%)
1	Y	0.74	0/4247	0.99	8/5790 (0.1%)
1	Z	0.71	0/4247	0.97	9/5790 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.67	0/4247	0.96	8/5790 (0.1%)
1	b	0.70	0/4247	0.94	7/5790 (0.1%)
1	c	0.67	0/4247	0.97	8/5790 (0.1%)
1	d	0.66	0/4247	0.96	9/5790 (0.2%)
1	e	0.71	0/4247	0.97	10/5790 (0.2%)
1	f	0.67	0/4247	0.93	7/5790 (0.1%)
1	g	0.73	1/4247 (0.0%)	0.96	9/5790 (0.2%)
1	h	0.69	0/4247	0.97	10/5790 (0.2%)
1	i	0.67	0/4247	0.95	13/5790 (0.2%)
1	j	0.72	0/4247	0.97	11/5790 (0.2%)
1	k	0.76	0/4247	0.97	12/5790 (0.2%)
1	l	0.74	0/4247	0.98	16/5790 (0.3%)
1	m	0.83	0/4247	1.00	11/5790 (0.2%)
1	n	0.78	0/4247	0.99	10/5790 (0.2%)
1	o	0.65	0/4247	0.94	11/5790 (0.2%)
1	p	0.69	0/4247	0.95	12/5790 (0.2%)
1	q	0.65	0/4247	0.95	12/5790 (0.2%)
1	r	0.68	0/4247	0.94	7/5790 (0.1%)
1	s	0.67	0/4247	0.95	8/5790 (0.1%)
1	t	0.66	0/4247	0.95	13/5790 (0.2%)
1	u	0.67	0/4247	0.93	8/5790 (0.1%)
1	v	0.68	0/4247	0.94	7/5790 (0.1%)
1	w	0.68	0/4247	0.95	11/5790 (0.2%)
1	x	0.68	0/4247	0.97	11/5790 (0.2%)
1	y	0.67	0/4247	0.95	10/5790 (0.2%)
1	z	0.68	0/4247	0.97	10/5790 (0.2%)
All	All	0.71	9/254820 (0.0%)	0.96	598/347400 (0.2%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	494	THR	CA-CB	-8.53	1.40	1.53
1	g	456	ALA	CA-CB	-5.89	1.43	1.53
1	A	630	HIS	C-O	5.80	1.26	1.23
1	U	251	THR	CA-CB	5.62	1.59	1.52
1	D	494	THR	CB-CG2	5.44	1.70	1.52

The worst 5 of 598 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	519	ASN	CA-C-N	-15.53	101.96	119.98
1	e	519	ASN	C-N-CA	-15.53	101.96	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	519	ASN	CA-C-N	-15.10	102.47	119.98
1	P	519	ASN	C-N-CA	-15.10	102.47	119.98
1	x	519	ASN	CA-C-N	-14.95	102.64	119.98

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	0	4121	0	3896	257	0
1	1	4121	0	3896	295	0
1	2	4121	0	3896	282	0
1	3	4121	0	3896	262	0
1	4	4121	0	3896	261	0
1	5	4121	0	3896	257	2
1	6	4121	0	3896	251	0
1	7	4121	0	3896	260	5
1	A	4121	0	3896	301	1
1	B	4121	0	3896	290	0
1	C	4121	0	3896	272	0
1	D	4121	0	3896	268	5
1	E	4121	0	3896	285	0
1	F	4121	0	3896	304	0
1	G	4121	0	3896	248	0
1	H	4121	0	3896	288	0
1	I	4121	0	3896	290	0
1	J	4121	0	3896	294	0
1	K	4121	0	3896	248	4
1	L	4121	0	3896	268	0
1	M	4121	0	3896	247	0
1	N	4121	0	3896	263	5
1	O	4121	0	3896	245	0
1	P	4121	0	3896	244	0
1	Q	4121	0	3896	272	0
1	R	4121	0	3896	257	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	4121	0	3896	265	0
1	T	4121	0	3896	264	1
1	U	4121	0	3896	290	5
1	V	4121	0	3896	284	0
1	W	4121	0	3896	306	0
1	X	4121	0	3896	291	0
1	Y	4121	0	3896	279	0
1	Z	4121	0	3896	270	0
1	a	4121	0	3896	262	0
1	b	4121	0	3896	255	0
1	c	4121	0	3896	265	0
1	d	4121	0	3896	252	0
1	e	4121	0	3896	253	0
1	f	4121	0	3896	258	0
1	g	4121	0	3896	283	6
1	h	4121	0	3896	276	0
1	i	4121	0	3896	262	0
1	j	4121	0	3896	263	0
1	k	4121	0	3896	256	3
1	l	4121	0	3896	261	2
1	m	4121	0	3896	270	0
1	n	4121	0	3896	257	1
1	o	4121	0	3896	287	0
1	p	4121	0	3896	272	2
1	q	4121	0	3896	273	0
1	r	4121	0	3896	256	0
1	s	4121	0	3896	258	0
1	t	4121	0	3896	255	1
1	u	4121	0	3896	254	0
1	v	4121	0	3896	267	0
1	w	4121	0	3896	281	0
1	x	4121	0	3896	267	0
1	y	4121	0	3896	269	0
1	z	4121	0	3896	274	1
All	All	247260	0	233760	12782	22

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 27.

The worst 5 of 12782 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:E:464:SER:HB3	1:g:551:SER:HA	1.35	1.09
1:M:464:SER:HB3	1:t:551:SER:HA	1.34	1.09
1:G:551:SER:HA	1:4:464:SER:HB3	1.34	1.07
1:L:551:SER:HA	1:u:464:SER:HB3	1.38	1.05
1:h:551:SER:HA	1:w:464:SER:HB3	1.38	1.05

The worst 5 of 22 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:265:THR:OG1	1:z:454:GLY:O[2_554]	1.28	0.92
1:K:590:ASP:OD1	1:N:455:SER:N[4_556]	1.38	0.82
1:l:455:SER:OG	1:p:661:GLU:OE2[4_556]	1.50	0.70
1:D:494:THR:OG1	1:U:329:GLY:CA[2_454]	1.58	0.62
1:g:456:ALA:CB	1:7:548:ALA:O[4_446]	1.64	0.56

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 X-ray entries followed by that with respect to entries of similar resolution.

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	0	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	3	19
1	1	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	3	20
1	2	518/520 (100%)	463 (89%)	43 (8%)	12 (2%)	5	25
1	3	518/520 (100%)	459 (89%)	46 (9%)	13 (2%)	4	23
1	4	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	4	23
1	5	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	4	23
1	6	518/520 (100%)	464 (90%)	42 (8%)	12 (2%)	5	25
1	7	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	3	20
1	A	518/520 (100%)	460 (89%)	43 (8%)	15 (3%)	3	20
1	B	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	3	19
1	D	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	4	22
1	E	518/520 (100%)	463 (89%)	41 (8%)	14 (3%)	4	22
1	F	518/520 (100%)	462 (89%)	42 (8%)	14 (3%)	4	22
1	G	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	4	22
1	H	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	3	20
1	I	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	3	20
1	J	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	3	20
1	K	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	4	23
1	L	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	3	20
1	M	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	4	23
1	N	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	4	22
1	O	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	4	22
1	P	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	4	22
1	Q	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	4	22
1	R	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	3	19
1	S	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	4	23
1	T	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	4	23
1	U	518/520 (100%)	471 (91%)	31 (6%)	16 (3%)	3	19
1	V	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	3	20
1	W	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	4	23
1	X	518/520 (100%)	461 (89%)	43 (8%)	14 (3%)	4	22
1	Y	518/520 (100%)	461 (89%)	44 (8%)	13 (2%)	4	23
1	Z	518/520 (100%)	462 (89%)	44 (8%)	12 (2%)	5	25
1	a	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	4	23
1	b	518/520 (100%)	467 (90%)	39 (8%)	12 (2%)	5	25
1	c	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	5	25
1	d	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	4	23
1	e	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	4	23
1	f	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	3	19
1	g	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h	518/520 (100%)	463 (89%)	44 (8%)	11 (2%)	5	27
1	i	518/520 (100%)	466 (90%)	37 (7%)	15 (3%)	3	20
1	j	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	4	23
1	k	518/520 (100%)	465 (90%)	37 (7%)	16 (3%)	3	19
1	l	518/520 (100%)	468 (90%)	38 (7%)	12 (2%)	5	25
1	m	518/520 (100%)	468 (90%)	37 (7%)	13 (2%)	4	23
1	n	518/520 (100%)	469 (90%)	36 (7%)	13 (2%)	4	23
1	o	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	4	22
1	p	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	3	19
1	q	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	3	19
1	r	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	3	19
1	s	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	4	23
1	t	518/520 (100%)	463 (89%)	40 (8%)	15 (3%)	3	20
1	u	518/520 (100%)	467 (90%)	37 (7%)	14 (3%)	4	22
1	v	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	3	20
1	w	518/520 (100%)	465 (90%)	38 (7%)	15 (3%)	3	20
1	x	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	5	25
1	y	518/520 (100%)	468 (90%)	35 (7%)	15 (3%)	3	20
1	z	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	4	23
All	All	31080/31200 (100%)	27915 (90%)	2328 (8%)	837 (3%)	4	22

5 of 837 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	LYS
1	A	519	ASN
1	A	531	LYS
1	A	545	LYS
1	B	459	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	0	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	1	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	2	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	3	452/452 (100%)	412 (91%)	40 (9%)	9	35
1	4	452/452 (100%)	411 (91%)	41 (9%)	9	33
1	5	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	6	452/452 (100%)	411 (91%)	41 (9%)	9	33
1	7	452/452 (100%)	411 (91%)	41 (9%)	9	33
1	A	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	B	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	C	452/452 (100%)	411 (91%)	41 (9%)	9	33
1	D	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	E	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	F	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	G	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	H	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	I	452/452 (100%)	405 (90%)	47 (10%)	7	28
1	J	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	K	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	L	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	M	452/452 (100%)	410 (91%)	42 (9%)	8	32
1	N	452/452 (100%)	412 (91%)	40 (9%)	9	35
1	O	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	P	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	Q	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	R	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	S	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	T	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	U	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	V	452/452 (100%)	409 (90%)	43 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	X	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	Y	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	Z	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	a	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	b	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	c	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	d	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	e	452/452 (100%)	405 (90%)	47 (10%)	7	28
1	f	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	g	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	h	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	i	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	j	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	k	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	l	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	m	452/452 (100%)	410 (91%)	42 (9%)	8	32
1	n	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	o	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	p	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	q	452/452 (100%)	405 (90%)	47 (10%)	7	28
1	r	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	s	452/452 (100%)	410 (91%)	42 (9%)	8	32
1	t	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	u	452/452 (100%)	410 (91%)	42 (9%)	8	32
1	v	452/452 (100%)	407 (90%)	45 (10%)	7	29
1	w	452/452 (100%)	409 (90%)	43 (10%)	8	31
1	x	452/452 (100%)	406 (90%)	46 (10%)	7	29
1	y	452/452 (100%)	408 (90%)	44 (10%)	8	30
1	z	452/452 (100%)	408 (90%)	44 (10%)	8	30
All	All	27120/27120 (100%)	24480 (90%)	2640 (10%)	8	30

5 of 2640 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	p	628	HIS
1	z	622	ILE
1	r	219	ASP
1	p	622	ILE
1	v	219	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1700 such sidechains are listed below:

Mol	Chain	Res	Type
1	g	696	ASN
1	o	498	ASN
1	4	457	GLN
1	h	691	ASN
1	g	691	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	520/520 (100%)	0.32	8 (1%) 72 49	45, 60, 92, 141	0
1	1	520/520 (100%)	0.47	16 (3%) 51 30	44, 61, 91, 139	0
1	2	520/520 (100%)	0.32	3 (0%) 85 69	46, 60, 93, 141	0
1	3	520/520 (100%)	0.24	14 (2%) 56 33	43, 59, 91, 138	0
1	4	520/520 (100%)	0.13	3 (0%) 85 69	44, 59, 92, 140	0
1	5	520/520 (100%)	0.16	8 (1%) 72 49	43, 57, 90, 138	0
1	6	520/520 (100%)	0.20	6 (1%) 76 55	42, 57, 90, 139	0
1	7	520/520 (100%)	0.13	4 (0%) 82 64	42, 58, 90, 138	0
1	A	520/520 (100%)	0.71	38 (7%) 21 11	45, 61, 92, 139	0
1	B	520/520 (100%)	0.64	25 (4%) 35 19	46, 61, 93, 139	0
1	C	520/520 (100%)	0.40	17 (3%) 49 28	45, 60, 92, 140	0
1	D	520/520 (100%)	0.42	13 (2%) 58 35	44, 61, 92, 139	0
1	E	520/520 (100%)	0.64	21 (4%) 42 23	46, 61, 93, 139	0
1	F	520/520 (100%)	0.63	25 (4%) 35 19	45, 61, 93, 138	0
1	G	520/520 (100%)	0.32	7 (1%) 75 53	46, 60, 91, 140	0
1	H	520/520 (100%)	0.34	5 (0%) 79 59	43, 60, 92, 137	0
1	I	520/520 (100%)	0.62	28 (5%) 31 16	45, 61, 92, 139	0
1	J	520/520 (100%)	0.73	29 (5%) 30 15	45, 62, 92, 141	0
1	K	520/520 (100%)	0.12	6 (1%) 76 55	43, 57, 91, 139	0
1	L	520/520 (100%)	0.08	4 (0%) 82 64	42, 58, 90, 141	0
1	M	520/520 (100%)	0.12	9 (1%) 69 45	43, 58, 90, 138	0
1	N	520/520 (100%)	0.12	9 (1%) 69 45	42, 58, 90, 138	0
1	O	520/520 (100%)	0.10	3 (0%) 85 69	42, 58, 91, 141	0
1	P	520/520 (100%)	0.19	4 (0%) 82 64	43, 58, 90, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Q	520/520 (100%)	0.29	12 (2%) 61 38	42, 59, 91, 138	0
1	R	520/520 (100%)	0.25	7 (1%) 75 53	43, 58, 91, 139	0
1	S	520/520 (100%)	0.26	12 (2%) 61 38	41, 57, 88, 141	0
1	T	520/520 (100%)	0.15	7 (1%) 75 53	42, 57, 90, 140	0
1	U	520/520 (100%)	0.34	8 (1%) 72 49	45, 60, 91, 139	0
1	V	520/520 (100%)	0.48	19 (3%) 45 25	45, 61, 92, 140	0
1	W	520/520 (100%)	0.75	41 (7%) 18 10	46, 61, 93, 139	0
1	X	520/520 (100%)	0.69	27 (5%) 33 17	44, 61, 93, 141	0
1	Y	520/520 (100%)	0.50	13 (2%) 58 35	45, 61, 92, 139	0
1	Z	520/520 (100%)	0.25	10 (1%) 66 43	44, 60, 91, 140	0
1	a	520/520 (100%)	0.21	2 (0%) 88 76	44, 59, 92, 139	0
1	b	520/520 (100%)	0.14	7 (1%) 75 53	42, 58, 90, 137	0
1	c	520/520 (100%)	0.13	8 (1%) 72 49	44, 59, 90, 141	0
1	d	520/520 (100%)	0.11	5 (0%) 79 59	45, 60, 91, 141	0
1	e	520/520 (100%)	0.16	9 (1%) 69 45	43, 58, 89, 141	0
1	f	520/520 (100%)	0.11	1 (0%) 91 83	45, 59, 92, 141	0
1	g	520/520 (100%)	0.46	18 (3%) 47 27	46, 60, 92, 134	0
1	h	520/520 (100%)	0.34	12 (2%) 61 38	45, 60, 91, 140	0
1	i	520/520 (100%)	0.15	4 (0%) 82 64	43, 59, 90, 138	0
1	j	520/520 (100%)	0.16	7 (1%) 75 53	43, 58, 90, 139	0
1	k	520/520 (100%)	0.28	9 (1%) 69 45	41, 58, 90, 135	0
1	l	520/520 (100%)	0.17	4 (0%) 82 64	42, 57, 90, 138	0
1	m	520/520 (100%)	0.26	10 (1%) 66 43	42, 57, 89, 138	0
1	n	520/520 (100%)	0.19	8 (1%) 72 49	42, 57, 90, 139	0
1	o	520/520 (100%)	0.18	2 (0%) 88 76	45, 60, 92, 139	0
1	p	520/520 (100%)	0.36	13 (2%) 58 35	46, 60, 91, 139	0
1	q	520/520 (100%)	0.16	4 (0%) 82 64	44, 60, 92, 139	0
1	r	520/520 (100%)	0.13	6 (1%) 76 55	43, 58, 90, 138	0
1	s	520/520 (100%)	0.06	5 (0%) 79 59	43, 59, 91, 139	0
1	t	520/520 (100%)	0.13	7 (1%) 75 53	43, 59, 91, 140	0
1	u	520/520 (100%)	0.13	9 (1%) 69 45	43, 58, 90, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	v	520/520 (100%)	0.21	5 (0%)	79 59	42, 59, 90, 141	0
1	w	520/520 (100%)	0.24	9 (1%)	69 45	43, 60, 92, 141	0
1	x	520/520 (100%)	0.22	7 (1%)	75 53	44, 60, 92, 140	0
1	y	520/520 (100%)	0.21	6 (1%)	76 55	43, 59, 90, 139	0
1	z	520/520 (100%)	0.29	13 (2%)	58 35	44, 59, 91, 141	0
All	All	31200/31200 (100%)	0.29	651 (2%)	63 40	41, 59, 91, 141	0

The worst 5 of 651 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	483	CYS	5.7
1	3	470	GLY	5.5
1	I	563	GLU	4.9
1	X	347	SER	4.8
1	I	356	GLY	4.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.