wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:57 PM GMT

PDB ID	:	4V86
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

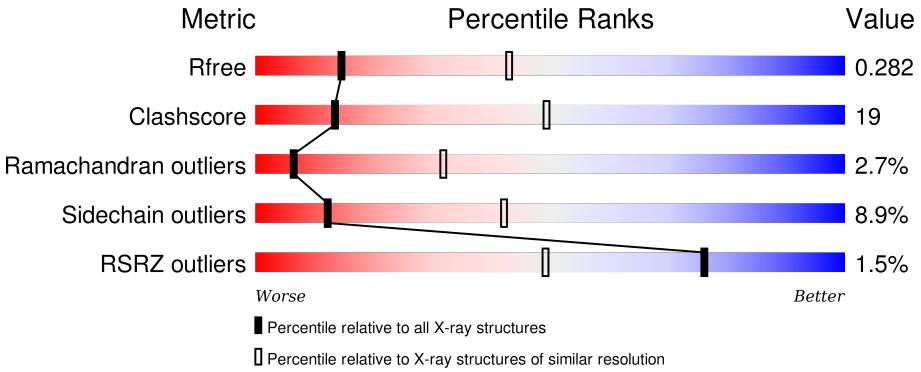
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower 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 <=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% 57% 37% 6%
1	1	520	% 53% 40% 8%
1	2	520	3% 56% 38% 6%
1	3	520	2% 57% 37% 6%
1	4	520	% 57% 38% 6%

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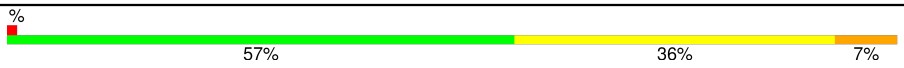
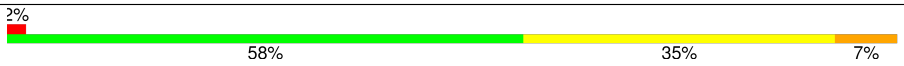
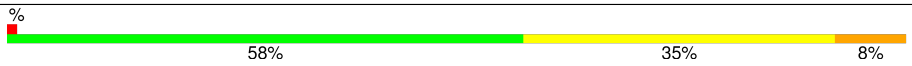
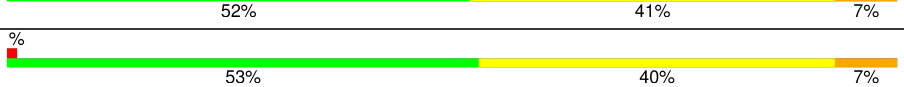
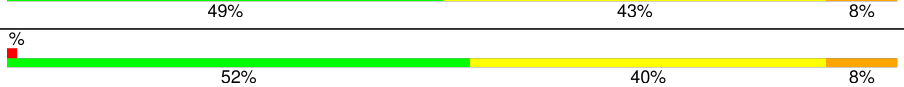
Mol	Chain	Length	Quality of chain
1	5	520	
1	6	520	
1	7	520	
1	A	520	
1	B	520	
1	C	520	
1	D	520	
1	E	520	
1	F	520	
1	G	520	
1	H	520	
1	I	520	
1	J	520	
1	K	520	
1	L	520	
1	M	520	
1	N	520	
1	O	520	
1	P	520	
1	Q	520	
1	R	520	
1	S	520	
1	T	520	
1	U	520	
1	V	520	

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Mol	Chain	Length	Quality of chain
1	W	520	2% 47% 46% 7%
1	X	520	3% 50% 43% 7%
1	Y	520	2% 51% 42% 7%
1	Z	520	2% 49% 44% 7%
1	a	520	2% 90% 10%
1	b	520	% 90% 10%
1	c	520	% 89% 11%
1	d	520	2% 90% 10%
1	e	520	% 89% 11%
1	f	520	% 90% 10%
1	g	520	89% 11%
1	h	520	% 91% 9%
1	i	520	% 89% 11%
1	j	520	% 90% 10%
1	k	520	% 88% 12%
1	l	520	90% 10%
1	m	520	% 90% 10%
1	n	520	% 89% 10%
1	o	520	% 90% 10%
1	p	520	3% 90% 10%
1	q	520	% 88% 12%
1	r	520	% 89% 11%
1	s	520	% 90% 10%
1	t	520	% 90% 10%
1	u	520	2% 90% 10%

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Mol	Chain	Length	Quality of chain
1	v	520	2% 89% 11%
1	w	520	2% 89% 11%
1	x	520	2% 91% 9%
1	y	520	% 90% 10%
1	z	520	2% 89% 11%

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	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	R	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	S	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	T	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	U	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	V	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	W	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	X	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	Y	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	Z	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
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			

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

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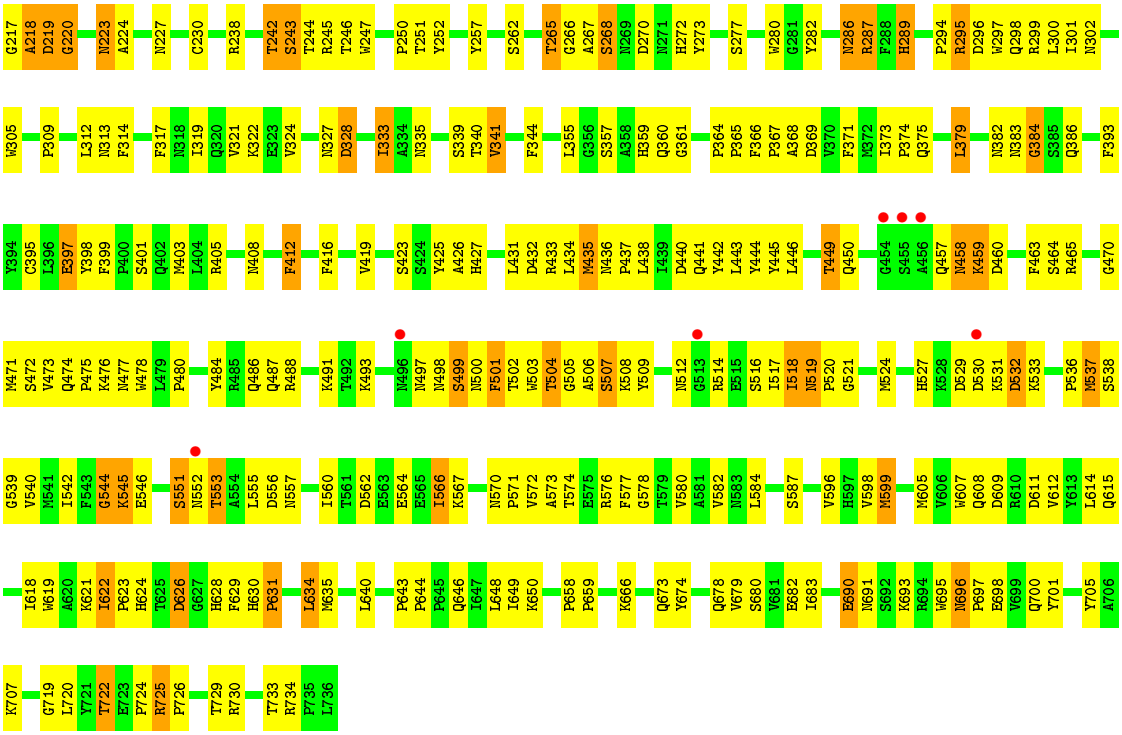
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	7	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

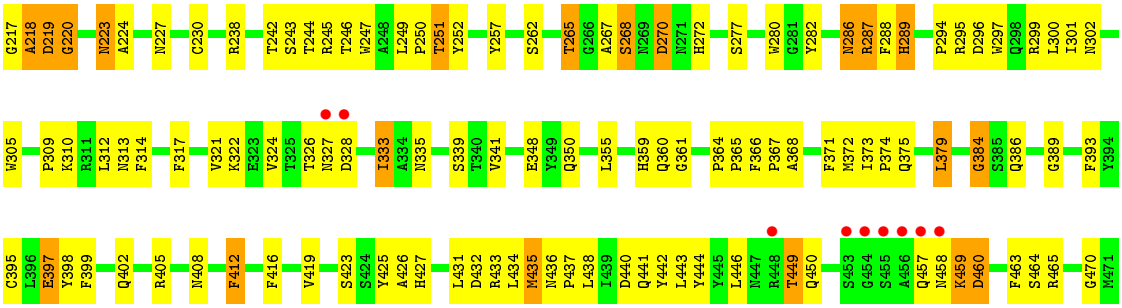
- Molecule 1: Capsid protein VP1

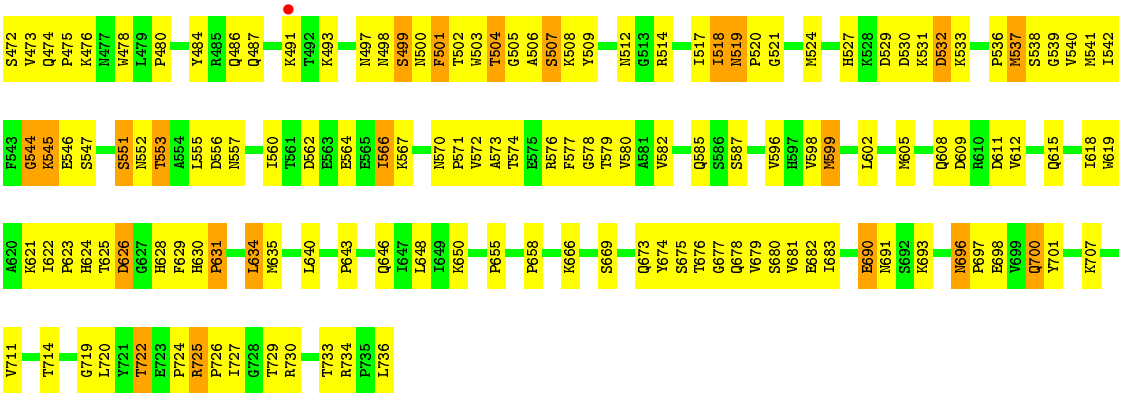
Chain A:



- Molecule 1: Capsid protein VP1

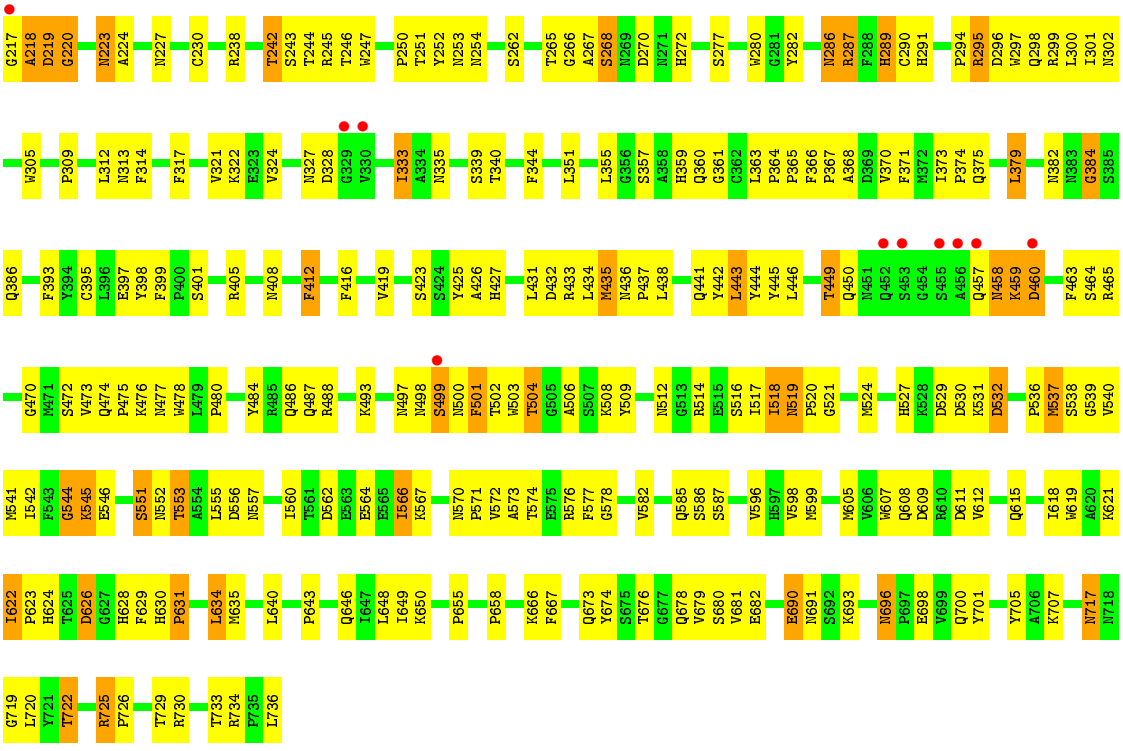
Chain B:





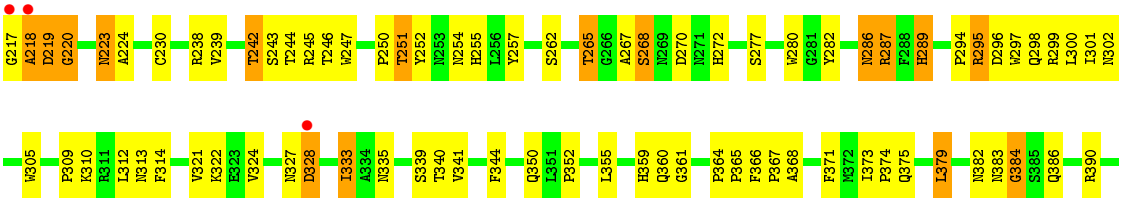
• Molecule 1: Capsid protein VP1

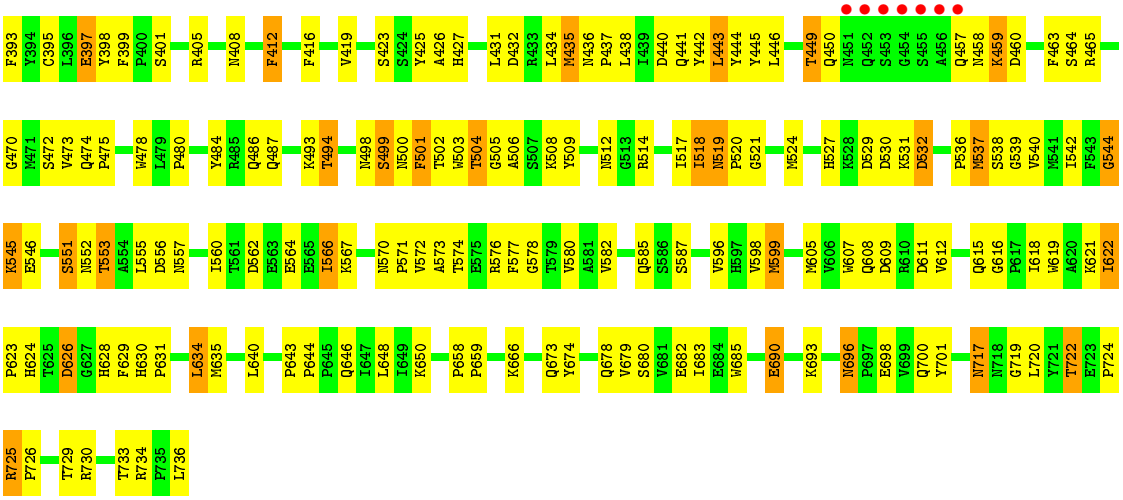
Chain C:



• Molecule 1: Capsid protein VP1

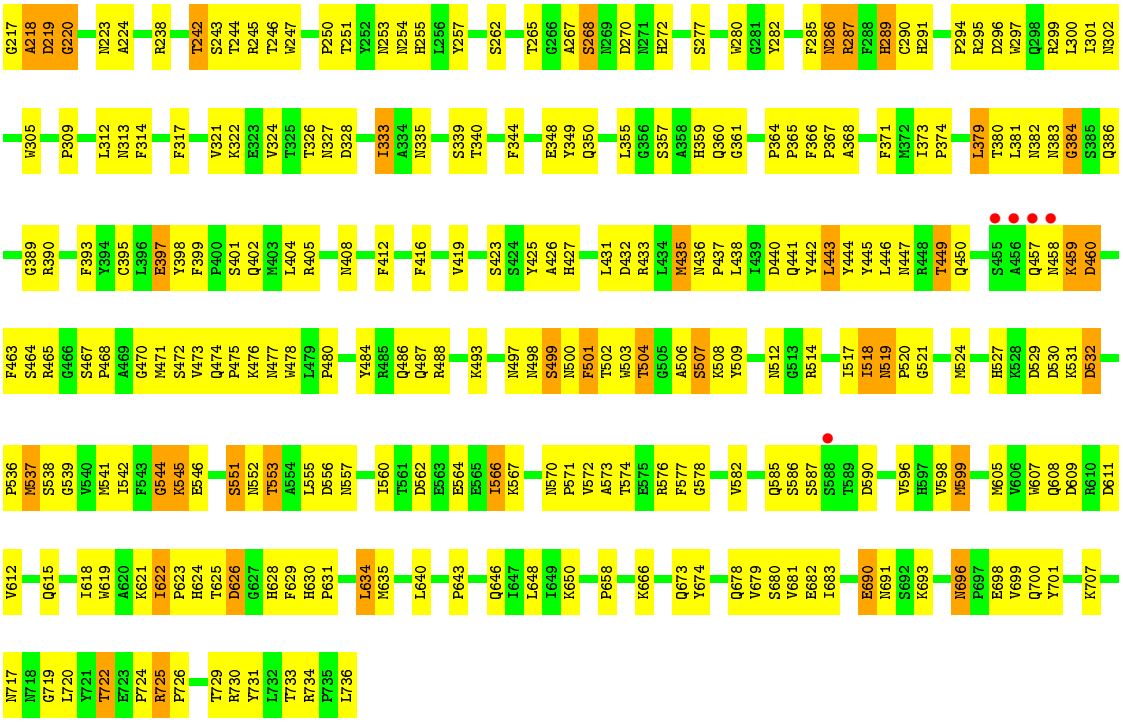
Chain D:





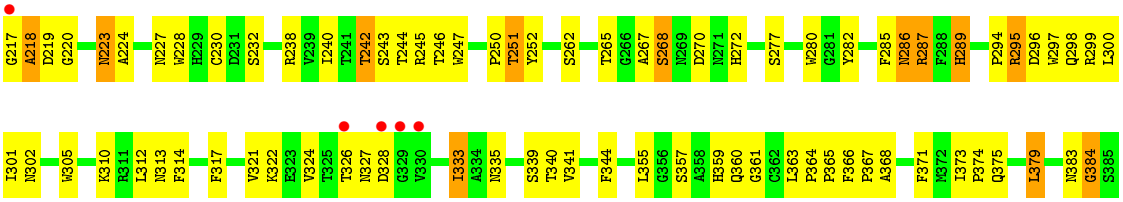
• Molecule 1: Capsid protein VP1

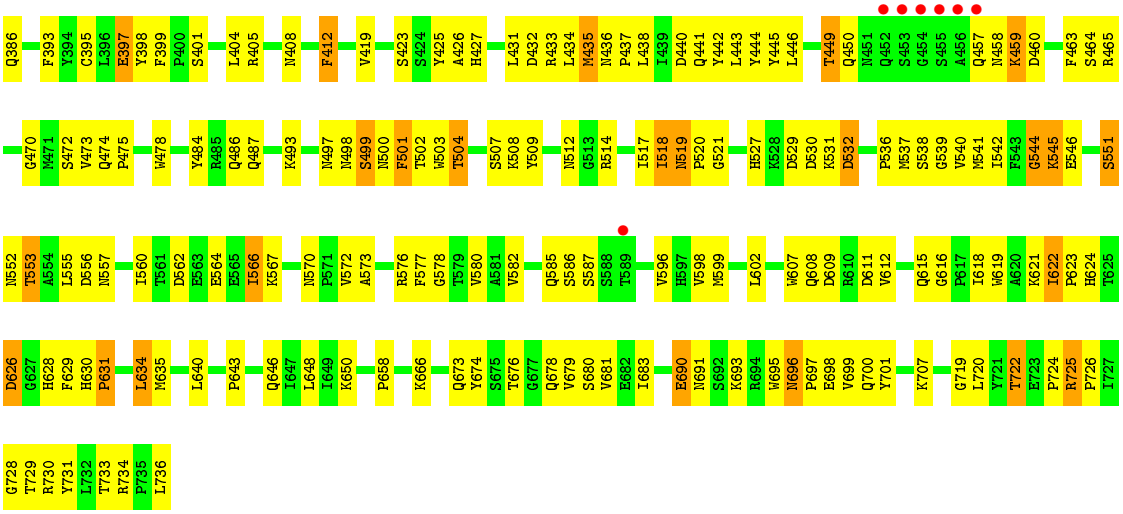
Chain E:



• Molecule 1: Capsid protein VP1

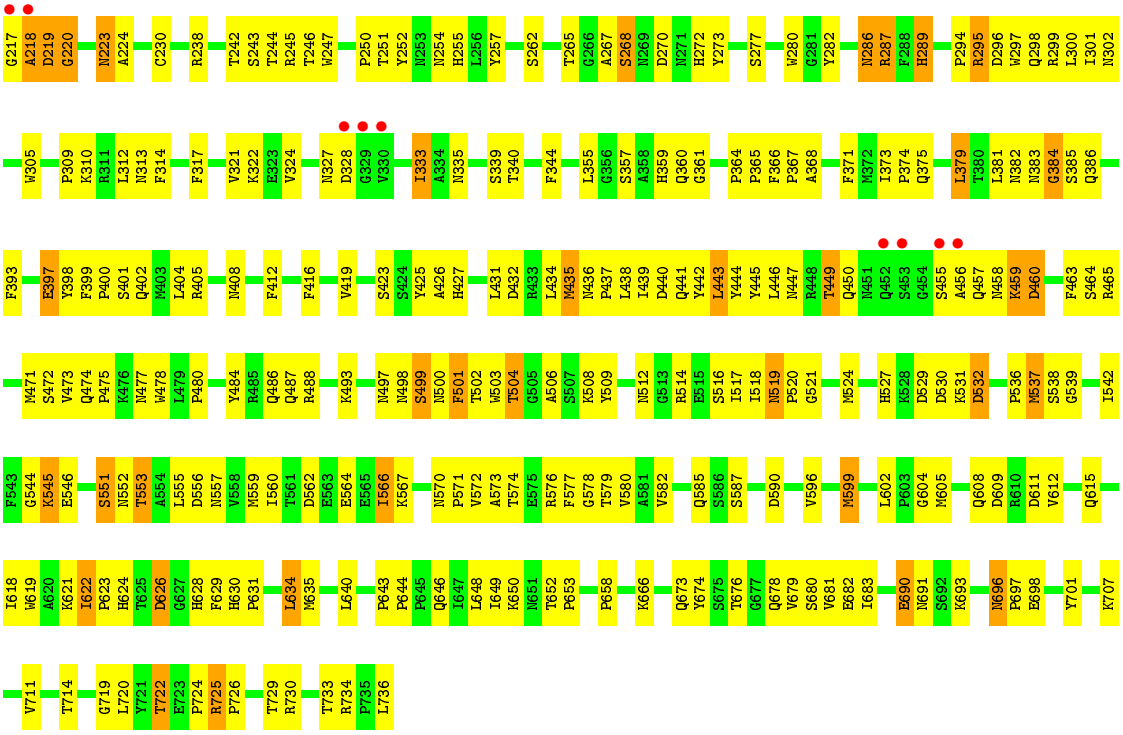
Chain F:





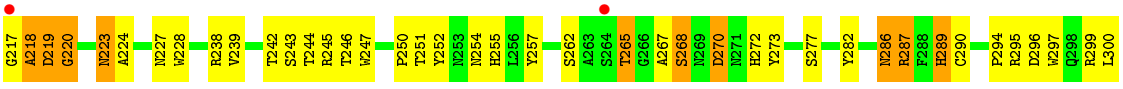
• Molecule 1: Capsid protein VP1

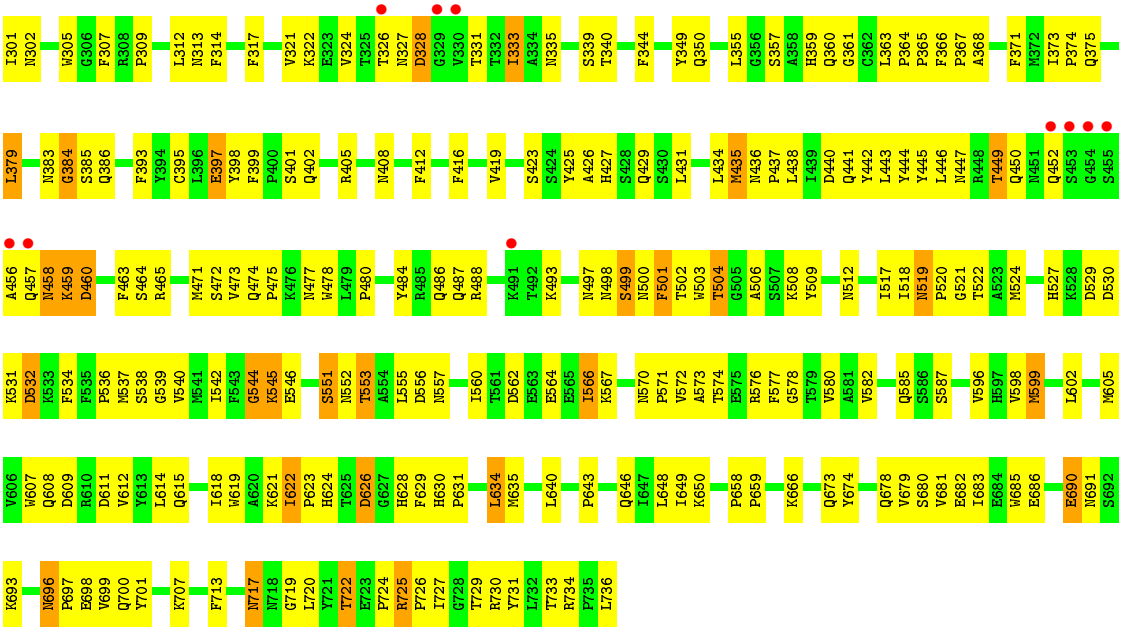
Chain G:



• Molecule 1: Capsid protein VP1

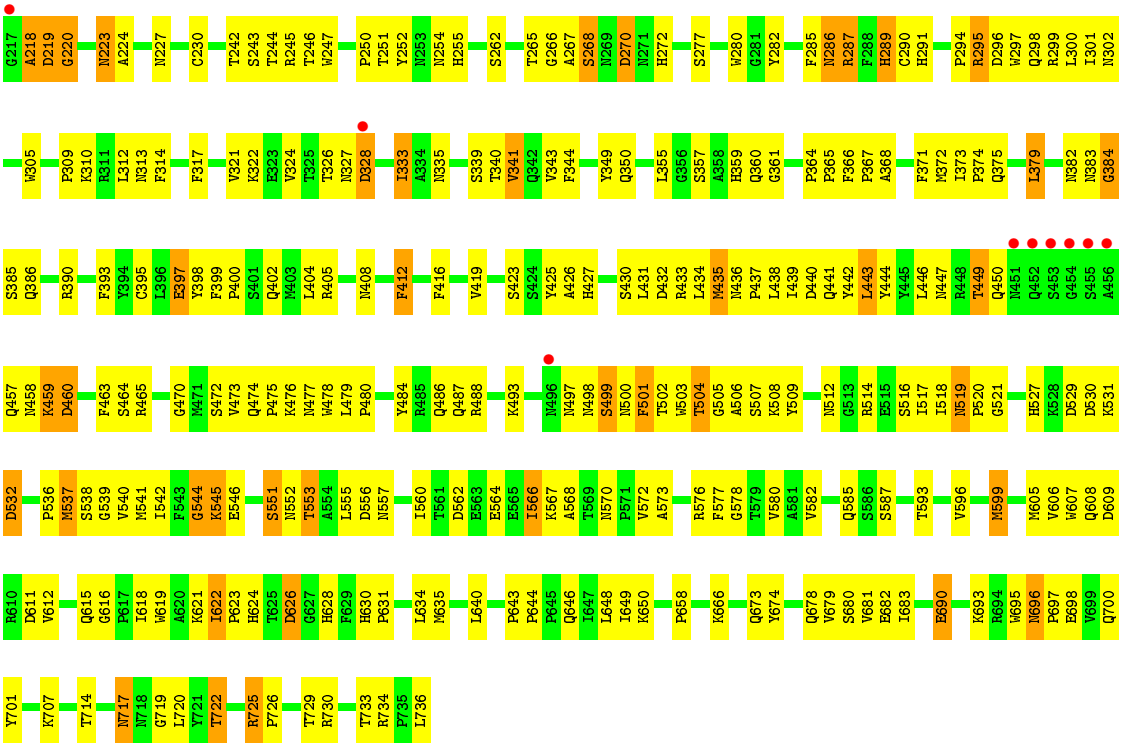
Chain H:





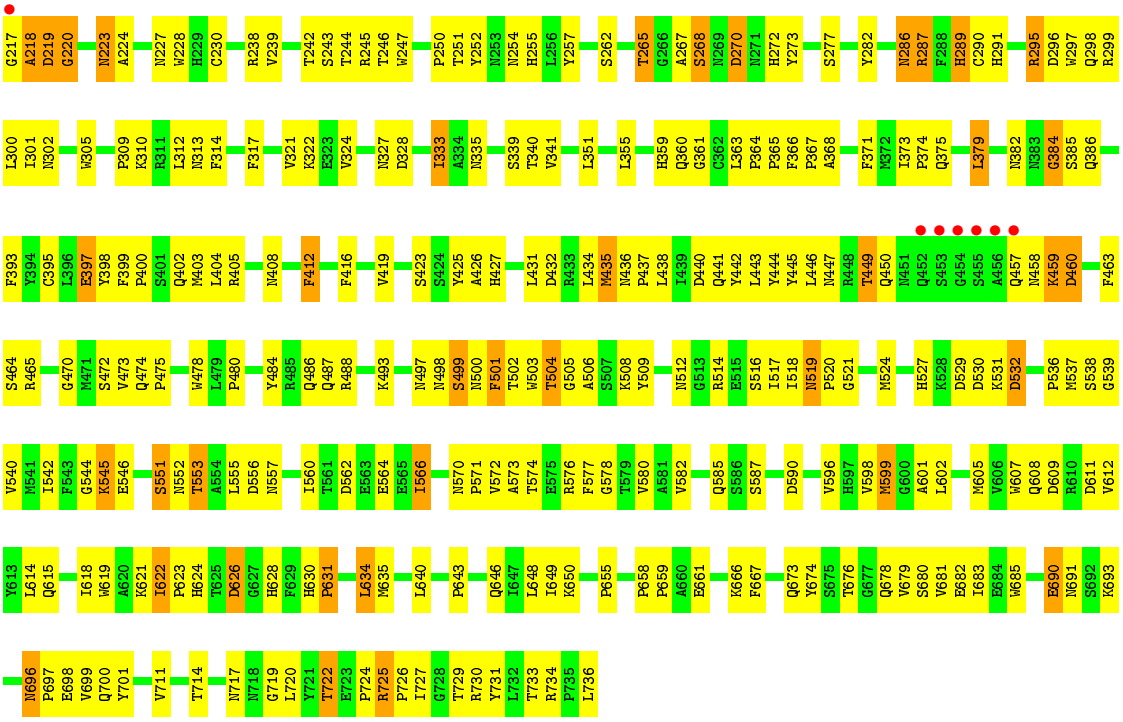
• Molecule 1: Capsid protein VP1

Chain I:



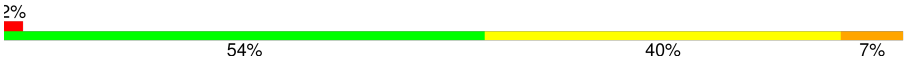
• Molecule 1: Capsid protein VP1

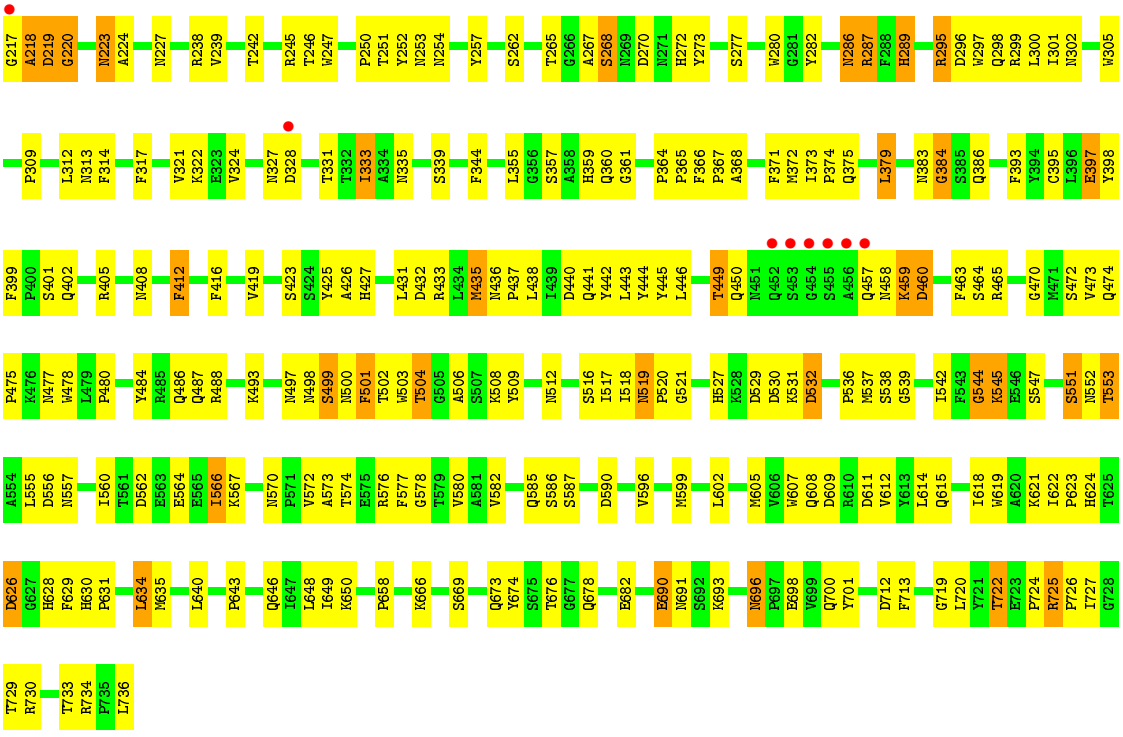
Chain J:



• Molecule 1: Capsid protein VP1

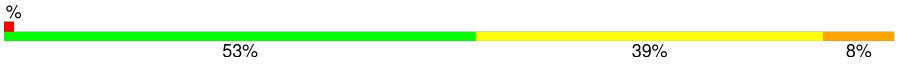
Chain K:

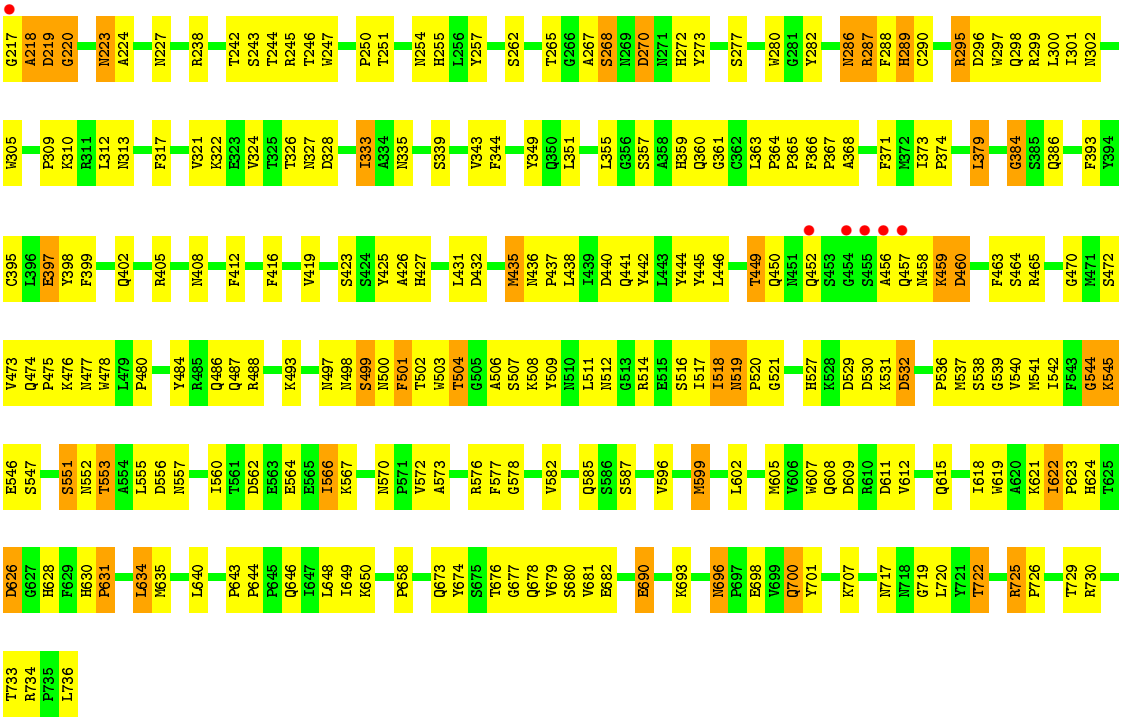




• Molecule 1: Capsid protein VP1

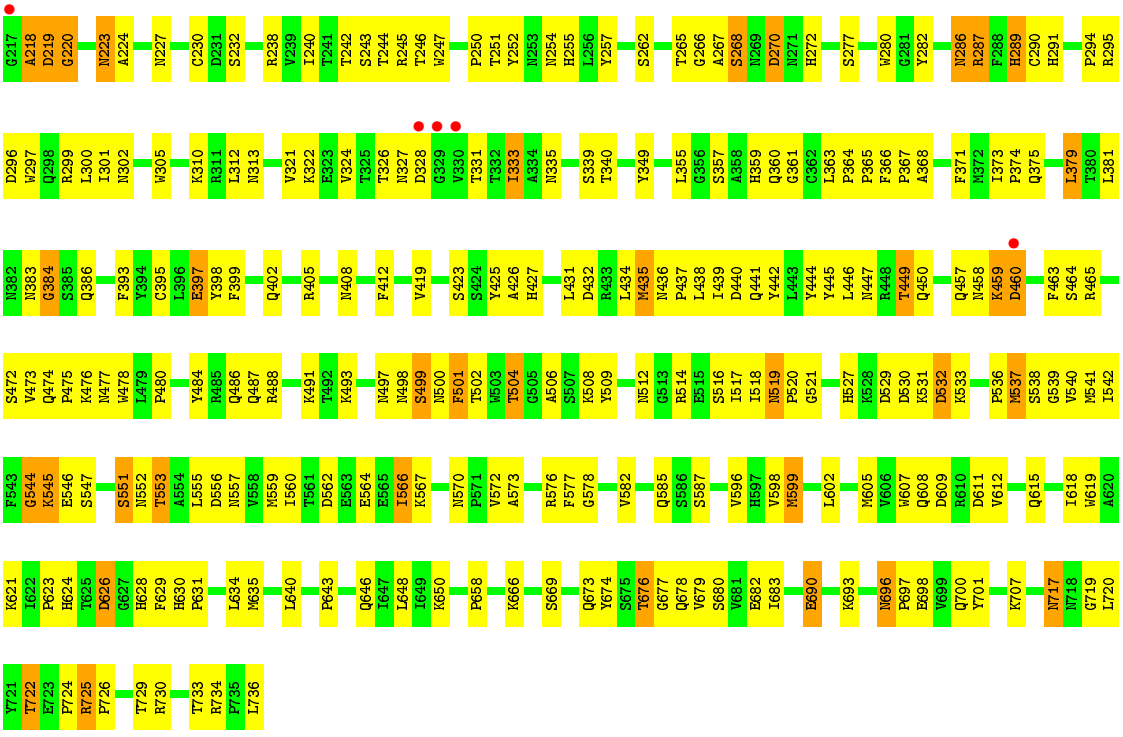
Chain L:





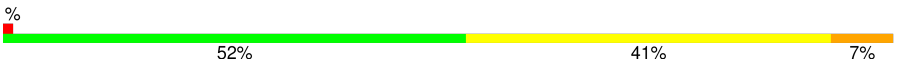
• Molecule 1: Capsid protein VP1

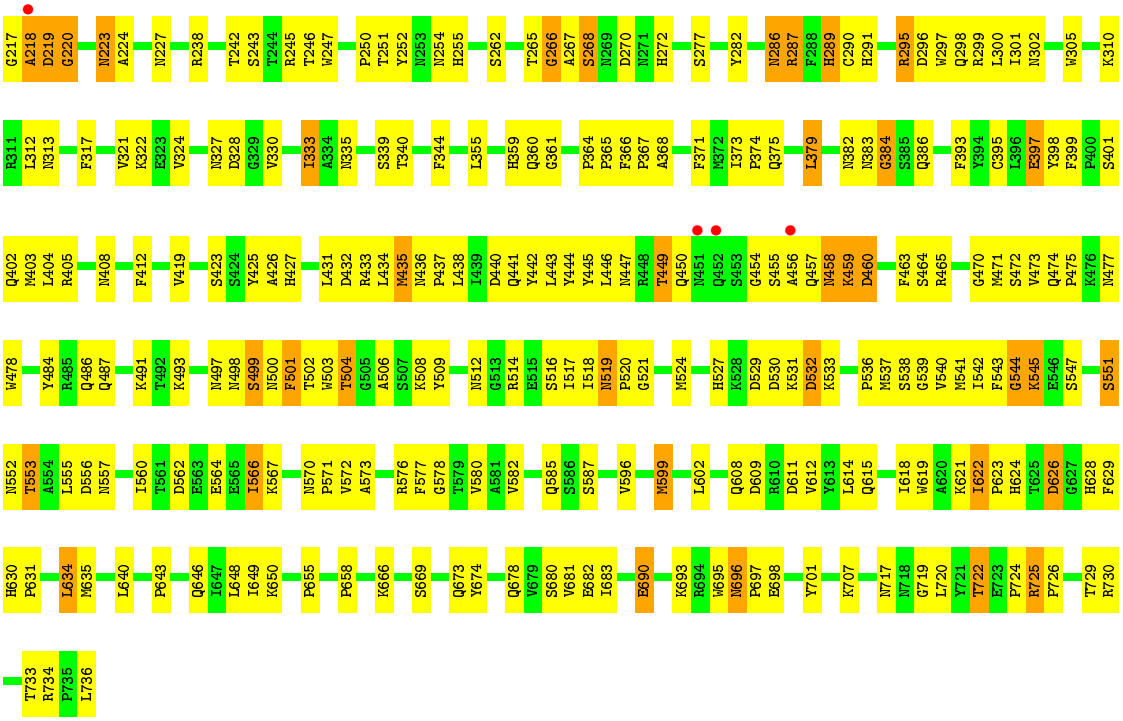
Chain M:



• Molecule 1: Capsid protein VP1

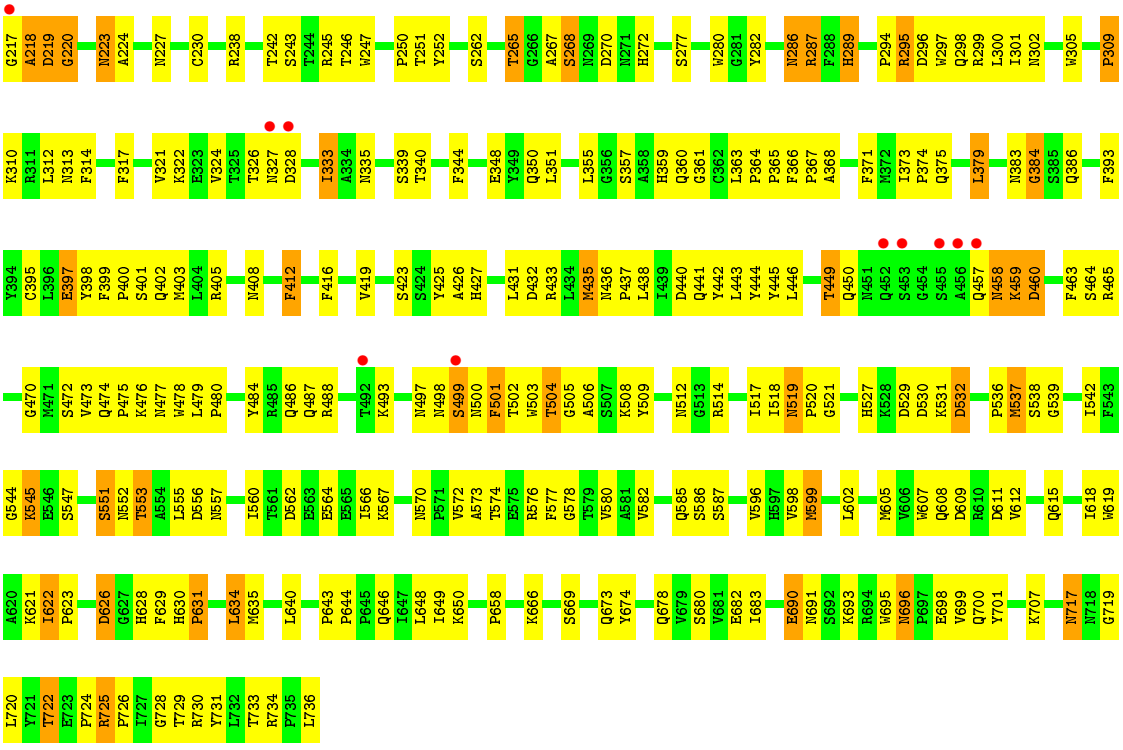
Chain N:





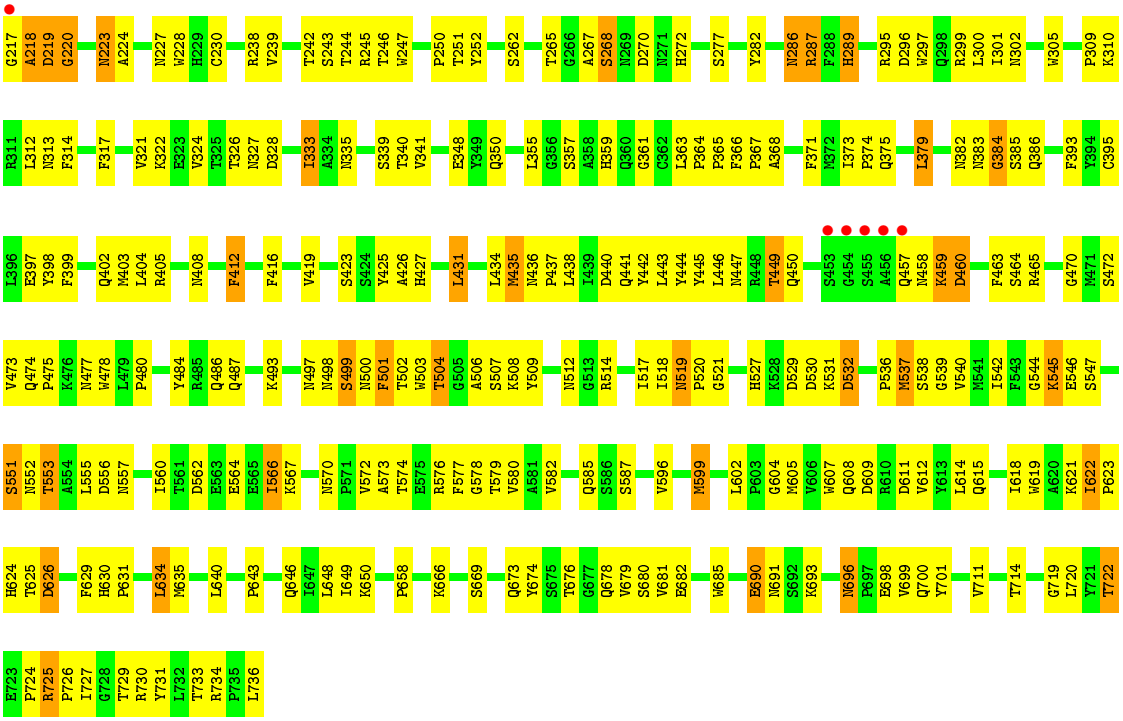
• Molecule 1: Capsid protein VP1

Chain O:



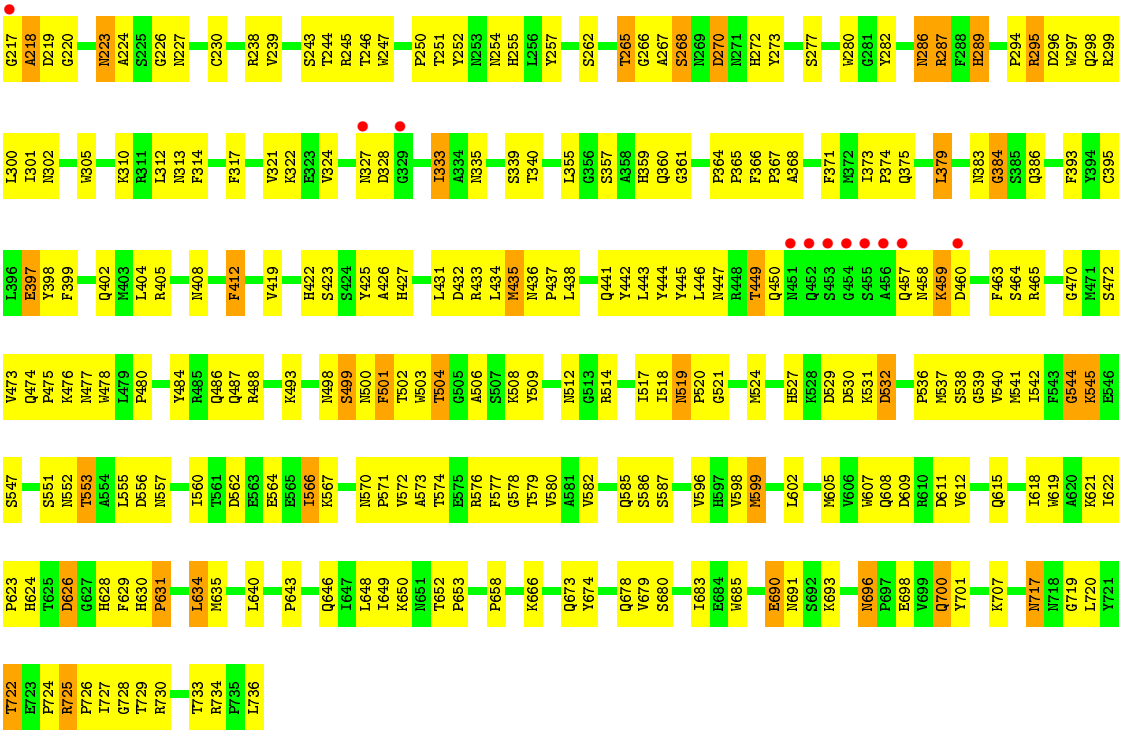
• Molecule 1: Capsid protein VP1

Chain P:



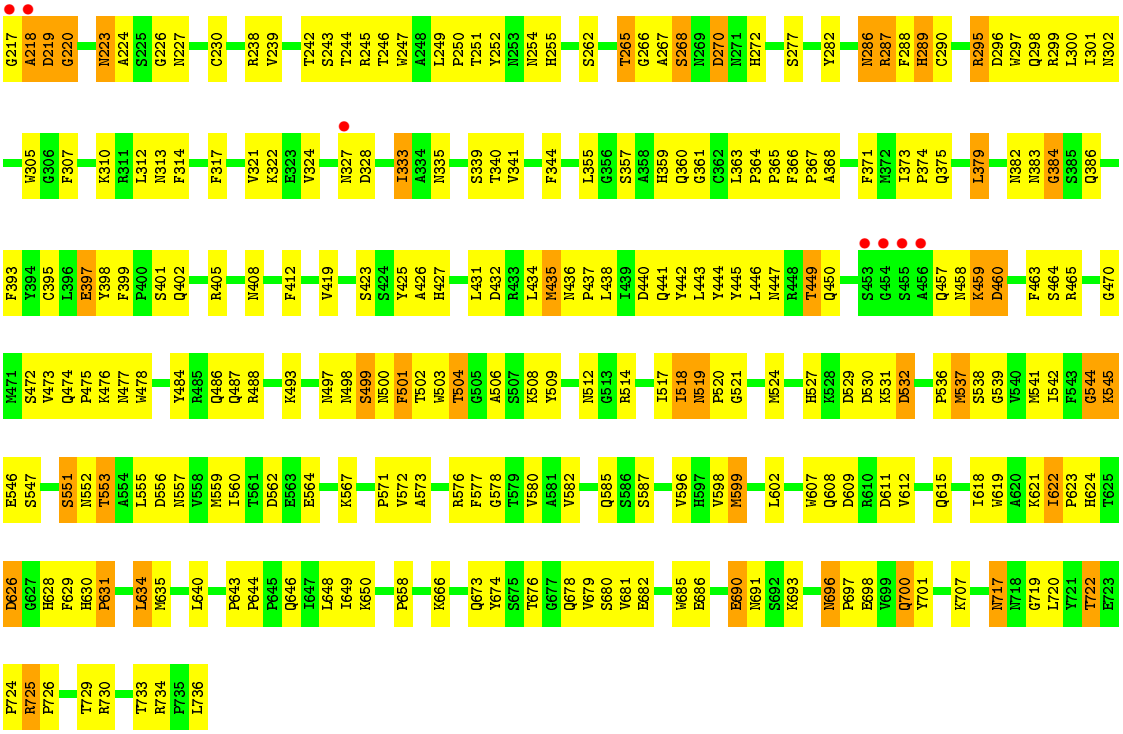
• Molecule 1: Capsid protein VP1

Chain Q:



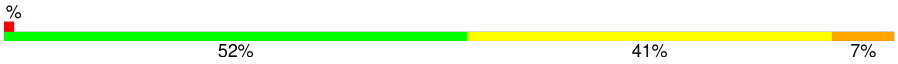
• Molecule 1: Capsid protein VP1

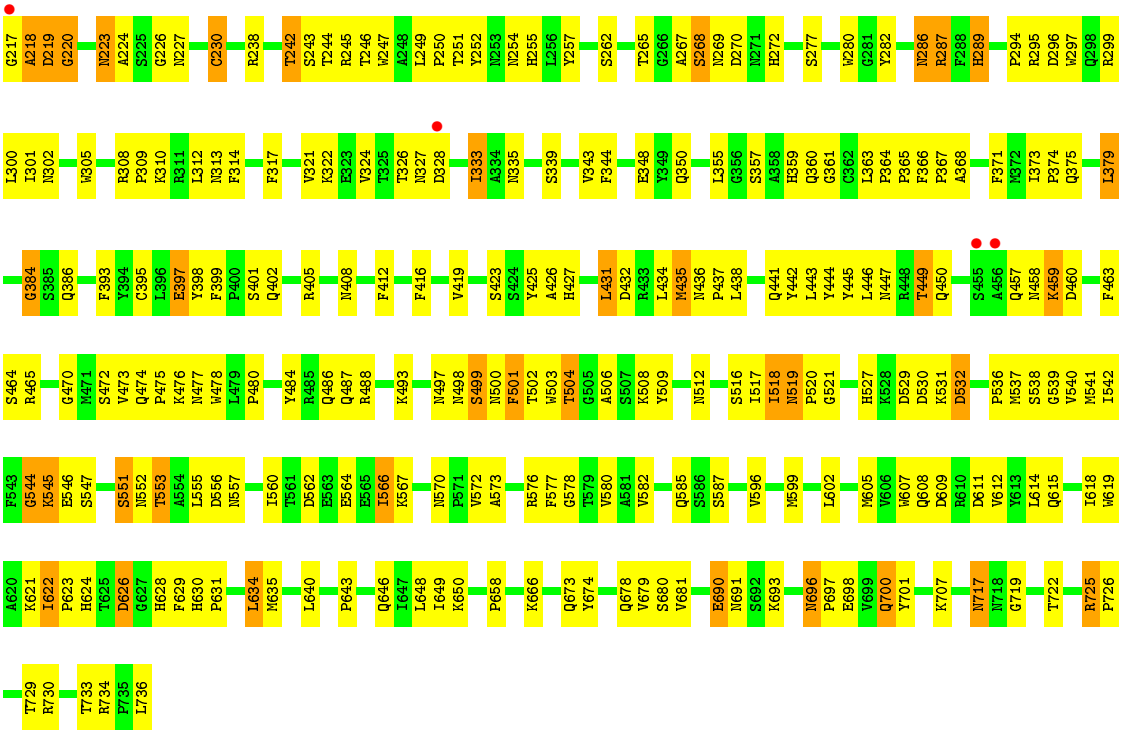
Chain R:



• Molecule 1: Capsid protein VP1

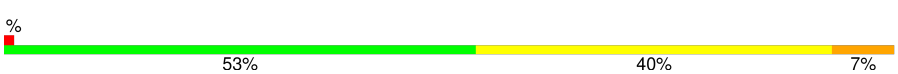
Chain S:

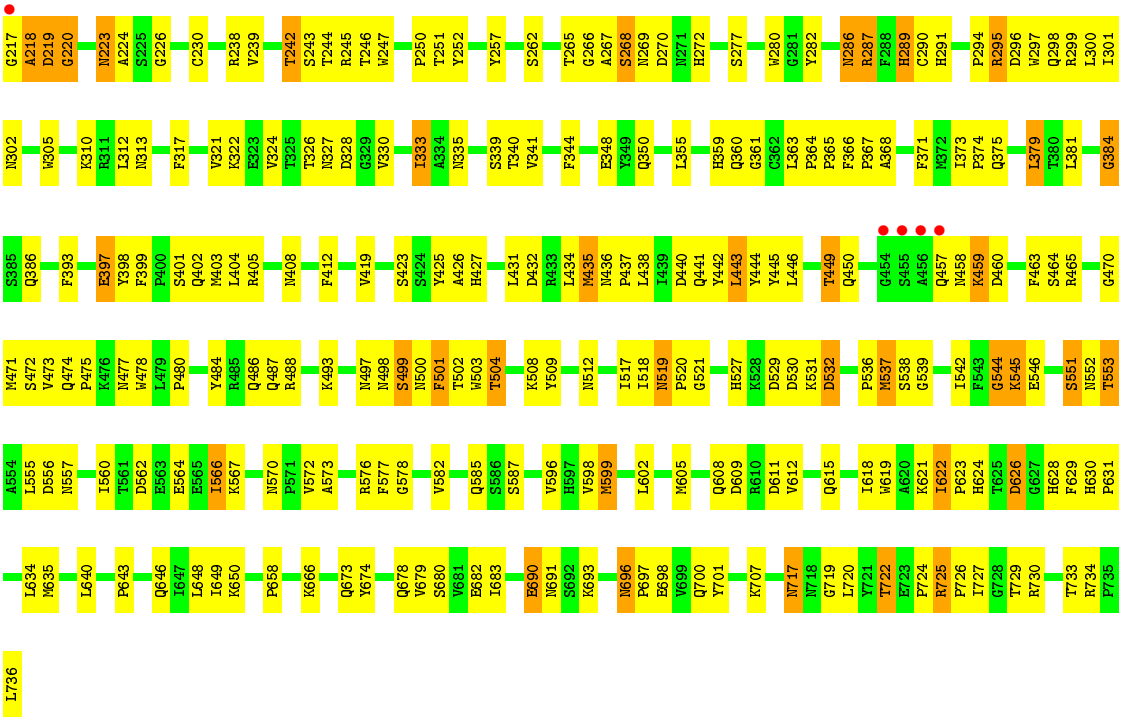




• Molecule 1: Capsid protein VP1

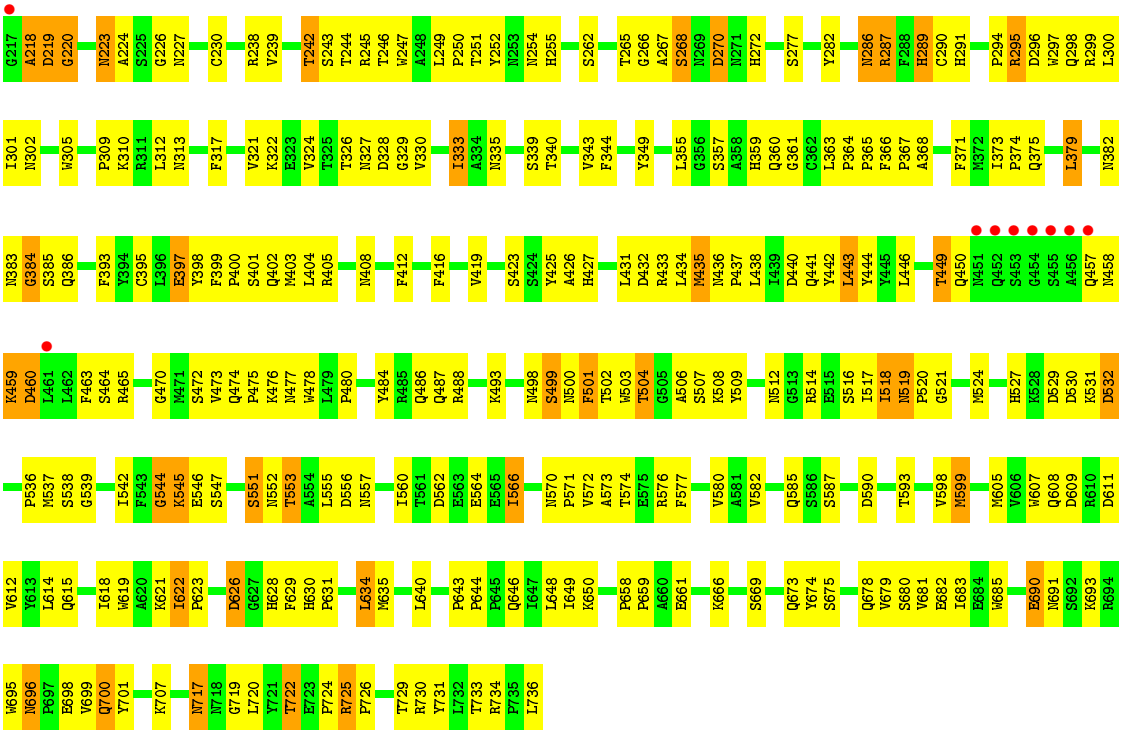
Chain T:





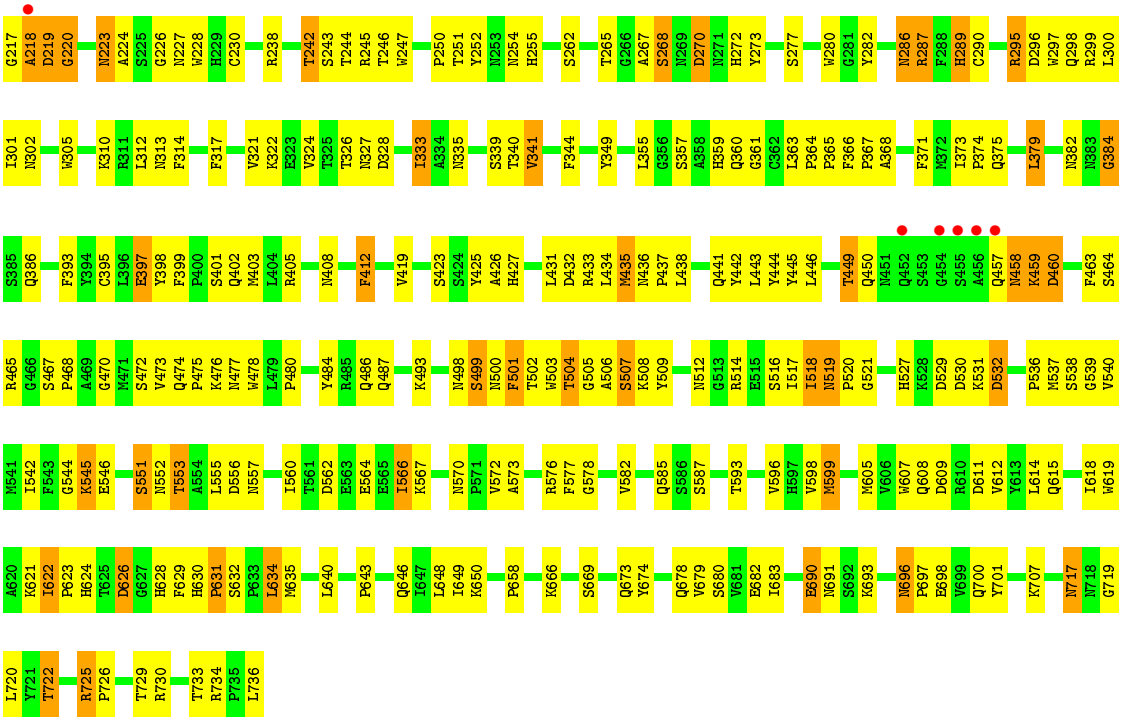
• Molecule 1: Capsid protein VP1

Chain U:



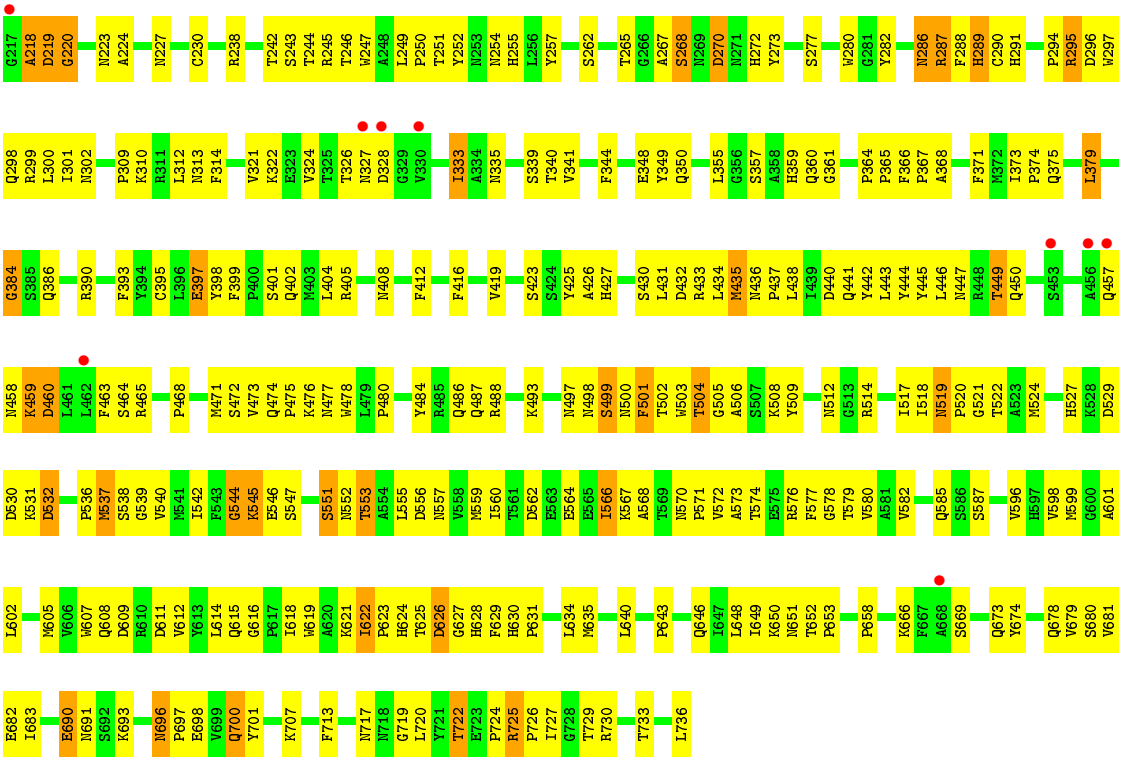
• Molecule 1: Capsid protein VP1

Chain V:



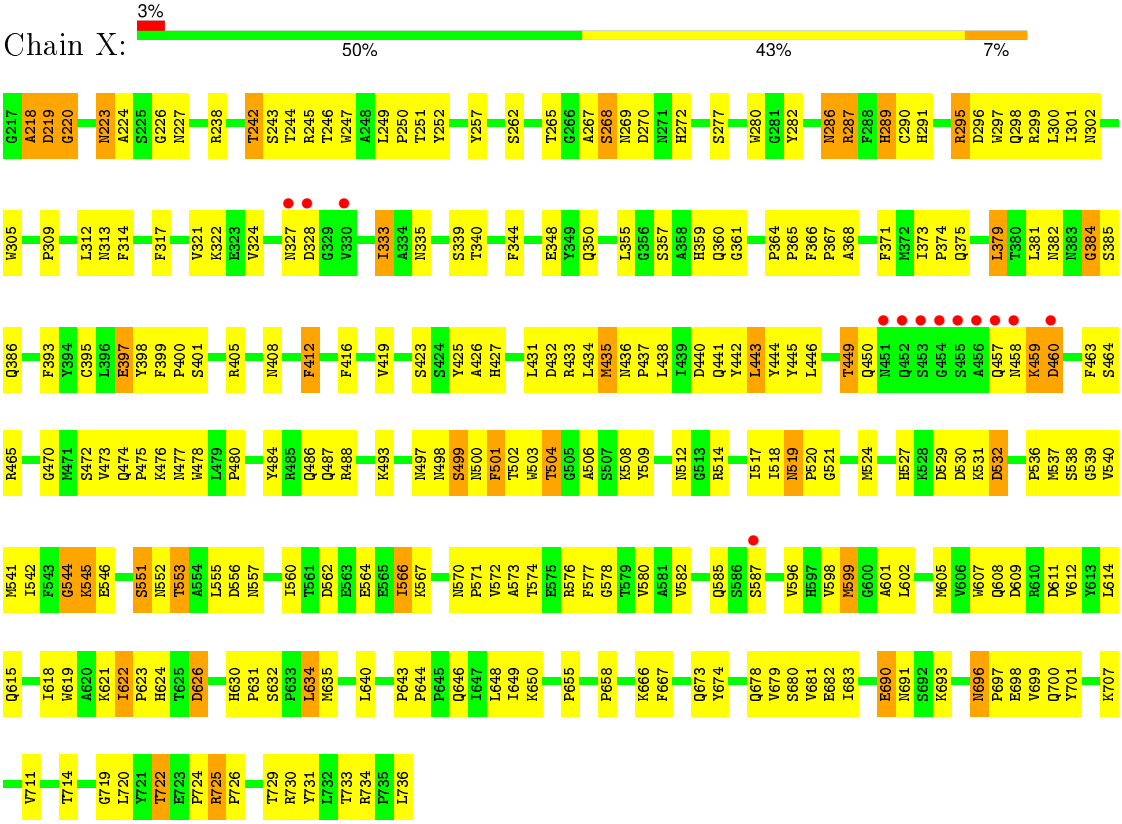
• Molecule 1: Capsid protein VP1

Chain W:



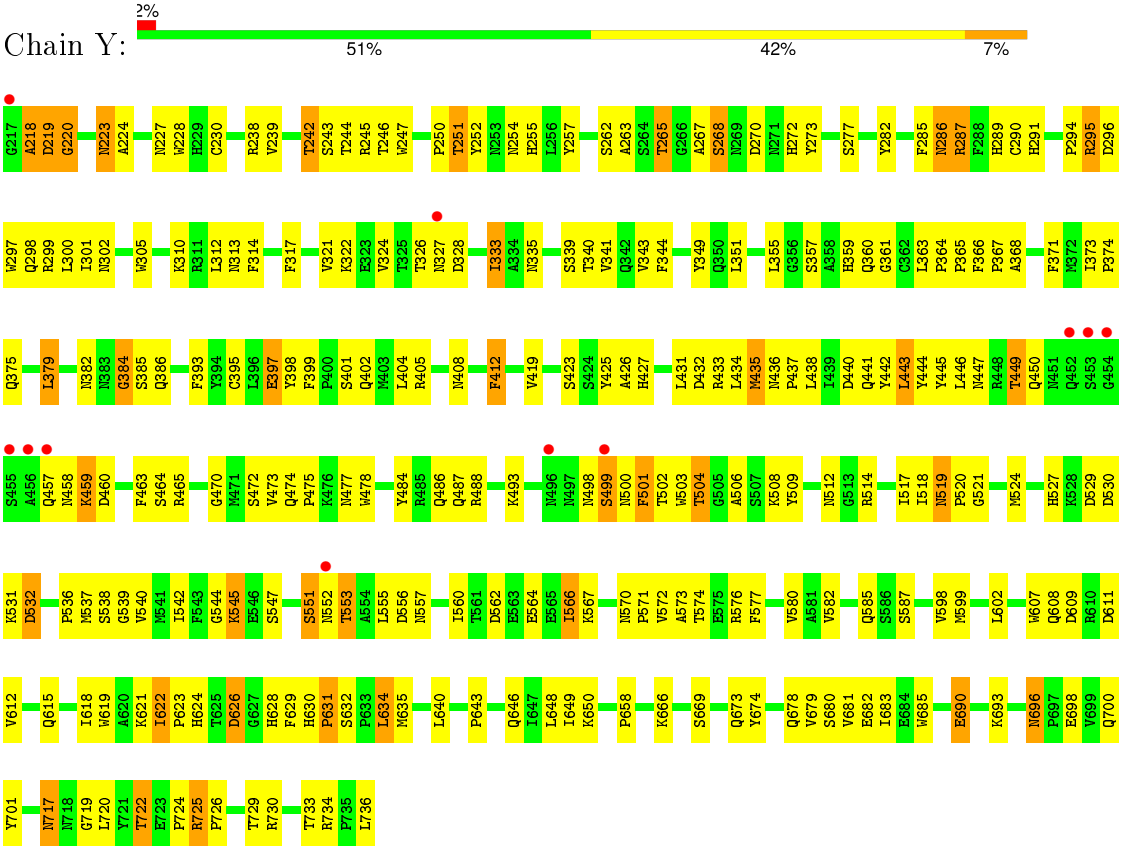
• Molecule 1: Capsid protein VP1

Chain X:



• Molecule 1: Capsid protein VP1

Chain Y:



• Molecule 1: Capsid protein VP1

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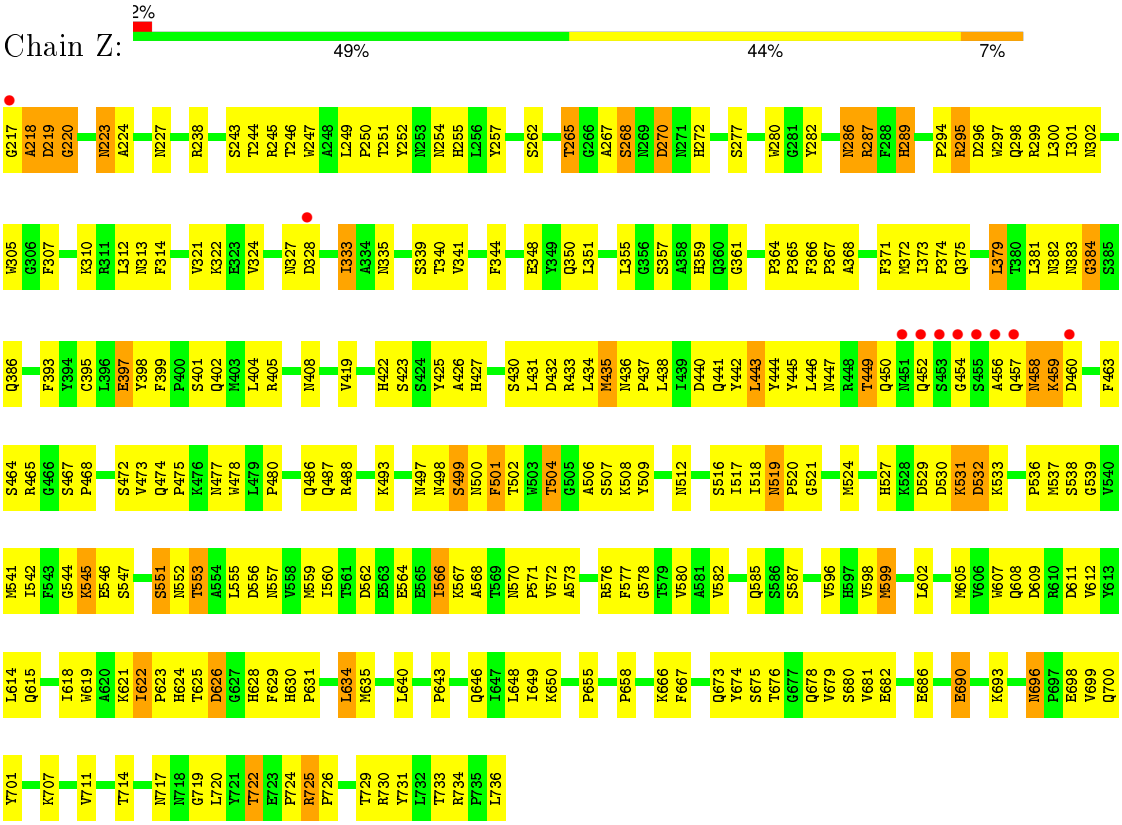
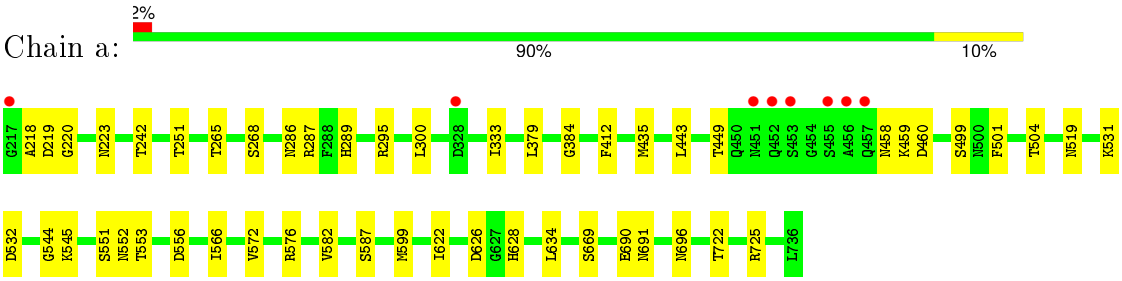


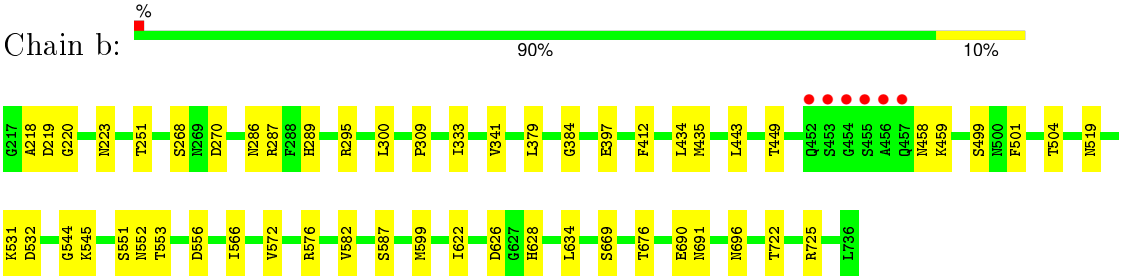
• Molecule 1: Capsid protein VP1

Chain a:



• Molecule 1: Capsid protein VP1

Chain b:



• Molecule 1: Capsid protein VP1

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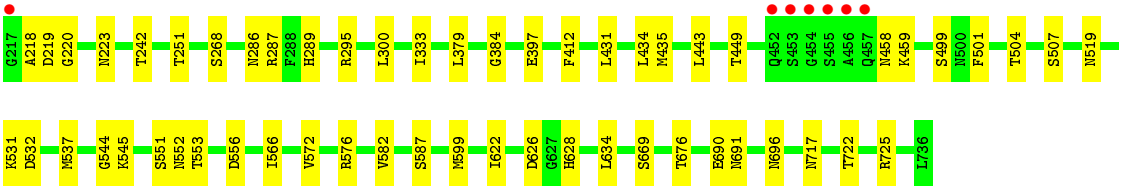
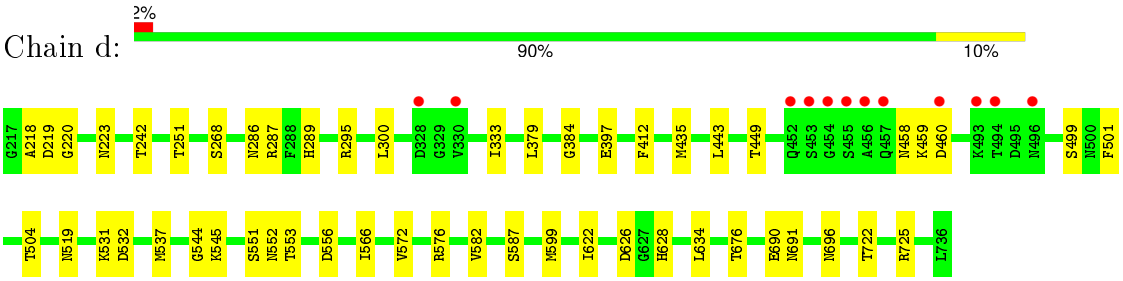


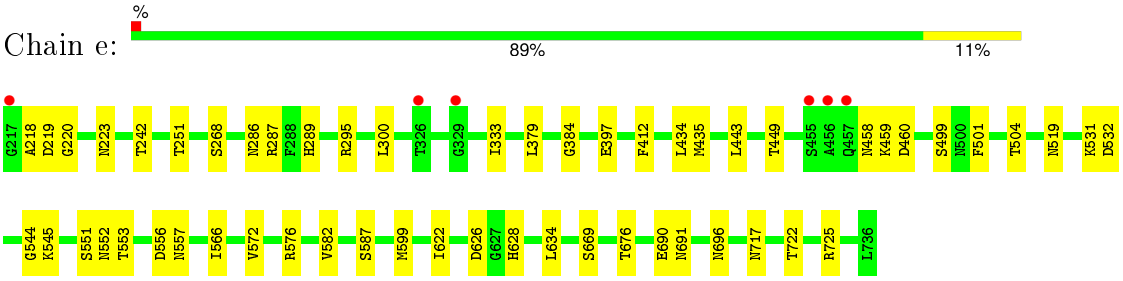
• Molecule 1: Capsid protein VP1

Chain d:



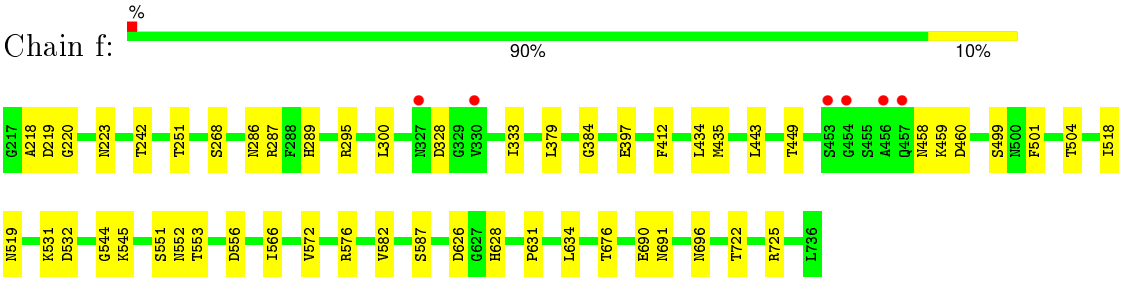
• Molecule 1: Capsid protein VP1

Chain e:



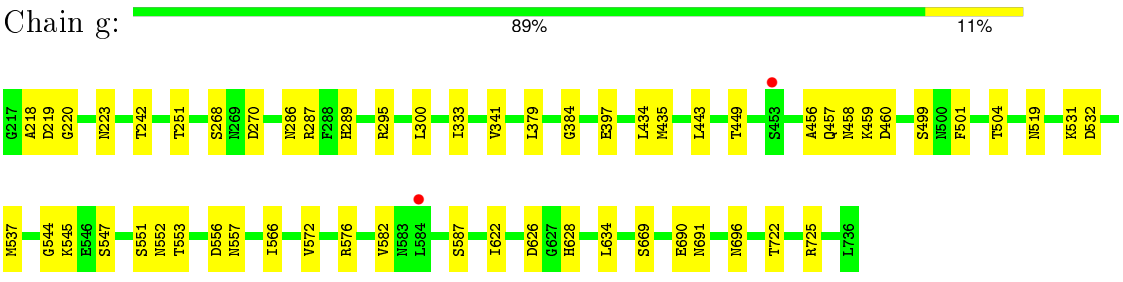
• Molecule 1: Capsid protein VP1

Chain f:



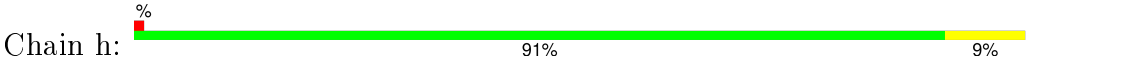
• Molecule 1: Capsid protein VP1

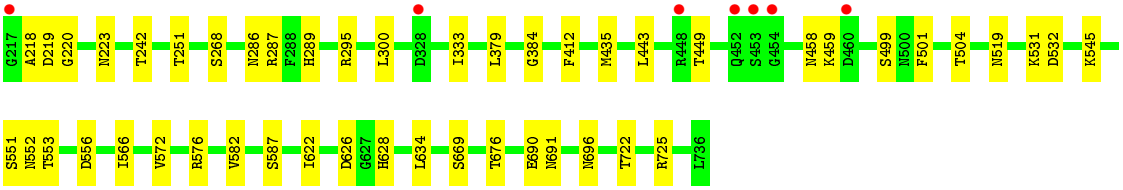
Chain g:



• Molecule 1: Capsid protein VP1

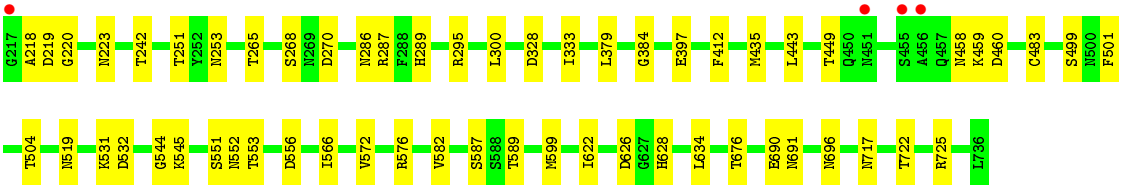
Chain h:





• Molecule 1: Capsid protein VP1

Chain i:



• Molecule 1: Capsid protein VP1

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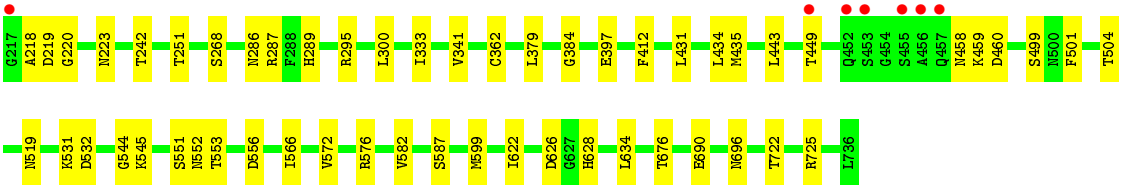
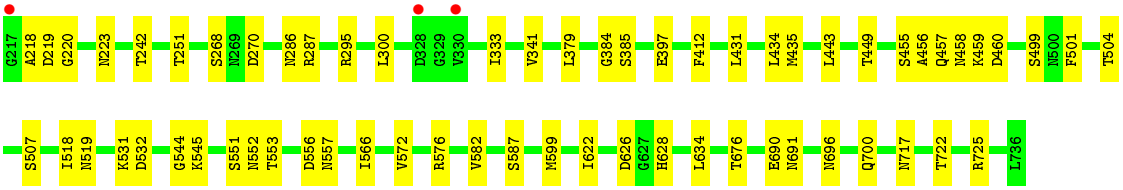


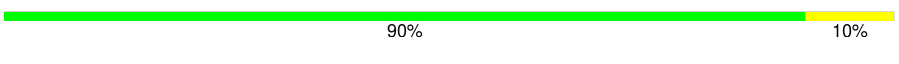
• Molecule 1: Capsid protein VP1

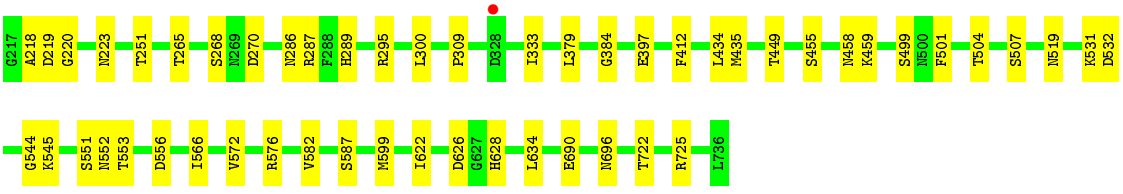
Chain k:



• Molecule 1: Capsid protein VP1

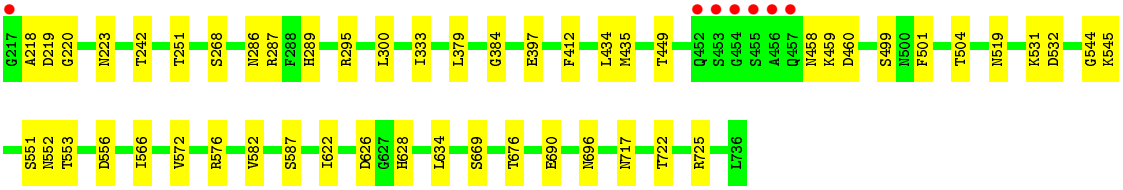
Chain l:



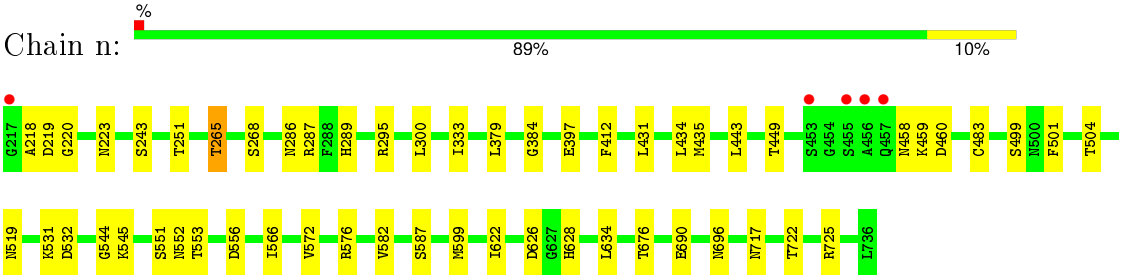


• Molecule 1: Capsid protein VP1

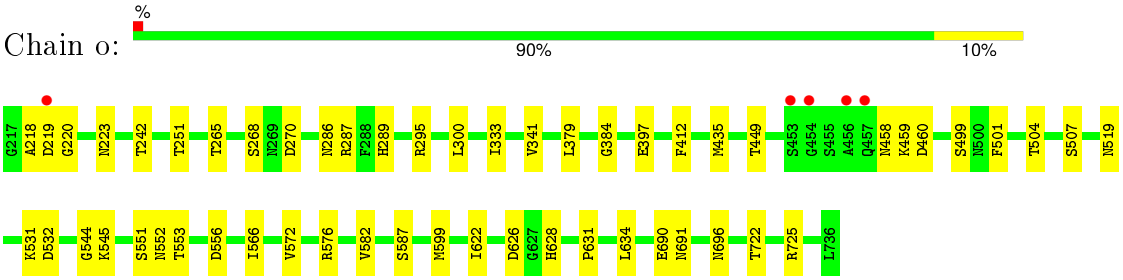
Chain m:



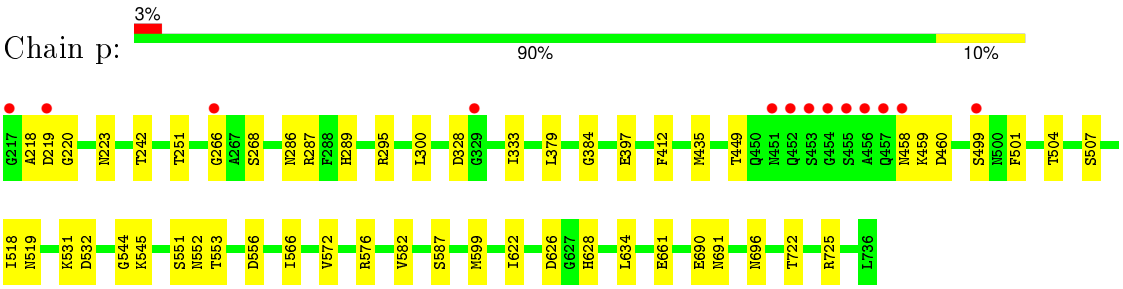
• Molecule 1: Capsid protein VP1



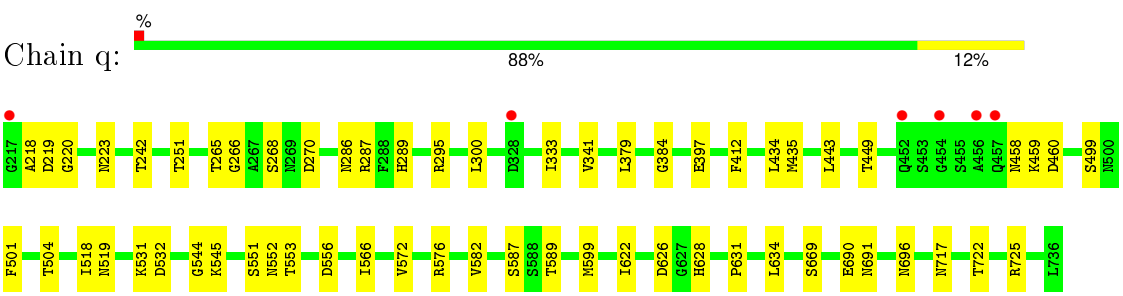
• Molecule 1: Capsid protein VP1



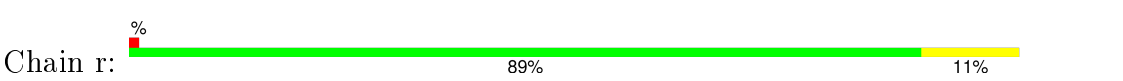
• Molecule 1: Capsid protein VP1

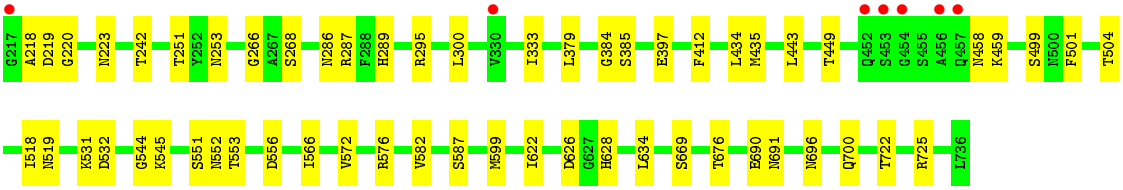


• Molecule 1: Capsid protein VP1



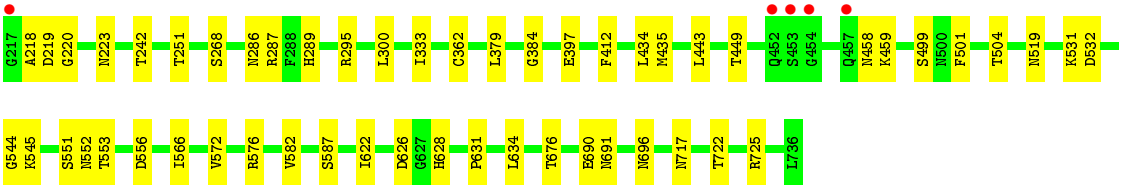
• Molecule 1: Capsid protein VP1





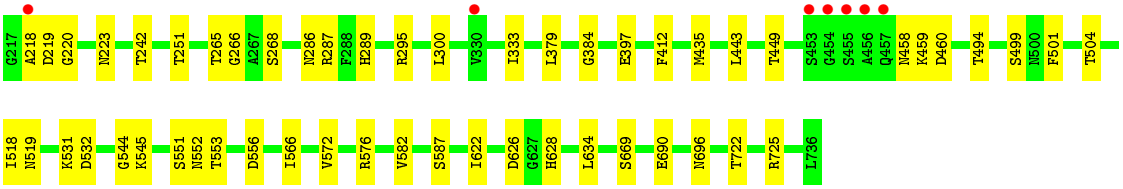
• Molecule 1: Capsid protein VP1

Chain s:



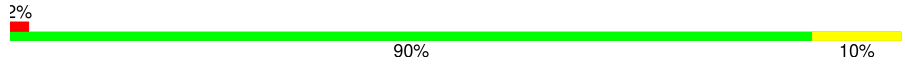
• Molecule 1: Capsid protein VP1

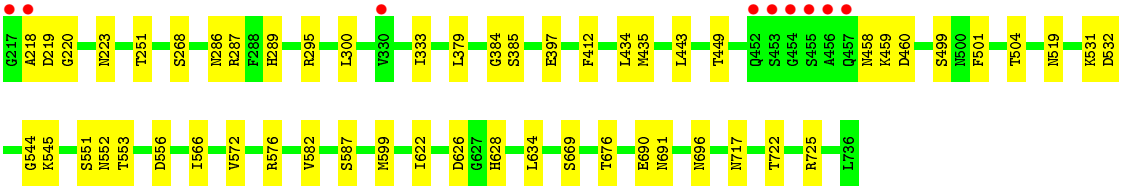
Chain t:



• Molecule 1: Capsid protein VP1

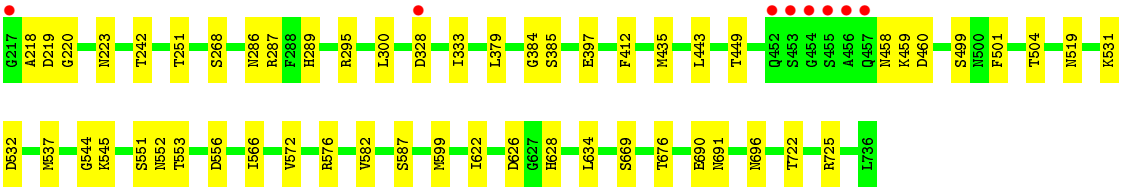
Chain u:





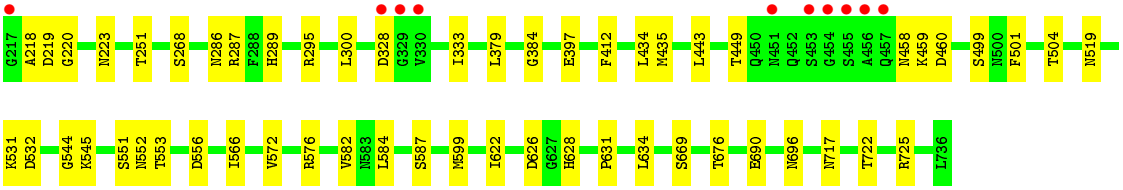
• Molecule 1: Capsid protein VP1

Chain v:



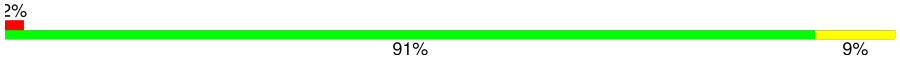
• Molecule 1: Capsid protein VP1

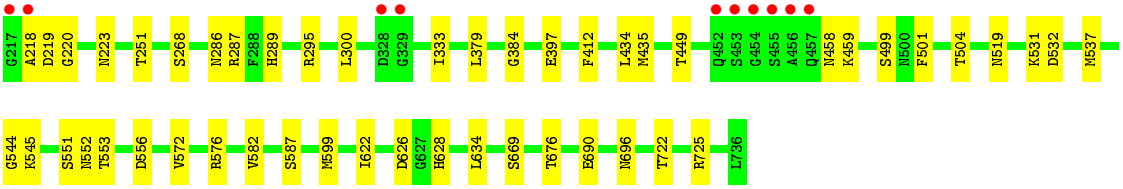
Chain w:



• Molecule 1: Capsid protein VP1

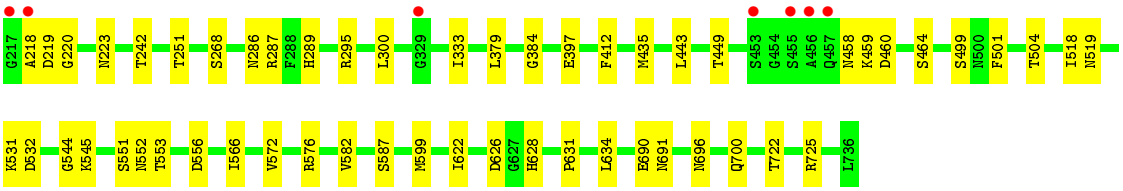
Chain x:





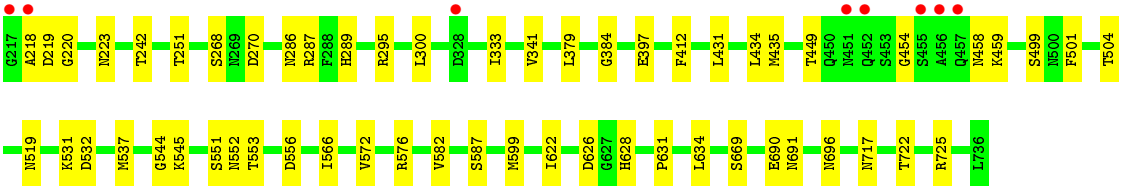
• Molecule 1: Capsid protein VP1

Chain y:



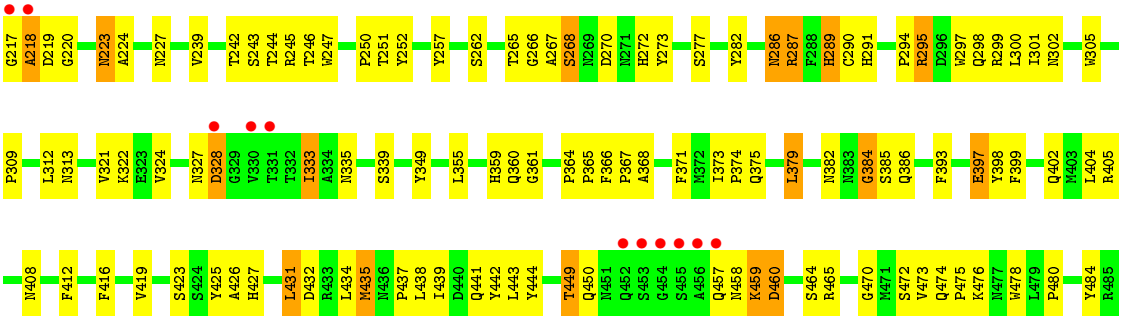
• Molecule 1: Capsid protein VP1

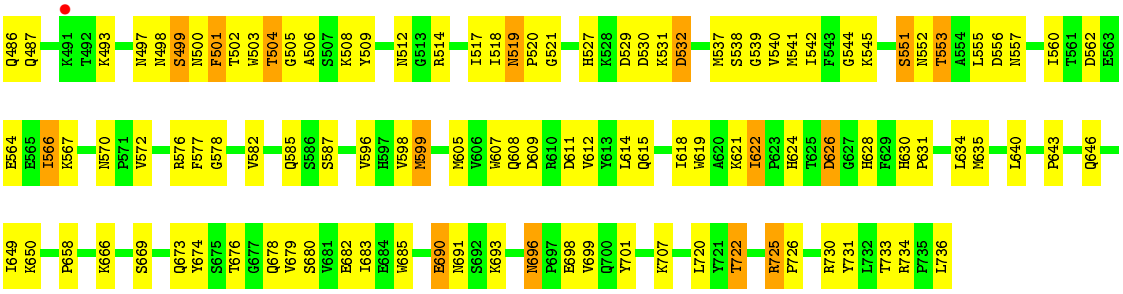
Chain z:



• Molecule 1: Capsid protein VP1

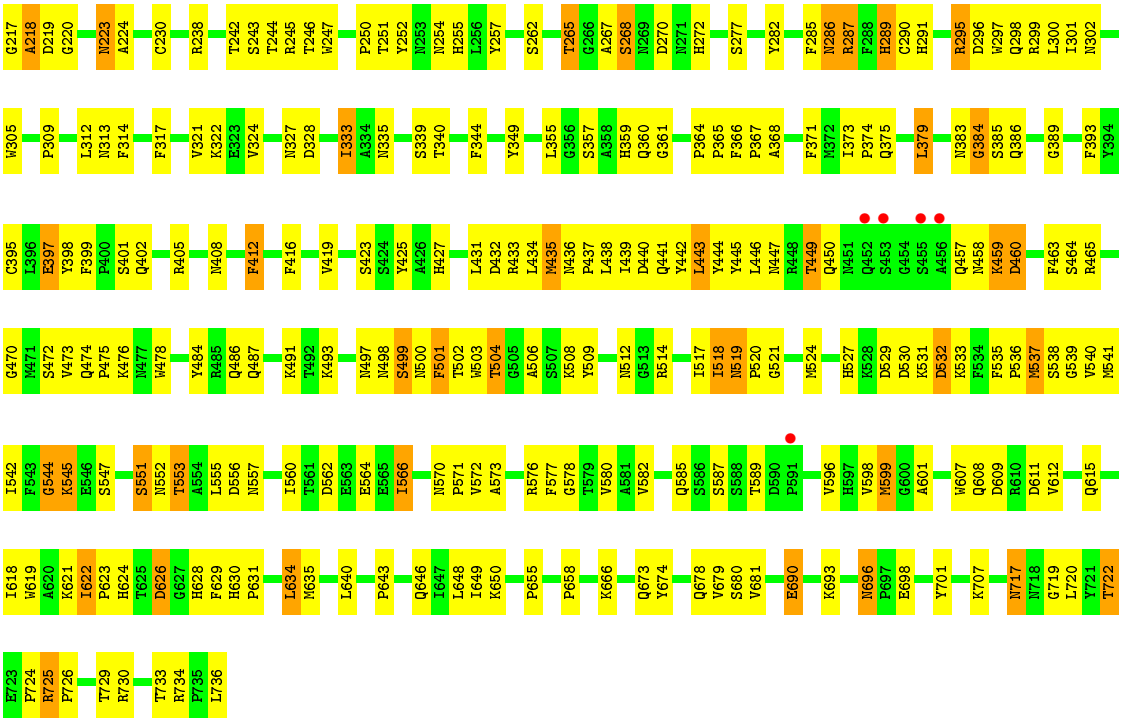
Chain 0:





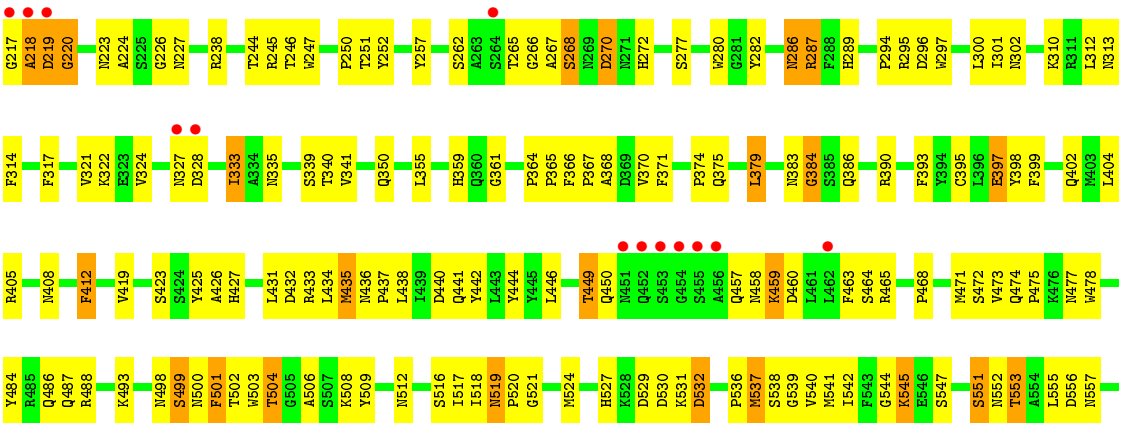
• Molecule 1: Capsid protein VP1

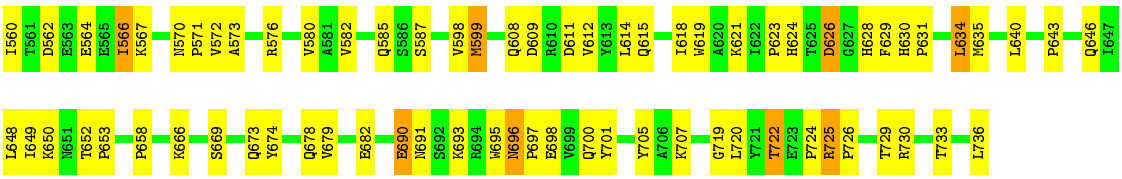
Chain 1:



• Molecule 1: Capsid protein VP1

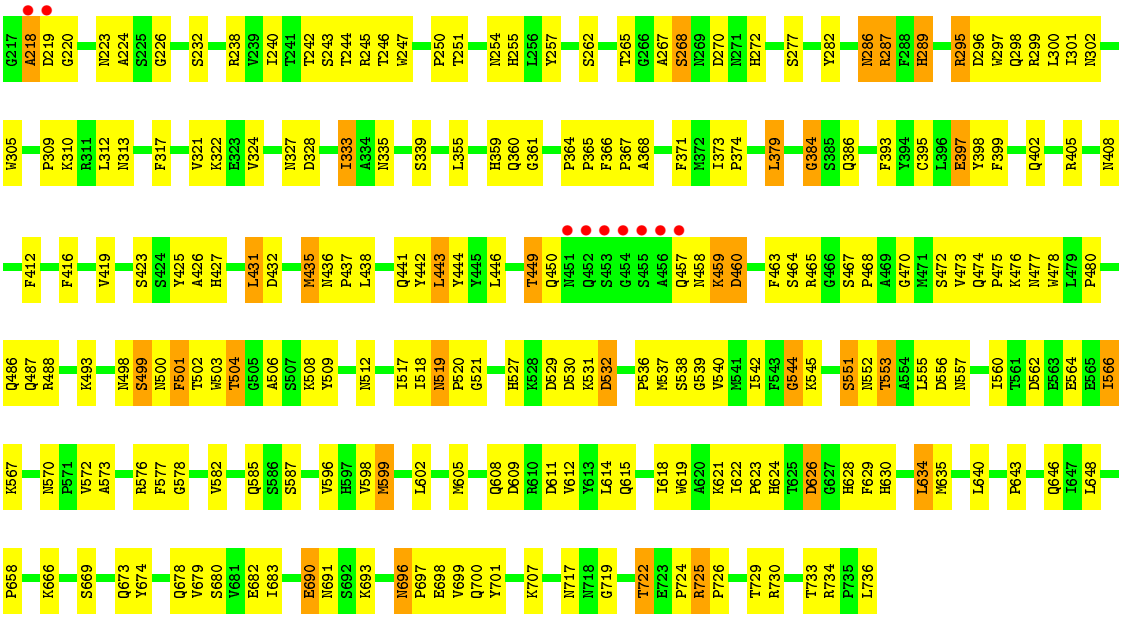
Chain 2:





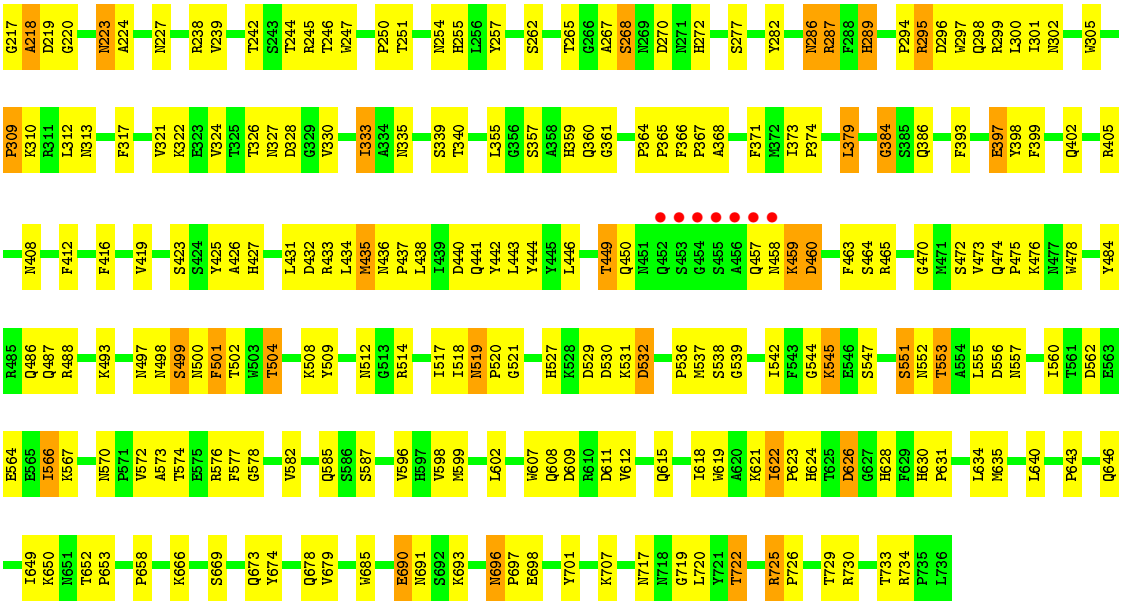
• Molecule 1: Capsid protein VP1

Chain 3:



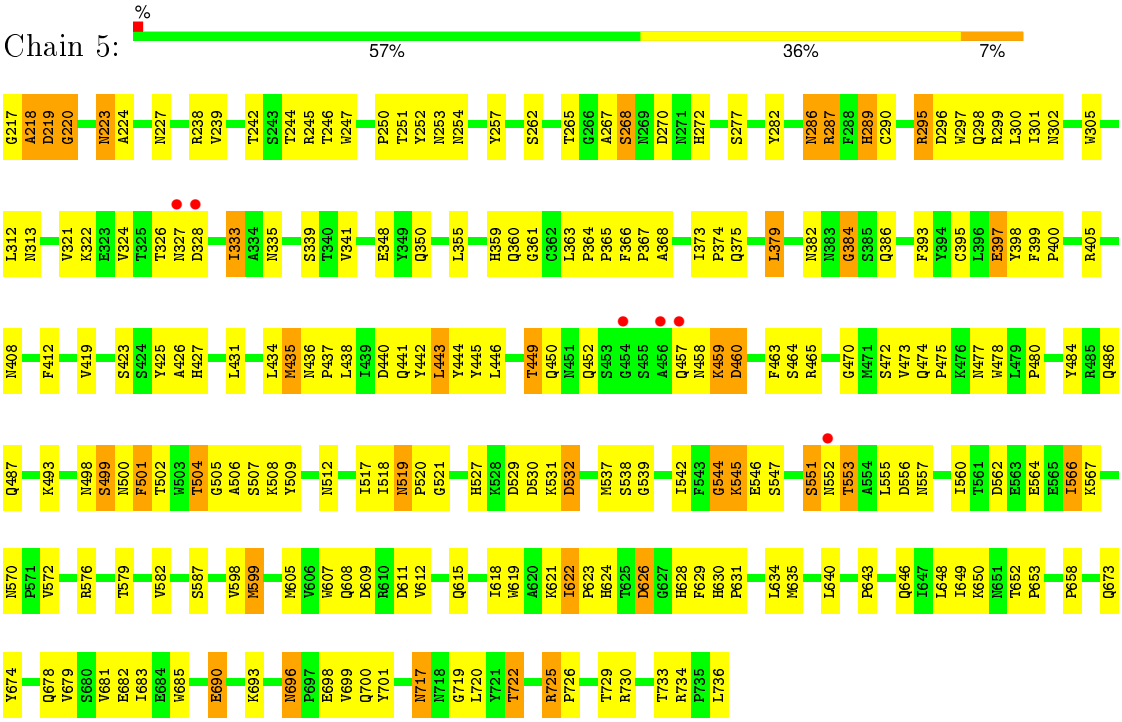
• Molecule 1: Capsid protein VP1

Chain 4:



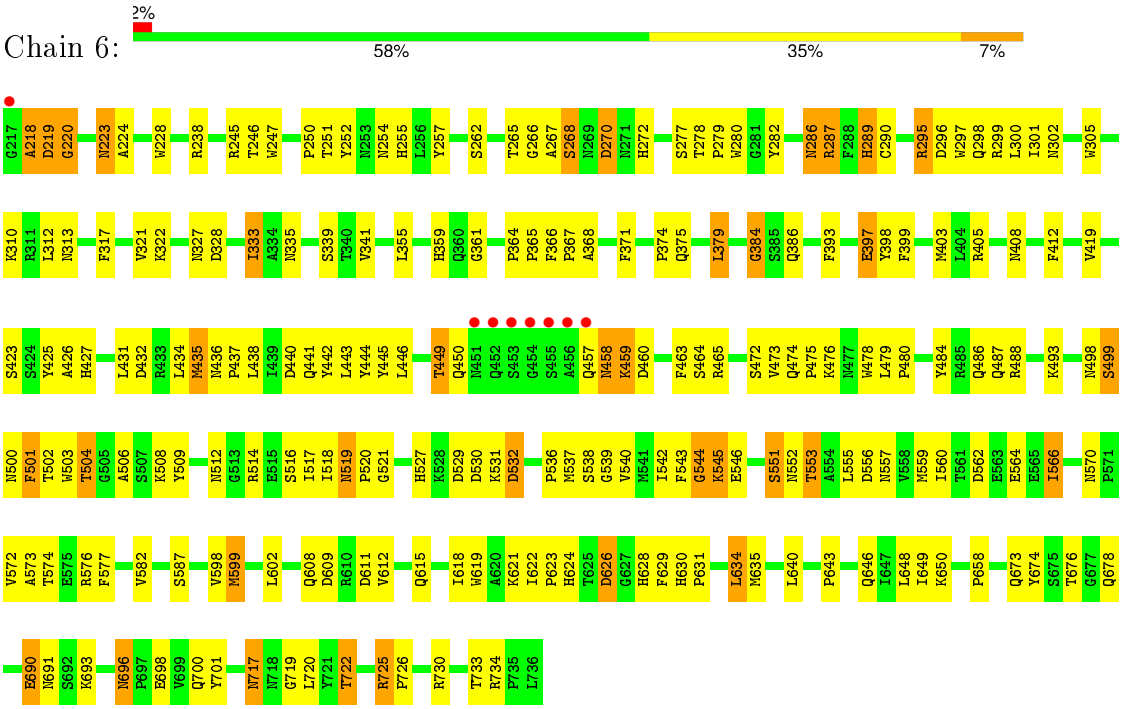
- Molecule 1: Capsid protein VP1

Chain 5:



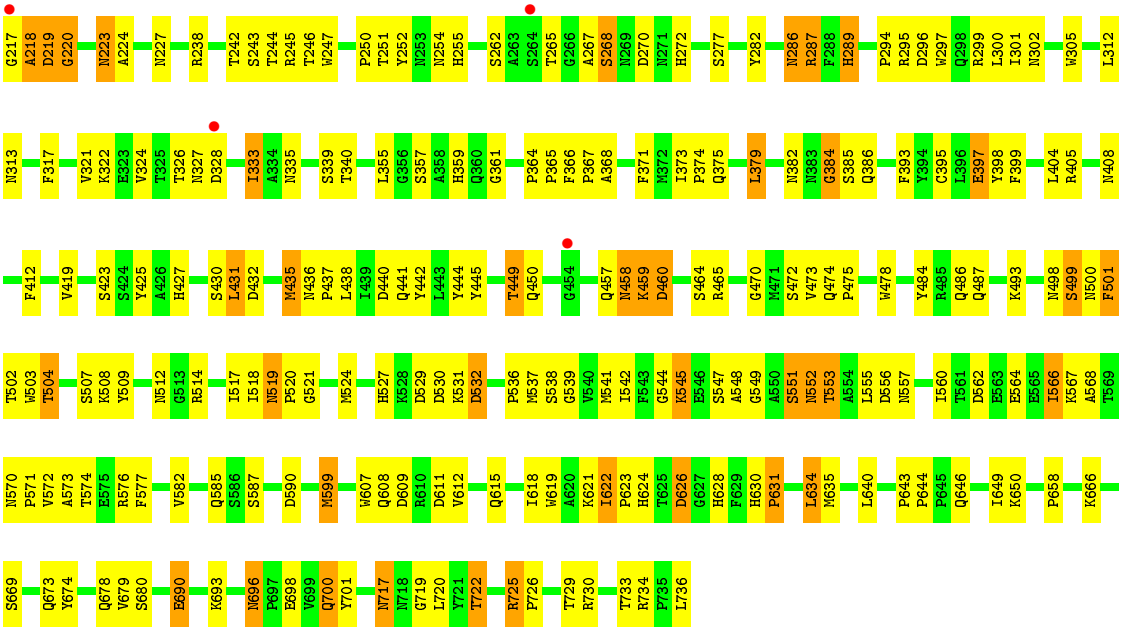
- Molecule 1: Capsid protein VP1

Chain 6:



- Molecule 1: Capsid protein VP1

Chain 7:


G217 A218 D219 G220 N223 A224 N227 R238 T242 S243 T244 R245 T246 W247 P250 T251 Y252 N253 N254 H255 S262 A263 S264 T265 G266 A267 S268 N269 D270 N271 H272 S277 Y282 N286 R287 F288 H289 P294 R295 D296 W297 Q298 R299 L300 I301 N302 W305 L312
N313 F317 V321 K322 E323 V324 T325 T326 N327 D328 I333 A334 N335 S339 T340 L355 G356 S357 A358 H359 Q360 G361 P364 P365 F366 P367 A368 F371 M372 I373 P374 Q375 L379 N382 N383 G384 S385 Q386 F393 Y394 C395 L396 E397 Y398 F399 L404 R405 N408
F412 V419 S423 S424 Y425 A426 H427 S430 L431 D432 M435 N436 P437 L438 I439 D440 Q441 Y442 L443 Y444 Y445 T449 Q450 G454 Q457 N458 K459 D460 S464 R465 G470 M471 S472 V473 Q474 P475 W478 Y484 R485 Q486 Q487 K493 N498 S499 N500 F501
T502 W503 T504 S507 K508 Y509 N512 G513 R514 I517 I518 N519 P520 G521 M524 H527 K528 D529 D530 K531 D532 P536 M537 S538 G539 V540 M541 I542 F543 G544 K545 E546 S547 A548 G549 A550 S551 N552 T553 A554 L555 D556 N557 I560 T561 D562 E563 E564 E565 I566 K567 A568 T569
N570 P571 V572 A573 T574 E575 R576 F577 V582 Q585 S586 S587 D590 M599 W607 Q608 D609 R610 D611 V612 Q615 I618 W619 A620 K621 I622 P623 H624 T625 D626 G627 H628 F629 H630 P631 L634 M635 L640 P643 P644 P645 Q646 I649 K650 P658 K666
S669 Q673 Y674 Q678 V679 S680 E690 K693 N696 P697 E698 V699 Q700 Y701 N717 N718 G719 L720 Y721 T722 R725 P726 T729 R730 T733 R734 P735 L736

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.251 , 0.286 0.246 , 0.282	Depositor DCC
R_{free} test set	3254 reflections (0.98%)	DCC
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 23.7	EDS
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
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 332221 reflections (0.000%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.60	0/4247	0.63	0/5790
1	1	0.63	0/4247	0.62	0/5790
1	2	0.56	0/4247	0.62	0/5790
1	3	0.55	0/4247	0.61	0/5790
1	4	0.54	0/4247	0.60	0/5790
1	5	0.59	0/4247	0.61	0/5790
1	6	0.62	0/4247	0.62	0/5790
1	7	0.55	0/4247	0.61	0/5790
1	A	0.68	0/4247	0.65	0/5790
1	B	0.66	0/4247	0.63	0/5790
1	C	0.58	0/4247	0.62	0/5790
1	D	0.60	2/4247 (0.0%)	0.63	2/5790 (0.0%)
1	E	0.65	0/4247	0.64	0/5790
1	F	0.62	0/4247	0.64	0/5790
1	G	0.58	0/4247	0.60	0/5790
1	H	0.56	0/4247	0.61	0/5790
1	I	0.65	0/4247	0.64	0/5790
1	J	0.70	0/4247	0.65	0/5790
1	K	0.58	0/4247	0.61	0/5790
1	L	0.55	0/4247	0.60	0/5790
1	M	0.55	0/4247	0.59	0/5790
1	N	0.57	0/4247	0.60	0/5790
1	O	0.56	1/4247 (0.0%)	0.60	0/5790
1	P	0.57	0/4247	0.62	0/5790
1	Q	0.56	0/4247	0.62	0/5790
1	R	0.56	0/4247	0.61	0/5790
1	S	0.63	1/4247 (0.0%)	0.62	0/5790
1	T	0.61	0/4247	0.61	0/5790
1	U	0.62	0/4247	0.63	0/5790
1	V	0.62	0/4247	0.62	0/5790
1	W	0.69	0/4247	0.64	0/5790
1	X	0.69	0/4247	0.65	0/5790
1	Y	0.64	0/4247	0.64	0/5790
1	Z	0.59	0/4247	0.62	0/5790

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.55	0/4247	0.61	0/5790
1	b	0.57	0/4247	0.60	0/5790
1	c	0.54	0/4247	0.62	0/5790
1	d	0.55	0/4247	0.61	0/5790
1	e	0.57	0/4247	0.61	0/5790
1	f	0.52	0/4247	0.60	0/5790
1	g	0.60	0/4247	0.62	0/5790
1	h	0.59	0/4247	0.61	0/5790
1	i	0.55	1/4247 (0.0%)	0.60	0/5790
1	j	0.58	1/4247 (0.0%)	0.61	0/5790
1	k	0.59	0/4247	0.61	0/5790
1	l	0.59	0/4247	0.60	0/5790
1	m	0.66	0/4247	0.63	0/5790
1	n	0.63	1/4247 (0.0%)	0.62	0/5790
1	o	0.53	0/4247	0.60	0/5790
1	p	0.58	0/4247	0.61	0/5790
1	q	0.55	0/4247	0.61	0/5790
1	r	0.55	0/4247	0.60	0/5790
1	s	0.55	1/4247 (0.0%)	0.61	0/5790
1	t	0.55	0/4247	0.60	0/5790
1	u	0.54	0/4247	0.59	0/5790
1	v	0.55	0/4247	0.60	0/5790
1	w	0.56	0/4247	0.61	0/5790
1	x	0.55	0/4247	0.60	0/5790
1	y	0.56	0/4247	0.61	0/5790
1	z	0.56	0/4247	0.61	0/5790
All	All	0.59	8/254820 (0.0%)	0.62	2/347400 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	j	362	CYS	CB-SG	-6.32	1.71	1.82
1	s	362	CYS	CB-SG	-6.18	1.71	1.82
1	S	230	CYS	CB-SG	-6.04	1.72	1.82
1	n	483	CYS	CB-SG	-5.67	1.72	1.81
1	D	494	THR	CB-CG2	5.50	1.70	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	494	THR	CA-CB-CG2	-5.89	104.15	112.40
1	D	494	THR	CB-CA-C	-5.82	95.88	111.60

There are no chirality outliers.

There are no planarity outliers.

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	0	4121	0	3896	252	0
1	1	4121	0	3896	285	0
1	2	4121	0	3896	267	0
1	3	4121	0	3896	252	0
1	4	4121	0	3896	245	0
1	5	4121	0	3896	242	2
1	6	4121	0	3896	244	0
1	7	4121	0	3896	244	5
1	A	4121	0	3896	415	1
1	B	4121	0	3896	392	0
1	C	4121	0	3896	379	0
1	D	4121	0	3896	369	5
1	E	4121	0	3896	407	0
1	F	4121	0	3896	377	0
1	G	4121	0	3896	342	0
1	H	4121	0	3896	403	0
1	I	4121	0	3896	403	0
1	J	4121	0	3896	418	0
1	K	4121	0	3896	341	4
1	L	4121	0	3896	334	0
1	M	4121	0	3896	373	0
1	N	4121	0	3896	383	5
1	O	4121	0	3896	397	0
1	P	4121	0	3896	381	0
1	Q	4121	0	3896	385	0
1	R	4121	0	3896	362	0
1	S	4121	0	3896	385	0
1	T	4121	0	3896	384	1
1	U	4121	0	3896	396	5
1	V	4121	0	3896	391	0
1	W	4121	0	3896	416	0
1	X	4121	0	3896	403	0
1	Y	4121	0	3896	402	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	4121	0	3896	403	0
1	a	4121	0	3896	0	0
1	b	4121	0	3896	0	0
1	c	4121	0	3896	0	0
1	d	4121	0	3896	0	0
1	e	4121	0	3896	0	0
1	f	4121	0	3896	0	0
1	g	4121	0	3896	0	6
1	h	4121	0	3896	0	0
1	i	4121	0	3896	0	0
1	j	4121	0	3896	0	0
1	k	4121	0	3896	0	3
1	l	4121	0	3896	0	2
1	m	4121	0	3896	0	0
1	n	4121	0	3896	0	1
1	o	4121	0	3896	0	0
1	p	4121	0	3896	0	2
1	q	4121	0	3896	0	0
1	r	4121	0	3896	0	0
1	s	4121	0	3896	0	0
1	t	4121	0	3896	0	1
1	u	4121	0	3896	0	0
1	v	4121	0	3896	0	0
1	w	4121	0	3896	0	0
1	x	4121	0	3896	0	0
1	y	4121	0	3896	0	0
1	z	4121	0	3896	0	1
All	All	247260	0	233760	9007	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 19.

The worst 5 of 9007 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	65.26	1.09
1:M:464:SER:HB3	1:T:551:SER:HA	177.77	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	175.30	1.05
1:H:551:SER:HA	1:W:464:SER:HB3	134.67	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:k:557:ASN:OD1	1:7:457:GLN:NE2[2_554]	1.64	0.56

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 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%)	5	28
1	1	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	6	29
1	2	518/520 (100%)	463 (89%)	43 (8%)	12 (2%)	8	36
1	3	518/520 (100%)	459 (89%)	46 (9%)	13 (2%)	7	34
1	4	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	7	34
1	5	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	7	34
1	6	518/520 (100%)	464 (90%)	42 (8%)	12 (2%)	8	36
1	7	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	6	29
1	A	518/520 (100%)	460 (89%)	43 (8%)	15 (3%)	6	29
1	B	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	6	29
1	C	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	5	28
1	D	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	6	32
1	E	518/520 (100%)	463 (89%)	41 (8%)	14 (3%)	6	32
1	F	518/520 (100%)	462 (89%)	42 (8%)	14 (3%)	6	32
1	G	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	6	32
1	H	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	6	29
1	J	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	6	29
1	K	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	7	34
1	L	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	6	29
1	M	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	7	34
1	N	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	6	32
1	O	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	6	32
1	P	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	6	32
1	Q	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	6	32
1	R	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	5	28
1	S	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	7	34
1	T	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	7	34
1	U	518/520 (100%)	471 (91%)	31 (6%)	16 (3%)	5	28
1	V	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	6	29
1	W	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	7	34
1	X	518/520 (100%)	461 (89%)	43 (8%)	14 (3%)	6	32
1	Y	518/520 (100%)	461 (89%)	44 (8%)	13 (2%)	7	34
1	Z	518/520 (100%)	462 (89%)	44 (8%)	12 (2%)	8	36
1	a	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	7	34
1	b	518/520 (100%)	467 (90%)	39 (8%)	12 (2%)	8	36
1	c	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	8	36
1	d	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	7	34
1	e	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	7	34
1	f	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	5	28
1	g	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	7	34
1	h	518/520 (100%)	463 (89%)	44 (8%)	11 (2%)	9	40
1	i	518/520 (100%)	466 (90%)	37 (7%)	15 (3%)	6	29
1	j	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	7	34
1	k	518/520 (100%)	465 (90%)	37 (7%)	16 (3%)	5	28
1	l	518/520 (100%)	468 (90%)	38 (7%)	12 (2%)	8	36
1	m	518/520 (100%)	468 (90%)	37 (7%)	13 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	n	518/520 (100%)	469 (90%)	36 (7%)	13 (2%)	7	34
1	o	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	6	32
1	p	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	5	28
1	q	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	5	28
1	r	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	5	28
1	s	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	7	34
1	t	518/520 (100%)	463 (89%)	40 (8%)	15 (3%)	6	29
1	u	518/520 (100%)	467 (90%)	37 (7%)	14 (3%)	6	32
1	v	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	6	29
1	w	518/520 (100%)	465 (90%)	38 (7%)	15 (3%)	6	29
1	x	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	8	36
1	y	518/520 (100%)	468 (90%)	35 (7%)	15 (3%)	6	29
1	z	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	7	34
All	All	31080/31200 (100%)	27915 (90%)	2328 (8%)	837 (3%)	6	32

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 (i)

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%)	412 (91%)	40 (9%)	12	42
1	1	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	2	452/452 (100%)	414 (92%)	38 (8%)	14	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	4	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	5	452/452 (100%)	411 (91%)	41 (9%)	12	41
1	6	452/452 (100%)	414 (92%)	38 (8%)	14	45
1	7	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	A	452/452 (100%)	408 (90%)	44 (10%)	10	37
1	B	452/452 (100%)	409 (90%)	43 (10%)	11	38
1	C	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	D	452/452 (100%)	411 (91%)	41 (9%)	12	41
1	E	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	F	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	G	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	H	452/452 (100%)	411 (91%)	41 (9%)	12	41
1	I	452/452 (100%)	410 (91%)	42 (9%)	11	39
1	J	452/452 (100%)	411 (91%)	41 (9%)	12	41
1	K	452/452 (100%)	415 (92%)	37 (8%)	14	46
1	L	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	M	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	N	452/452 (100%)	414 (92%)	38 (8%)	14	45
1	O	452/452 (100%)	411 (91%)	41 (9%)	12	41
1	P	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	Q	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	R	452/452 (100%)	408 (90%)	44 (10%)	10	37
1	S	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	T	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	U	452/452 (100%)	410 (91%)	42 (9%)	11	39
1	V	452/452 (100%)	409 (90%)	43 (10%)	11	38
1	W	452/452 (100%)	410 (91%)	42 (9%)	11	39
1	X	452/452 (100%)	415 (92%)	37 (8%)	14	46
1	Y	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	Z	452/452 (100%)	413 (91%)	39 (9%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	452/452 (100%)	414 (92%)	38 (8%)	14	45
1	b	452/452 (100%)	410 (91%)	42 (9%)	11	39
1	c	452/452 (100%)	408 (90%)	44 (10%)	10	37
1	d	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	e	452/452 (100%)	410 (91%)	42 (9%)	11	39
1	f	452/452 (100%)	415 (92%)	37 (8%)	14	46
1	g	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	h	452/452 (100%)	415 (92%)	37 (8%)	14	46
1	i	452/452 (100%)	410 (91%)	42 (9%)	11	39
1	j	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	k	452/452 (100%)	408 (90%)	44 (10%)	10	37
1	l	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	m	452/452 (100%)	414 (92%)	38 (8%)	14	45
1	n	452/452 (100%)	411 (91%)	41 (9%)	12	41
1	o	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	p	452/452 (100%)	415 (92%)	37 (8%)	14	46
1	q	452/452 (100%)	408 (90%)	44 (10%)	10	37
1	r	452/452 (100%)	411 (91%)	41 (9%)	12	41
1	s	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	t	452/452 (100%)	415 (92%)	37 (8%)	14	46
1	u	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	v	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	w	452/452 (100%)	412 (91%)	40 (9%)	12	42
1	x	452/452 (100%)	415 (92%)	37 (8%)	14	46
1	y	452/452 (100%)	413 (91%)	39 (9%)	13	44
1	z	452/452 (100%)	409 (90%)	43 (10%)	11	38
All	All	27120/27120 (100%)	24715 (91%)	2405 (9%)	12	42

5 of 2405 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	219	ASP
1	h	458	ASN

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Mol	Chain	Res	Type
1	3	443	LEU
1	b	626	ASP
1	e	333	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1634 such sidechains are listed below:

Mol	Chain	Res	Type
1	b	427	HIS
1	h	624	HIS
1	3	458	ASN
1	c	302	ASN
1	e	512	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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, 95^{th} 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%)	-0.44	12 (2%)	64	33	45, 60, 92, 141	0
1	1	520/520 (100%)	-0.42	5 (0%)	84	60	44, 61, 91, 139	0
1	2	520/520 (100%)	-0.42	13 (2%)	61	30	46, 60, 93, 141	0
1	3	520/520 (100%)	-0.49	9 (1%)	73	45	43, 59, 91, 138	0
1	4	520/520 (100%)	-0.61	7 (1%)	79	53	44, 59, 92, 140	0
1	5	520/520 (100%)	-0.51	6 (1%)	81	55	43, 57, 90, 138	0
1	6	520/520 (100%)	-0.46	8 (1%)	76	49	42, 57, 90, 139	0
1	7	520/520 (100%)	-0.57	4 (0%)	87	67	42, 58, 90, 138	0
1	A	520/520 (100%)	-0.29	7 (1%)	79	53	45, 61, 92, 139	0
1	B	520/520 (100%)	-0.43	10 (1%)	70	41	46, 61, 93, 139	0
1	C	520/520 (100%)	-0.41	10 (1%)	70	41	45, 60, 92, 140	0
1	D	520/520 (100%)	-0.42	10 (1%)	70	41	44, 61, 92, 139	0
1	E	520/520 (100%)	-0.44	5 (0%)	84	60	46, 61, 93, 139	0
1	F	520/520 (100%)	-0.35	12 (2%)	64	33	45, 61, 93, 138	0
1	G	520/520 (100%)	-0.50	9 (1%)	73	45	46, 60, 91, 140	0
1	H	520/520 (100%)	-0.46	12 (2%)	64	33	43, 60, 92, 137	0
1	I	520/520 (100%)	-0.38	9 (1%)	73	45	45, 61, 92, 139	0
1	J	520/520 (100%)	-0.32	7 (1%)	79	53	45, 62, 92, 141	0
1	K	520/520 (100%)	-0.51	8 (1%)	76	49	43, 57, 91, 139	0
1	L	520/520 (100%)	-0.56	6 (1%)	81	55	42, 58, 90, 141	0
1	M	520/520 (100%)	-0.50	5 (0%)	84	60	43, 58, 90, 138	0
1	N	520/520 (100%)	-0.58	4 (0%)	87	67	42, 58, 90, 138	0
1	O	520/520 (100%)	-0.52	10 (1%)	70	41	42, 58, 91, 141	0
1	P	520/520 (100%)	-0.51	6 (1%)	81	55	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%)	-0.45	11 (2%) 67 36	42, 59, 91, 138	0
1	R	520/520 (100%)	-0.51	7 (1%) 79 53	43, 58, 91, 139	0
1	S	520/520 (100%)	-0.52	4 (0%) 87 67	41, 57, 88, 141	0
1	T	520/520 (100%)	-0.49	5 (0%) 84 60	42, 57, 90, 140	0
1	U	520/520 (100%)	-0.45	9 (1%) 73 45	45, 60, 91, 139	0
1	V	520/520 (100%)	-0.41	6 (1%) 81 55	45, 61, 92, 140	0
1	W	520/520 (100%)	-0.34	9 (1%) 73 45	46, 61, 93, 139	0
1	X	520/520 (100%)	-0.33	13 (2%) 61 30	44, 61, 93, 141	0
1	Y	520/520 (100%)	-0.39	11 (2%) 67 36	45, 61, 92, 139	0
1	Z	520/520 (100%)	-0.45	10 (1%) 70 41	44, 60, 91, 140	0
1	a	520/520 (100%)	-0.47	8 (1%) 76 49	44, 59, 92, 139	0
1	b	520/520 (100%)	-0.55	6 (1%) 81 55	42, 58, 90, 137	0
1	c	520/520 (100%)	-0.55	7 (1%) 79 53	44, 59, 90, 141	0
1	d	520/520 (100%)	-0.50	12 (2%) 64 33	45, 60, 91, 141	0
1	e	520/520 (100%)	-0.53	6 (1%) 81 55	43, 58, 89, 141	0
1	f	520/520 (100%)	-0.51	6 (1%) 81 55	45, 59, 92, 141	0
1	g	520/520 (100%)	-0.50	2 (0%) 93 80	46, 60, 92, 134	0
1	h	520/520 (100%)	-0.48	7 (1%) 79 53	45, 60, 91, 140	0
1	i	520/520 (100%)	-0.55	4 (0%) 87 67	43, 59, 90, 138	0
1	j	520/520 (100%)	-0.51	7 (1%) 79 53	43, 58, 90, 139	0
1	k	520/520 (100%)	-0.53	3 (0%) 90 73	41, 58, 90, 135	0
1	l	520/520 (100%)	-0.54	1 (0%) 95 87	42, 57, 90, 138	0
1	m	520/520 (100%)	-0.55	7 (1%) 79 53	42, 57, 89, 138	0
1	n	520/520 (100%)	-0.50	5 (0%) 84 60	42, 57, 90, 139	0
1	o	520/520 (100%)	-0.53	5 (0%) 84 60	45, 60, 92, 139	0
1	p	520/520 (100%)	-0.43	13 (2%) 61 30	46, 60, 91, 139	0
1	q	520/520 (100%)	-0.49	6 (1%) 81 55	45, 60, 92, 139	0
1	r	520/520 (100%)	-0.56	7 (1%) 79 53	43, 58, 90, 138	0
1	s	520/520 (100%)	-0.52	5 (0%) 84 60	43, 59, 91, 139	0
1	t	520/520 (100%)	-0.52	7 (1%) 79 53	43, 59, 91, 140	0
1	u	520/520 (100%)	-0.49	9 (1%) 73 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%)	-0.53	8 (1%) 76 49	42, 59, 90, 141	0
1	w	520/520 (100%)	-0.46	10 (1%) 70 41	43, 60, 92, 141	0
1	x	520/520 (100%)	-0.47	10 (1%) 70 41	44, 60, 92, 140	0
1	y	520/520 (100%)	-0.53	7 (1%) 79 53	43, 59, 90, 139	0
1	z	520/520 (100%)	-0.44	8 (1%) 76 49	45, 59, 91, 141	0
All	All	31200/31200 (100%)	-0.48	455 (1%) 76 49	41, 59, 91, 141	0

The worst 5 of 455 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	x	217	GLY	7.9
1	2	217	GLY	6.4
1	P	453	SER	5.7
1	T	217	GLY	5.7
1	U	217	GLY	5.3

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 carbohydrates 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.