wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:22 PM GMT

PDB ID	:	3SHM
Title	:	Structure-function Analysis of Receptor Binding in Adeno-Associated Virus Serotype 6 (AAV-6)
Authors	:	Xie, Q.; Lerch, T.F.; Meyer, N.L.; Chapman, M.S.
Deposited on	:	2011-06-16
Resolution	:	3.02 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:

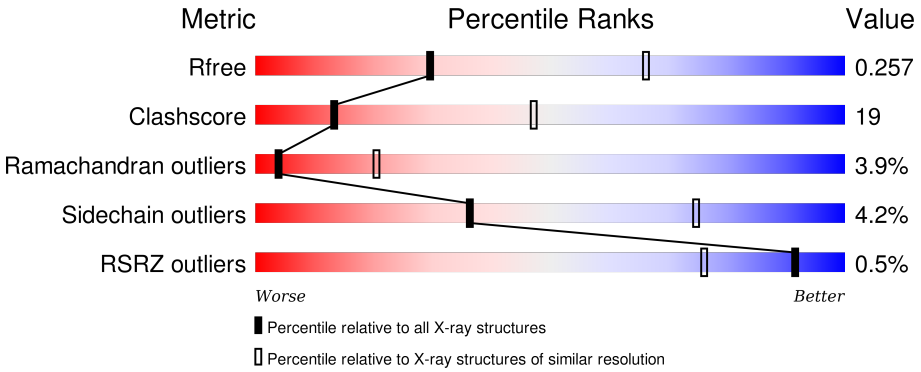
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.02 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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	A	516	63% 33% ·
1	B	516	61% 35% ·
1	C	516	64% 33% ·
1	D	516	% 61% 35% ·
1	E	516	61% 35% ·

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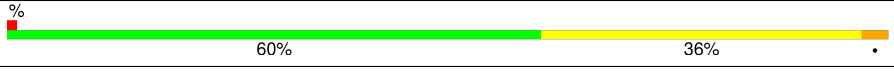
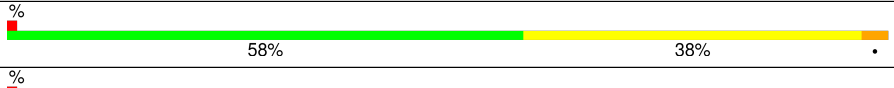
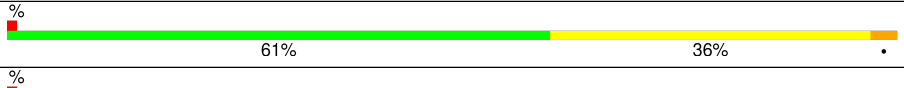
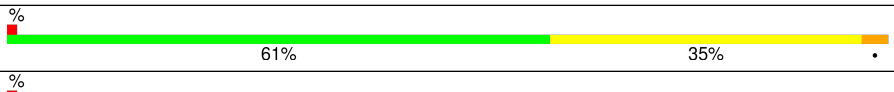
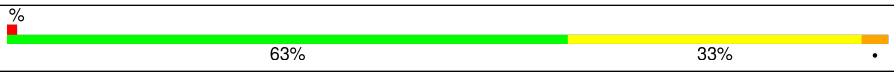
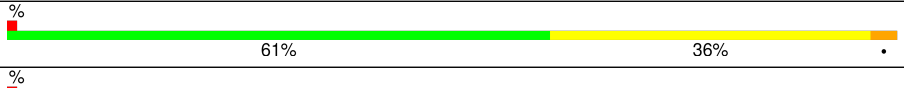
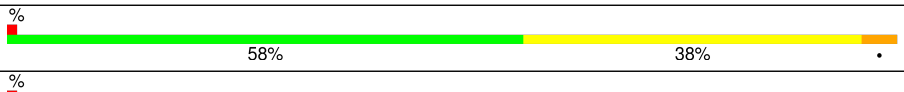
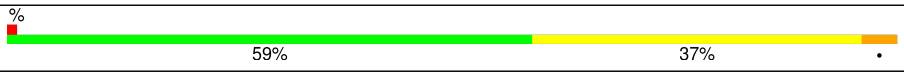
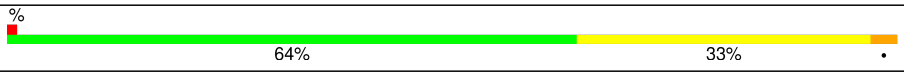
Mol	Chain	Length	Quality of chain
1	F	516	
1	G	516	
1	H	516	
1	I	516	
1	J	516	
1	K	516	
1	L	516	
1	M	516	
1	N	516	
1	O	516	
1	P	516	
1	Q	516	
1	R	516	
1	S	516	
1	T	516	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 82000 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	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	B	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	C	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	D	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	E	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	F	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	G	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	H	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	I	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	J	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	K	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	L	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	M	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	N	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	O	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	P	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			

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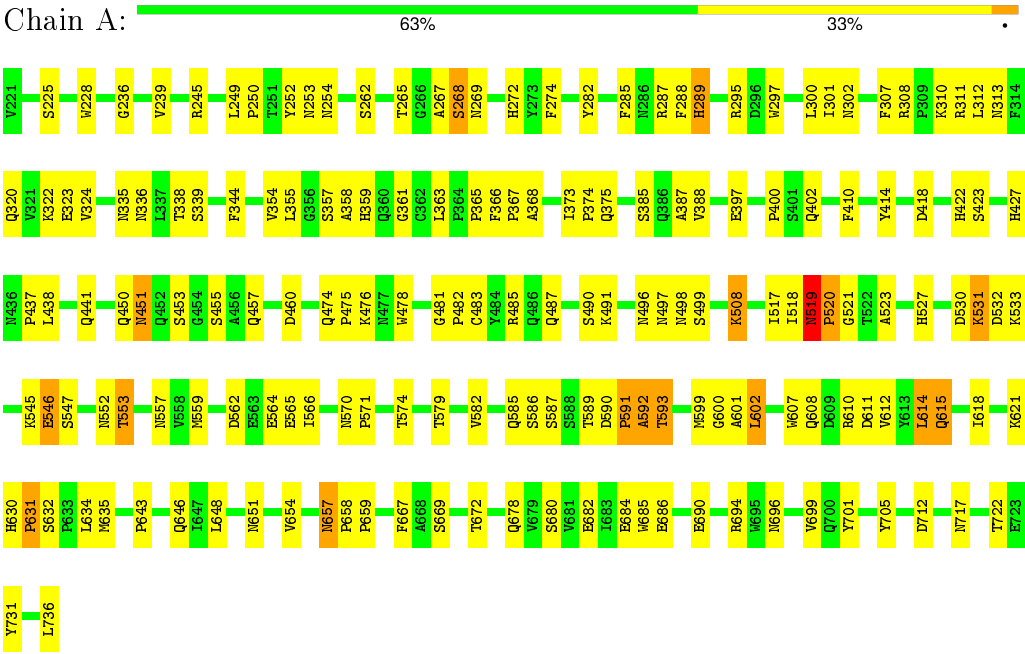
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	R	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	S	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			
1	T	516	Total	C	N	O	S	0	0	0
			4100	2596	708	780	16			

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.

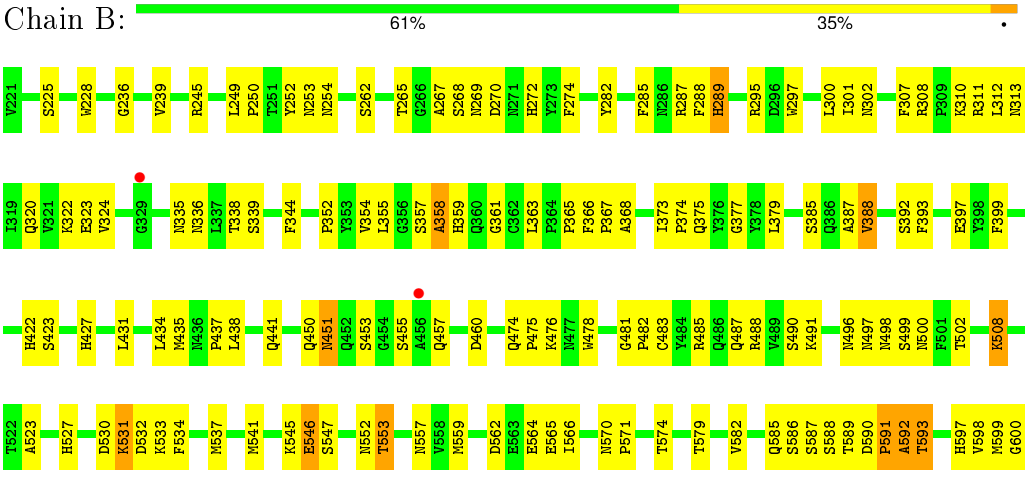
- Molecule 1: Capsid protein VP1

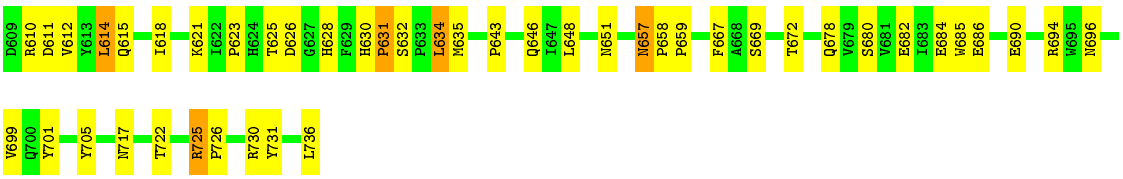
Chain A:



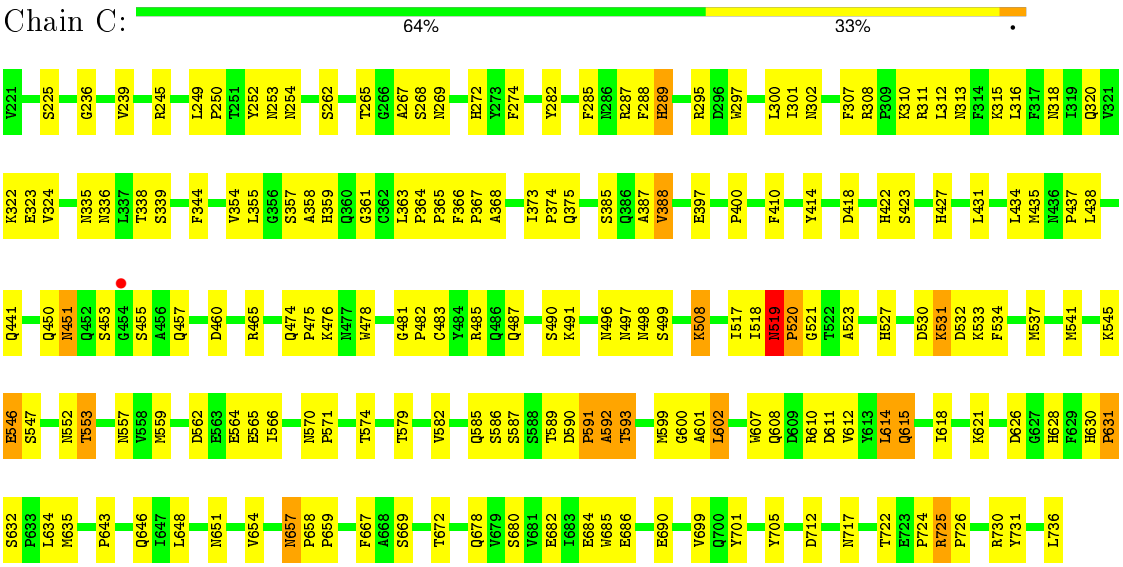
- Molecule 1: Capsid protein VP1

Chain B:

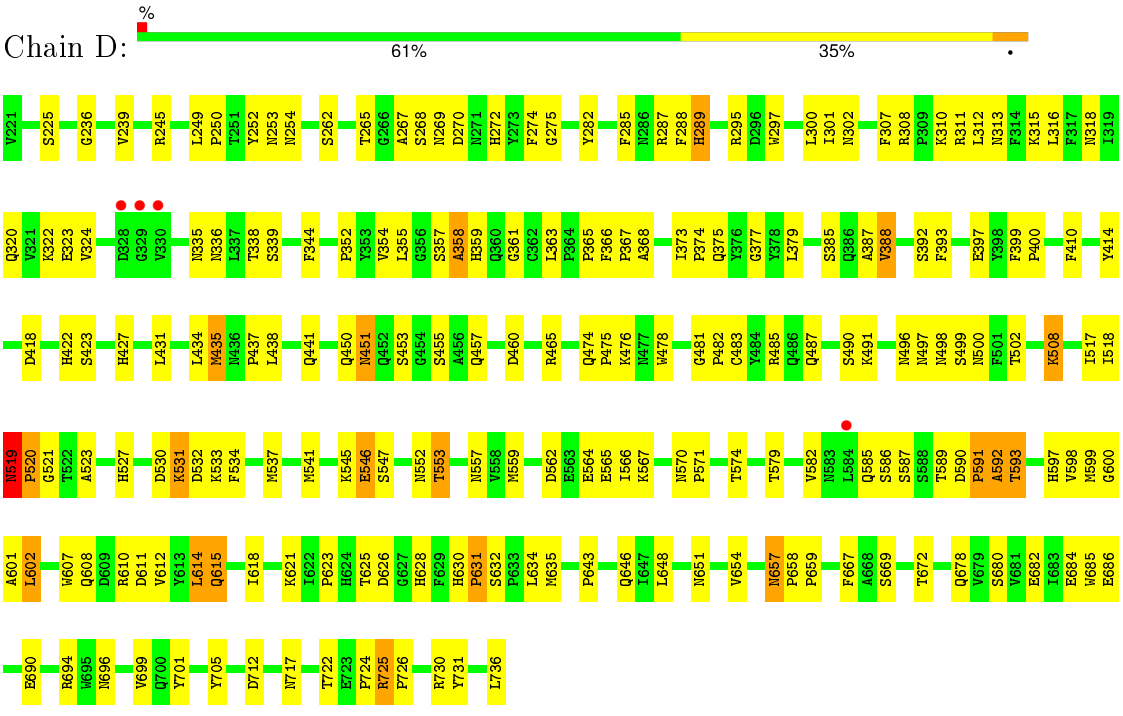




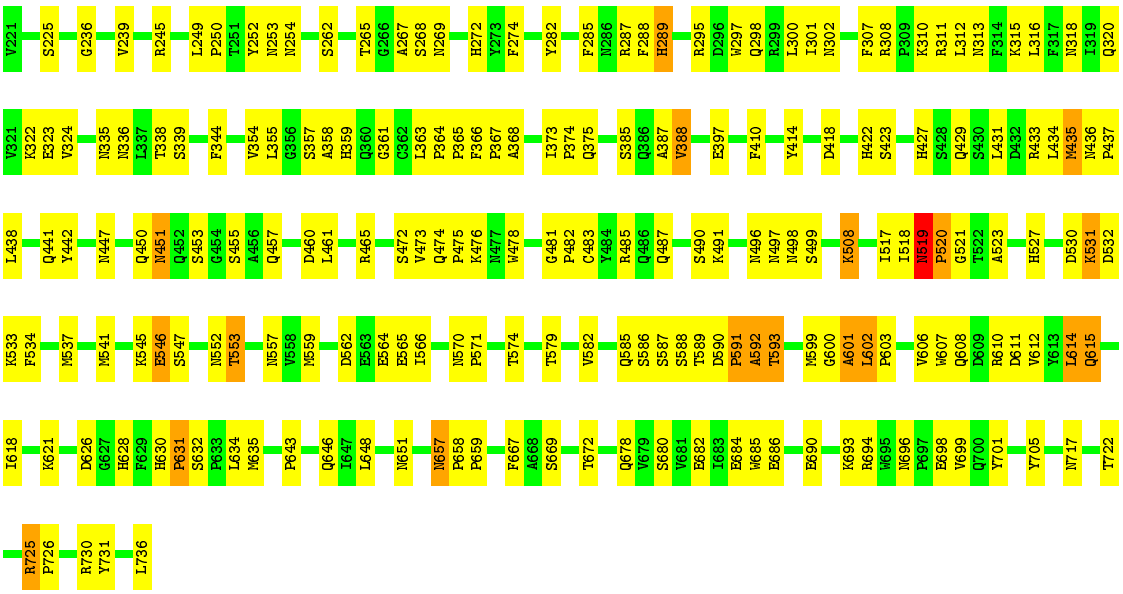
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

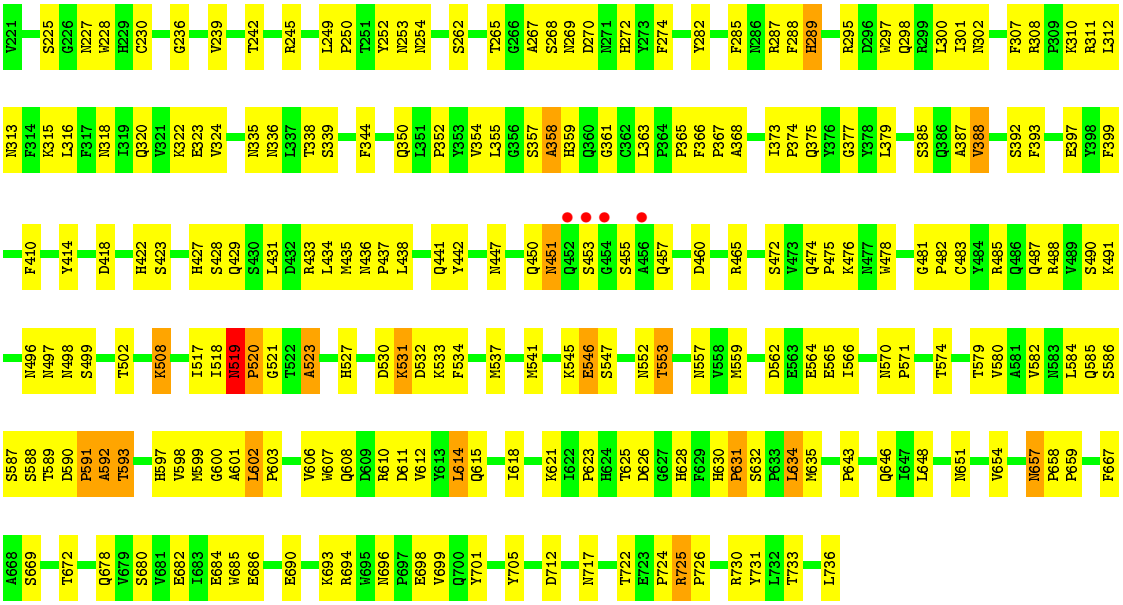


• Molecule 1: Capsid protein VP1



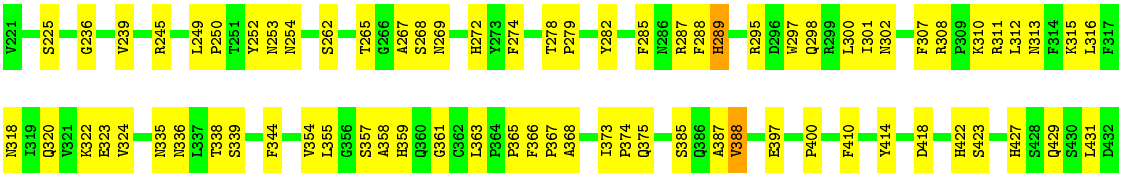
- Molecule 1: Capsid protein VP1

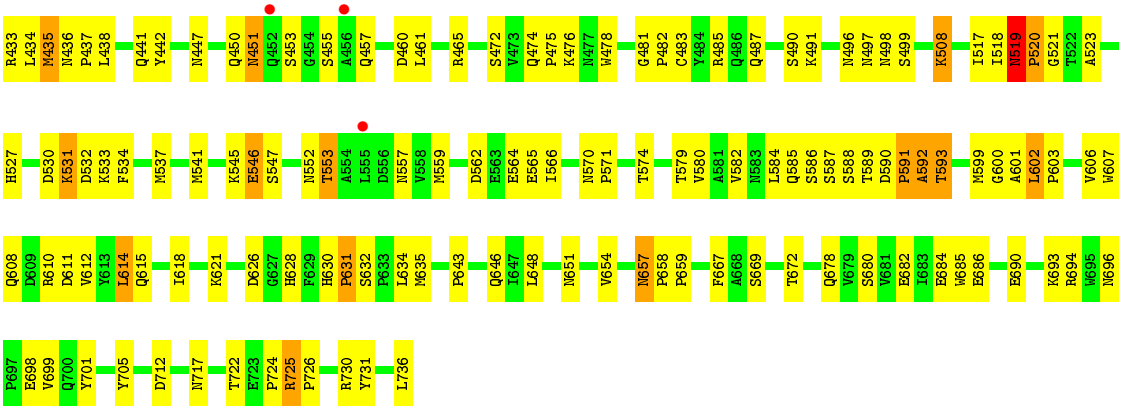
Chain F:



- Molecule 1: Capsid protein VP1

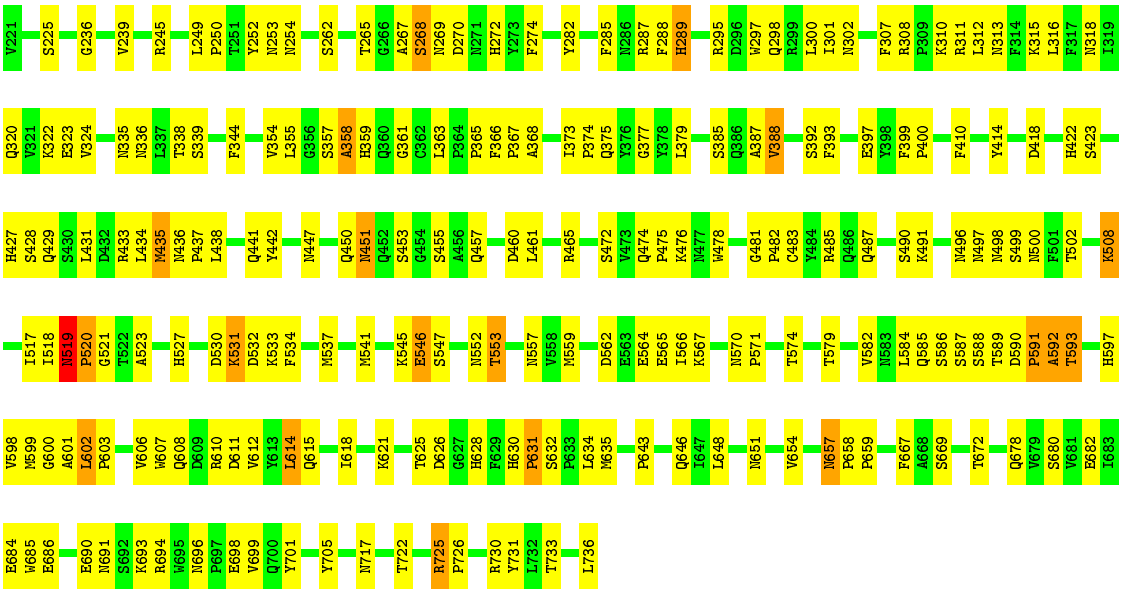
Chain G:





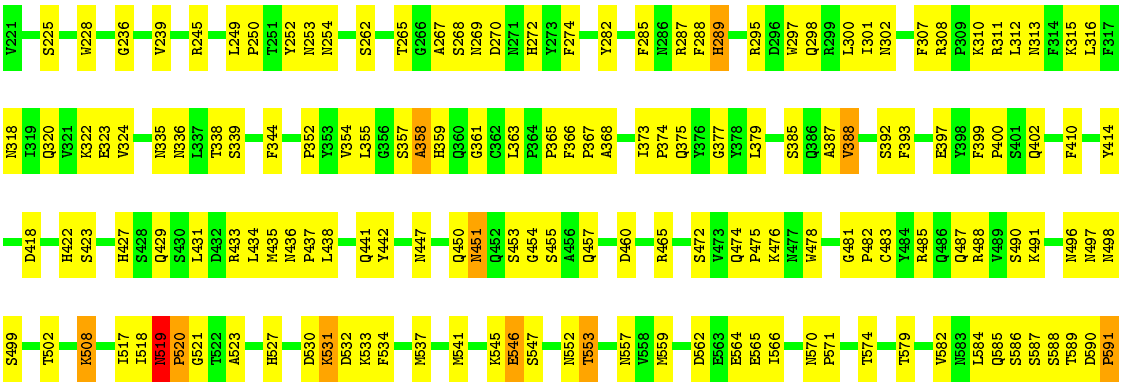
- Molecule 1: Capsid protein VP1

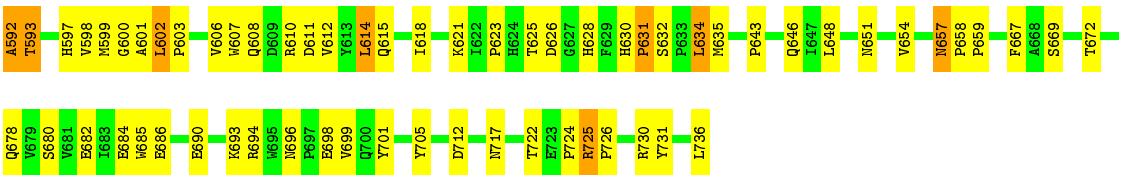
Chain H:



- Molecule 1: Capsid protein VP1

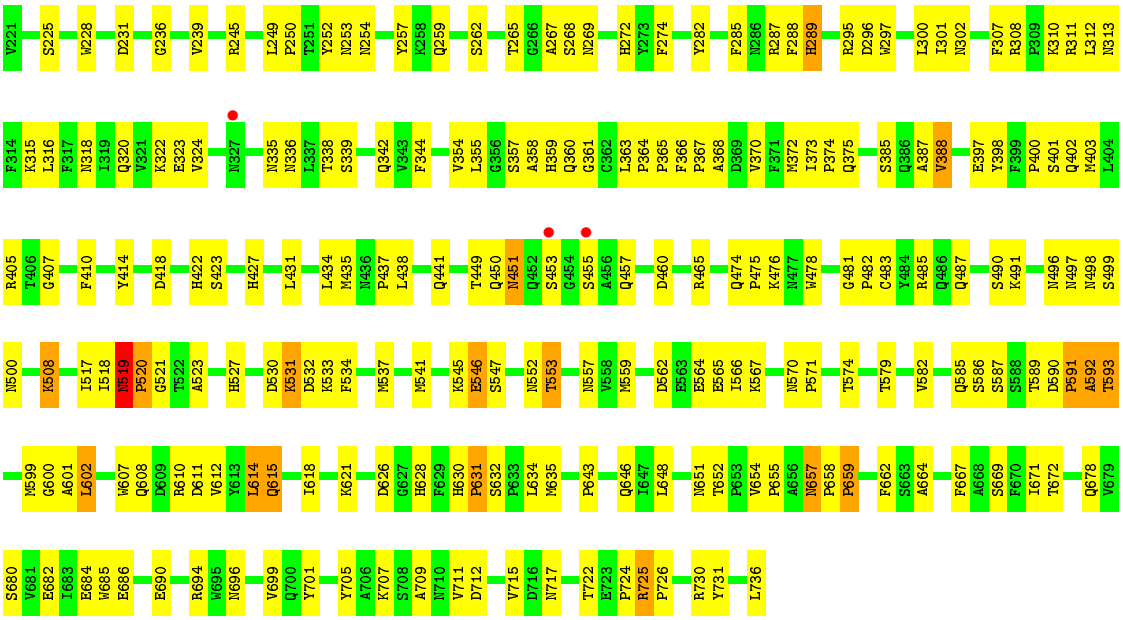
Chain I:





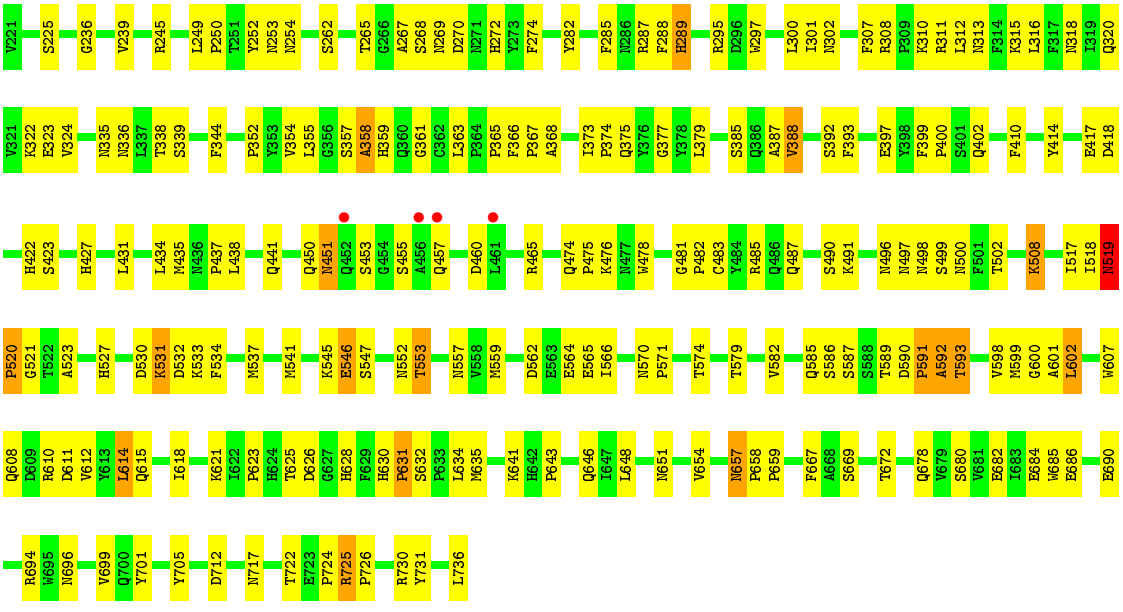
• Molecule 1: Capsid protein VP1

Chain J:



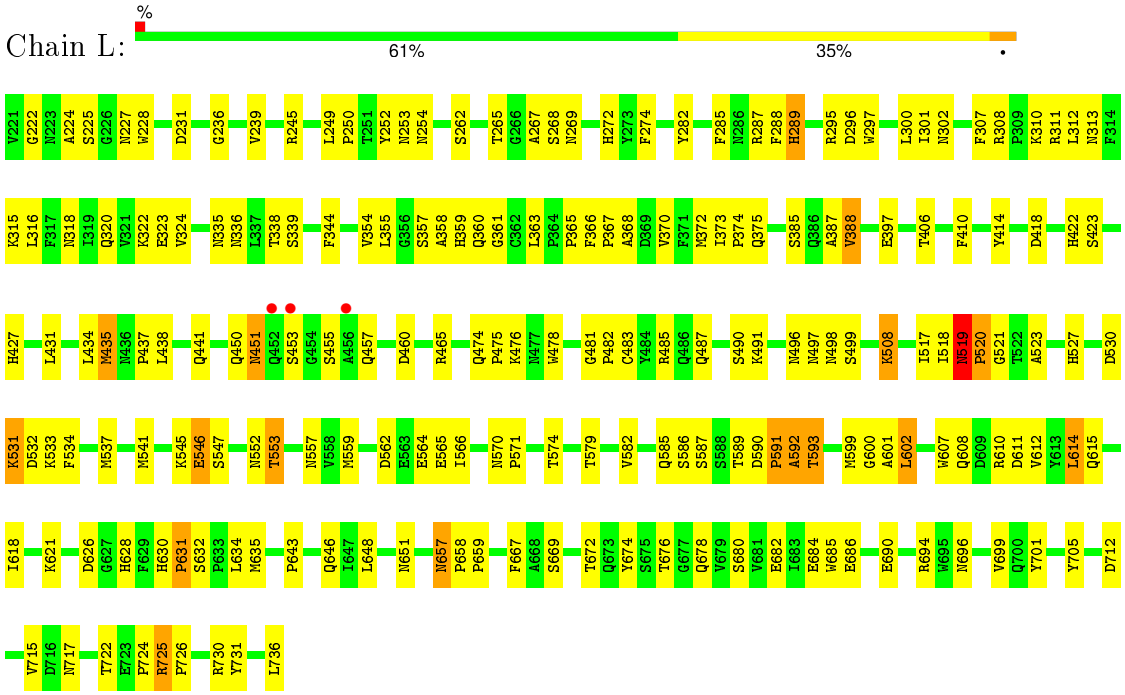
• Molecule 1: Capsid protein VP1

Chain K:



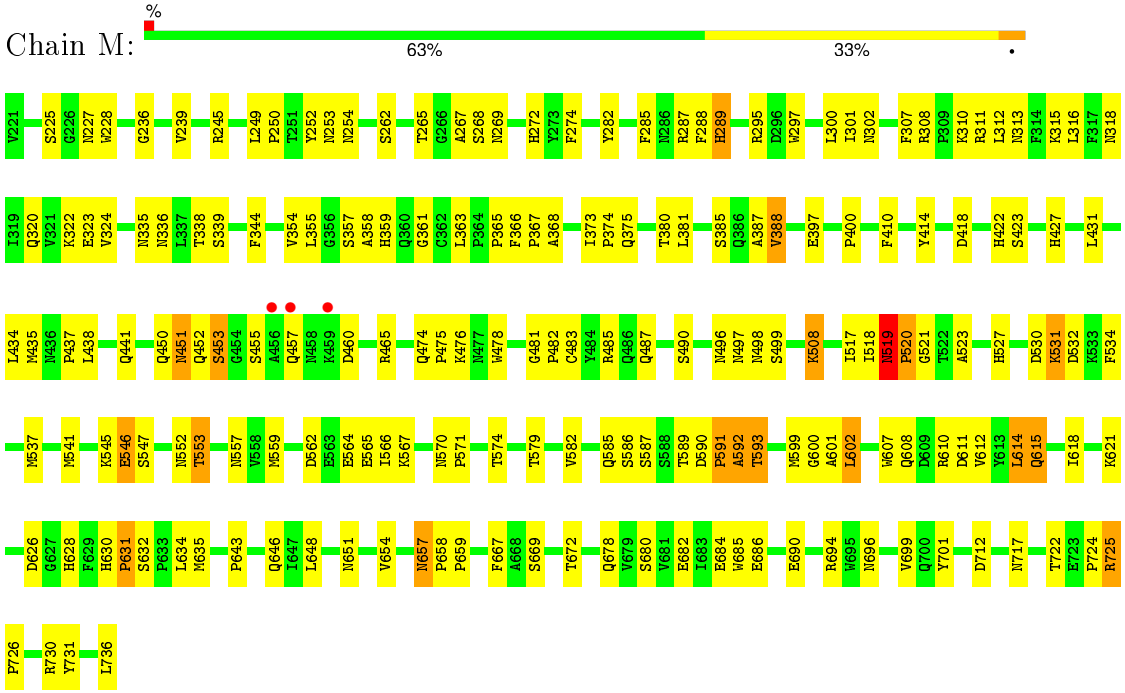
- Molecule 1: Capsid protein VP1

Chain L:



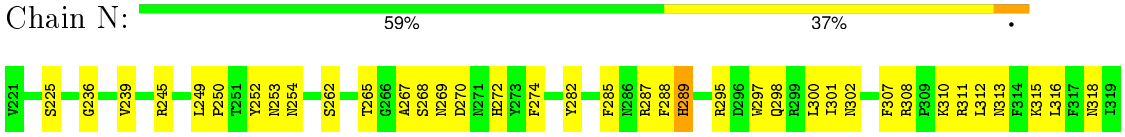
- Molecule 1: Capsid protein VP1

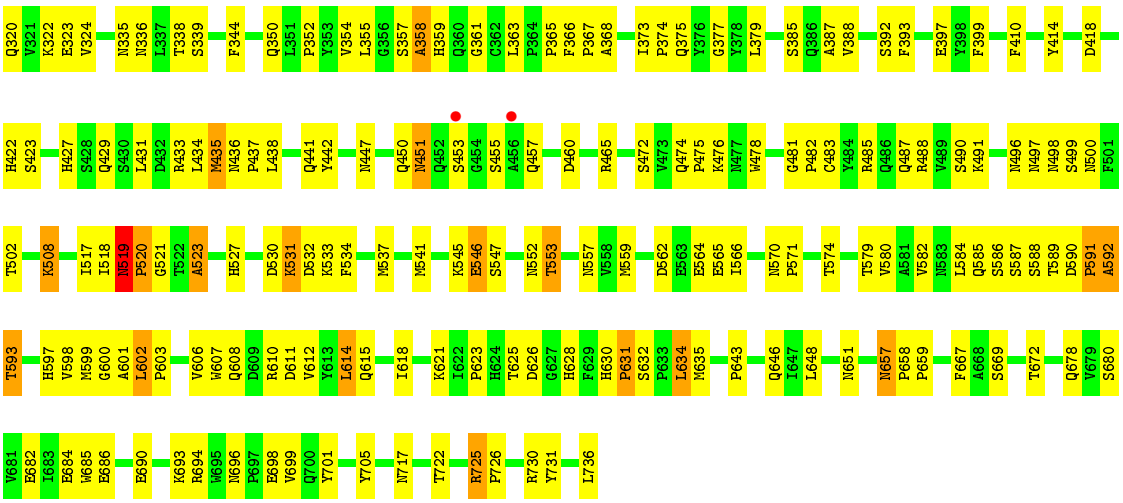
Chain M:



- Molecule 1: Capsid protein VP1

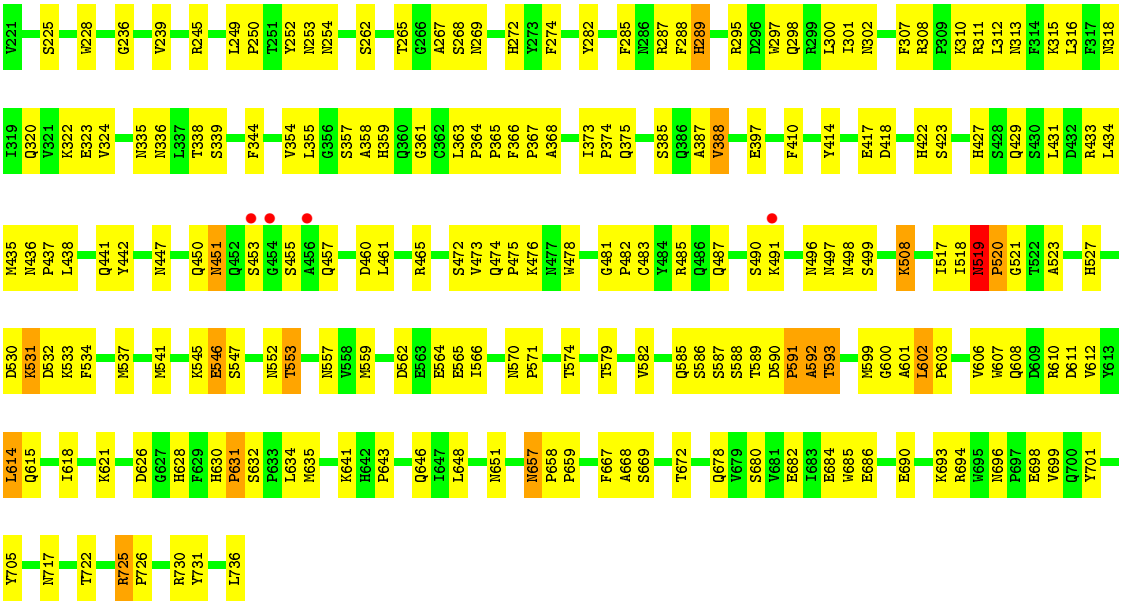
Chain N:





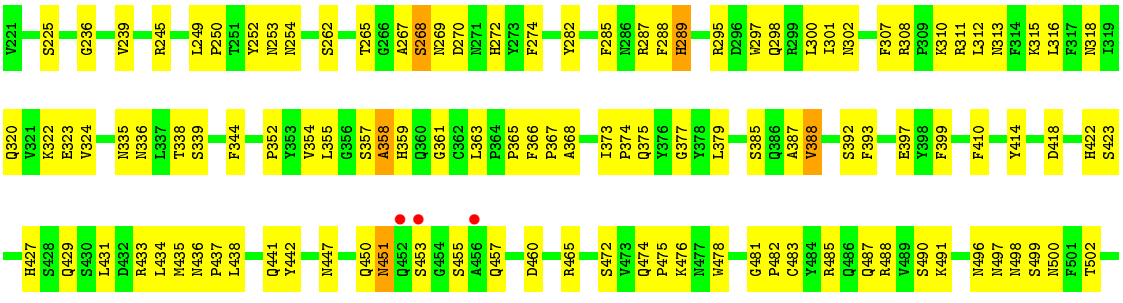
• Molecule 1: Capsid protein VP1

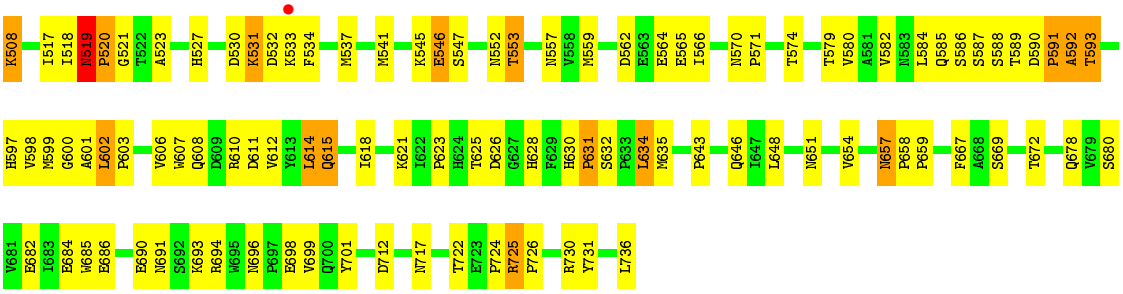
Chain O:

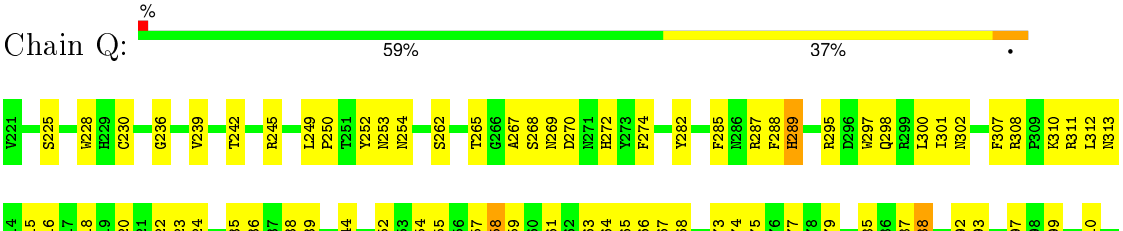


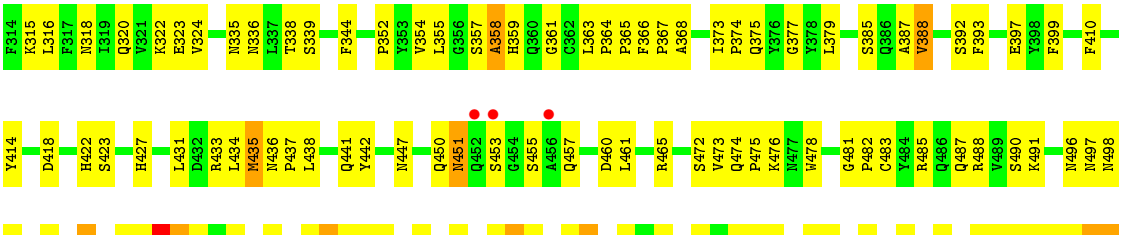
• Molecule 1: Capsid protein VP1

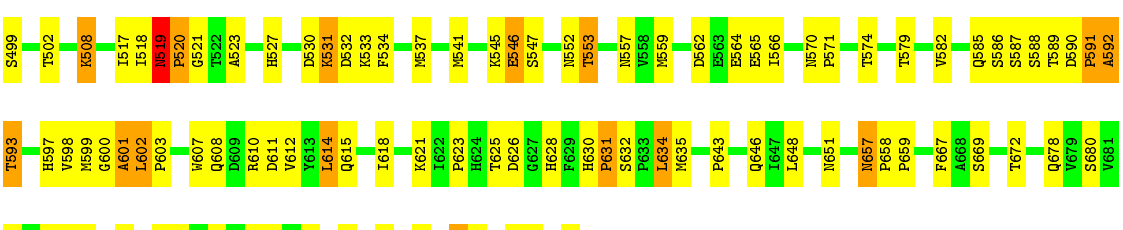
Chain P:

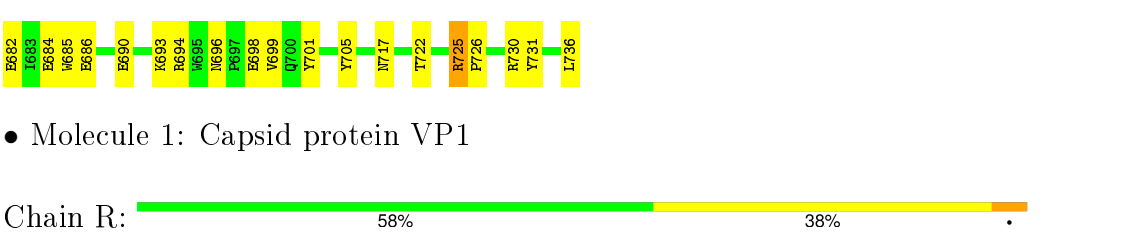


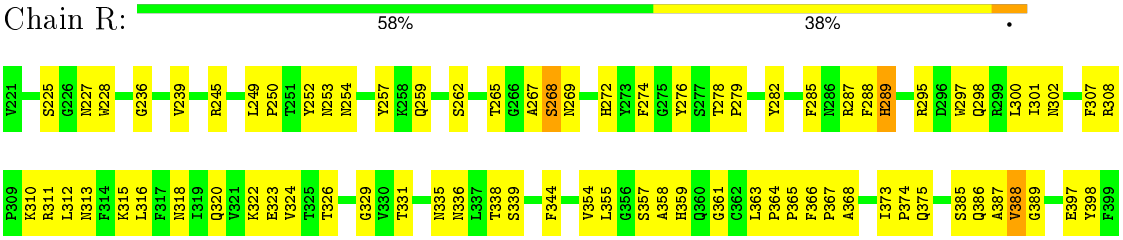


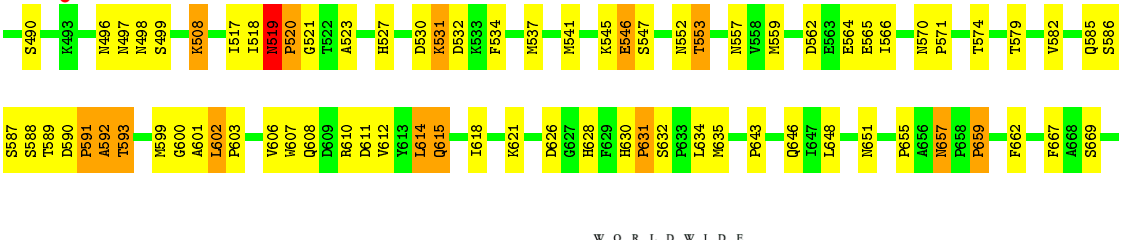










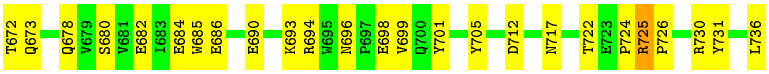


• Molecule 1: Capsid protein VP1

Chain Q:

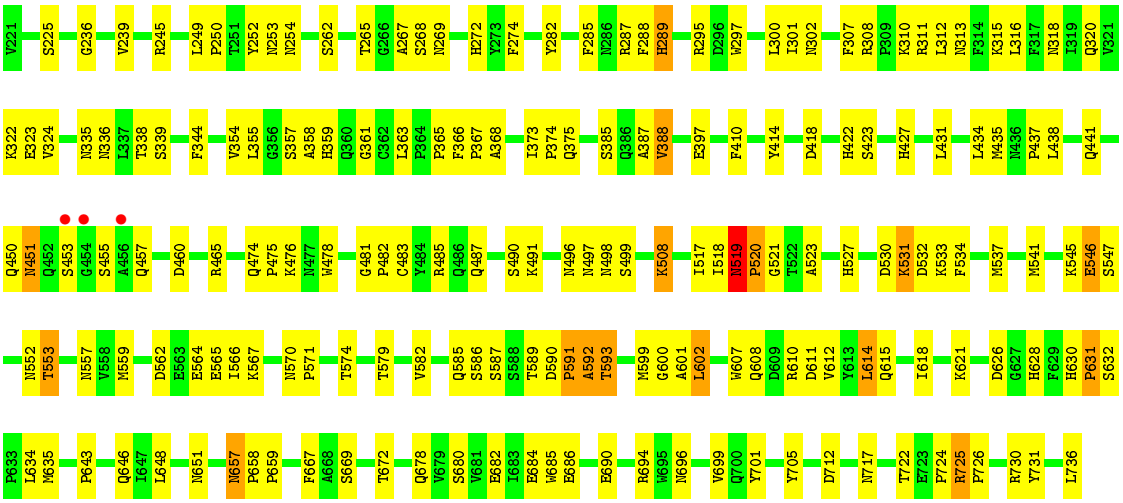
• Molecule 1: Capsid protein VP1

Chain R:



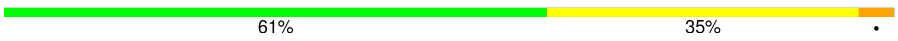
• Molecule 1: Capsid protein VP1

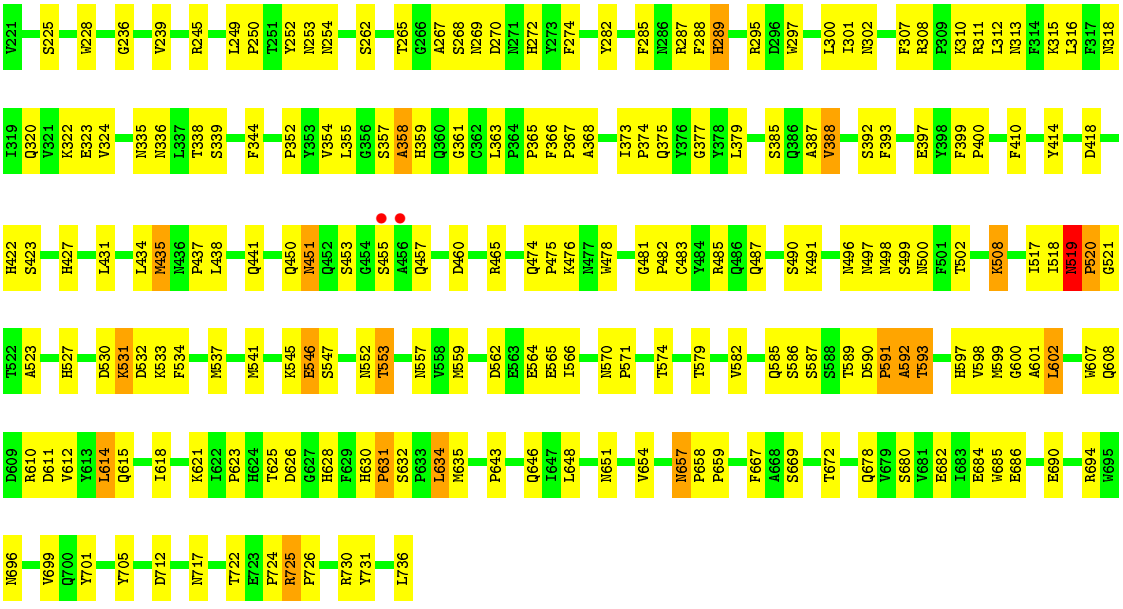
Chain S:



• Molecule 1: Capsid protein VP1

Chain T:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	258.36Å 258.36Å 612.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.67 – 3.02 48.67 – 3.02	Depositor EDS
% Data completeness (in resolution range)	23.0 (48.67-3.02) 23.0 (48.67-3.02)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.273 , 0.286 0.241 , 0.257	Depositor DCC
R_{free} test set	977 reflections (1.42%)	DCC
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.6	EDS
Estimated twinning fraction	0.078 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.060 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.048 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.049 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.059 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.057 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.136 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 68828 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	82000	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.62% 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	A	0.21	0/4226	0.37	0/5762
1	B	0.21	0/4226	0.37	0/5762
1	C	0.21	0/4226	0.37	0/5762
1	D	0.22	0/4226	0.37	0/5762
1	E	0.21	0/4226	0.37	0/5762
1	F	0.21	0/4226	0.37	0/5762
1	G	0.21	0/4226	0.37	0/5762
1	H	0.22	0/4226	0.37	0/5762
1	I	0.22	0/4226	0.37	0/5762
1	J	0.22	0/4226	0.37	0/5762
1	K	0.21	0/4226	0.37	0/5762
1	L	0.22	0/4226	0.37	0/5762
1	M	0.22	0/4226	0.37	0/5762
1	N	0.21	0/4226	0.37	0/5762
1	O	0.21	0/4226	0.37	0/5762
1	P	0.22	0/4226	0.37	0/5762
1	Q	0.21	0/4226	0.37	0/5762
1	R	0.22	0/4226	0.37	0/5762
1	S	0.21	0/4226	0.37	0/5762
1	T	0.21	0/4226	0.37	0/5762
All	All	0.21	0/84520	0.37	0/115240

There are no bond length outliers.

There are no bond angle outliers.

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	A	4100	0	3881	137	1
1	B	4100	0	3881	167	2
1	C	4100	0	3881	133	2
1	D	4100	0	3881	170	1
1	E	4100	0	3881	173	1
1	F	4100	0	3881	213	0
1	G	4100	0	3881	174	1
1	H	4100	0	3881	208	0
1	I	4100	0	3881	207	1
1	J	4100	0	3881	194	2
1	K	4100	0	3881	166	1
1	L	4100	0	3881	167	2
1	M	4100	0	3881	137	5
1	N	4100	0	3881	204	0
1	O	4100	0	3881	168	2
1	P	4100	0	3881	204	0
1	Q	4100	0	3881	203	0
1	R	4100	0	3881	197	3
1	S	4100	0	3881	134	2
1	T	4100	0	3881	170	1
All	All	82000	0	77620	2997	15

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 2997 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:J:658:PRO:HG2	1:L:250:PRO:HB3	1.19	1.14
1:J:705:TYR:O	1:R:388:VAL:HG12	1.59	1.03
1:J:397:GLU:HB2	1:L:367:PRO:HB2	1.45	0.98
1:D:359:HIS:HE1	1:E:436:ASN:H	1.03	0.96
1:B:359:HIS:HE1	1:G:436:ASN:H	1.01	0.95

The worst 5 of 15 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:I:454:GLY:O	1:O:668:ALA:O[3_545]	1.88	0.32
1:M:453:SER:OG	1:R:326:THR:OG1[4_455]	1.94	0.26
1:G:626:ASP:OD1	1:M:423:SER:OG[2_555]	2.07	0.13
1:B:423:SER:OG	1:M:626:ASP:OD1[2_555]	2.09	0.11
1:M:452:GLN:O	1:R:329:GLY:CA[4_455]	2.10	0.10

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	A	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	B	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	C	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	D	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	4	20
1	E	514/516 (100%)	438 (85%)	55 (11%)	21 (4%)	3	19
1	F	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	G	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	H	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	I	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	J	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	K	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	L	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	4	20
1	M	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	4	20
1	N	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	O	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	P	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4	20
1	Q	514/516 (100%)	438 (85%)	55 (11%)	21 (4%)	3	19
1	R	514/516 (100%)	437 (85%)	57 (11%)	20 (4%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	S	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4 20
1	T	514/516 (100%)	438 (85%)	56 (11%)	20 (4%)	4 20
All	All	10280/10320 (100%)	8756 (85%)	1122 (11%)	402 (4%)	4 20

5 of 402 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ALA
1	A	519	ASN
1	A	531	LYS
1	A	552	ASN
1	A	586	SER

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	A	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	B	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	C	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	D	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	E	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	F	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	G	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	H	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	I	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	J	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	K	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	L	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	M	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	N	451/451 (100%)	432 (96%)	19 (4%)	36 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	P	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	Q	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	R	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	S	451/451 (100%)	432 (96%)	19 (4%)	36 75
1	T	451/451 (100%)	432 (96%)	19 (4%)	36 75
All	All	9020/9020 (100%)	8640 (96%)	380 (4%)	36 75

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	289	HIS
1	L	388	VAL
1	S	593	THR
1	J	435	MET
1	K	323	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 464 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	651	ASN
1	L	302	ASN
1	S	342	GLN
1	J	302	ASN
1	K	313	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 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	A	516/516 (100%)	-0.55	0 100 100	72, 88, 112, 147	0
1	B	516/516 (100%)	-0.54	2 (0%) 93 79	71, 87, 112, 144	0
1	C	516/516 (100%)	-0.54	1 (0%) 95 87	70, 87, 110, 145	0
1	D	516/516 (100%)	-0.54	4 (0%) 87 67	71, 88, 112, 144	0
1	E	516/516 (100%)	-0.59	0 100 100	71, 87, 111, 148	0
1	F	516/516 (100%)	-0.56	4 (0%) 87 67	70, 87, 111, 147	0
1	G	516/516 (100%)	-0.47	3 (0%) 90 73	73, 87, 112, 145	0
1	H	516/516 (100%)	-0.58	0 100 100	70, 86, 112, 145	0
1	I	516/516 (100%)	-0.53	0 100 100	71, 87, 112, 146	0
1	J	516/516 (100%)	-0.49	3 (0%) 90 73	73, 89, 112, 147	0
1	K	516/516 (100%)	-0.52	4 (0%) 87 67	70, 88, 113, 146	0
1	L	516/516 (100%)	-0.45	3 (0%) 90 73	73, 88, 112, 146	0
1	M	516/516 (100%)	-0.50	3 (0%) 90 73	70, 88, 112, 145	0
1	N	516/516 (100%)	-0.53	2 (0%) 93 79	71, 87, 111, 147	0
1	O	516/516 (100%)	-0.52	4 (0%) 87 67	70, 87, 111, 147	0
1	P	516/516 (100%)	-0.55	4 (0%) 87 67	67, 86, 111, 146	0
1	Q	516/516 (100%)	-0.56	3 (0%) 90 73	70, 87, 111, 146	0
1	R	516/516 (100%)	-0.51	2 (0%) 93 79	72, 88, 112, 146	0
1	S	516/516 (100%)	-0.55	3 (0%) 90 73	71, 87, 111, 145	0
1	T	516/516 (100%)	-0.54	2 (0%) 93 79	72, 87, 111, 145	0
All	All	10320/10320 (100%)	-0.53	47 (0%) 91 76	67, 87, 112, 148	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	454	GLY	3.9
1	F	453	SER	3.6
1	T	456	ALA	3.2
1	G	456	ALA	3.2
1	F	456	ALA	3.0

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.