wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:09 AM GMT

PDB ID	:	3KIC
Title	:	Crystal structure of adeno-associated virus serotype 3B
Authors	:	Lerch, T.F.; Xie, Q.; Chapman, M.S.
Deposited on	:	2009-11-01
Resolution	:	2.60 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:

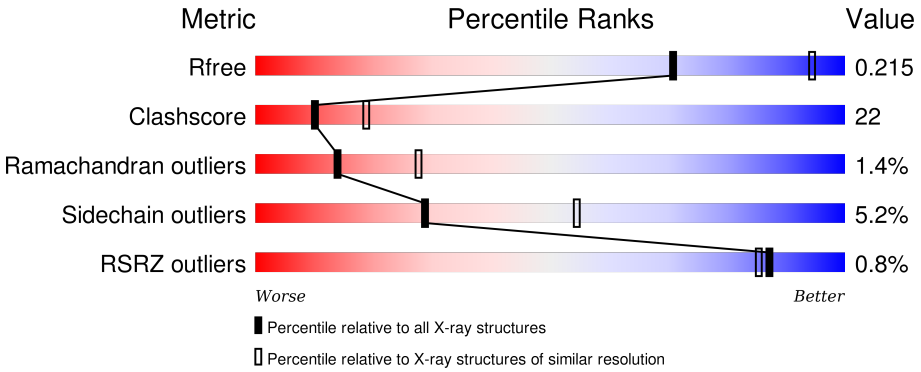
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	736	41% 27% • 29%
1	B	736	% 42% 26% • 29%
1	C	736	% 40% 28% • 29%
1	D	736	% 41% 27% • 29%
1	E	736	% 41% 27% • 29%

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Mol	Chain	Length	Quality of chain
1	F	736	43% 25% 29%
1	G	736	45% 24% 29%
1	H	736	42% 27% 29%
1	I	736	41% 26% 29%
1	J	736	42% 26% 29%
1	K	736	43% 26% 29%
1	L	736	44% 25% 29%
1	M	736	44% 25% 29%
1	N	736	44% 25% 29%
1	O	736	42% 26% 29%
1	P	736	42% 26% 29%
1	Q	736	40% 28% 29%
1	R	736	43% 25% 29%
1	S	736	45% 24% 29%
1	T	736	44% 24% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	D5M	A	999	-	-	-	X
2	D5M	B	999	-	-	-	X
2	D5M	D	999	-	-	-	X
2	D5M	E	999	-	-	-	X
2	D5M	F	999	-	-	-	X
2	D5M	G	999	-	-	-	X
2	D5M	H	999	-	-	-	X
2	D5M	I	999	-	-	-	X
2	D5M	L	999	-	-	-	X
2	D5M	M	999	-	-	-	X
2	D5M	N	999	-	-	-	X
2	D5M	O	999	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	D5M	R	999	-	-	-	X
2	D5M	S	999	-	-	-	X
2	D5M	T	999	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 83520 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
			4154	2618	723	798	15			
1	B	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	C	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	D	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	E	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	F	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	G	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	H	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	I	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	J	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	K	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	L	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	M	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	N	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	O	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	P	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			

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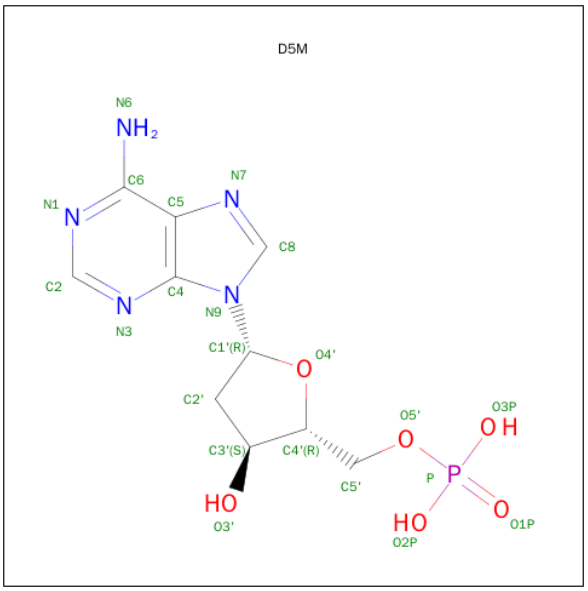
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	R	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	S	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			
1	T	520	Total	C	N	O	S	0	0	0
			4154	2618	723	798	15			

- Molecule 2 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: D5M) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	G	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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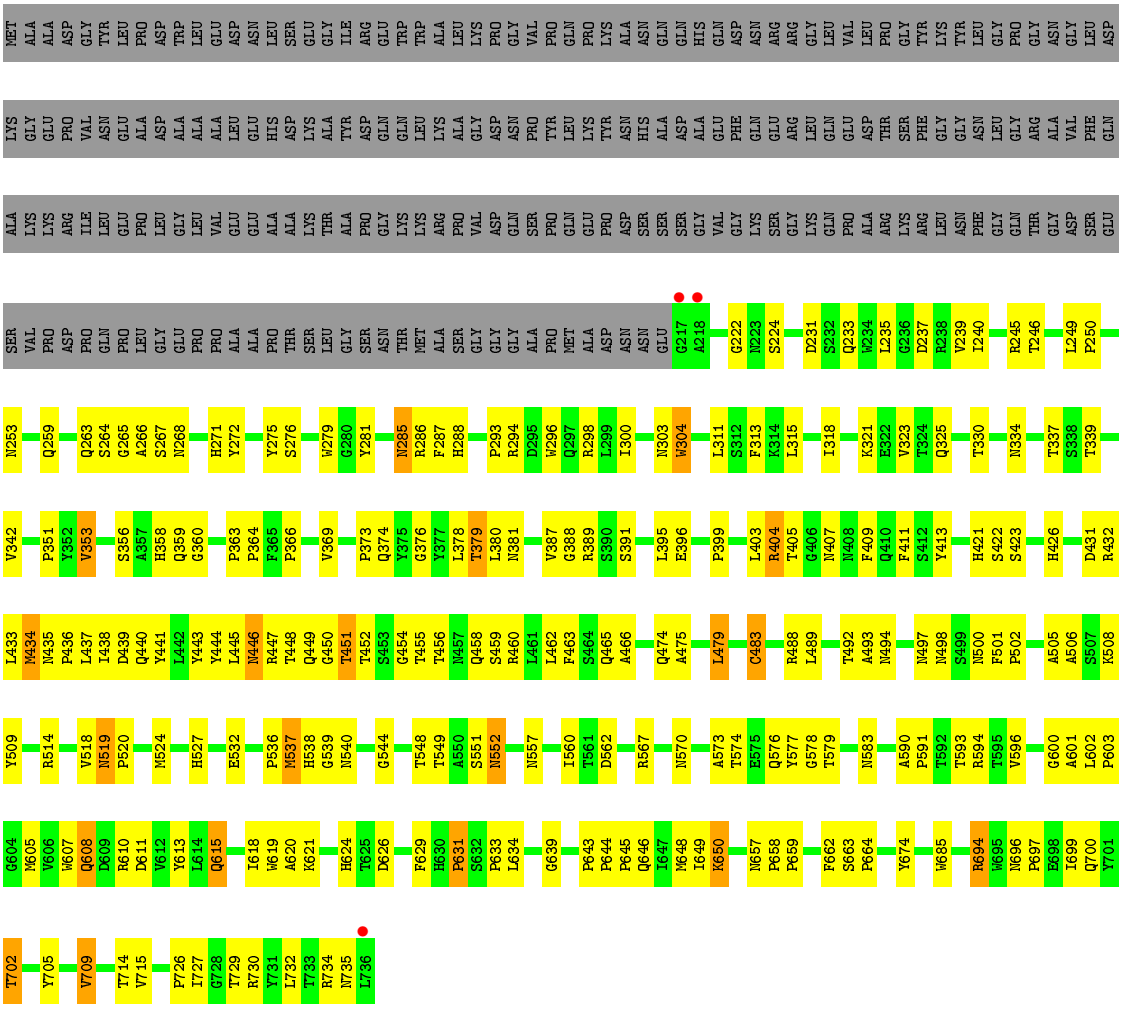
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	I	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	J	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	K	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	L	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	M	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	N	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	O	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	P	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	Q	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	R	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	S	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	T	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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.

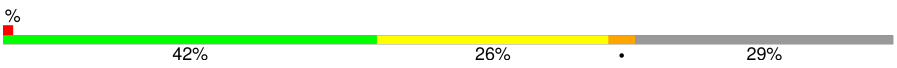
- Molecule 1: Capsid protein VP1

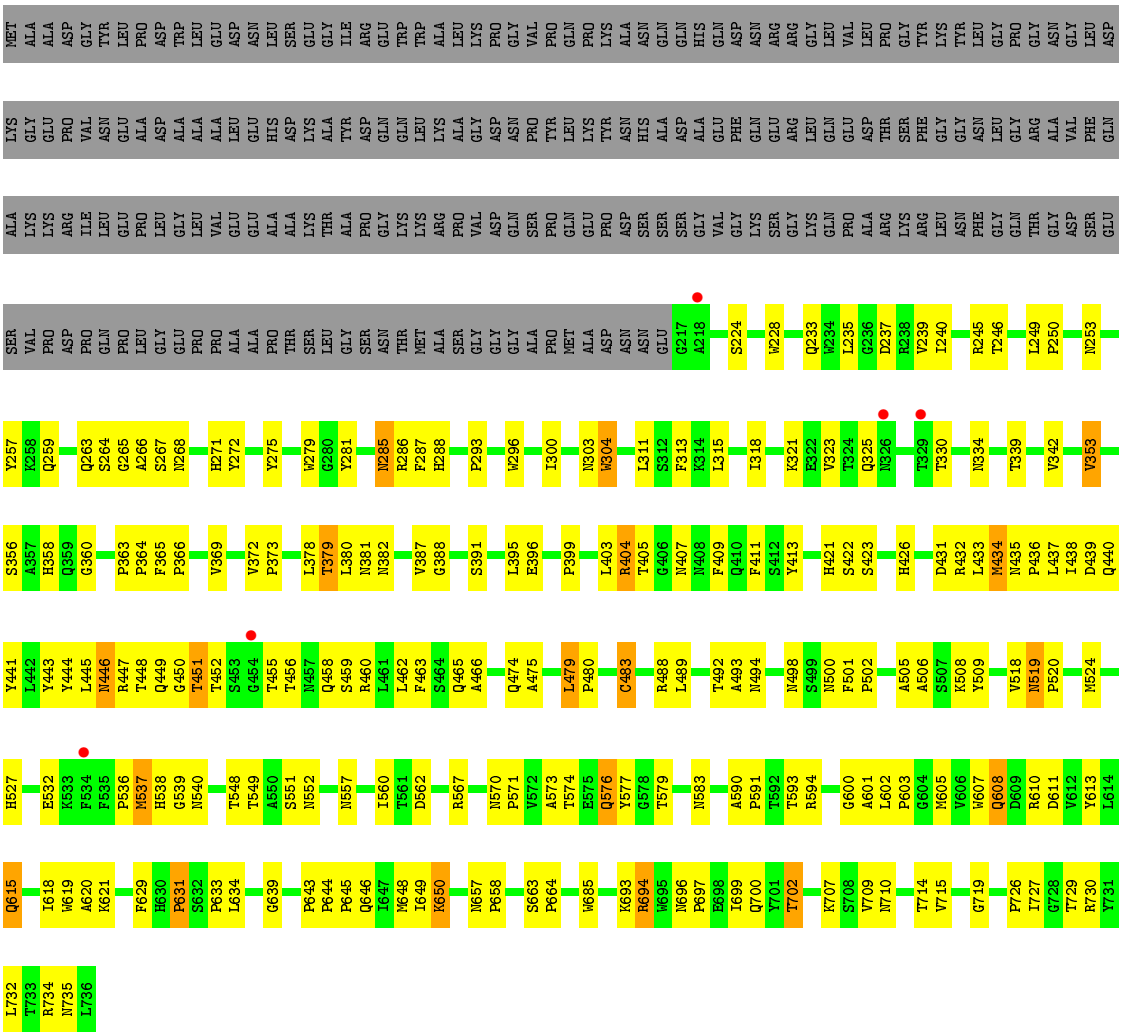
Chain A:



- Molecule 1: Capsid protein VP1

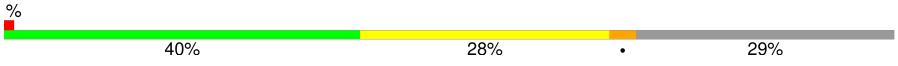
Chain B:

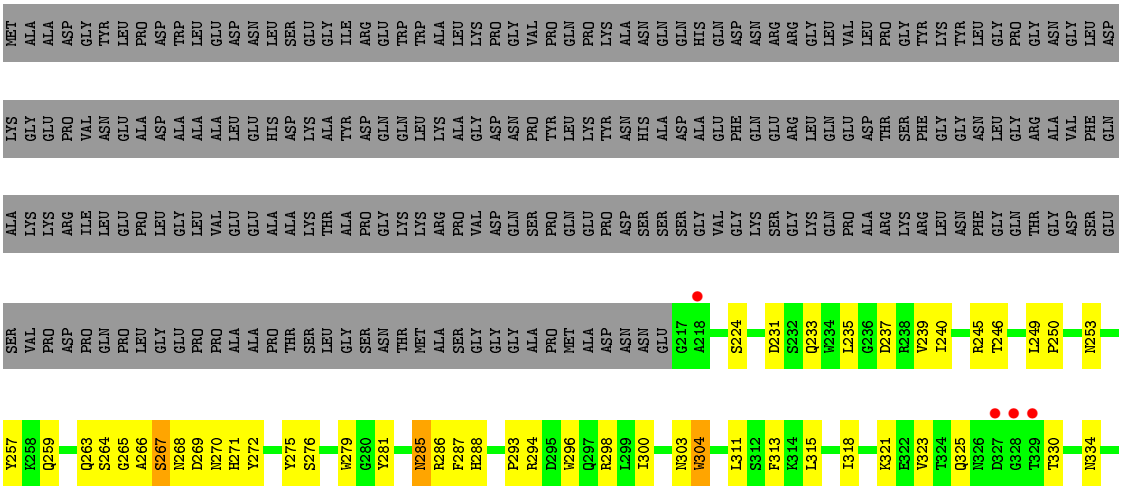


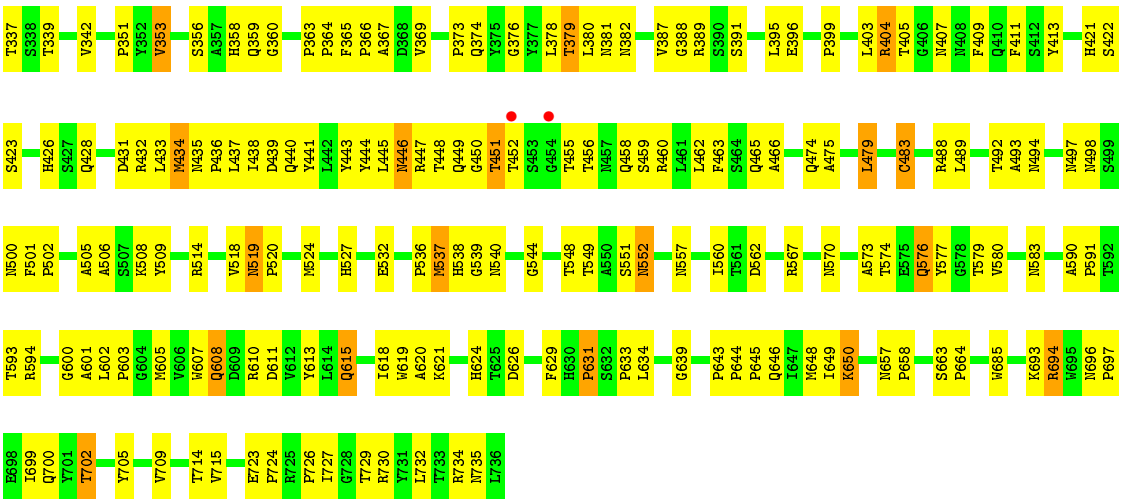


• Molecule 1: Capsid protein VP1

Chain C:

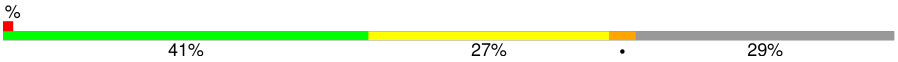


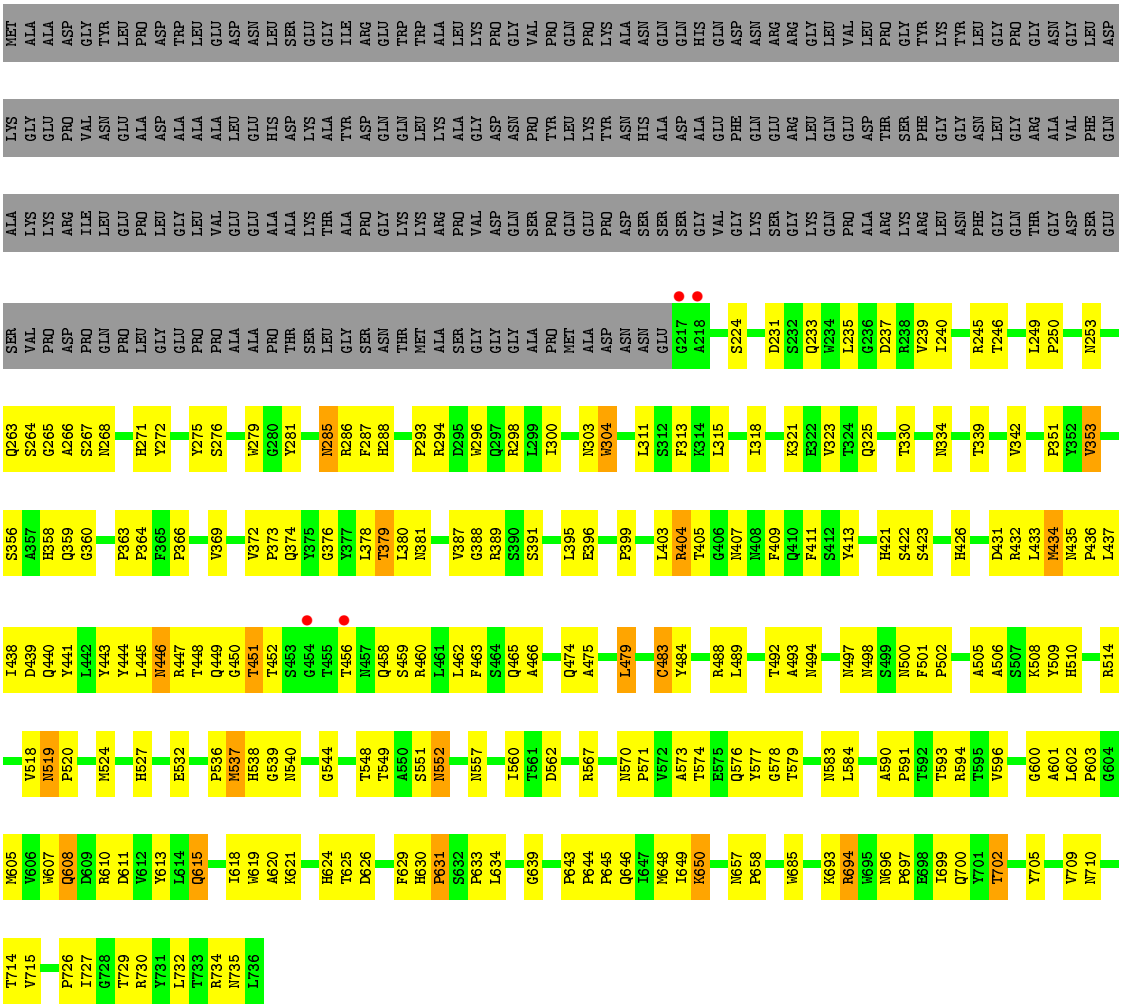




• Molecule 1: Capsid protein VP1

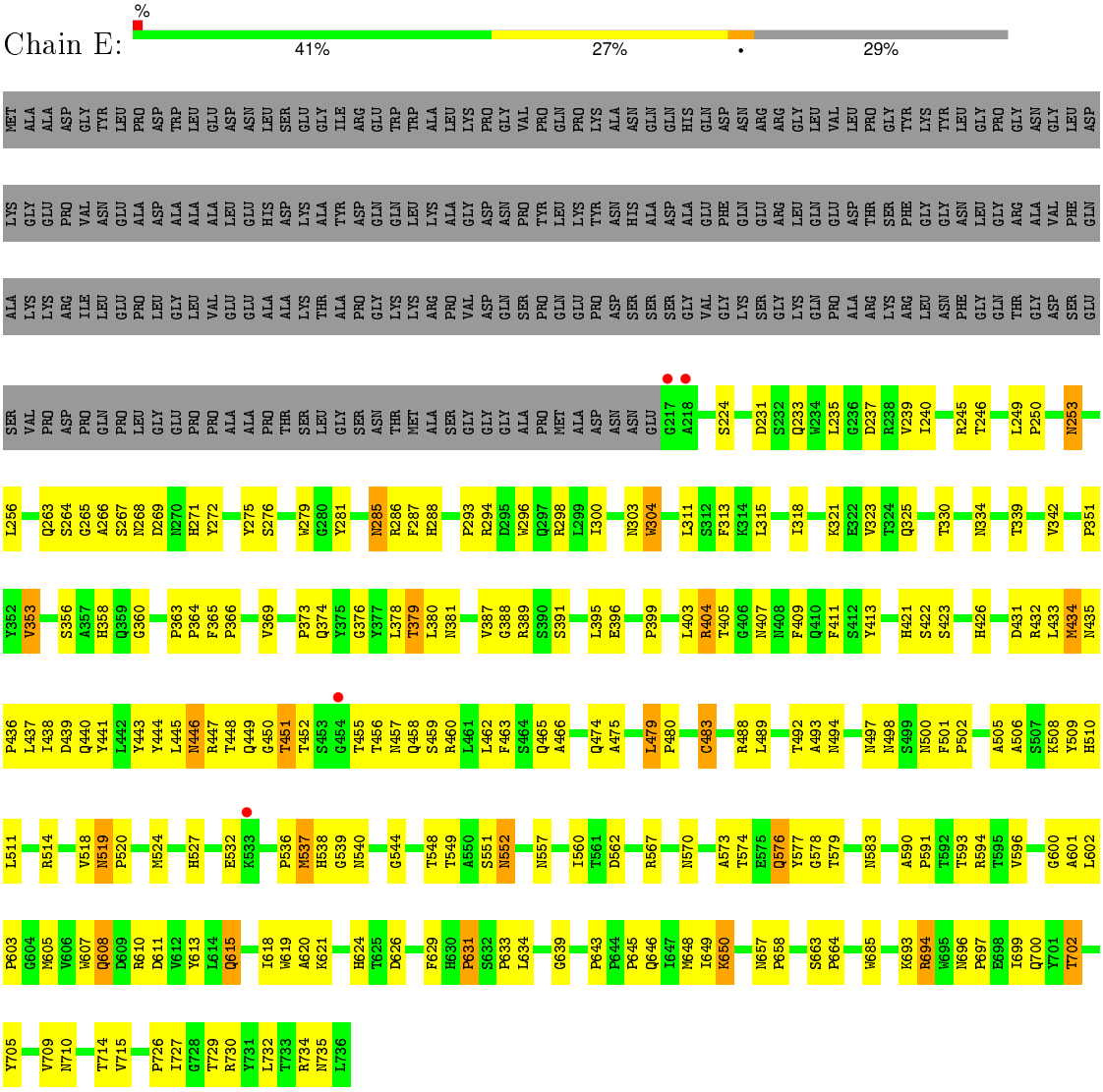
Chain D:





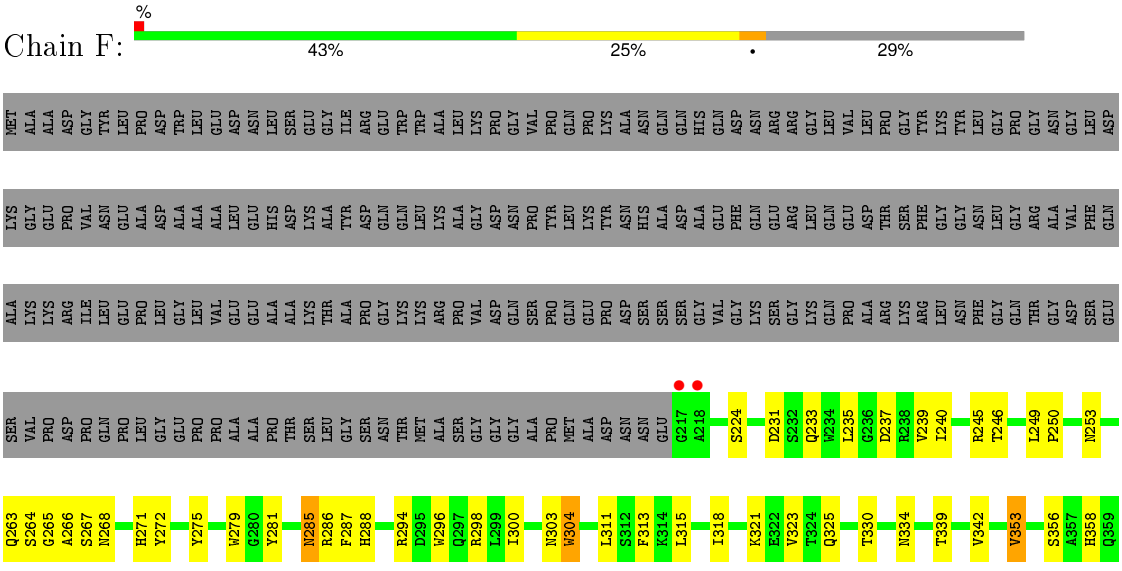
• Molecule 1: Capsid protein VP1

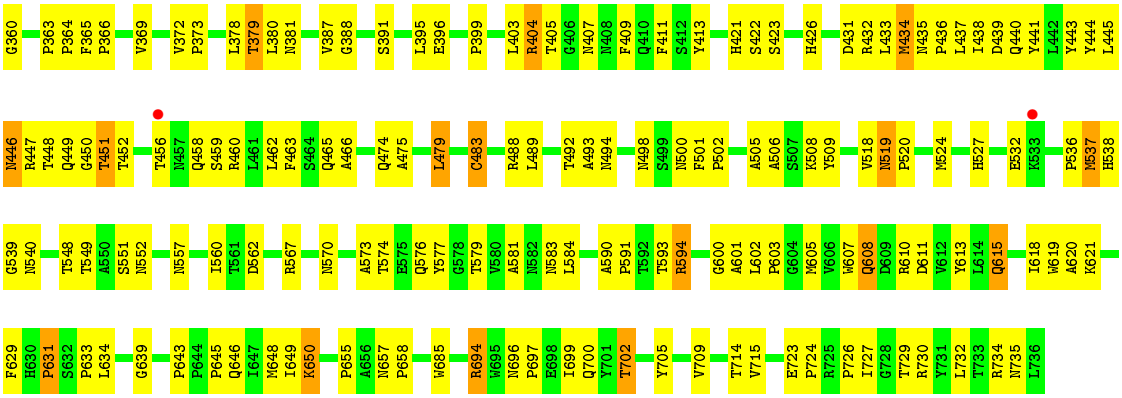
Chain E:



• Molecule 1: Capsid protein VP1

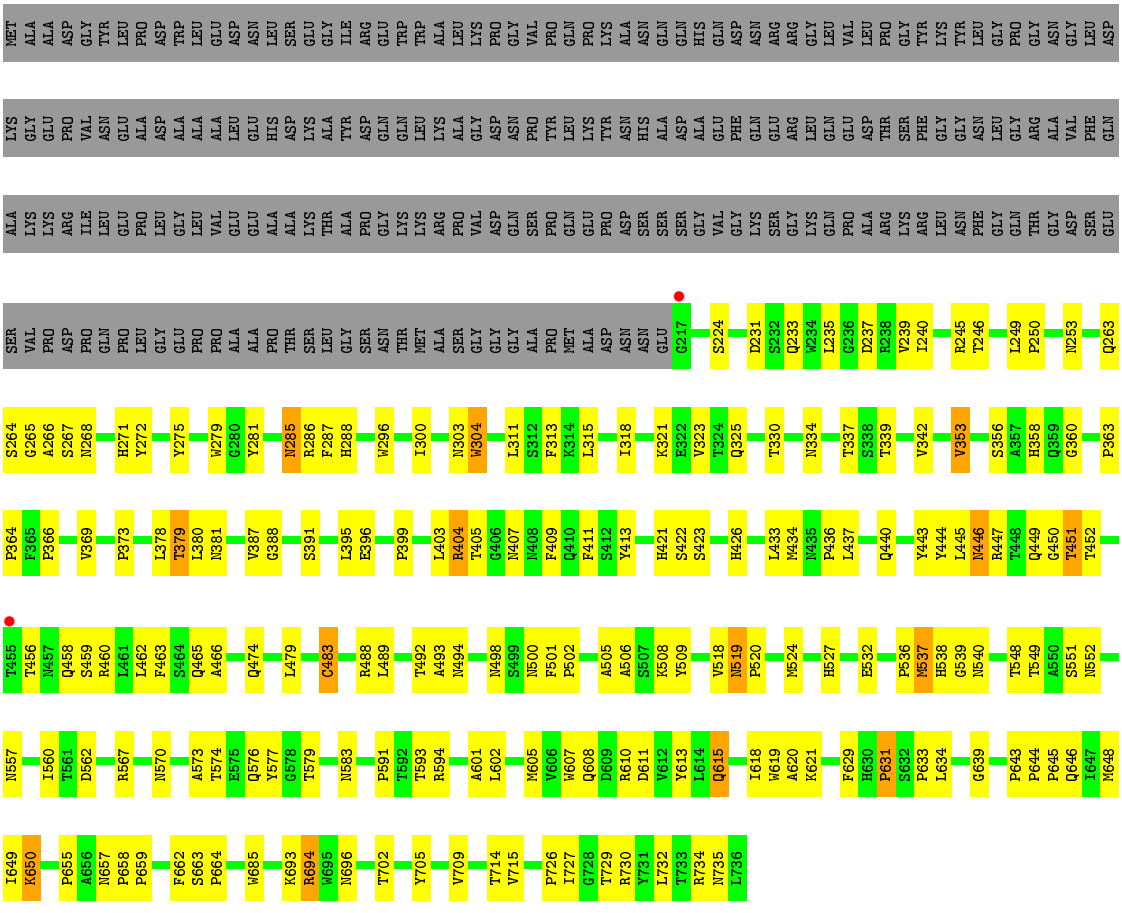
Chain F:





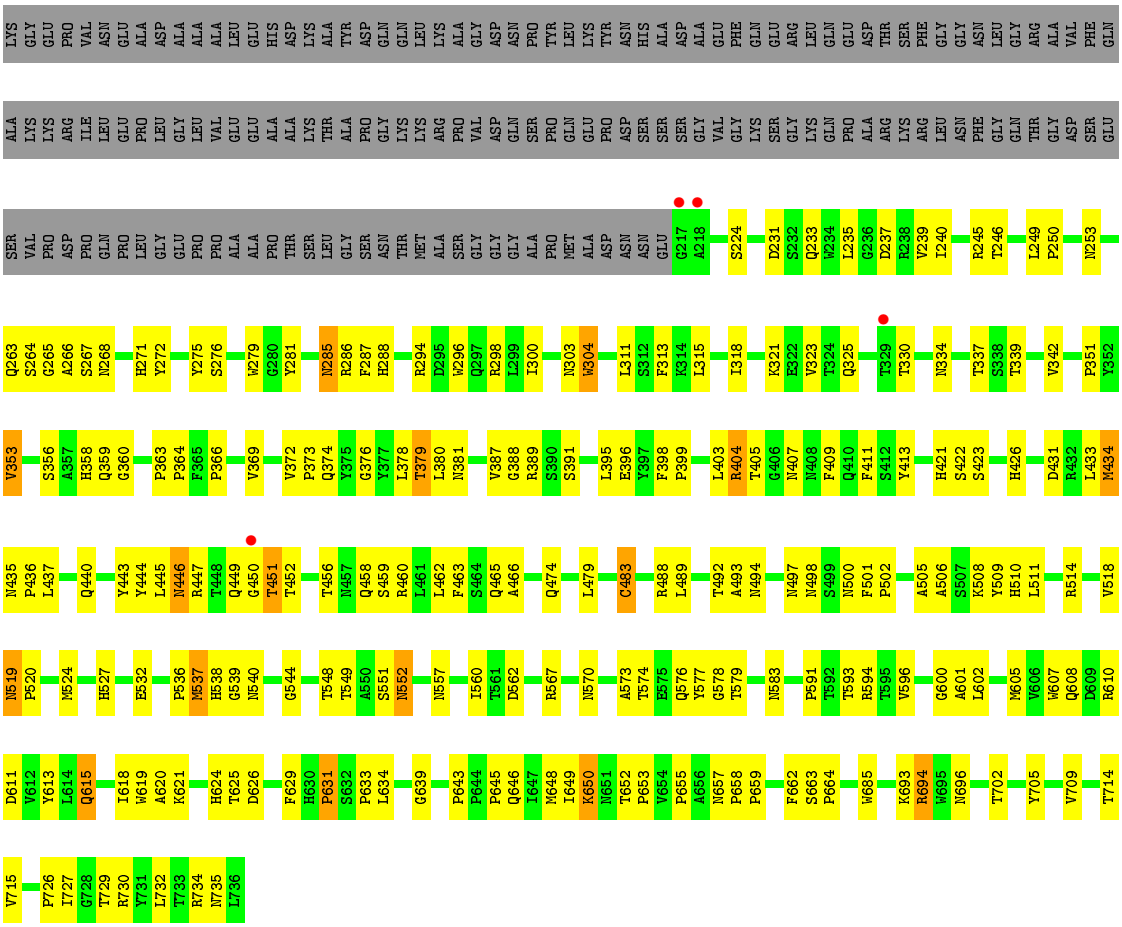
• Molecule 1: Capsid protein VP1

Chain G:



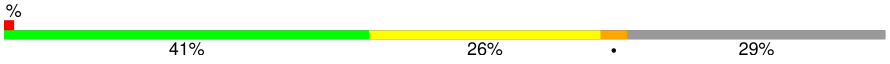
• Molecule 1: Capsid protein VP1

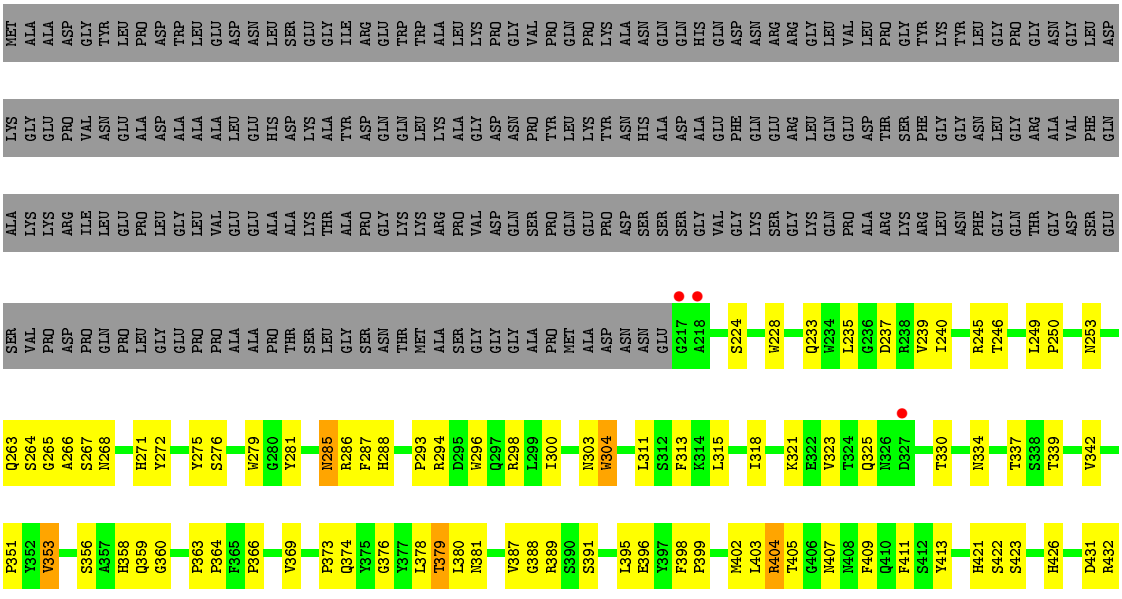
Chain H:

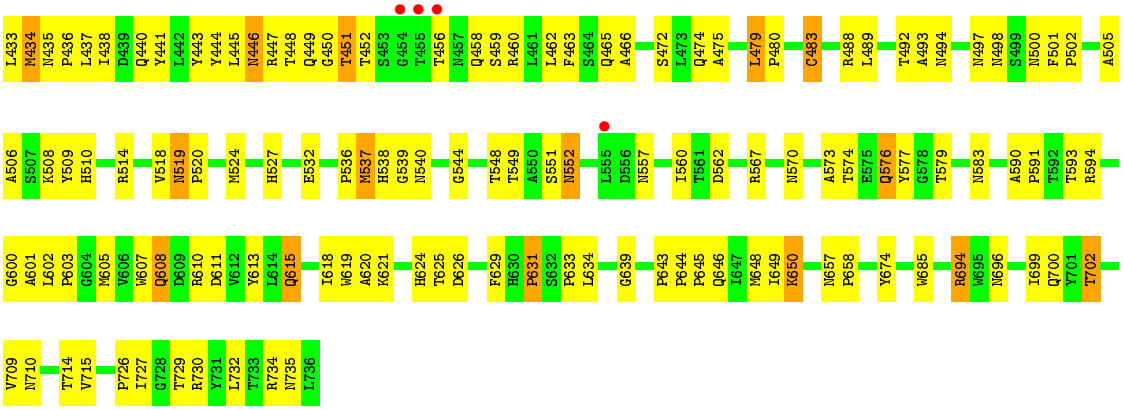


• Molecule 1: Capsid protein VP1

Chain I:

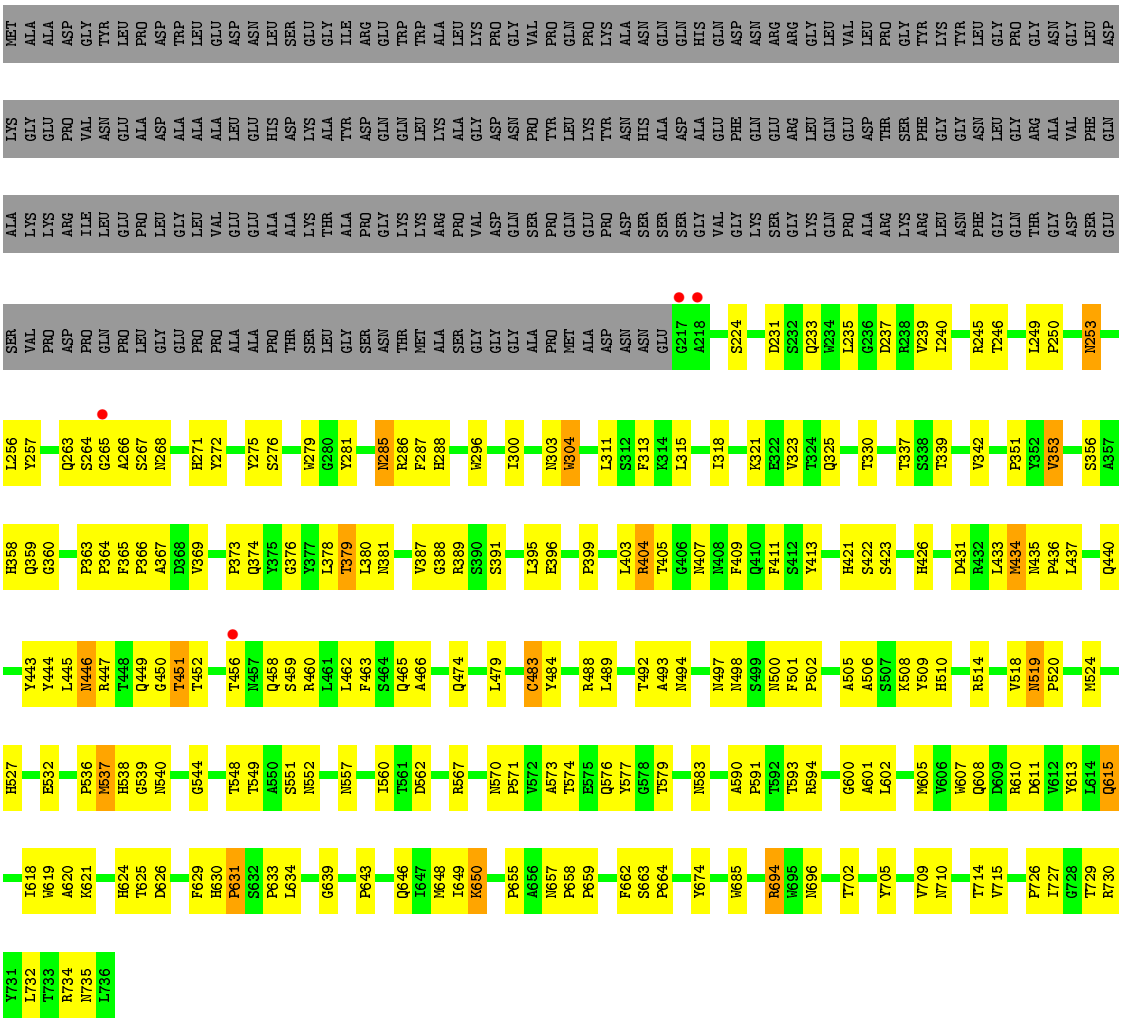






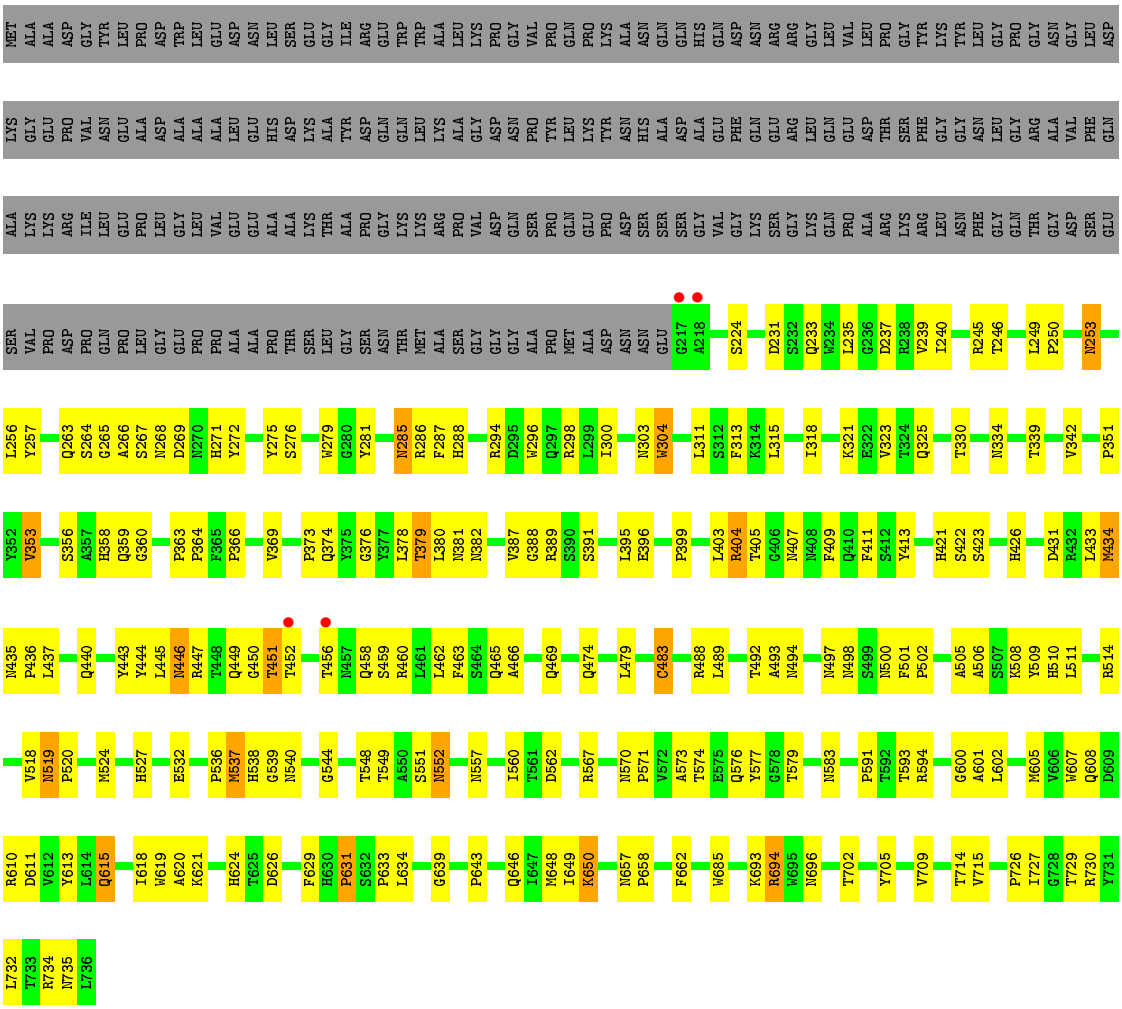
• Molecule 1: Capsid protein VP1

Chain J:



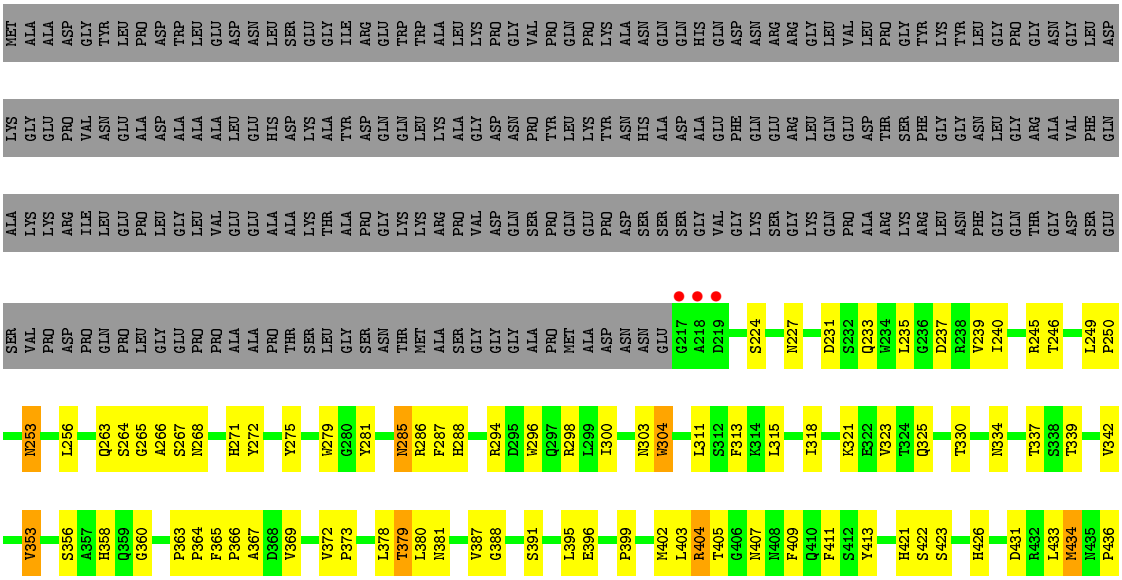
• Molecule 1: Capsid protein VP1

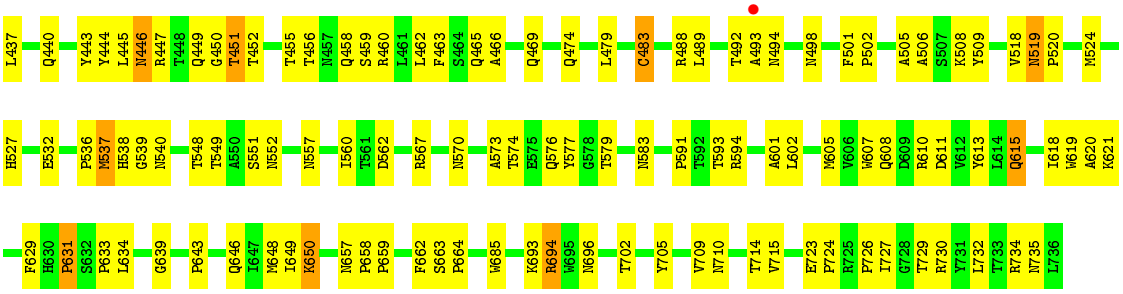
Chain K:



• Molecule 1: Capsid protein VP1

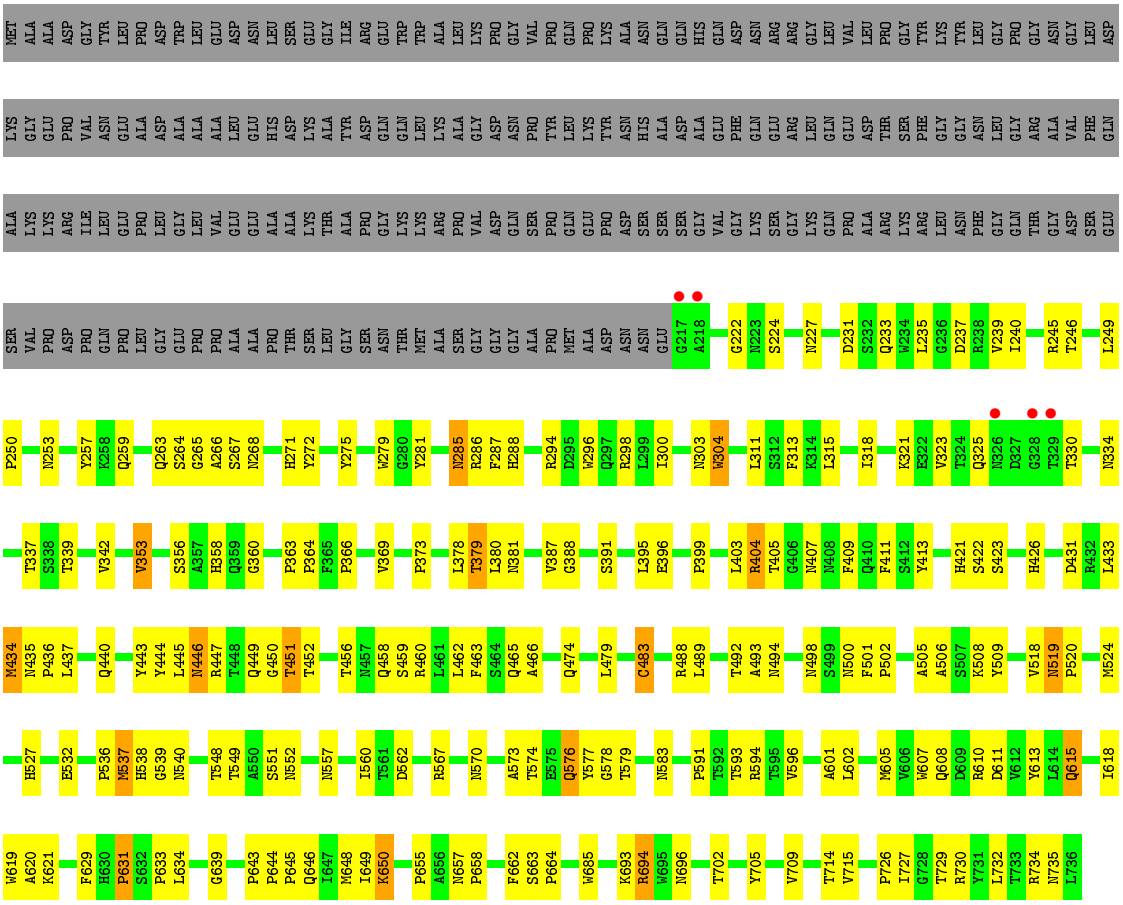
Chain L:





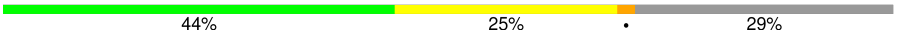
• Molecule 1: Capsid protein VP1

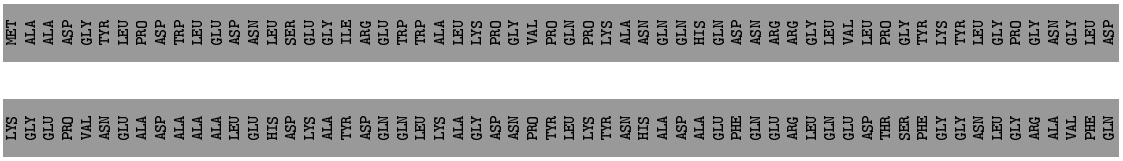
Chain M:

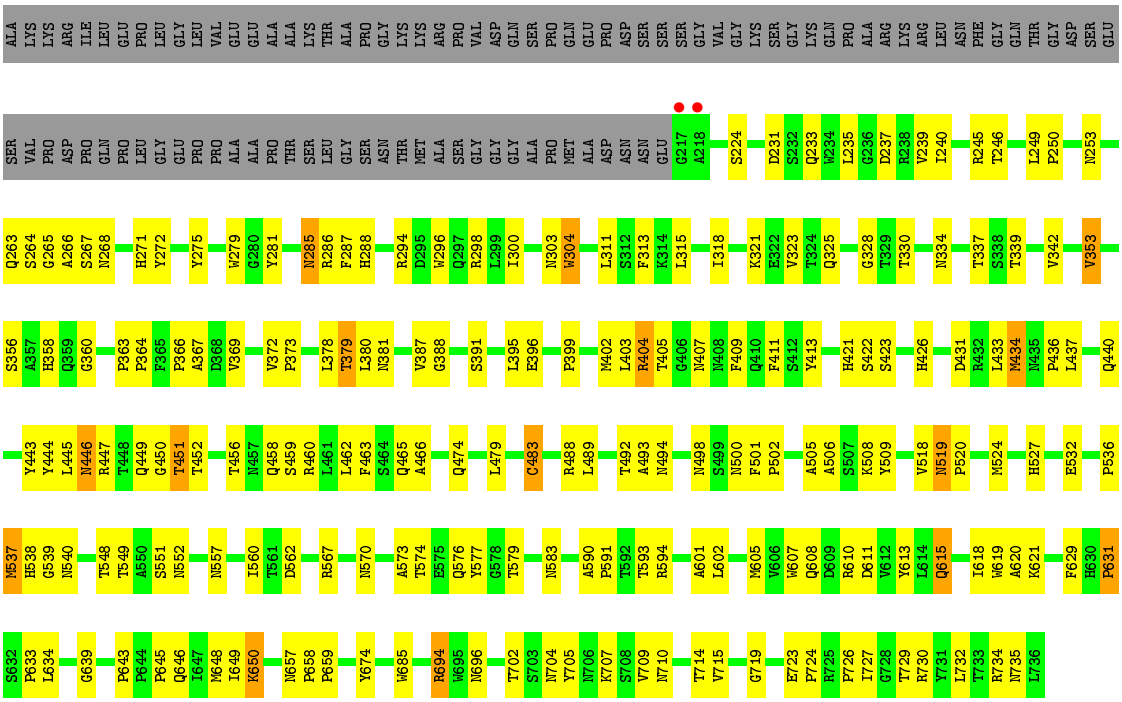


• Molecule 1: Capsid protein VP1

Chain N:

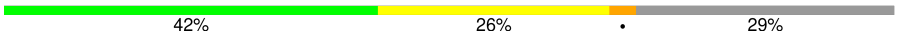


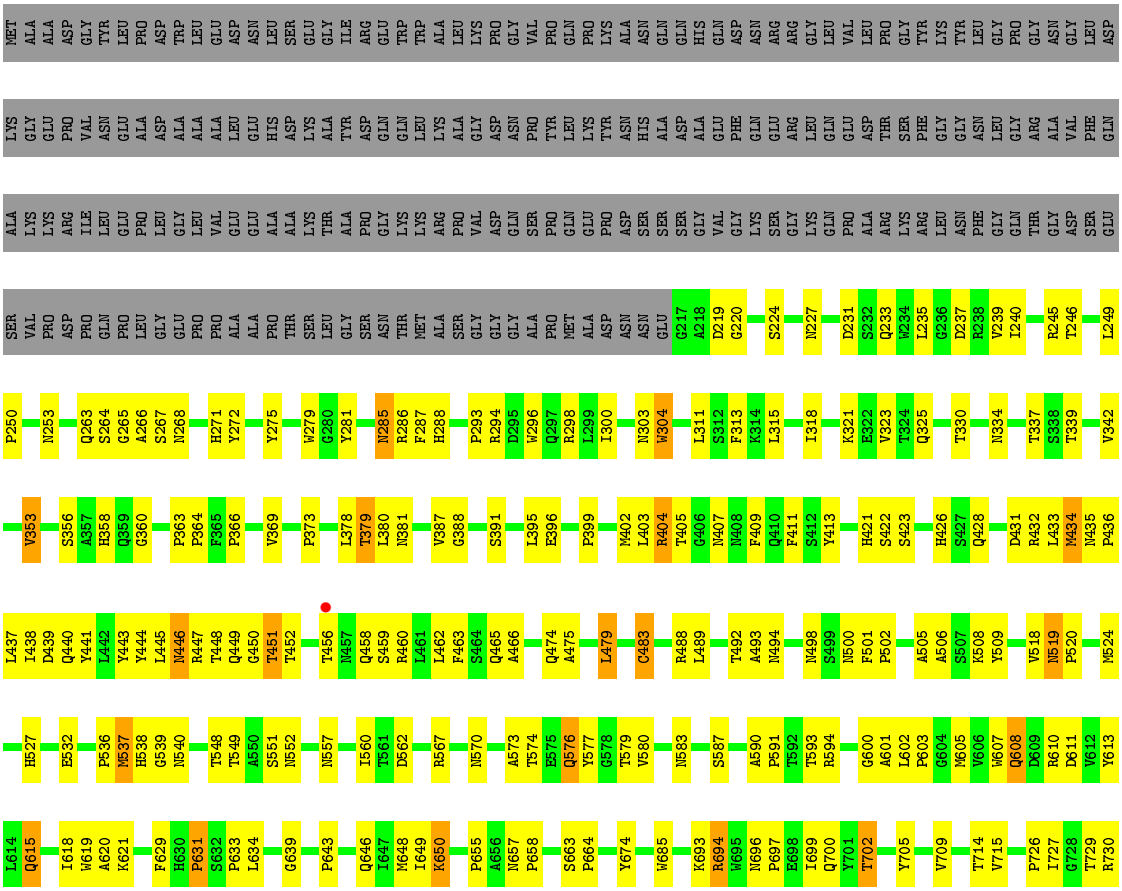




• Molecule 1: Capsid protein VP1

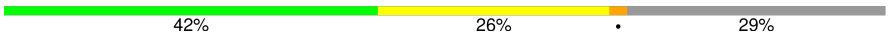
Chain O:

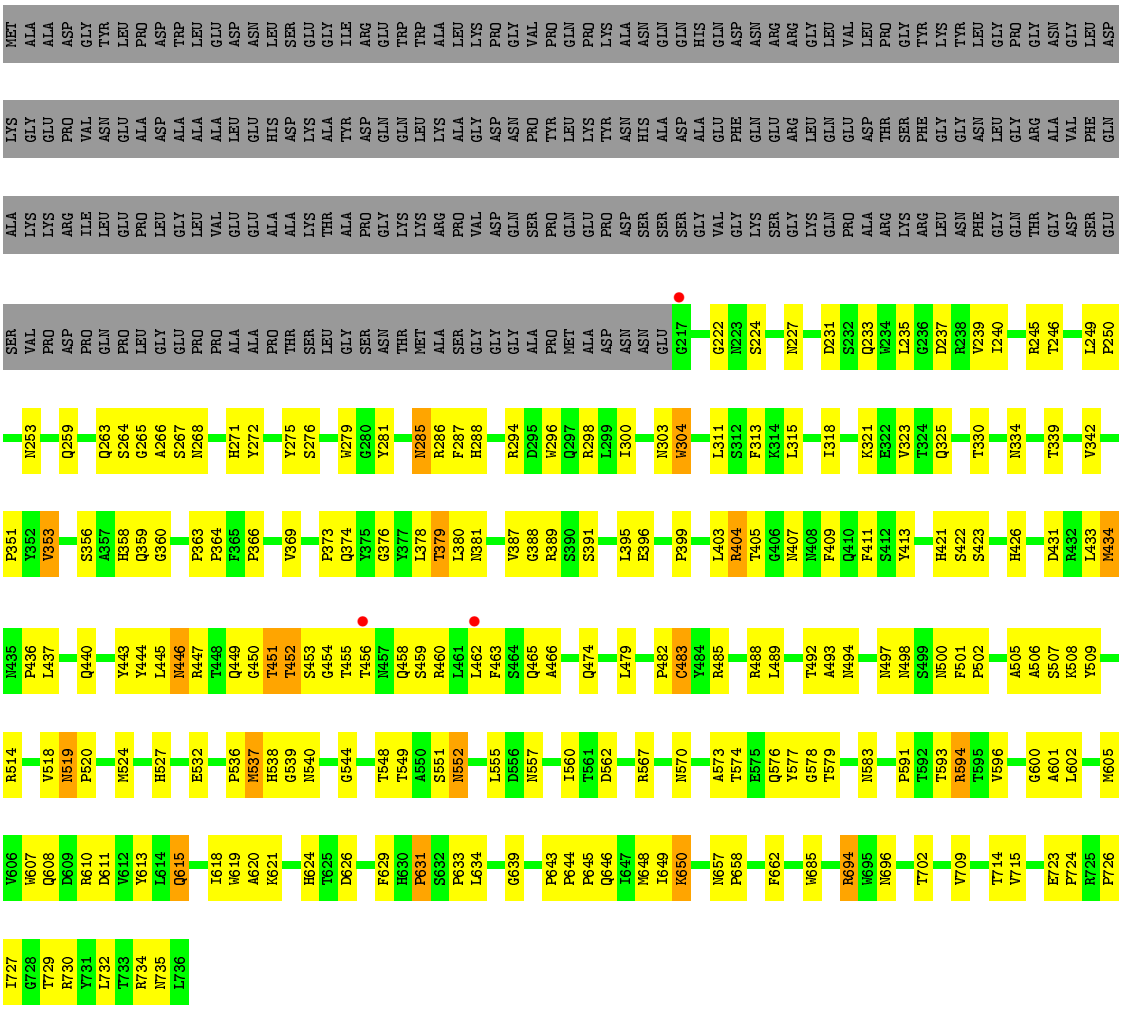




• Molecule 1: Capsid protein VP1

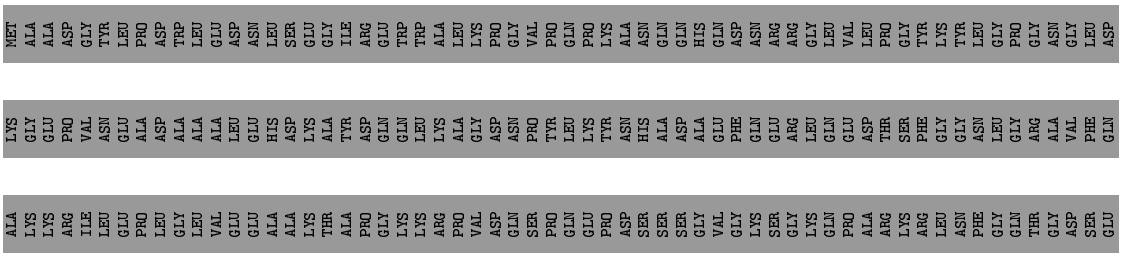
Chain P:

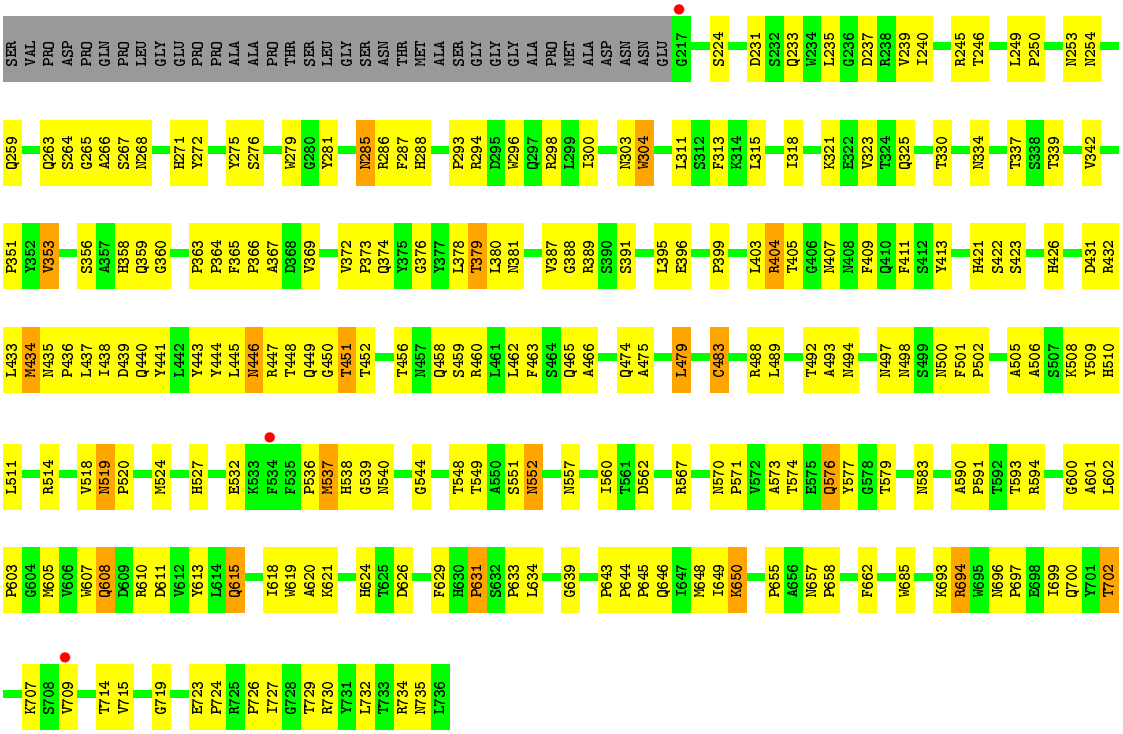




• Molecule 1: Capsid protein VP1

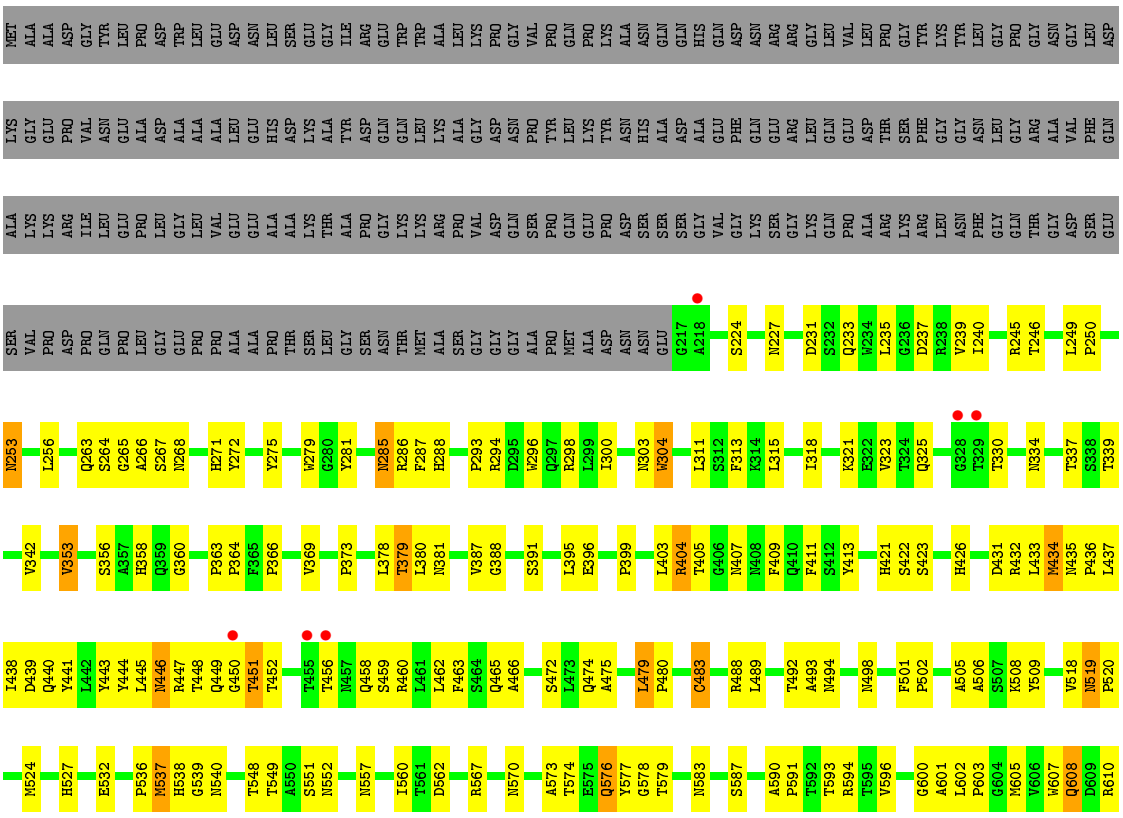
Chain Q:





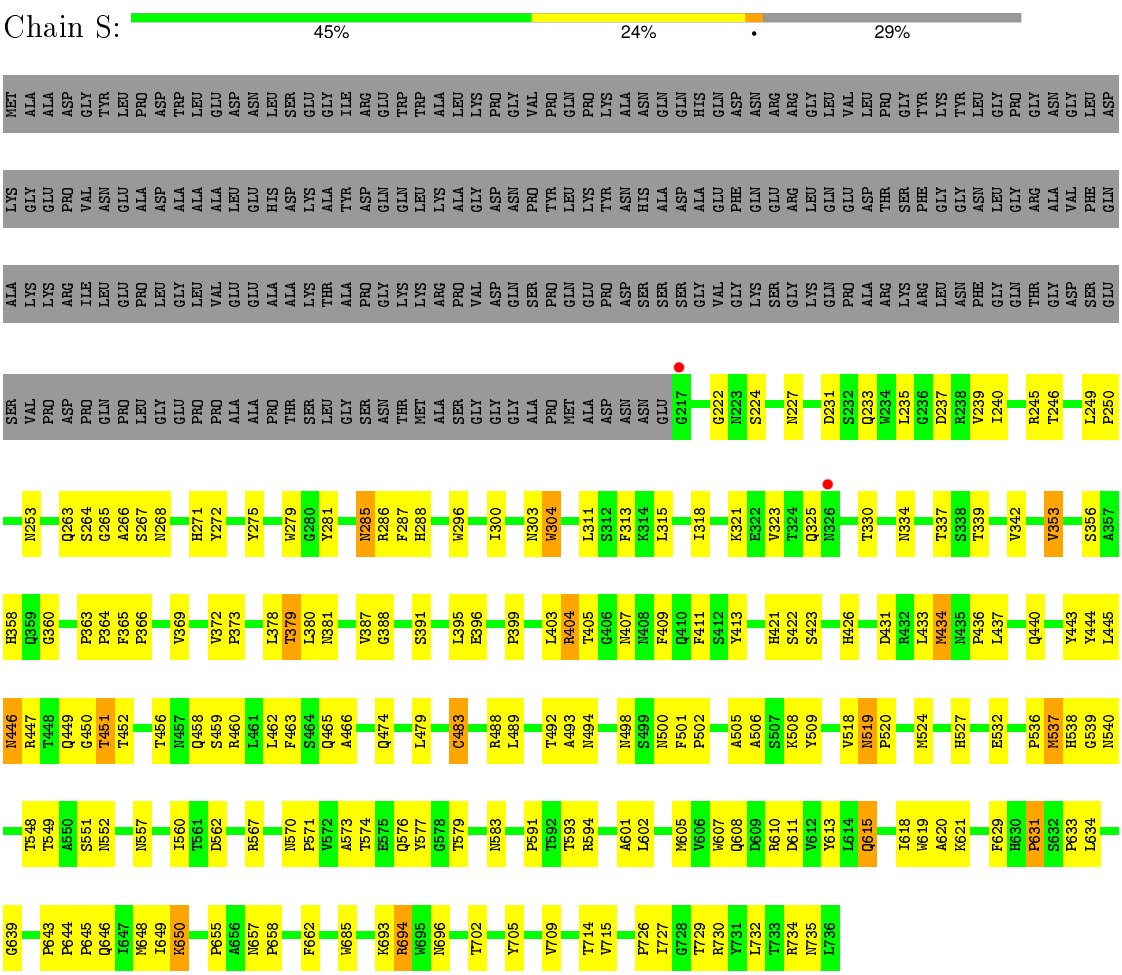
- Molecule 1: Capsid protein VP1

Chain R:



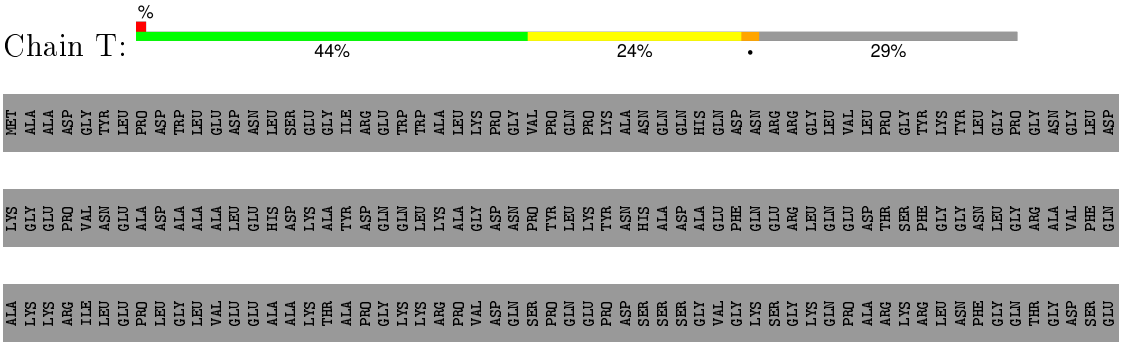
• Molecule 1: Capsid protein VP1

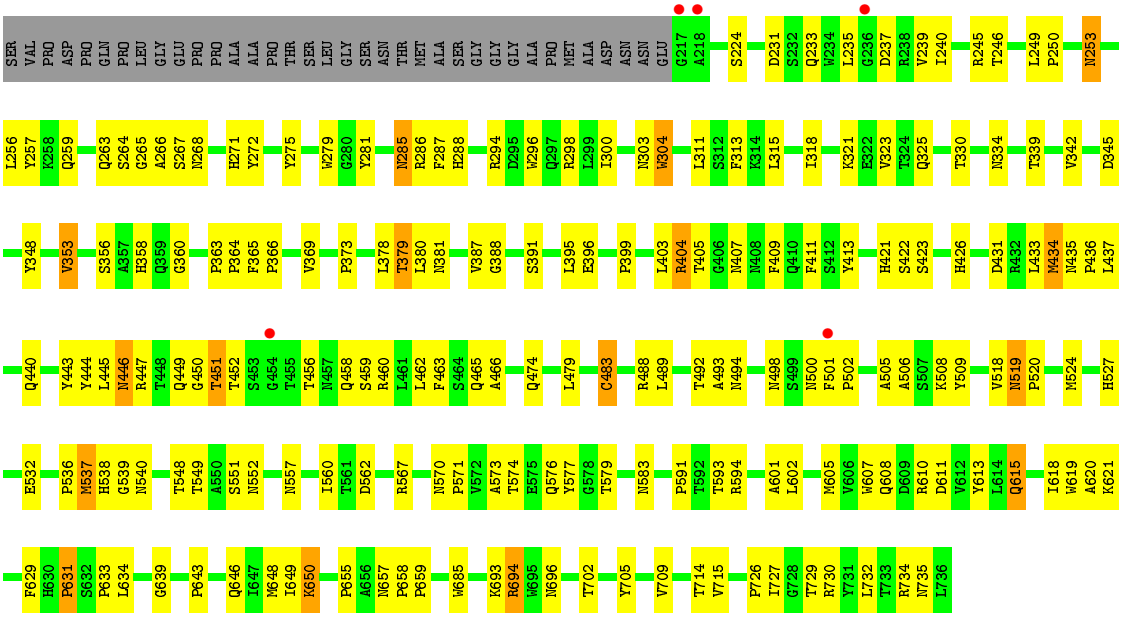
Chain S:



• Molecule 1: Capsid protein VP1

Chain T:




SER VAL PRO ASP PRO GLN PRO LEU GLY GLU PRO PRO ALA ALA PRO THR SER LEU GLY SER ASN THR MET ALA SER GLY GLY GLY ALA PRO MET ALA ASP ASN ASN GLU G217 A218 S224 D231 S232 Q233 W234 L235 G236 D237 R238 V239 I240 R245 T246 L249 P250 N253
L256 Y257 K258 Q259 Q263 S264 G265 A266 S267 N268 H271 Y272 Y275 W279 G280 Y281 N285 R286 F287 H288 R294 D295 W296 Q297 R298 L299 I300 N303 W304 L311 S312 F313 K314 L315 I318 K321 E322 V323 T324 Q325 T330 N334 T339 V342 D345
Y348 V353 S356 A357 H358 Q359 G360 P363 P364 F365 P366 V369 P373 L378 T379 L380 N381 V387 G388 S391 L395 E396 P399 L403 R404 T405 G406 N407 N408 F409 Q410 F411 S412 Y413 H421 S422 S423 H426 D431 R432 L433 M434 N435 P436 L437
Q440 Y443 Y444 L445 N446 R447 T448 Q449 G450 T451 T452 S453 G454 T455 T456 N457 Q458 S459 R460 L461 L462 F463 S464 Q465 A466 Q474 L479 C483 R488 L489 T492 A493 N494 N498 S499 N500 F501 P502 A505 A506 S507 K508 Y509 V518 N519 P520 M524 H527
E532 P536 M537 H538 G539 N540 T548 T549 A550 S551 N552 N557 I560 T561 D562 R567 N570 P571 V572 A573 T574 E575 Q576 Y577 G578 T579 N583 P591 T592 T593 R594 A601 L602 M605 V606 W607 Q608 D609 R610 D611 V612 Y613 L614 Q615 I618 W619 A620 K621
F629 H630 P631 S632 P633 L634 G639 P643 Q646 I647 W648 I649 K650 P655 A656 N657 P658 P659 W685 K693 R694 W695 N696 T702 Y705 V709 T714 V715 P726 I727 G728 T729 R730 Y731 L732 T733 R734 N735 L736

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	257.70Å 257.70Å 603.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.99 – 2.60 48.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	28.1 (14.99-2.60) 28.0 (48.70-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.190 , 0.218 0.190 , 0.215	Depositor DCC
R_{free} test set	3318 reflections (2.67%)	DCC
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.5	EDS
Estimated twinning fraction	0.475 for h,-h-k,-l 0.119 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.125 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.116 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 0.119 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.119 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 0.135 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.429 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.475 for h,-h-k,-l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 128434 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	83520	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

[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.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.66% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D5M

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	0.25	0/4282	0.43	0/5843
1	B	0.25	0/4282	0.43	0/5843
1	C	0.25	0/4282	0.43	0/5843
1	D	0.25	0/4282	0.43	0/5843
1	E	0.25	0/4282	0.43	0/5843
1	F	0.25	0/4282	0.43	0/5843
1	G	0.25	0/4282	0.43	0/5843
1	H	0.25	0/4282	0.43	0/5843
1	I	0.25	0/4282	0.43	0/5843
1	J	0.25	0/4282	0.43	0/5843
1	K	0.25	0/4282	0.43	0/5843
1	L	0.25	0/4282	0.43	0/5843
1	M	0.25	0/4282	0.43	0/5843
1	N	0.25	0/4282	0.43	0/5843
1	O	0.25	0/4282	0.43	0/5843
1	P	0.25	0/4282	0.43	0/5843
1	Q	0.25	0/4282	0.43	0/5843
1	R	0.25	0/4282	0.43	0/5843
1	S	0.25	0/4282	0.43	0/5843
1	T	0.25	0/4282	0.43	0/5843
All	All	0.25	0/85640	0.43	0/116860

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 (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	A	4154	0	3899	243	8
1	B	4154	0	3899	214	4
1	C	4154	0	3899	247	19
1	D	4154	0	3899	244	0
1	E	4154	0	3899	243	4
1	F	4154	0	3899	211	0
1	G	4154	0	3899	163	3
1	H	4154	0	3899	208	0
1	I	4154	0	3899	238	0
1	J	4154	0	3899	212	0
1	K	4154	0	3899	201	1
1	L	4154	0	3899	172	25
1	M	4154	0	3899	173	0
1	N	4154	0	3899	171	7
1	O	4154	0	3899	215	0
1	P	4154	0	3899	208	9
1	Q	4154	0	3899	247	2
1	R	4154	0	3899	209	0
1	S	4154	0	3899	168	0
1	T	4154	0	3899	168	0
2	A	22	0	12	1	0
2	B	22	0	12	2	0
2	C	22	0	12	2	0
2	D	22	0	12	2	0
2	E	22	0	12	2	0
2	F	22	0	12	2	0
2	G	22	0	12	2	0
2	H	22	0	12	2	0
2	I	22	0	12	1	0
2	J	22	0	12	1	0
2	K	22	0	12	2	0
2	L	22	0	12	2	0
2	M	22	0	12	2	0
2	N	22	0	12	2	0
2	O	22	0	12	2	0
2	P	22	0	12	1	0
2	Q	22	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	22	0	12	1	0
2	S	22	0	12	1	0
2	T	22	0	12	2	0
All	All	83520	0	78220	3544	41

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 22.

The worst 5 of 3544 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:C:519:ASN:HB3	1:C:520:PRO:HD3	1.46	0.98
1:S:519:ASN:HB3	1:S:520:PRO:HD3	1.46	0.98
1:P:519:ASN:HB3	1:P:520:PRO:HD3	1.45	0.98
1:G:519:ASN:HB3	1:G:520:PRO:HD3	1.45	0.98
1:F:519:ASN:HB3	1:F:520:PRO:HD3	1.45	0.97

The worst 5 of 41 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:E:456:THR:OG1	1:K:469:GLN:O[3_445]	1.58	0.62
1:C:267:SER:C	1:L:455:THR:CG2[4_445]	1.59	0.61
1:C:267:SER:O	1:L:456:THR:OG1[4_445]	1.62	0.58
1:C:267:SER:CA	1:L:455:THR:O[4_445]	1.65	0.55
1:C:268:ASN:N	1:L:456:THR:N[4_445]	1.66	0.54

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	518/736 (70%)	467 (90%)	44 (8%)	7 (1%)	14	28
1	B	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	C	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	D	518/736 (70%)	467 (90%)	44 (8%)	7 (1%)	14	28
1	E	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	F	518/736 (70%)	465 (90%)	46 (9%)	7 (1%)	14	28
1	G	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	H	518/736 (70%)	467 (90%)	44 (8%)	7 (1%)	14	28
1	I	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	J	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	K	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	L	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	M	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	N	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	O	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	P	518/736 (70%)	466 (90%)	44 (8%)	8 (2%)	13	26
1	Q	518/736 (70%)	465 (90%)	46 (9%)	7 (1%)	14	28
1	R	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	S	518/736 (70%)	466 (90%)	45 (9%)	7 (1%)	14	28
1	T	518/736 (70%)	465 (90%)	46 (9%)	7 (1%)	14	28
All	All	10360/14720 (70%)	9320 (90%)	899 (9%)	141 (1%)	14	28

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	SER
1	B	264	SER
1	C	264	SER
1	D	264	SER
1	E	264	SER

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	A	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	B	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	C	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	D	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	E	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	F	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	G	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	H	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	I	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	J	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	K	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	L	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	M	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	N	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	O	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	P	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	Q	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	R	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	S	459/627 (73%)	435 (95%)	24 (5%)	29	54
1	T	459/627 (73%)	435 (95%)	24 (5%)	29	54
All	All	9180/12540 (73%)	8700 (95%)	480 (5%)	29	54

5 of 480 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	253	ASN
1	L	304	TRP
1	S	451	THR
1	J	404	ARG
1	K	285	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 481 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	540	ASN
1	K	608	GLN
1	S	374	GLN
1	I	710	ASN
1	J	608	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	D5M	A	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	B	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	C	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	D	999	-	20,24,24	0.98	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	E	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	F	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	G	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	H	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	D5M	I	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.91	3 (13%)
2	D5M	J	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.91	3 (13%)
2	D5M	K	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	L	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	M	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	N	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	O	999	-	20,24,24	0.96	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	P	999	-	20,24,24	0.97	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	Q	999	-	20,24,24	0.96	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	R	999	-	20,24,24	0.96	1 (5%)	23,36,36	1.92	3 (13%)
2	D5M	S	999	-	20,24,24	0.96	1 (5%)	23,36,36	1.93	3 (13%)
2	D5M	T	999	-	20,24,24	0.96	1 (5%)	23,36,36	1.92	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D5M	A	999	-	-	0/6/22/22	0/3/3/3
2	D5M	B	999	-	-	0/6/22/22	0/3/3/3
2	D5M	C	999	-	-	0/6/22/22	0/3/3/3
2	D5M	D	999	-	-	0/6/22/22	0/3/3/3
2	D5M	E	999	-	-	0/6/22/22	0/3/3/3
2	D5M	F	999	-	-	0/6/22/22	0/3/3/3
2	D5M	G	999	-	-	0/6/22/22	0/3/3/3
2	D5M	H	999	-	-	0/6/22/22	0/3/3/3
2	D5M	I	999	-	-	0/6/22/22	0/3/3/3
2	D5M	J	999	-	-	0/6/22/22	0/3/3/3
2	D5M	K	999	-	-	0/6/22/22	0/3/3/3
2	D5M	L	999	-	-	0/6/22/22	0/3/3/3
2	D5M	M	999	-	-	0/6/22/22	0/3/3/3
2	D5M	N	999	-	-	0/6/22/22	0/3/3/3
2	D5M	O	999	-	-	0/6/22/22	0/3/3/3
2	D5M	P	999	-	-	0/6/22/22	0/3/3/3
2	D5M	Q	999	-	-	0/6/22/22	0/3/3/3
2	D5M	R	999	-	-	0/6/22/22	0/3/3/3
2	D5M	S	999	-	-	0/6/22/22	0/3/3/3
2	D5M	T	999	-	-	0/6/22/22	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	999	D5M	C5-C4	3.22	1.47	1.40
2	P	999	D5M	C5-C4	3.22	1.47	1.40
2	Q	999	D5M	C5-C4	3.23	1.47	1.40
2	B	999	D5M	C5-C4	3.24	1.47	1.40
2	M	999	D5M	C5-C4	3.25	1.47	1.40

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	999	D5M	N3-C2-N1	-6.98	123.55	128.89
2	A	999	D5M	N3-C2-N1	-6.97	123.55	128.89
2	O	999	D5M	N3-C2-N1	-6.97	123.55	128.89
2	N	999	D5M	N3-C2-N1	-6.97	123.56	128.89
2	L	999	D5M	N3-C2-N1	-6.97	123.56	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	D5M	1	0
2	B	999	D5M	2	0
2	C	999	D5M	2	0
2	D	999	D5M	2	0
2	E	999	D5M	2	0
2	F	999	D5M	2	0
2	G	999	D5M	2	0
2	H	999	D5M	2	0
2	I	999	D5M	1	0
2	J	999	D5M	1	0
2	K	999	D5M	2	0
2	L	999	D5M	2	0
2	M	999	D5M	2	0
2	N	999	D5M	2	0
2	O	999	D5M	2	0
2	P	999	D5M	1	0
2	Q	999	D5M	1	0
2	R	999	D5M	1	0
2	S	999	D5M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	999	D5M	2	0

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	520/736 (70%)	-0.04	3 (0%)	90	88	65, 88, 125, 152	0
1	B	520/736 (70%)	-0.06	5 (0%)	84	81	65, 88, 125, 152	0
1	C	520/736 (70%)	-0.07	6 (1%)	81	77	65, 88, 125, 152	0
1	D	520/736 (70%)	-0.04	4 (0%)	87	85	65, 88, 125, 152	0
1	E	520/736 (70%)	-0.02	4 (0%)	87	85	65, 88, 125, 152	0
1	F	520/736 (70%)	-0.01	4 (0%)	87	85	65, 88, 125, 152	0
1	G	520/736 (70%)	0.03	2 (0%)	93	91	65, 88, 125, 152	0
1	H	520/736 (70%)	-0.02	4 (0%)	87	85	65, 88, 125, 152	0
1	I	520/736 (70%)	-0.00	7 (1%)	79	75	65, 88, 125, 152	0
1	J	520/736 (70%)	-0.10	4 (0%)	87	85	65, 88, 125, 152	0
1	K	520/736 (70%)	0.02	4 (0%)	87	85	65, 88, 125, 152	0
1	L	520/736 (70%)	-0.07	4 (0%)	87	85	65, 88, 125, 152	0
1	M	520/736 (70%)	-0.09	5 (0%)	84	81	65, 88, 125, 152	0
1	N	520/736 (70%)	-0.10	2 (0%)	93	91	65, 88, 125, 152	0
1	O	520/736 (70%)	-0.07	1 (0%)	95	95	65, 88, 125, 152	0
1	P	520/736 (70%)	-0.04	3 (0%)	90	88	65, 88, 125, 152	0
1	Q	520/736 (70%)	0.01	3 (0%)	90	88	65, 88, 125, 152	0
1	R	520/736 (70%)	-0.02	6 (1%)	81	77	65, 88, 125, 152	0
1	S	520/736 (70%)	-0.04	2 (0%)	93	91	65, 88, 125, 152	0
1	T	520/736 (70%)	-0.04	5 (0%)	84	81	65, 88, 125, 152	0
All	All	10400/14720 (70%)	-0.04	78 (0%)	87	85	65, 88, 125, 152	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	GLY	5.1
1	N	217	GLY	5.0
1	Q	217	GLY	4.8
1	R	218	ALA	4.6
1	I	217	GLY	4.5

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	D5M	E	999	22/22	0.87	0.30	4.92	81,81,81,81	22
2	D5M	T	999	22/22	0.92	0.30	4.05	81,81,81,81	22
2	D5M	M	999	22/22	0.93	0.31	3.96	81,81,81,81	22
2	D5M	N	999	22/22	0.90	0.28	3.94	81,81,81,81	22
2	D5M	L	999	22/22	0.94	0.27	3.61	81,81,81,81	22
2	D5M	D	999	22/22	0.91	0.23	3.45	81,81,81,81	22
2	D5M	I	999	22/22	0.93	0.23	3.34	81,81,81,81	22
2	D5M	B	999	22/22	0.93	0.25	3.30	81,81,81,81	22
2	D5M	O	999	22/22	0.94	0.26	3.20	81,81,81,81	22
2	D5M	R	999	22/22	0.93	0.25	3.09	81,81,81,81	22
2	D5M	A	999	22/22	0.94	0.23	2.51	81,81,81,81	22
2	D5M	F	999	22/22	0.93	0.26	2.44	81,81,81,81	22
2	D5M	S	999	22/22	0.93	0.22	2.40	81,81,81,81	22
2	D5M	G	999	22/22	0.93	0.23	2.19	81,81,81,81	22
2	D5M	H	999	22/22	0.93	0.24	2.18	81,81,81,81	22
2	D5M	C	999	22/22	0.94	0.22	1.92	81,81,81,81	22
2	D5M	Q	999	22/22	0.94	0.22	1.77	81,81,81,81	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	D5M	J	999	22/22	0.94	0.19	1.26	81,81,81,81	22
2	D5M	P	999	22/22	0.92	0.19	0.95	81,81,81,81	22
2	D5M	K	999	22/22	0.92	0.19	0.83	81,81,81,81	22

6.5 Other polymers (i)

There are no such residues in this entry.