



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:46 PM BST

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 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/ValidationPDFNotes.html>

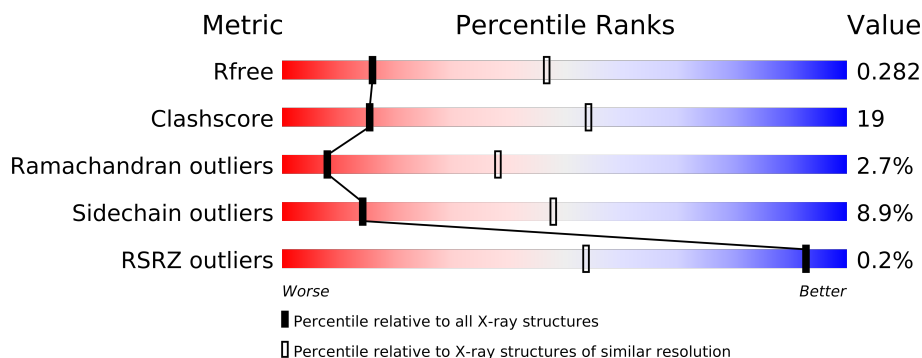
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	520	
1	1	520	
1	2	520	
1	3	520	
1	4	520	
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	





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

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Mol	Chain	Length	Quality of chain
1	w	520	
1	x	520	
1	y	520	
1	z	520	

2 Entry composition

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

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

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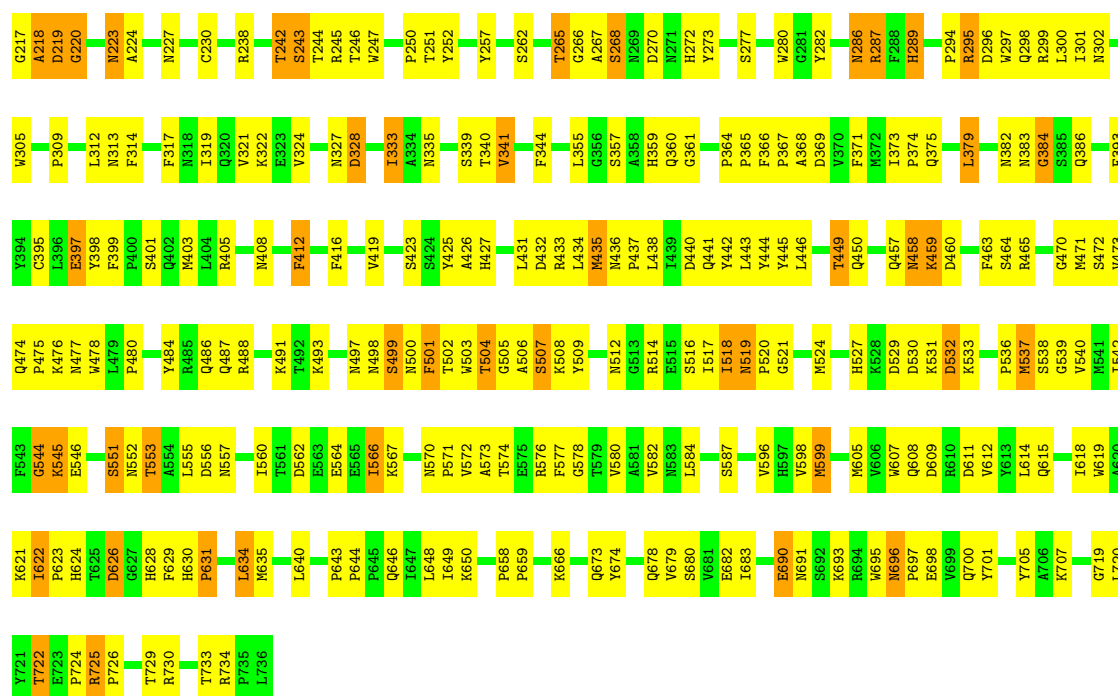
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			
1	7	520	Total	C	N	O	S	0	0	0
			4121	2607	712	786	16			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

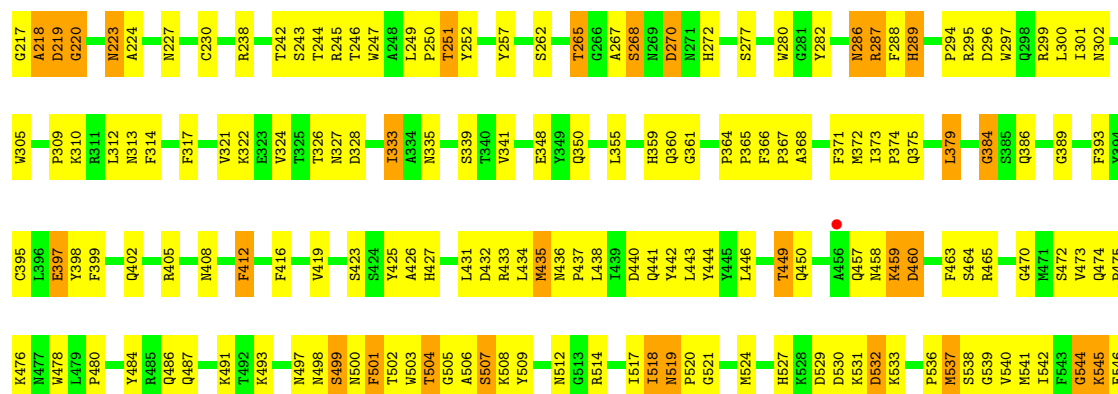
• Molecule 1: Capsid protein VP1

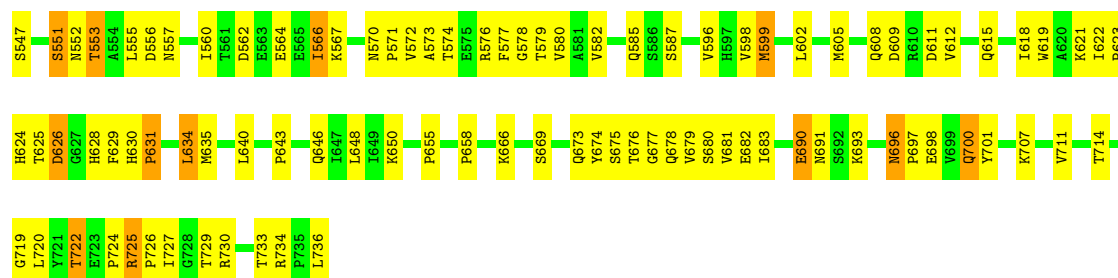
Chain A:



• Molecule 1: Capsid protein VP1

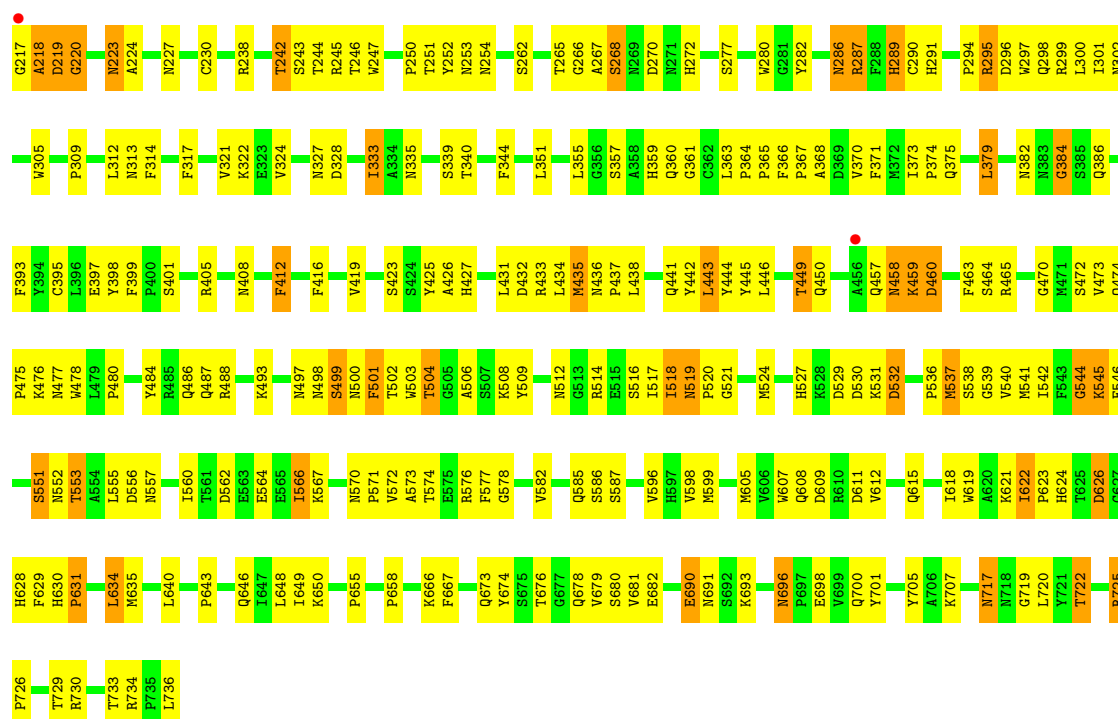
Chain B:





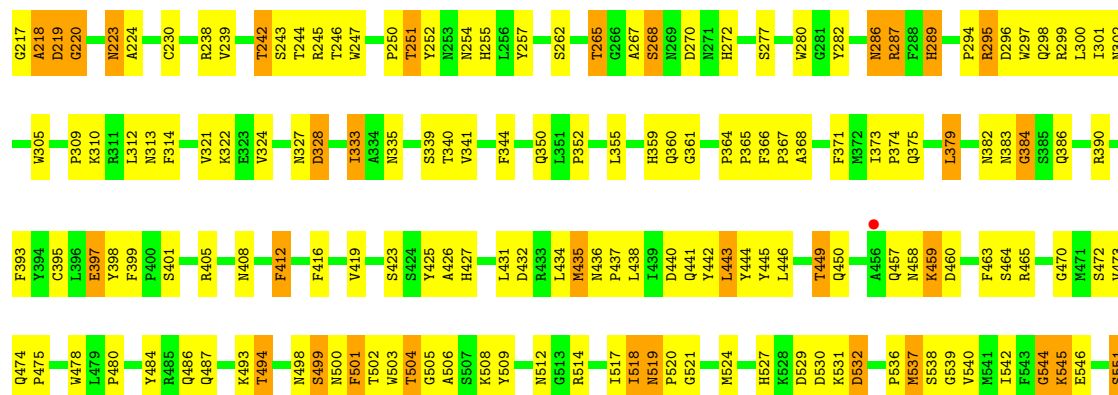
• Molecule 1: Capsid protein VP1

Chain C:



• Molecule 1: Capsid protein VP1

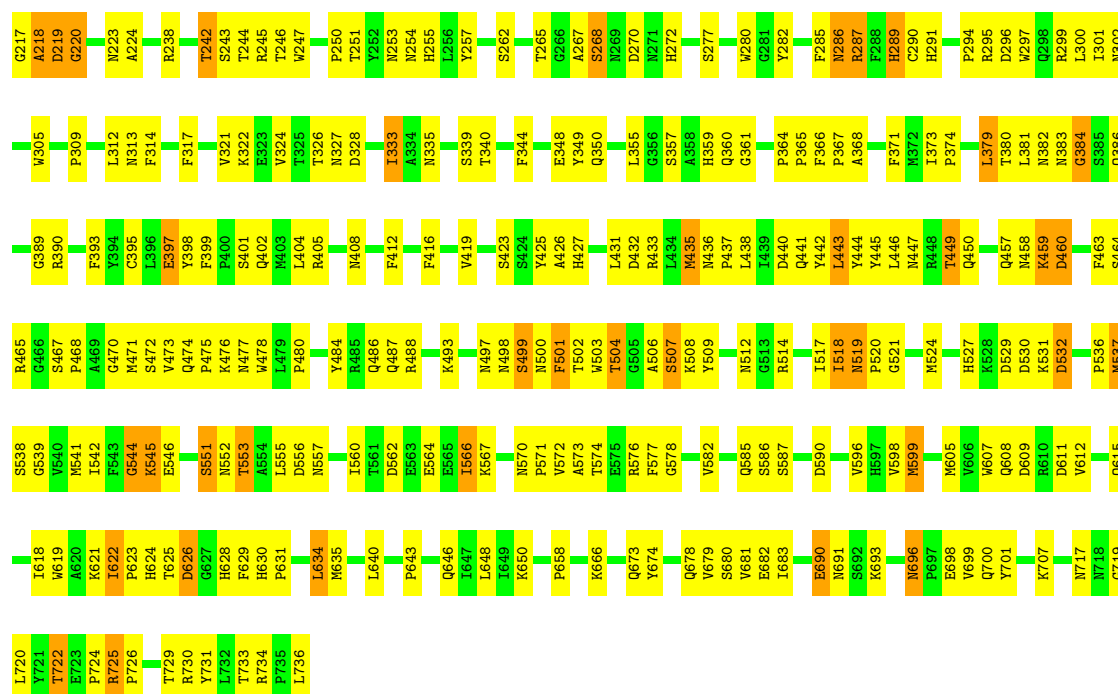
Chain D:





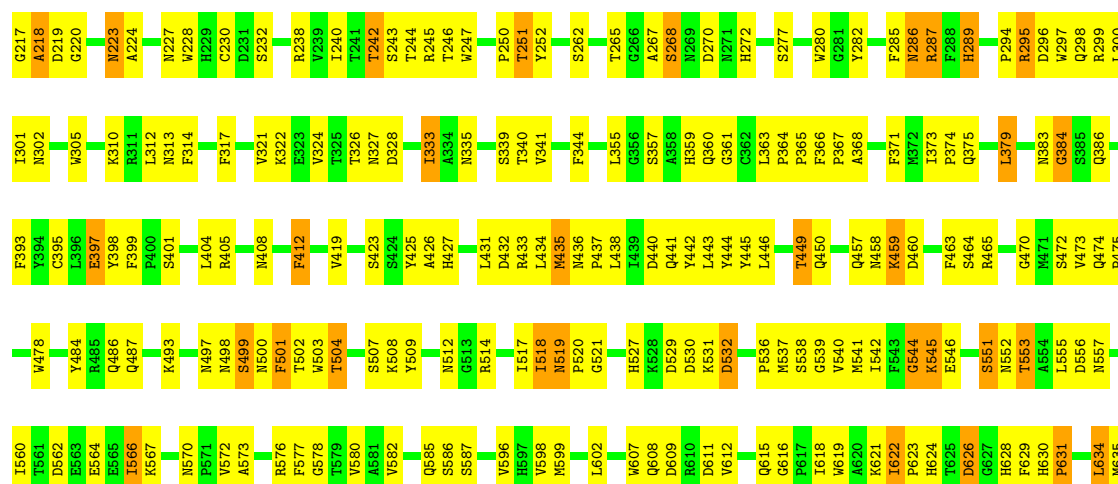
• Molecule 1: Capsid protein VP1

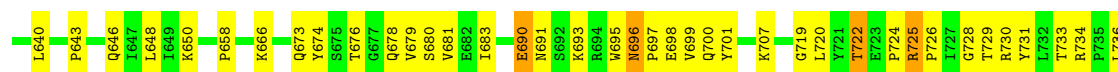
Chain E:



• Molecule 1: Capsid protein VP1

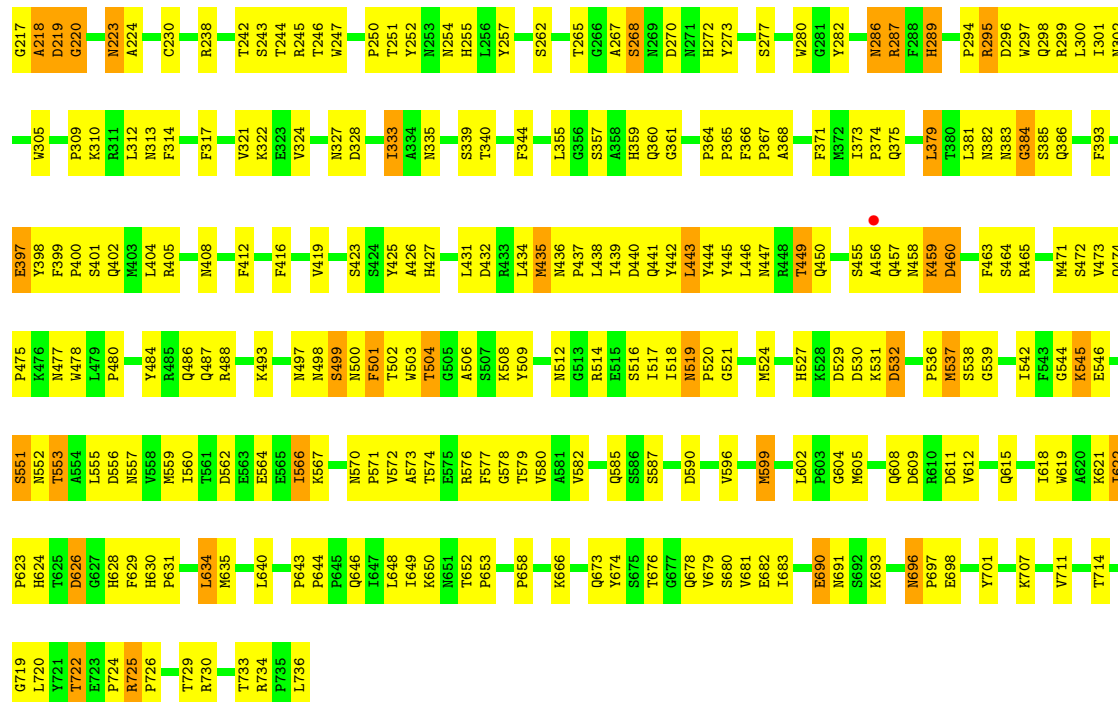
Chain F:





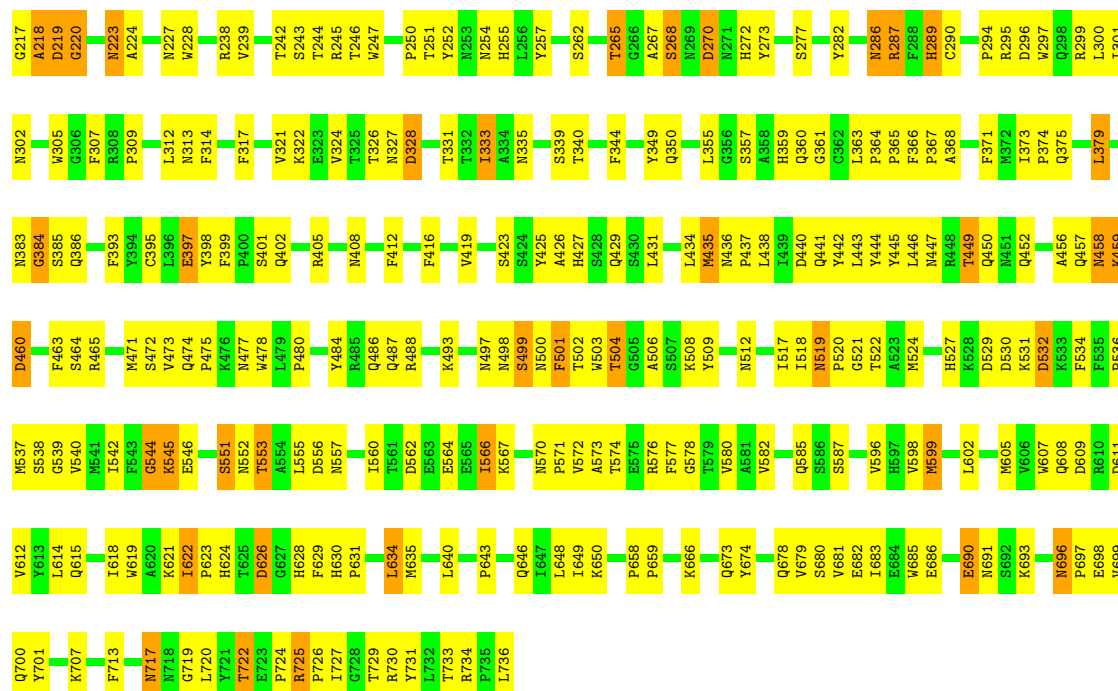
● Molecule 1: Capsid protein VP1

Chain G:

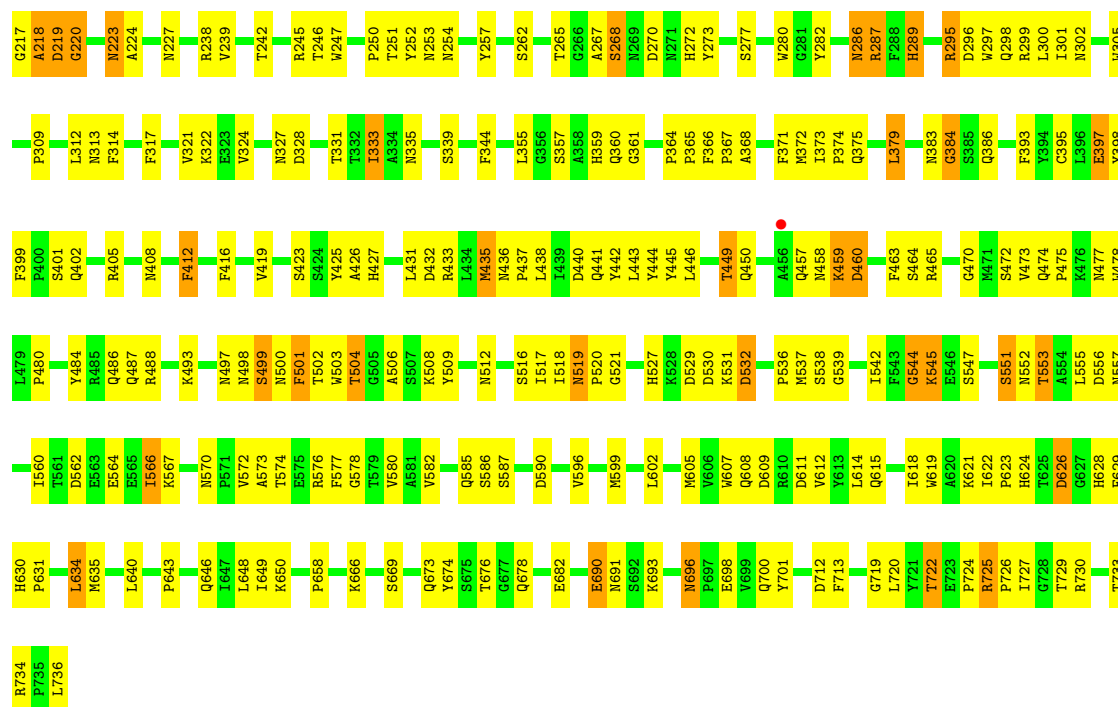


● Molecule 1: Capsid protein VP1

Chain H:

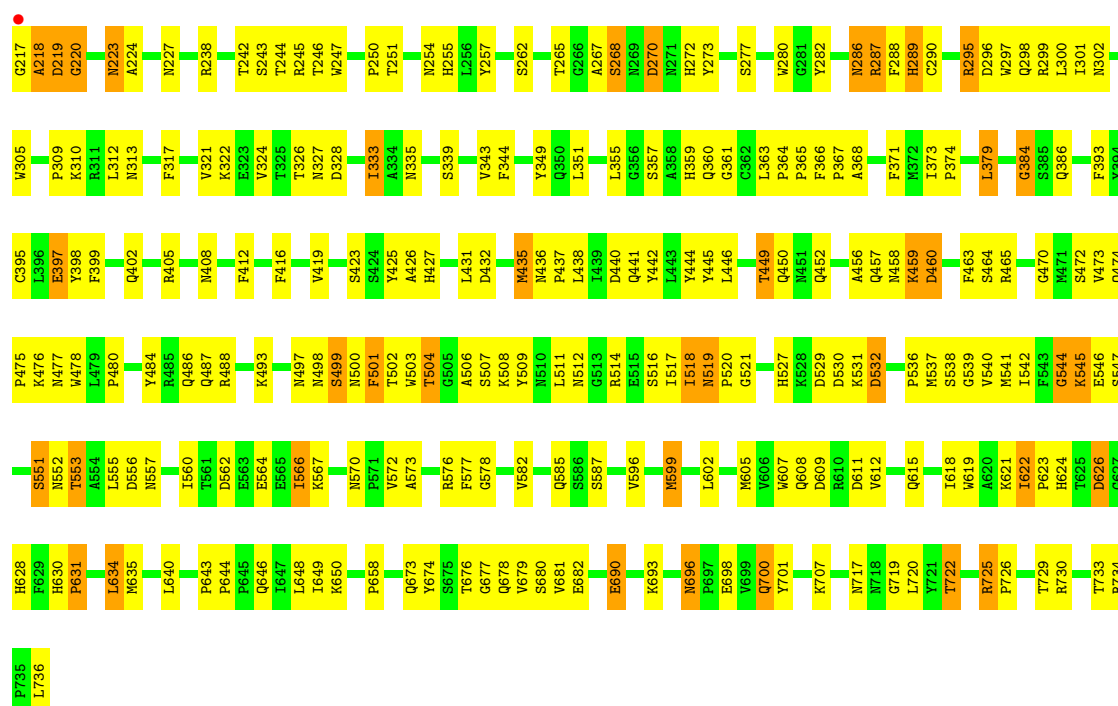






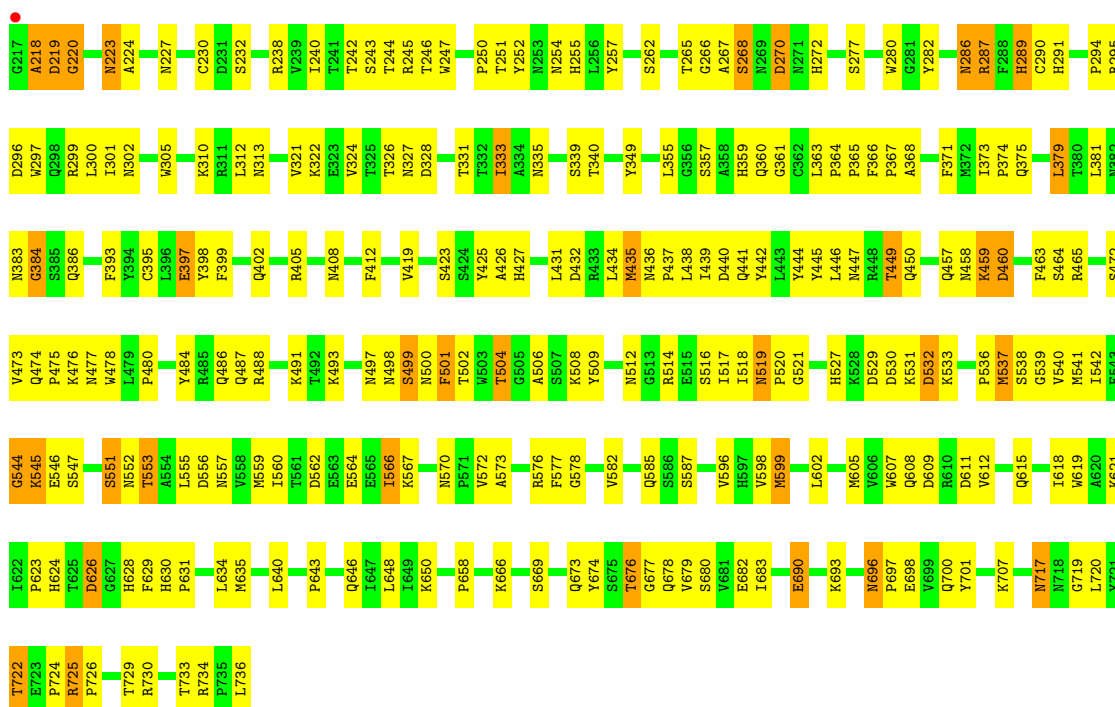
• Molecule 1: Capsid protein VP1

Chain L:



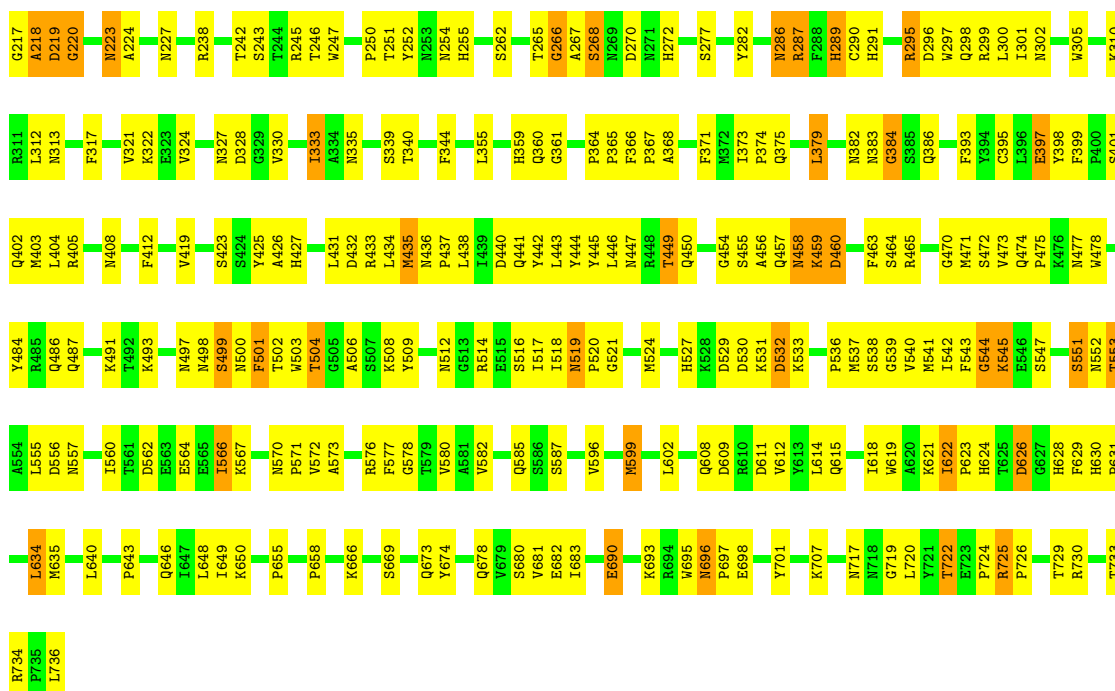
• Molecule 1: Capsid protein VP1

Chain M:



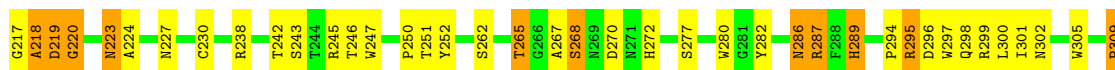
• Molecule 1: Capsid protein VP1

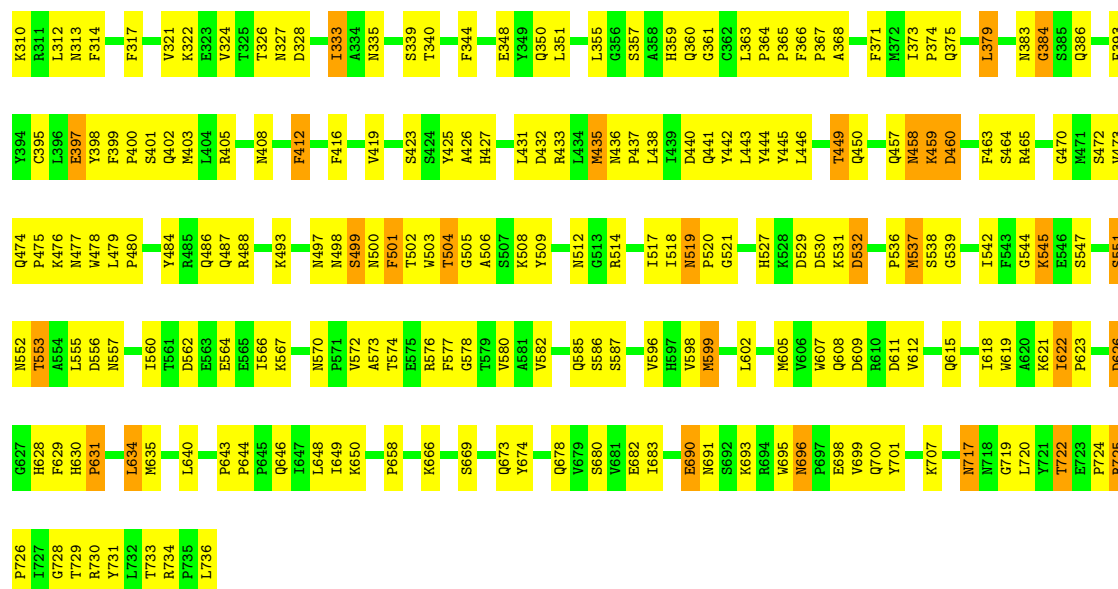
Chain N:



• Molecule 1: Capsid protein VP1

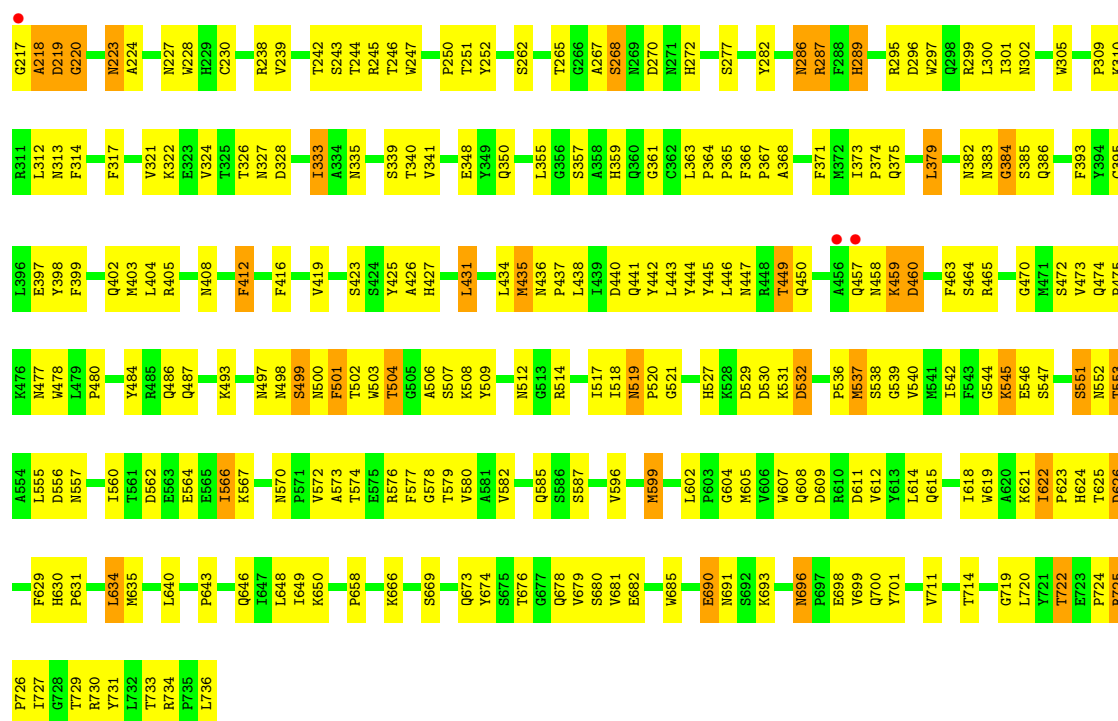
Chain O:





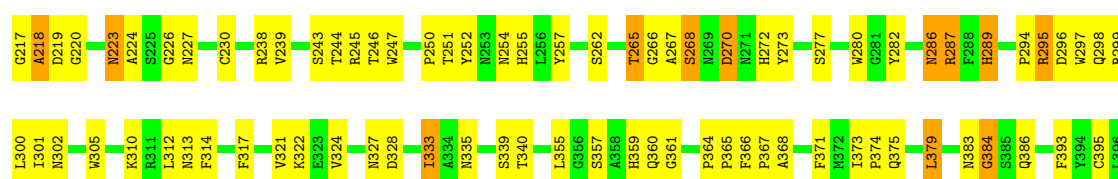
• Molecule 1: Capsid protein VP1

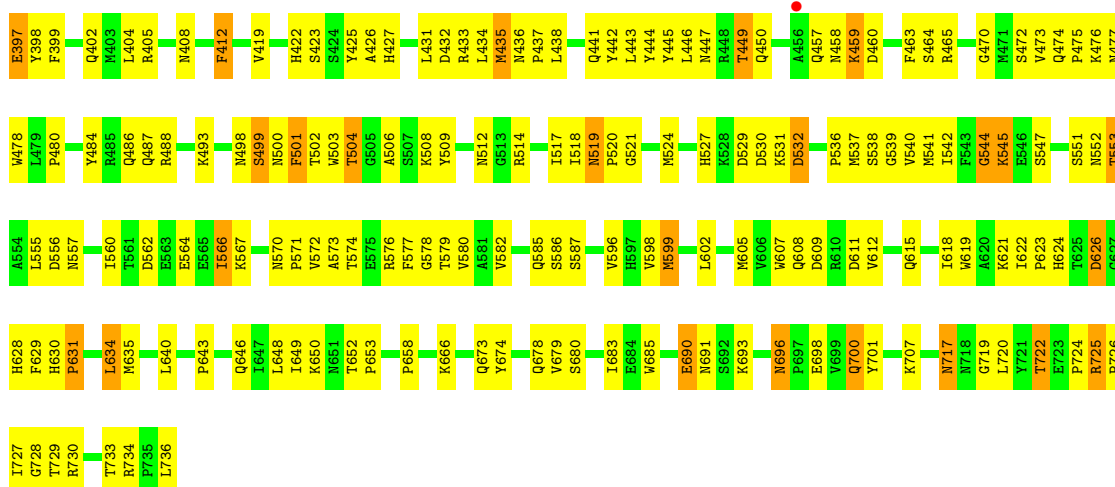
Chain P:



• Molecule 1: Capsid protein VP1

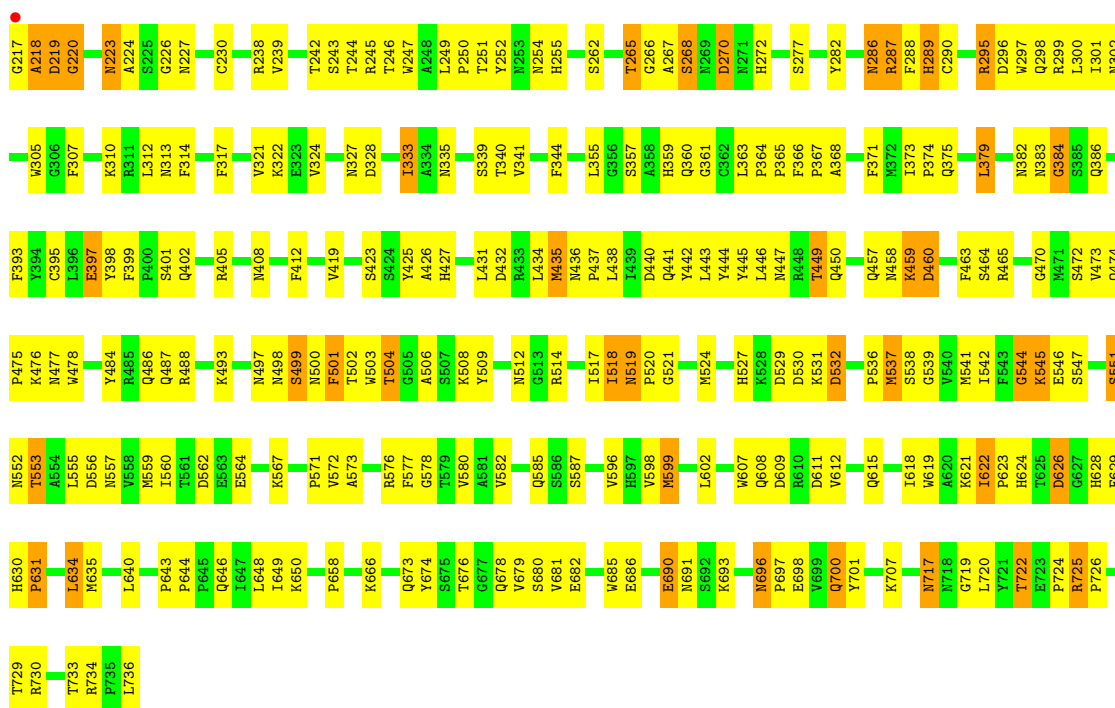
Chain Q:





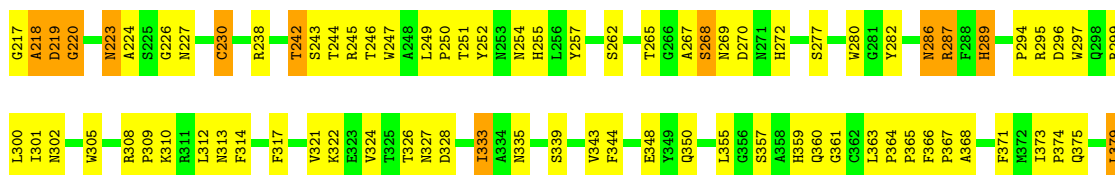
• Molecule 1: Capsid protein VP1

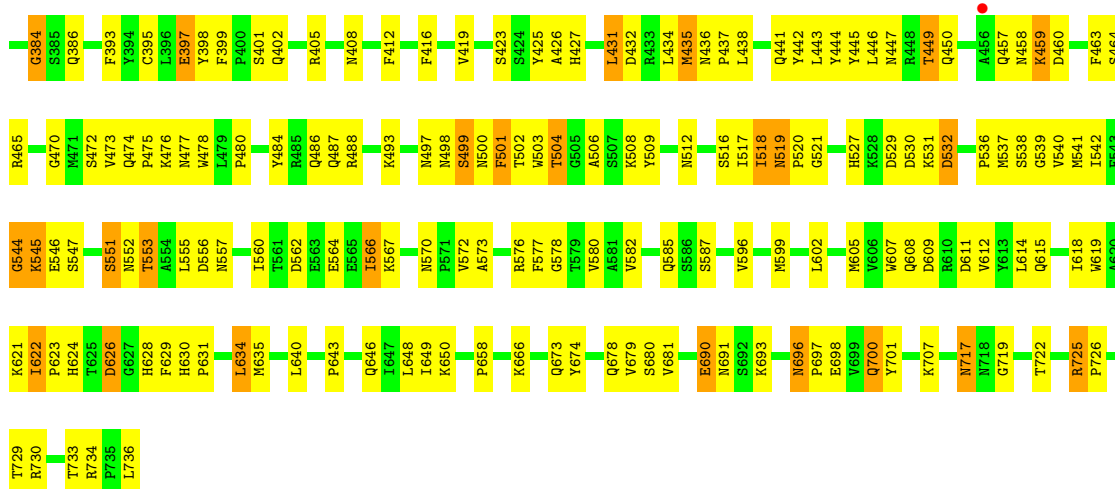
Chain R:



• Molecule 1: Capsid protein VP1

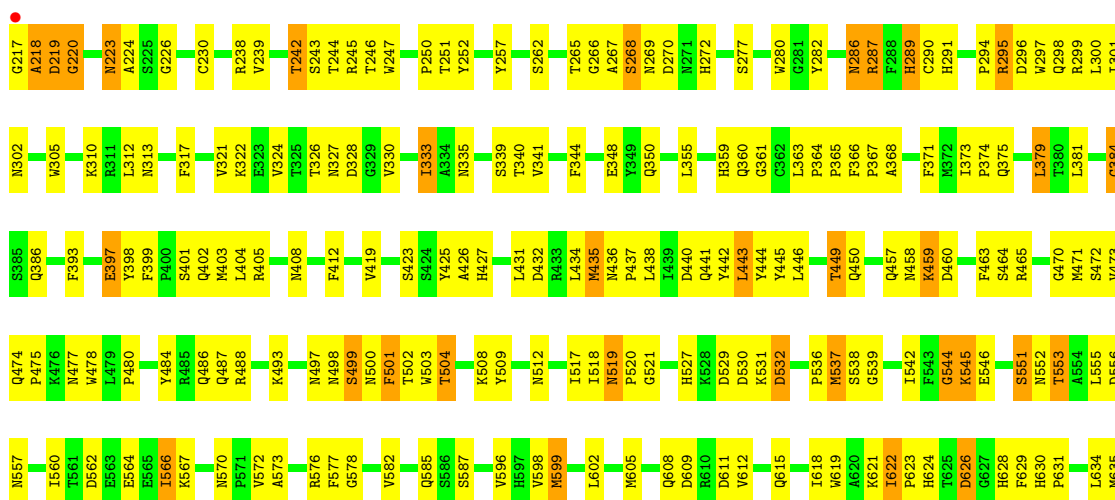
Chain S:





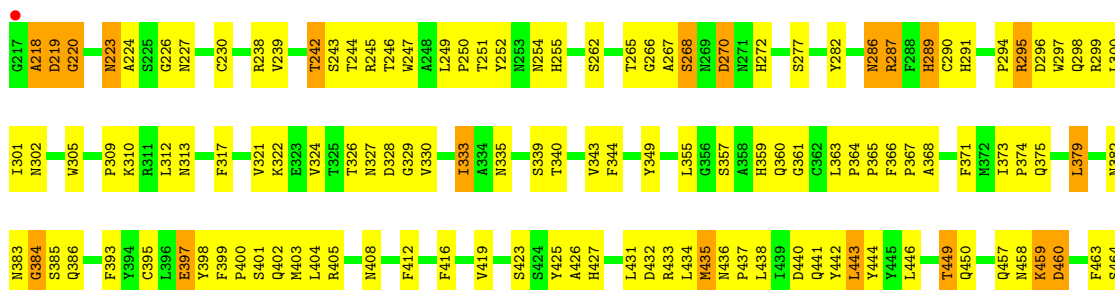
• Molecule 1: Capsid protein VP1

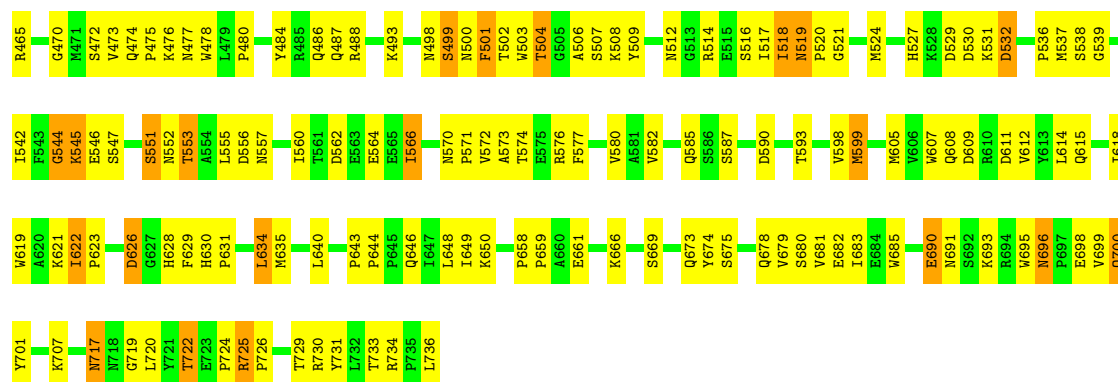
Chain T:



• Molecule 1: Capsid protein VP1

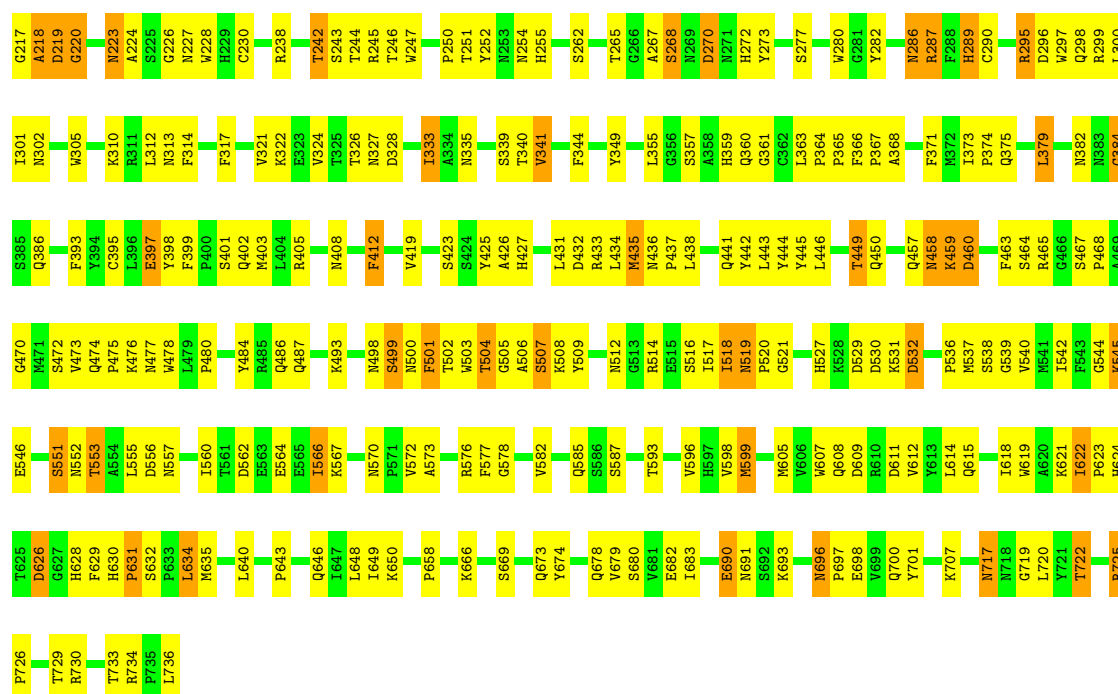
Chain U:





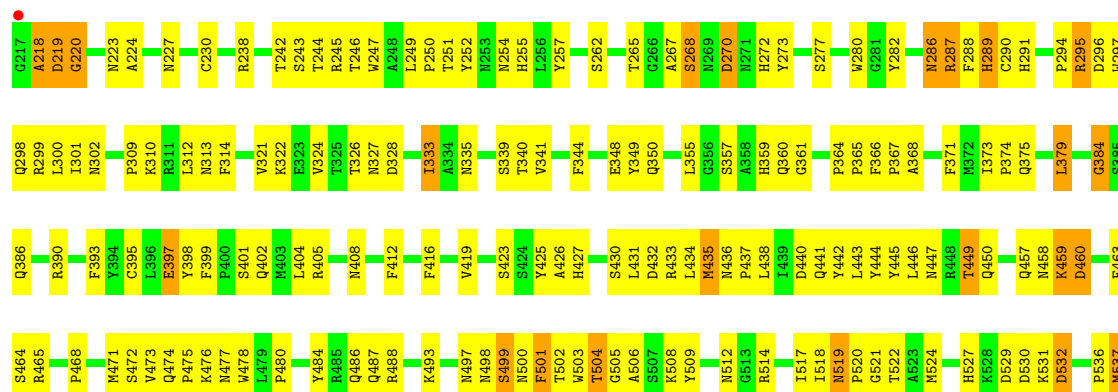
• Molecule 1: Capsid protein VP1

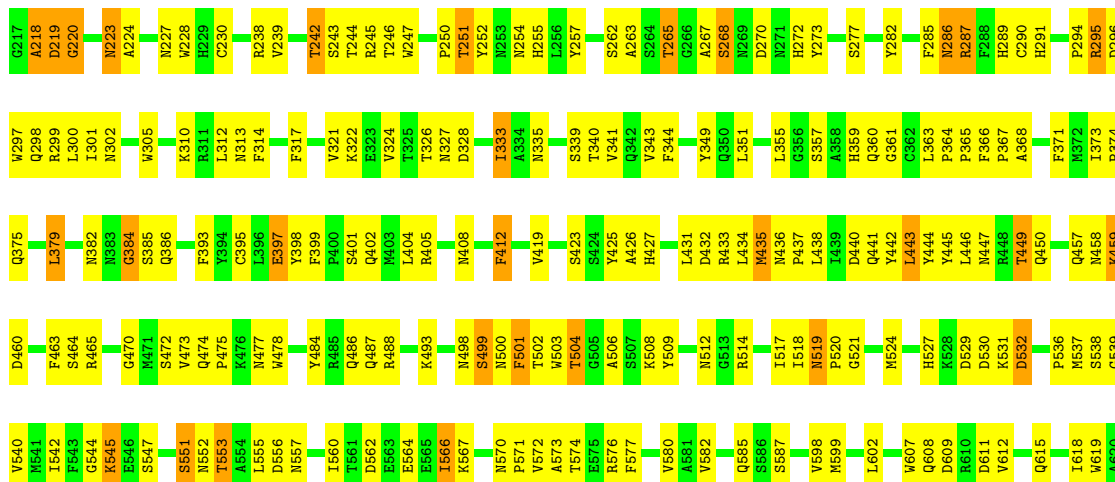
Chain V:

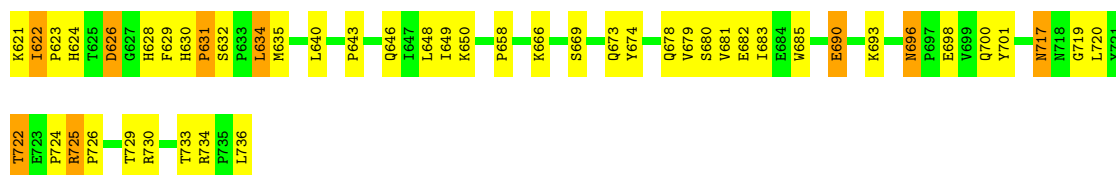


• Molecule 1: Capsid protein VP1

Chain W:

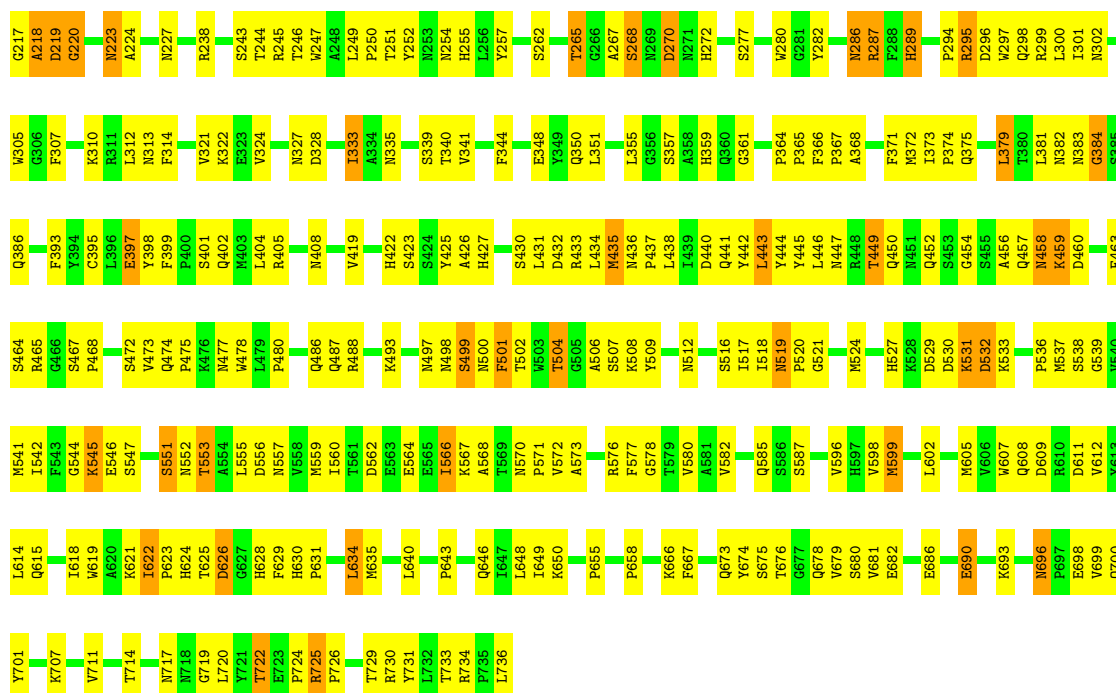






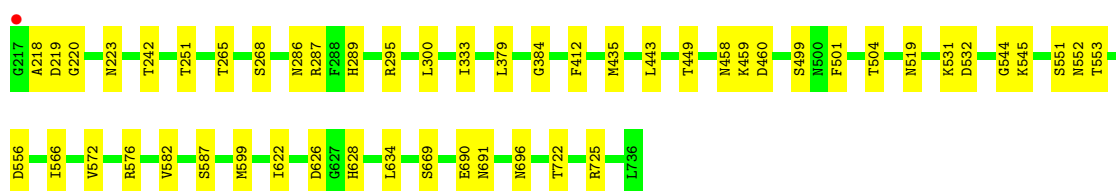
• Molecule 1: Capsid protein VP1

Chain Z:



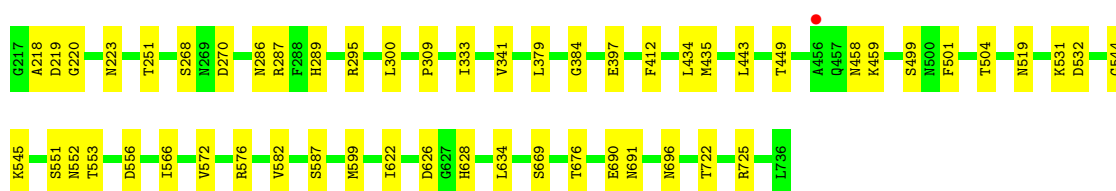
• Molecule 1: Capsid protein VP1

Chain a:

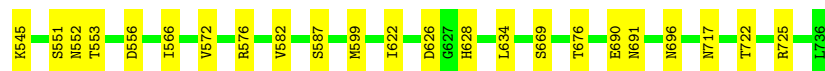


• Molecule 1: Capsid protein VP1

Chain b:



• Molecule 1: Capsid protein VP1



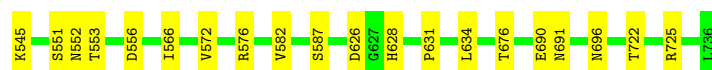
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- Downloaded from <http://www.sagepub.com> at NANYANG TECH UNIV LIBRARY on June 11, 2015



- _____



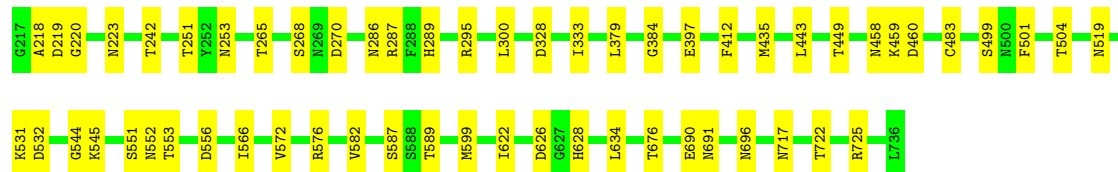
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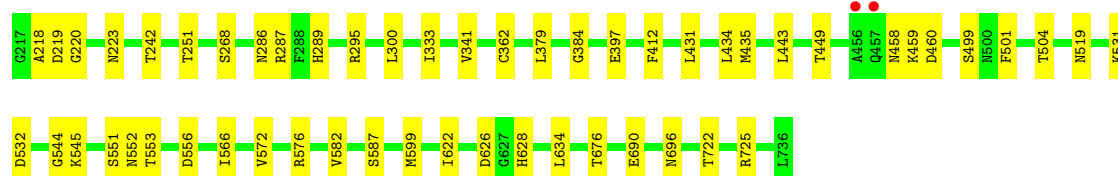
- Molecule 1: Capsid protein VP1

Chain i:



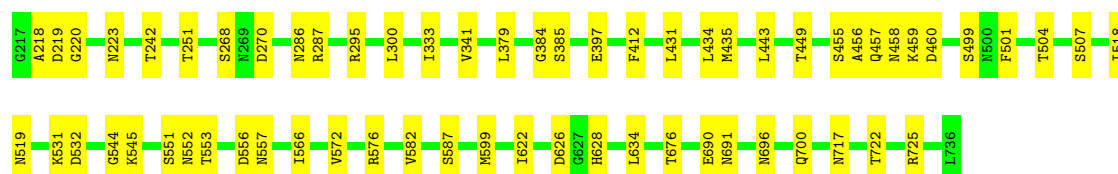
- Molecule 1: Capsid protein VP1

Chain j:



- Molecule 1: Capsid protein VP1

Chain k:



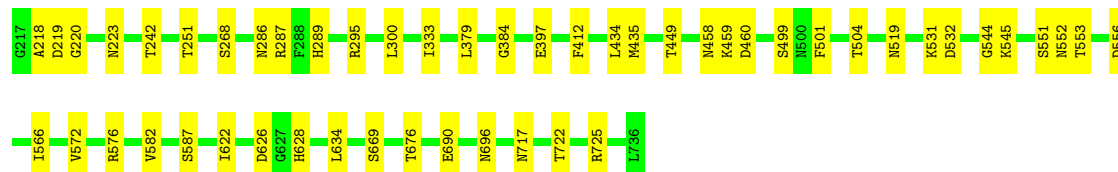
- Molecule 1: Capsid protein VP1

Chain l:

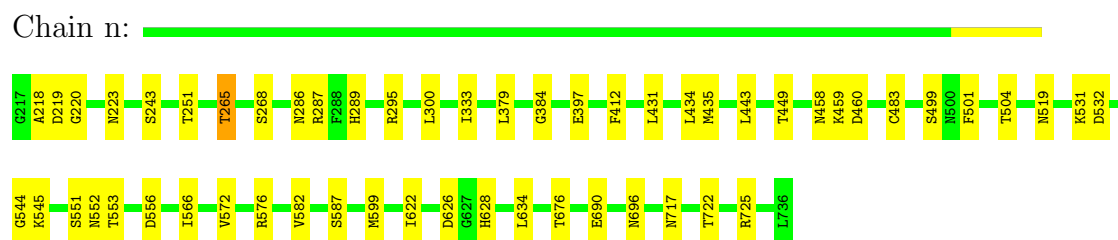


- Molecule 1: Capsid protein VP1

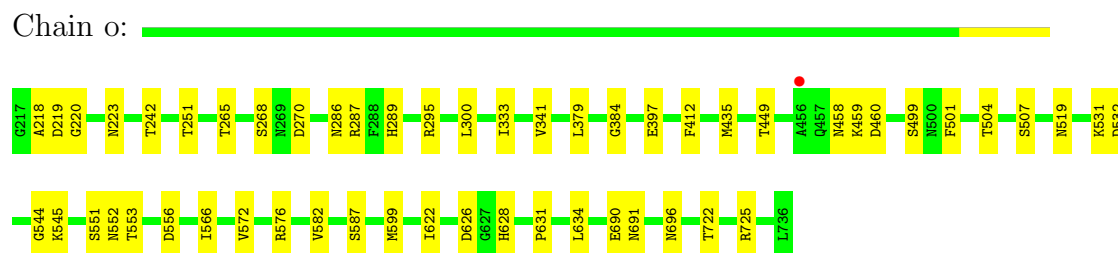
Chain m:



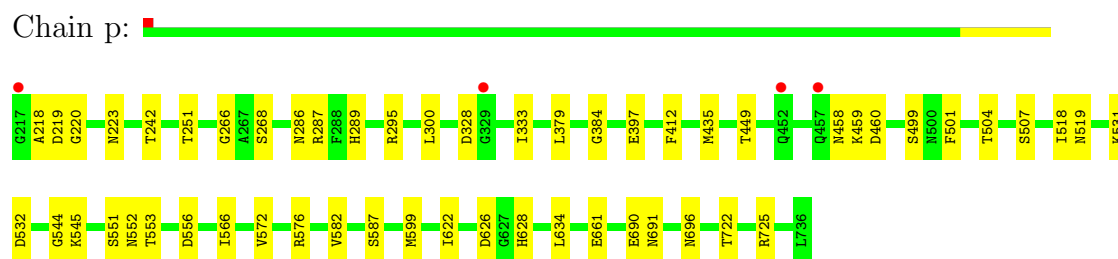
- Molecule 1: Capsid protein VP1



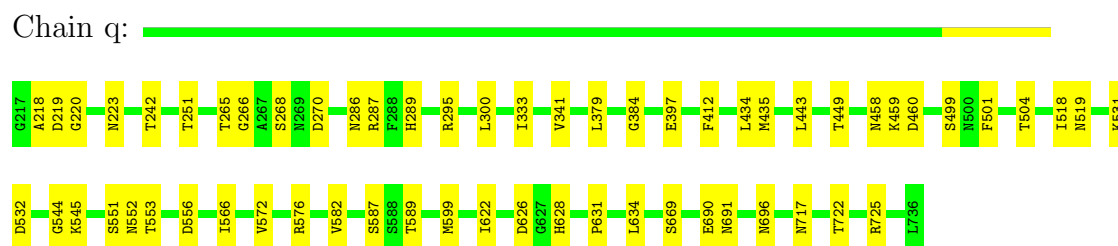
- Molecule 1: Capsid protein VP1



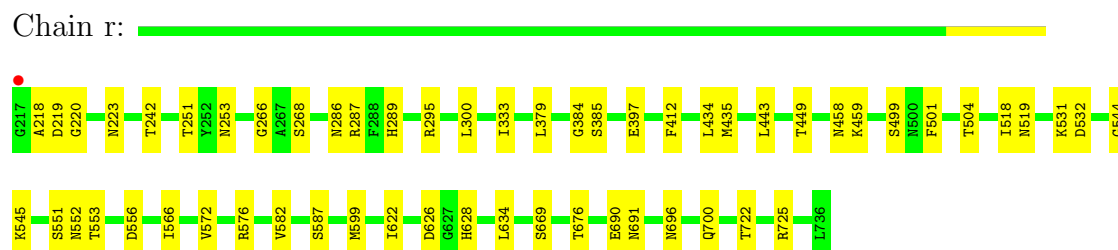
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

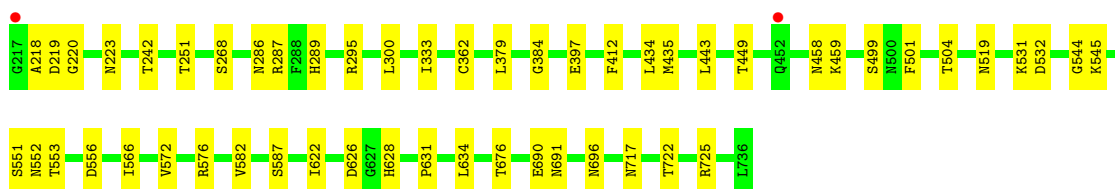


- Molecule 1: Capsid protein VP1



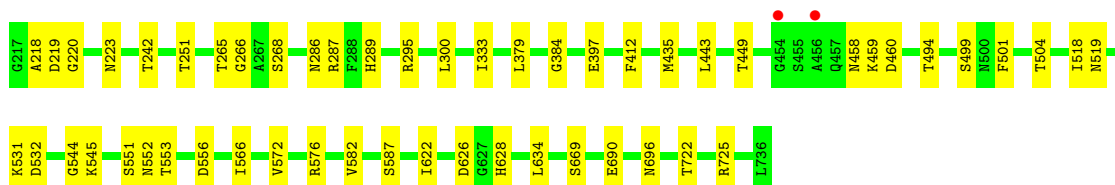
- Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

Chain t:



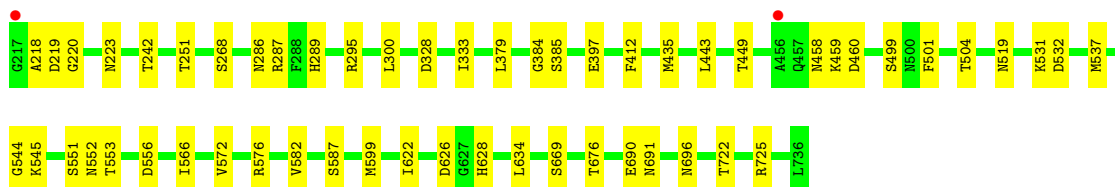
• Molecule 1: Capsid protein VP1

Chain u:



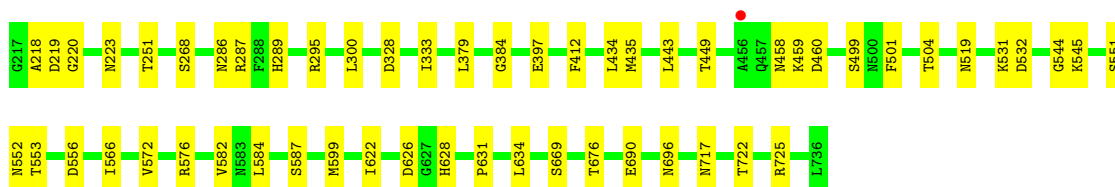
• Molecule 1: Capsid protein VP1

Chain v:



• Molecule 1: Capsid protein VP1

Chain w:



• Molecule 1: Capsid protein VP1

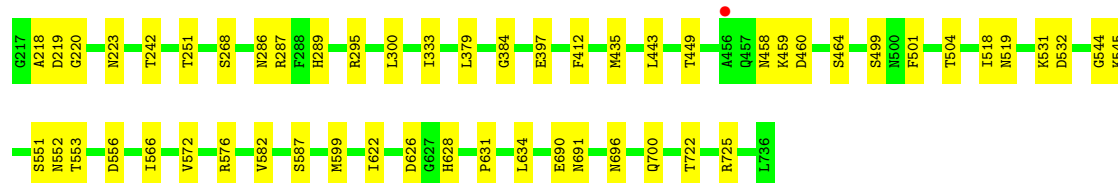
Chain x:





• Molecule 1: Capsid protein VP1

Chain y:



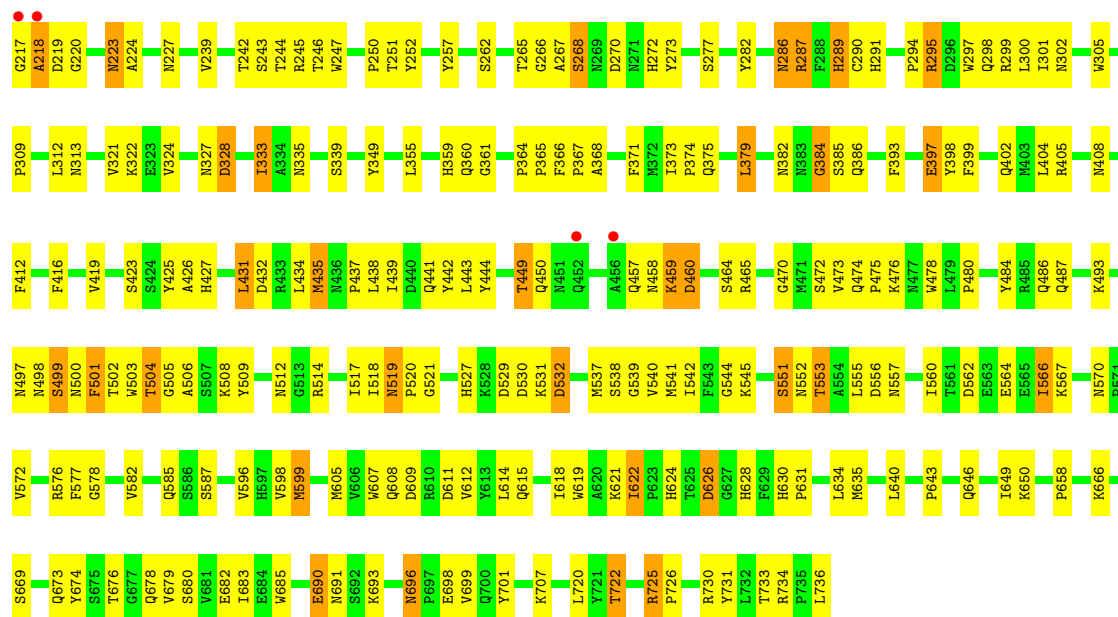
• Molecule 1: Capsid protein VP1

Chain z:



• Molecule 1: Capsid protein VP1

Chain 0:

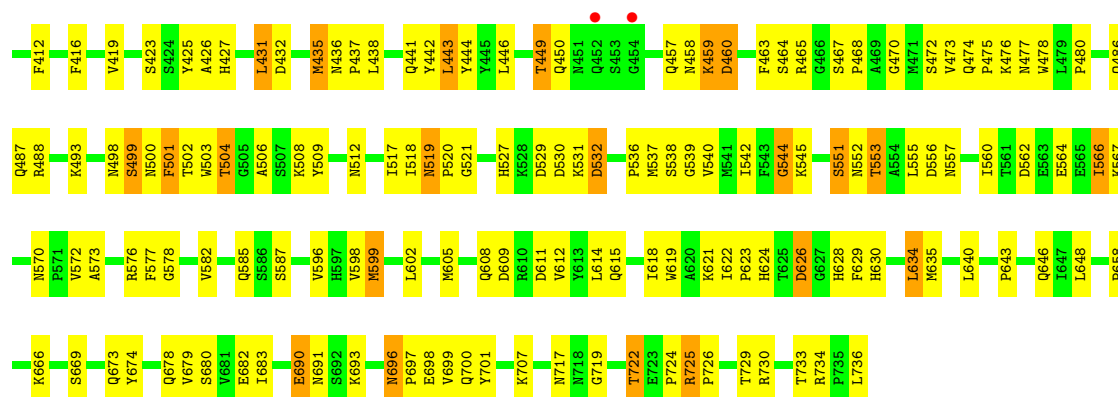


• Molecule 1: Capsid protein VP1

Chain 1:

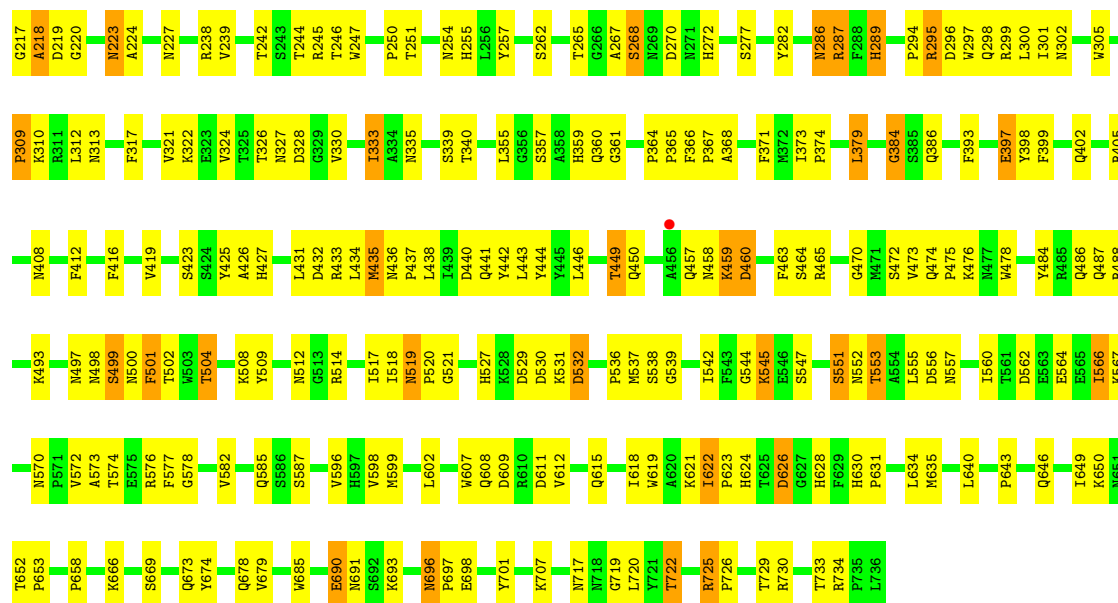


[illegible]



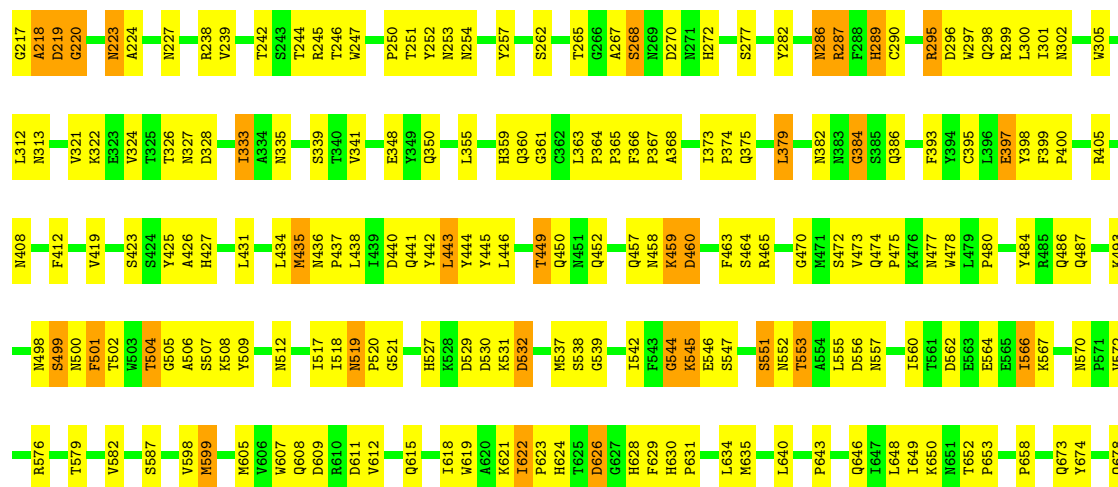
• Molecule 1: Capsid protein VP1

Chain 4:



• Molecule 1: Capsid protein VP1

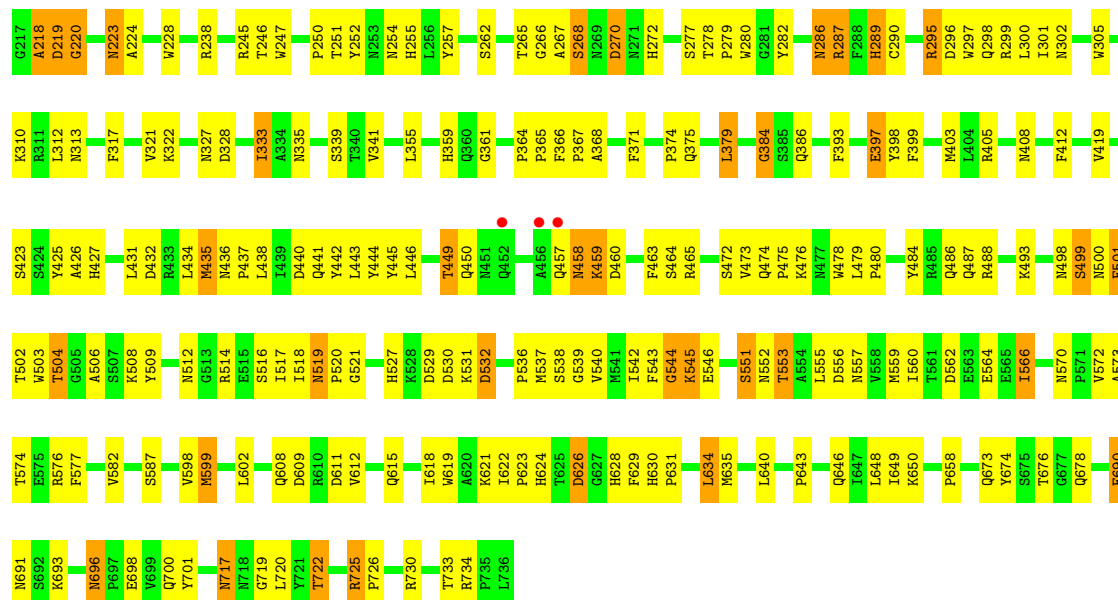
Chain 5:





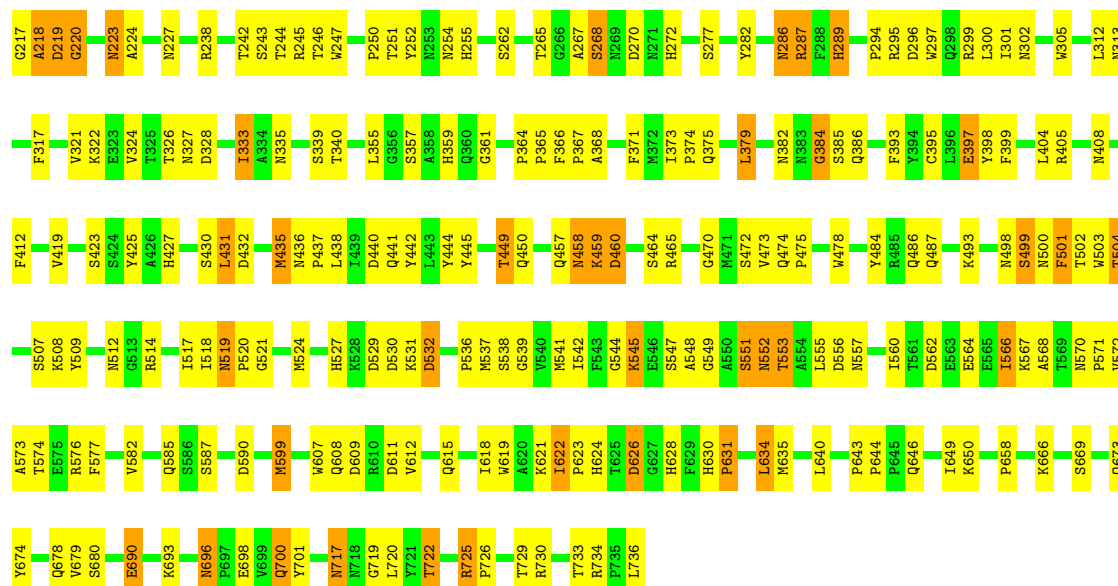
• Molecule 1: Capsid protein VP1

Chain 6:



• Molecule 1: Capsid protein VP1

Chain 7:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	354.79Å 363.90Å 371.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.00 49.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	35.1 (49.21-3.00) 35.1 (49.21-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.251 , 0.286 0.247 , 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 , 20.0	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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	4121	0	3896	403	0
1	Y	4121	0	3896	402	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 9007 close contacts within the same asymmetric unit are listed below.

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

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	7	34
1	1	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	7	35
1	2	518/520 (100%)	463 (89%)	43 (8%)	12 (2%)	10	43
1	3	518/520 (100%)	459 (89%)	46 (9%)	13 (2%)	9	40
1	4	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	9	40
1	5	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	9	40
1	6	518/520 (100%)	464 (90%)	42 (8%)	12 (2%)	10	43
1	7	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	7	35
1	A	518/520 (100%)	460 (89%)	43 (8%)	15 (3%)	7	35
1	B	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	7	35
1	C	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	7	34
1	D	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	8	38
1	E	518/520 (100%)	463 (89%)	41 (8%)	14 (3%)	8	38
1	F	518/520 (100%)	462 (89%)	42 (8%)	14 (3%)	8	38
1	G	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	8	38
1	H	518/520 (100%)	462 (89%)	41 (8%)	15 (3%)	7	35
1	I	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	7	35
1	K	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	9	40
1	L	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	7	35
1	M	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	9	40
1	N	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	8	38
1	O	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	8	38
1	P	518/520 (100%)	466 (90%)	38 (7%)	14 (3%)	8	38
1	Q	518/520 (100%)	465 (90%)	39 (8%)	14 (3%)	8	38
1	R	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	7	34
1	S	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	9	40
1	T	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	9	40
1	U	518/520 (100%)	471 (91%)	31 (6%)	16 (3%)	7	34
1	V	518/520 (100%)	464 (90%)	39 (8%)	15 (3%)	7	35
1	W	518/520 (100%)	463 (89%)	42 (8%)	13 (2%)	9	40
1	X	518/520 (100%)	461 (89%)	43 (8%)	14 (3%)	8	38
1	Y	518/520 (100%)	461 (89%)	44 (8%)	13 (2%)	9	40
1	Z	518/520 (100%)	462 (89%)	44 (8%)	12 (2%)	10	43
1	a	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	9	40
1	b	518/520 (100%)	467 (90%)	39 (8%)	12 (2%)	10	43
1	c	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	10	43
1	d	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	9	40
1	e	518/520 (100%)	471 (91%)	34 (7%)	13 (2%)	9	40
1	f	518/520 (100%)	466 (90%)	36 (7%)	16 (3%)	7	34
1	g	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	9	40
1	h	518/520 (100%)	463 (89%)	44 (8%)	11 (2%)	11	47
1	i	518/520 (100%)	466 (90%)	37 (7%)	15 (3%)	7	35
1	j	518/520 (100%)	467 (90%)	38 (7%)	13 (2%)	9	40
1	k	518/520 (100%)	465 (90%)	37 (7%)	16 (3%)	7	34
1	l	518/520 (100%)	468 (90%)	38 (7%)	12 (2%)	10	43
1	m	518/520 (100%)	468 (90%)	37 (7%)	13 (2%)	9	40
1	n	518/520 (100%)	469 (90%)	36 (7%)	13 (2%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	o	518/520 (100%)	464 (90%)	40 (8%)	14 (3%)	8	38
1	p	518/520 (100%)	463 (89%)	39 (8%)	16 (3%)	7	34
1	q	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	7	34
1	r	518/520 (100%)	464 (90%)	38 (7%)	16 (3%)	7	34
1	s	518/520 (100%)	465 (90%)	40 (8%)	13 (2%)	9	40
1	t	518/520 (100%)	463 (89%)	40 (8%)	15 (3%)	7	35
1	u	518/520 (100%)	467 (90%)	37 (7%)	14 (3%)	8	38
1	v	518/520 (100%)	469 (90%)	34 (7%)	15 (3%)	7	35
1	w	518/520 (100%)	465 (90%)	38 (7%)	15 (3%)	7	35
1	x	518/520 (100%)	465 (90%)	41 (8%)	12 (2%)	10	43
1	y	518/520 (100%)	468 (90%)	35 (7%)	15 (3%)	7	35
1	z	518/520 (100%)	466 (90%)	39 (8%)	13 (2%)	9	40
All	All	31080/31200 (100%)	27915 (90%)	2328 (8%)	837 (3%)	8	38

5 of 837 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	1	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	2	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	3	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	4	452/452 (100%)	413 (91%)	39 (9%)	15	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	6	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	7	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	A	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	B	452/452 (100%)	409 (90%)	43 (10%)	12	44
1	C	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	D	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	E	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	F	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	G	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	H	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	I	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	J	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	K	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	L	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	M	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	N	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	O	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	P	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	Q	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	R	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	S	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	T	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	U	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	V	452/452 (100%)	409 (90%)	43 (10%)	12	44
1	W	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	X	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	Y	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	Z	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	a	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	b	452/452 (100%)	410 (91%)	42 (9%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	d	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	e	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	f	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	g	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	h	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	i	452/452 (100%)	410 (91%)	42 (9%)	13	45
1	j	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	k	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	l	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	m	452/452 (100%)	414 (92%)	38 (8%)	16	51
1	n	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	o	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	p	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	q	452/452 (100%)	408 (90%)	44 (10%)	12	42
1	r	452/452 (100%)	411 (91%)	41 (9%)	14	46
1	s	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	t	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	u	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	v	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	w	452/452 (100%)	412 (91%)	40 (9%)	14	48
1	x	452/452 (100%)	415 (92%)	37 (8%)	17	52
1	y	452/452 (100%)	413 (91%)	39 (9%)	15	50
1	z	452/452 (100%)	409 (90%)	43 (10%)	12	44
All	All	27120/27120 (100%)	24715 (91%)	2405 (9%)	14	48

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

Mol	Chain	Res	Type
1	b	219	ASP
1	h	458	ASN
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 chains 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	520/520 (100%)	-0.34	4 (0%) 83 26	45, 60, 92, 141	0
1	1	520/520 (100%)	-0.31	0 100 100	44, 61, 91, 139	0
1	2	520/520 (100%)	-0.32	2 (0%) 90 41	46, 60, 93, 141	0
1	3	520/520 (100%)	-0.35	2 (0%) 90 41	43, 59, 91, 138	0
1	4	520/520 (100%)	-0.42	1 (0%) 93 54	44, 59, 92, 140	0
1	5	520/520 (100%)	-0.36	0 100 100	43, 57, 90, 138	0
1	6	520/520 (100%)	-0.34	3 (0%) 86 32	42, 57, 90, 139	0
1	7	520/520 (100%)	-0.40	0 100 100	42, 58, 90, 138	0
1	A	520/520 (100%)	-0.25	0 100 100	45, 61, 92, 139	0
1	B	520/520 (100%)	-0.30	1 (0%) 93 54	46, 61, 93, 139	0
1	C	520/520 (100%)	-0.32	2 (0%) 90 41	45, 60, 92, 140	0
1	D	520/520 (100%)	-0.32	1 (0%) 93 54	44, 61, 92, 139	0
1	E	520/520 (100%)	-0.32	0 100 100	46, 61, 93, 139	0
1	F	520/520 (100%)	-0.27	0 100 100	45, 61, 93, 138	0
1	G	520/520 (100%)	-0.35	1 (0%) 93 54	46, 60, 91, 140	0
1	H	520/520 (100%)	-0.34	0 100 100	43, 60, 92, 137	0
1	I	520/520 (100%)	-0.29	1 (0%) 93 54	45, 61, 92, 139	0
1	J	520/520 (100%)	-0.25	1 (0%) 93 54	45, 62, 92, 141	0
1	K	520/520 (100%)	-0.37	1 (0%) 93 54	43, 57, 91, 139	0
1	L	520/520 (100%)	-0.38	1 (0%) 93 54	42, 58, 90, 141	0
1	M	520/520 (100%)	-0.36	1 (0%) 93 54	43, 58, 90, 138	0
1	N	520/520 (100%)	-0.40	0 100 100	42, 58, 90, 138	0
1	O	520/520 (100%)	-0.37	0 100 100	42, 58, 91, 141	0
1	P	520/520 (100%)	-0.38	3 (0%) 86 32	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%)	-0.33	1 (0%) 93 54	42, 59, 91, 138	0
1	R	520/520 (100%)	-0.37	1 (0%) 93 54	43, 58, 91, 139	0
1	S	520/520 (100%)	-0.37	1 (0%) 93 54	41, 57, 88, 141	0
1	T	520/520 (100%)	-0.37	1 (0%) 93 54	42, 57, 90, 140	0
1	U	520/520 (100%)	-0.33	1 (0%) 93 54	45, 60, 91, 139	0
1	V	520/520 (100%)	-0.31	0 100 100	45, 61, 92, 140	0
1	W	520/520 (100%)	-0.26	1 (0%) 93 54	46, 61, 93, 139	0
1	X	520/520 (100%)	-0.26	1 (0%) 93 54	44, 61, 93, 141	0
1	Y	520/520 (100%)	-0.31	0 100 100	45, 61, 92, 139	0
1	Z	520/520 (100%)	-0.34	0 100 100	44, 60, 91, 140	0
1	a	520/520 (100%)	-0.34	1 (0%) 93 54	44, 59, 92, 139	0
1	b	520/520 (100%)	-0.38	1 (0%) 93 54	42, 58, 90, 137	0
1	c	520/520 (100%)	-0.38	0 100 100	44, 59, 90, 141	0
1	d	520/520 (100%)	-0.36	0 100 100	45, 60, 91, 141	0
1	e	520/520 (100%)	-0.37	1 (0%) 93 54	43, 58, 89, 141	0
1	f	520/520 (100%)	-0.37	1 (0%) 93 54	45, 59, 92, 141	0
1	g	520/520 (100%)	-0.35	0 100 100	46, 60, 92, 134	0
1	h	520/520 (100%)	-0.34	1 (0%) 93 54	45, 60, 91, 140	0
1	i	520/520 (100%)	-0.38	0 100 100	43, 59, 90, 138	0
1	j	520/520 (100%)	-0.36	2 (0%) 90 41	43, 58, 90, 139	0
1	k	520/520 (100%)	-0.36	0 100 100	41, 58, 90, 135	0
1	l	520/520 (100%)	-0.38	0 100 100	42, 57, 90, 138	0
1	m	520/520 (100%)	-0.39	0 100 100	42, 57, 89, 138	0
1	n	520/520 (100%)	-0.35	0 100 100	42, 57, 90, 139	0
1	o	520/520 (100%)	-0.36	1 (0%) 93 54	45, 60, 92, 139	0
1	p	520/520 (100%)	-0.32	4 (0%) 83 26	46, 60, 91, 139	0
1	q	520/520 (100%)	-0.35	0 100 100	45, 60, 92, 139	0
1	r	520/520 (100%)	-0.39	1 (0%) 93 54	43, 58, 90, 138	0
1	s	520/520 (100%)	-0.37	2 (0%) 90 41	43, 59, 91, 139	0
1	t	520/520 (100%)	-0.36	2 (0%) 90 41	43, 59, 91, 140	0
1	u	520/520 (100%)	-0.35	3 (0%) 86 32	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%)	-0.37	2 (0%)	90	41	42, 59, 90, 141	0
1	w	520/520 (100%)	-0.33	1 (0%)	93	54	43, 60, 92, 141	0
1	x	520/520 (100%)	-0.33	3 (0%)	86	32	44, 60, 92, 140	0
1	y	520/520 (100%)	-0.37	1 (0%)	93	54	43, 59, 90, 139	0
1	z	520/520 (100%)	-0.33	1 (0%)	93	54	45, 59, 91, 141	0
All	All	31200/31200 (100%)	-0.35	60 (0%)	93	54	41, 59, 91, 141	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	x	217	GLY	4.5
1	U	217	GLY	3.4
1	s	217	GLY	3.1
1	u	217	GLY	3.0
1	2	217	GLY	2.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.