



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 17, 2018 – 05:46 PM EST

PDB ID : 6BWX
EMDB ID: : EMD-7300
Title : Atomic resolution structure of human bufavirus 1
Authors : Mietzsch, M.; Agbandje-McKenna, M.
Deposited on : 2017-12-15
Resolution : 2.84 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

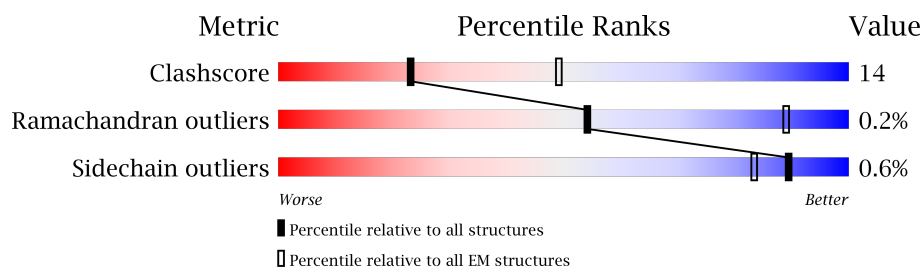
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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.
















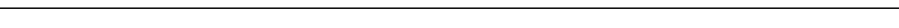











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	537	
1	1	537	
1	2	537	
1	3	537	
1	4	537	
1	5	537	
1	6	537	
1	7	537	
1	A	537	

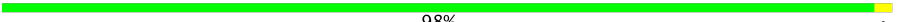
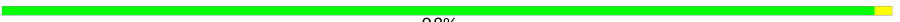
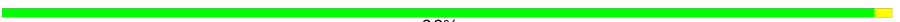












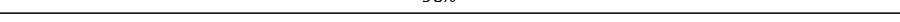
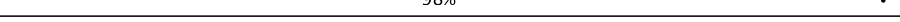
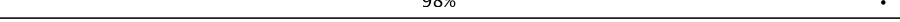
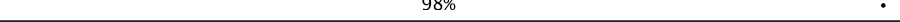
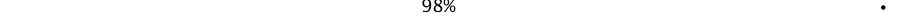
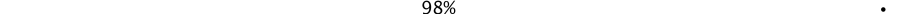
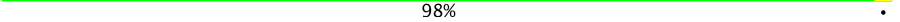
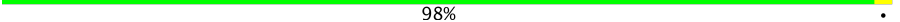
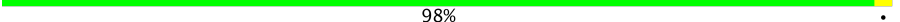
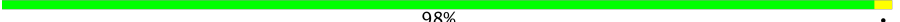
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Mol	Chain	Length	Quality of chain
1	B	537	 63% 36% .
1	C	537	 63% 36% .
1	D	537	 64% 36% .
1	E	537	 63% 36% .
1	F	537	 63% 36% .
1	G	537	 62% 37% .
1	H	537	 63% 36% .
1	I	537	 63% 36% .
1	J	537	 64% 35% .
1	K	537	 63% 36% .
1	L	537	 63% 37% .
1	M	537	 64% 35% .
1	N	537	 63% 37% .
1	O	537	 63% 36% .
1	P	537	 62% 37% .
1	Q	537	 63% 36% .
1	R	537	 64% 36% .
1	S	537	 63% 36% .
1	T	537	 64% 36% .
1	U	537	 64% 36% .
1	V	537	 63% 36% .
1	W	537	 64% 35% .
1	X	537	 64% 35% .
1	Y	537	 63% 36% .
1	Z	537	 63% 36% .

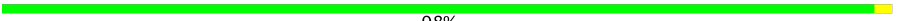
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Mol	Chain	Length	Quality of chain
1	a	537	 98%
1	b	537	 98%
1	c	537	 98%
1	d	537	 98%
1	e	537	 98%
1	f	537	 98%
1	g	537	 98%
1	h	537	 98%
1	i	537	 98%
1	j	537	 98%
1	k	537	 98%
1	l	537	 98%
1	m	537	 98%
1	n	537	 98%
1	o	537	 98%
1	p	537	 98%
1	q	537	 98%
1	r	537	 98%
1	s	537	 98%
1	t	537	 98%
1	u	537	 98%
1	v	537	 98%
1	w	537	 98%
1	x	537	 98%
1	y	537	 98%

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Mol	Chain	Length	Quality of chain
1	z	537	 98%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 261180 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	B	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	C	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	D	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	E	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	F	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	G	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	H	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	I	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	J	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	K	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	L	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	M	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	N	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	O	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	P	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	Q	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	S	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	T	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	U	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	V	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	W	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	X	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	Y	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	Z	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	1	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	2	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	3	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	4	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	5	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	6	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	a	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	b	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	c	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	d	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	e	537	Total 4353	C 2754	N 764	O 821	S 14	0	0
1	f	537	Total 4353	C 2754	N 764	O 821	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	h	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	i	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	j	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	k	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	l	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	m	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	n	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	o	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	p	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	q	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	r	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	s	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	t	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	u	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	v	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	w	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	x	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	y	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	z	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		
1	7	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	537	Total	C	N	O	S	0	0
			4353	2754	764	821	14		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	VAL	ILE	conflict	UNP A0A097PIK3
B	35	VAL	ILE	conflict	UNP A0A097PIK3
C	35	VAL	ILE	conflict	UNP A0A097PIK3
D	35	VAL	ILE	conflict	UNP A0A097PIK3
E	35	VAL	ILE	conflict	UNP A0A097PIK3
F	35	VAL	ILE	conflict	UNP A0A097PIK3
G	35	VAL	ILE	conflict	UNP A0A097PIK3
H	35	VAL	ILE	conflict	UNP A0A097PIK3
I	35	VAL	ILE	conflict	UNP A0A097PIK3
J	35	VAL	ILE	conflict	UNP A0A097PIK3
K	35	VAL	ILE	conflict	UNP A0A097PIK3
L	35	VAL	ILE	conflict	UNP A0A097PIK3
M	35	VAL	ILE	conflict	UNP A0A097PIK3
N	35	VAL	ILE	conflict	UNP A0A097PIK3
O	35	VAL	ILE	conflict	UNP A0A097PIK3
P	35	VAL	ILE	conflict	UNP A0A097PIK3
Q	35	VAL	ILE	conflict	UNP A0A097PIK3
R	35	VAL	ILE	conflict	UNP A0A097PIK3
S	35	VAL	ILE	conflict	UNP A0A097PIK3
T	35	VAL	ILE	conflict	UNP A0A097PIK3
U	35	VAL	ILE	conflict	UNP A0A097PIK3
V	35	VAL	ILE	conflict	UNP A0A097PIK3
W	35	VAL	ILE	conflict	UNP A0A097PIK3
X	35	VAL	ILE	conflict	UNP A0A097PIK3
Y	35	VAL	ILE	conflict	UNP A0A097PIK3
Z	35	VAL	ILE	conflict	UNP A0A097PIK3
1	35	VAL	ILE	conflict	UNP A0A097PIK3
2	35	VAL	ILE	conflict	UNP A0A097PIK3
3	35	VAL	ILE	conflict	UNP A0A097PIK3
4	35	VAL	ILE	conflict	UNP A0A097PIK3
5	35	VAL	ILE	conflict	UNP A0A097PIK3
6	35	VAL	ILE	conflict	UNP A0A097PIK3
a	35	VAL	ILE	conflict	UNP A0A097PIK3
b	35	VAL	ILE	conflict	UNP A0A097PIK3
c	35	VAL	ILE	conflict	UNP A0A097PIK3
d	35	VAL	ILE	conflict	UNP A0A097PIK3

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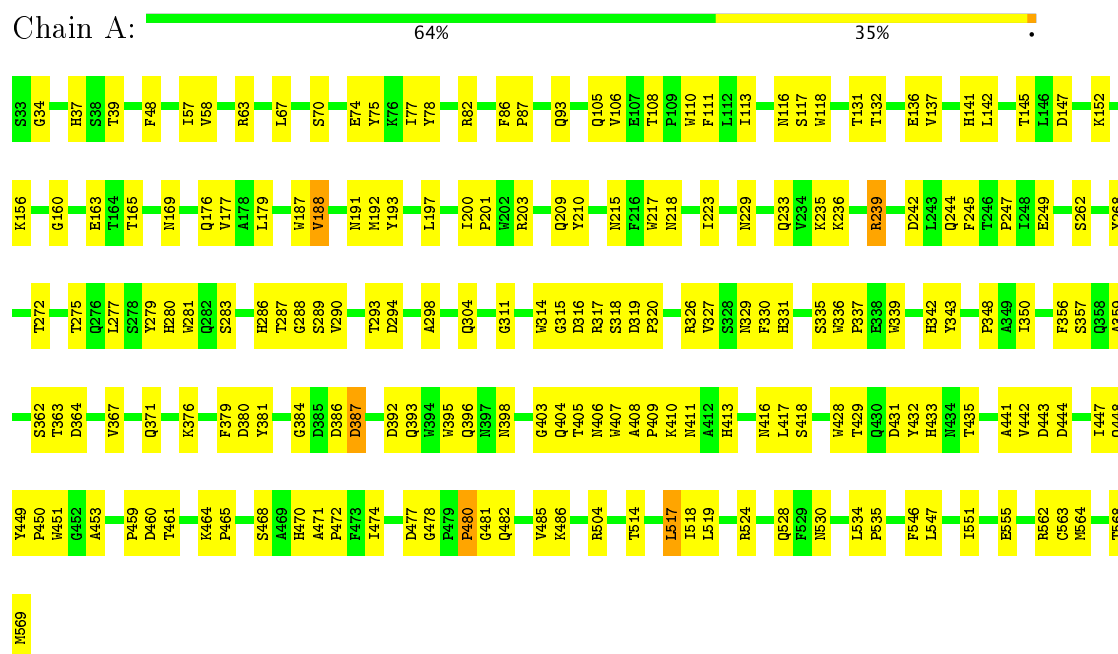
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Chain	Residue	Modelled	Actual	Comment	Reference
e	35	VAL	ILE	conflict	UNP A0A097PIK3
f	35	VAL	ILE	conflict	UNP A0A097PIK3
g	35	VAL	ILE	conflict	UNP A0A097PIK3
h	35	VAL	ILE	conflict	UNP A0A097PIK3
i	35	VAL	ILE	conflict	UNP A0A097PIK3
j	35	VAL	ILE	conflict	UNP A0A097PIK3
k	35	VAL	ILE	conflict	UNP A0A097PIK3
l	35	VAL	ILE	conflict	UNP A0A097PIK3
m	35	VAL	ILE	conflict	UNP A0A097PIK3
n	35	VAL	ILE	conflict	UNP A0A097PIK3
o	35	VAL	ILE	conflict	UNP A0A097PIK3
p	35	VAL	ILE	conflict	UNP A0A097PIK3
q	35	VAL	ILE	conflict	UNP A0A097PIK3
r	35	VAL	ILE	conflict	UNP A0A097PIK3
s	35	VAL	ILE	conflict	UNP A0A097PIK3
t	35	VAL	ILE	conflict	UNP A0A097PIK3
u	35	VAL	ILE	conflict	UNP A0A097PIK3
v	35	VAL	ILE	conflict	UNP A0A097PIK3
w	35	VAL	ILE	conflict	UNP A0A097PIK3
x	35	VAL	ILE	conflict	UNP A0A097PIK3
y	35	VAL	ILE	conflict	UNP A0A097PIK3
z	35	VAL	ILE	conflict	UNP A0A097PIK3
7	35	VAL	ILE	conflict	UNP A0A097PIK3
0	35	VAL	ILE	conflict	UNP A0A097PIK3

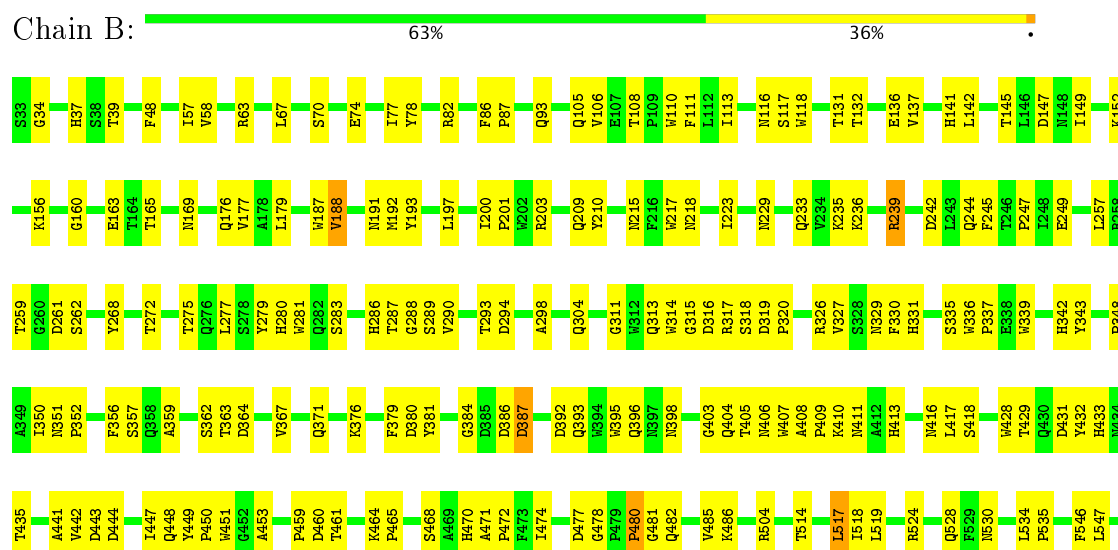
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: VP2



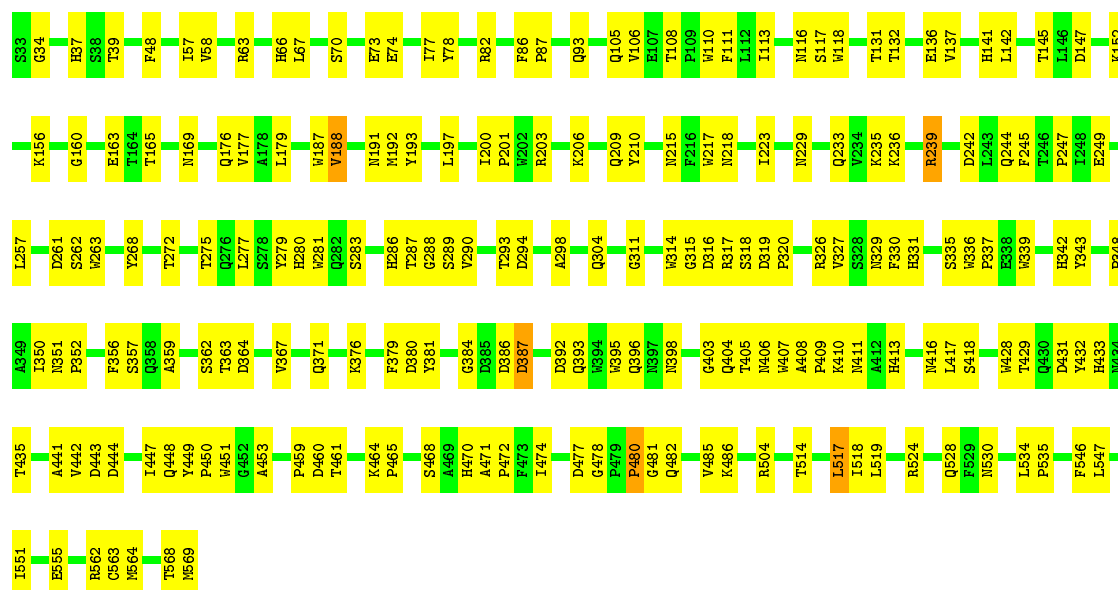
• Molecule 1: VP2





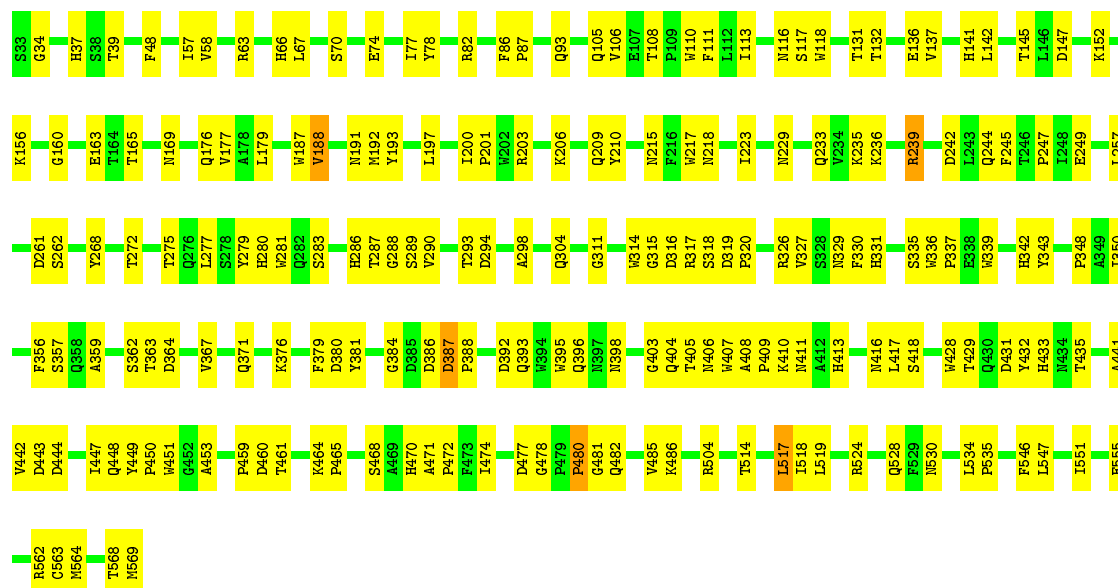
• Molecule 1: VP2

Chain C:  63% 36%



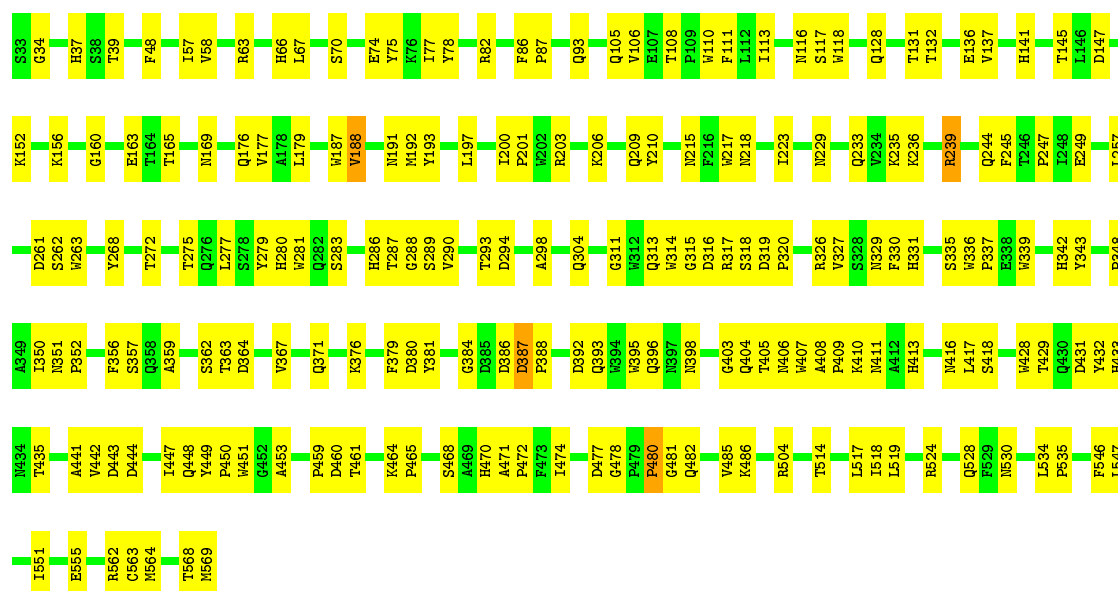
• Molecule 1: VP2

Chain D:  64% 36%



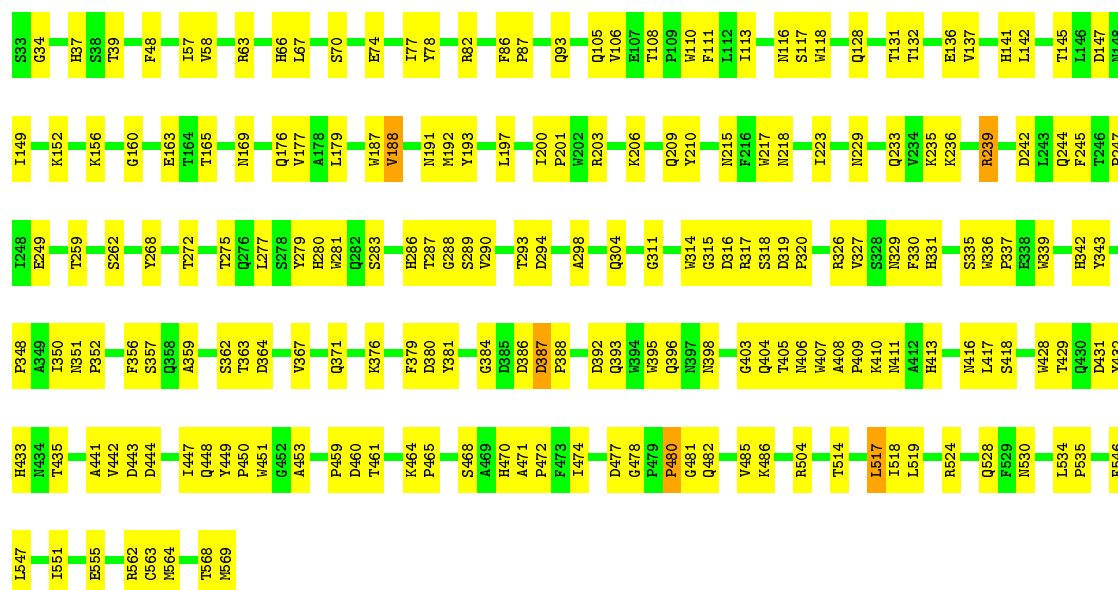
• Molecule 1: VP2

Chain E:  63% 36%



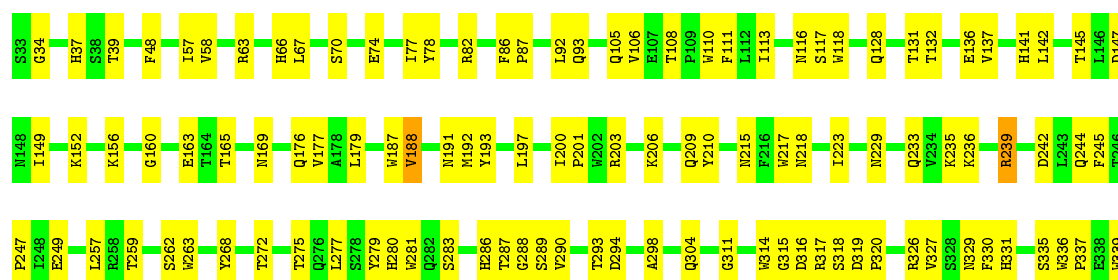
• Molecule 1: VP2

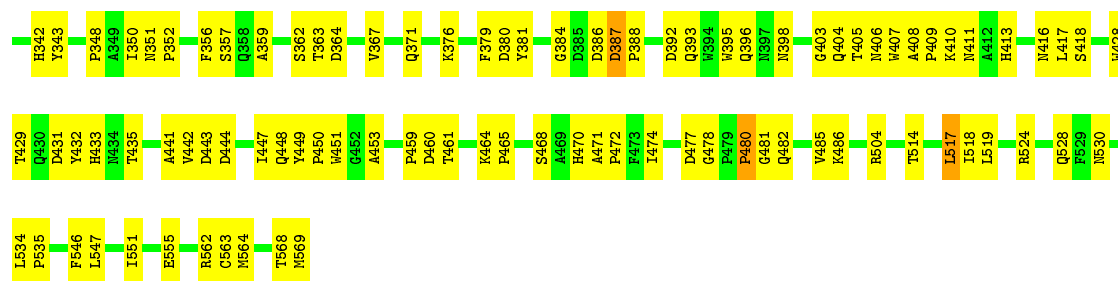
Chain F: 63% 36% .



• Molecule 1: VP2

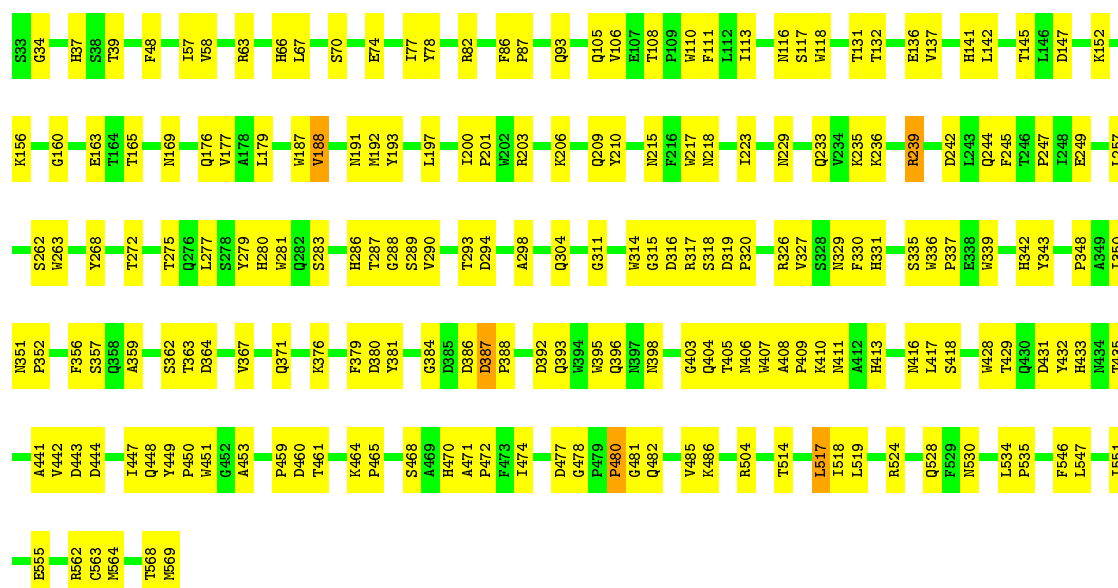
Chain G: 62% 37% .





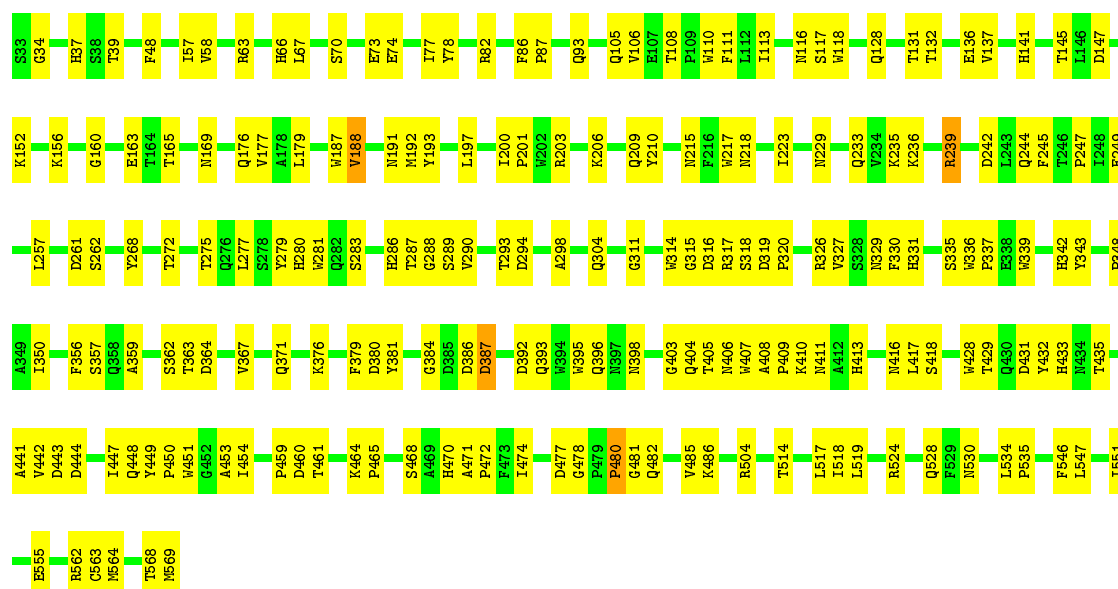
• Molecule 1: VP2

Chain H: 63% 36%

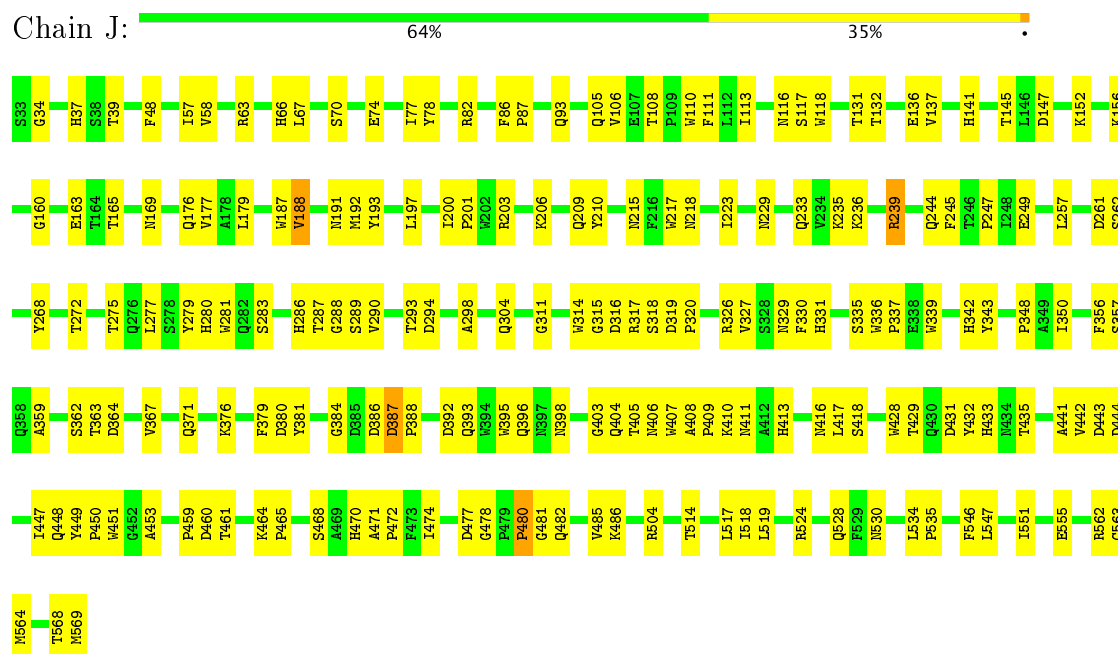


• Molecule 1: VP2

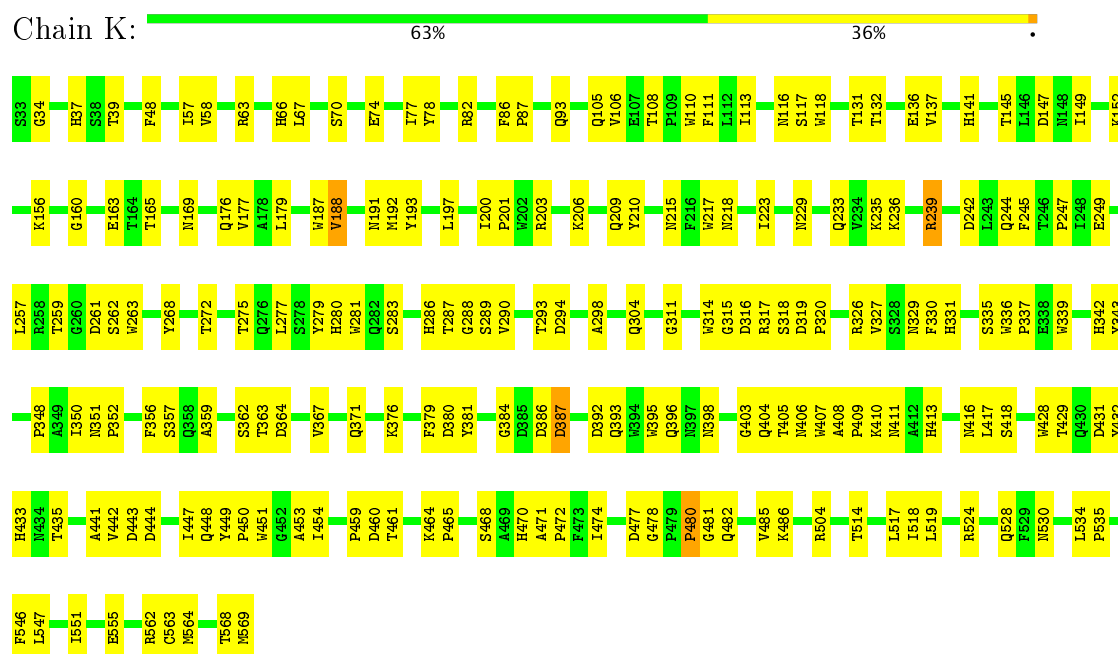
Chain I: 63% 36%



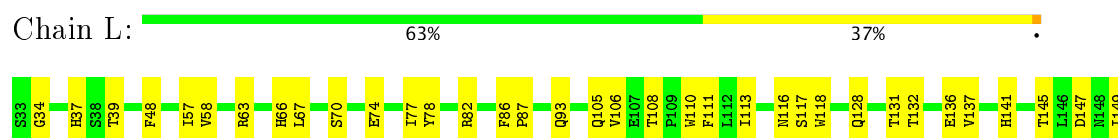
- Molecule 1: VP2

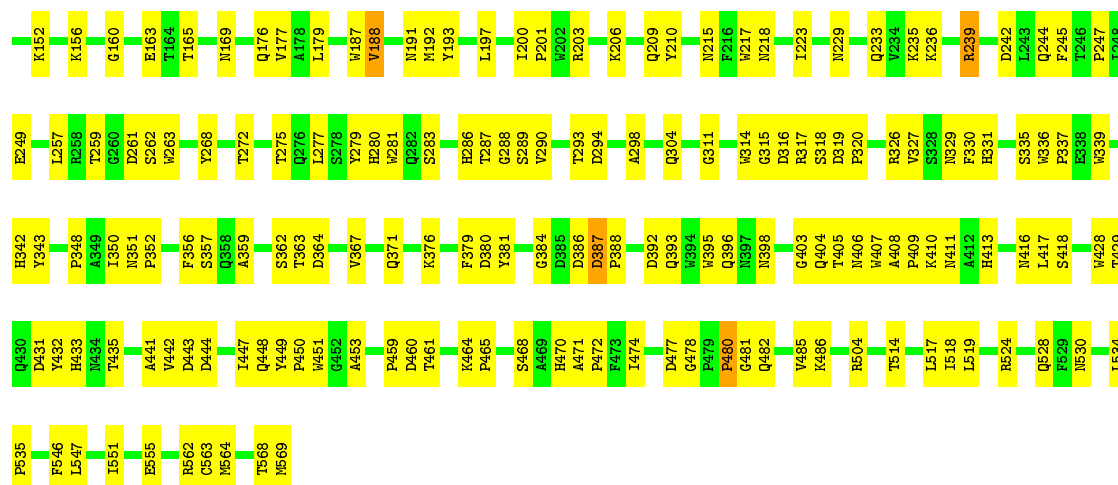


- Molecule 1: VP2



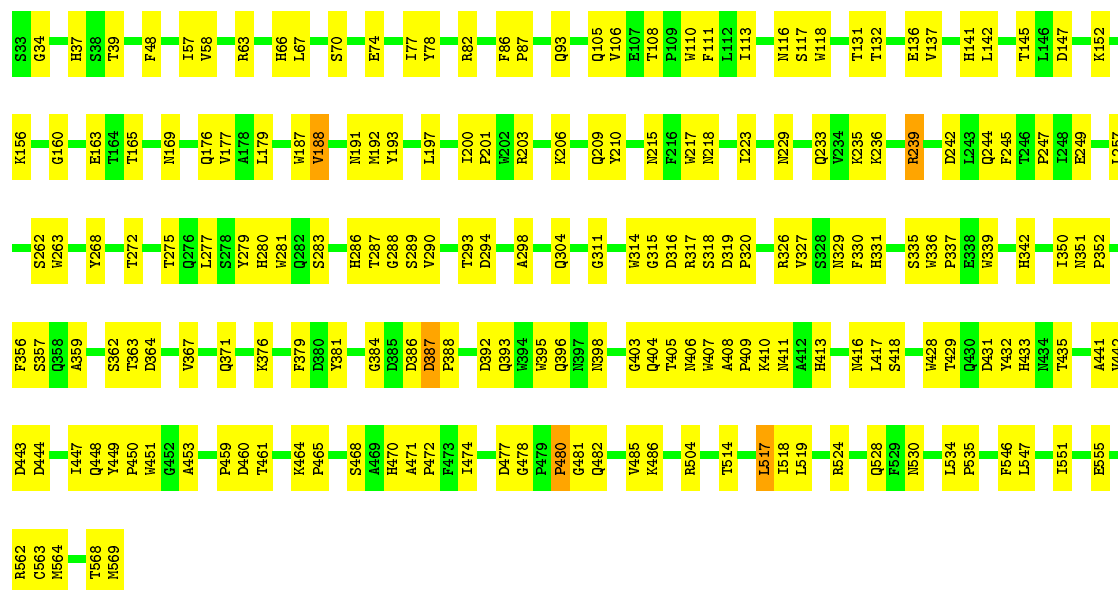
- Molecule 1: VP2





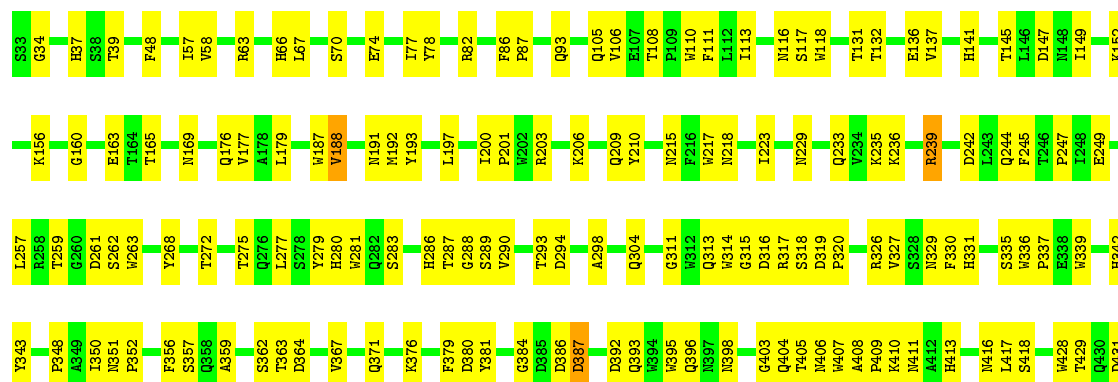
• Molecule 1: VP2

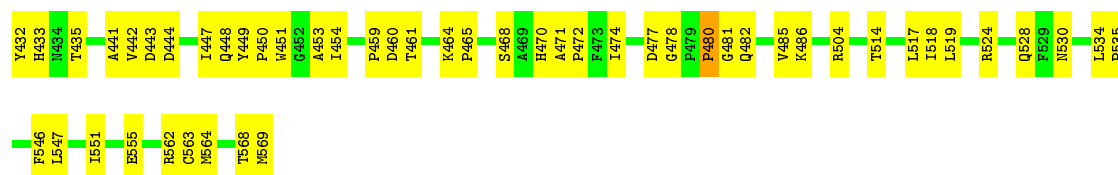
Chain M: •



• Molecule 1: VP2

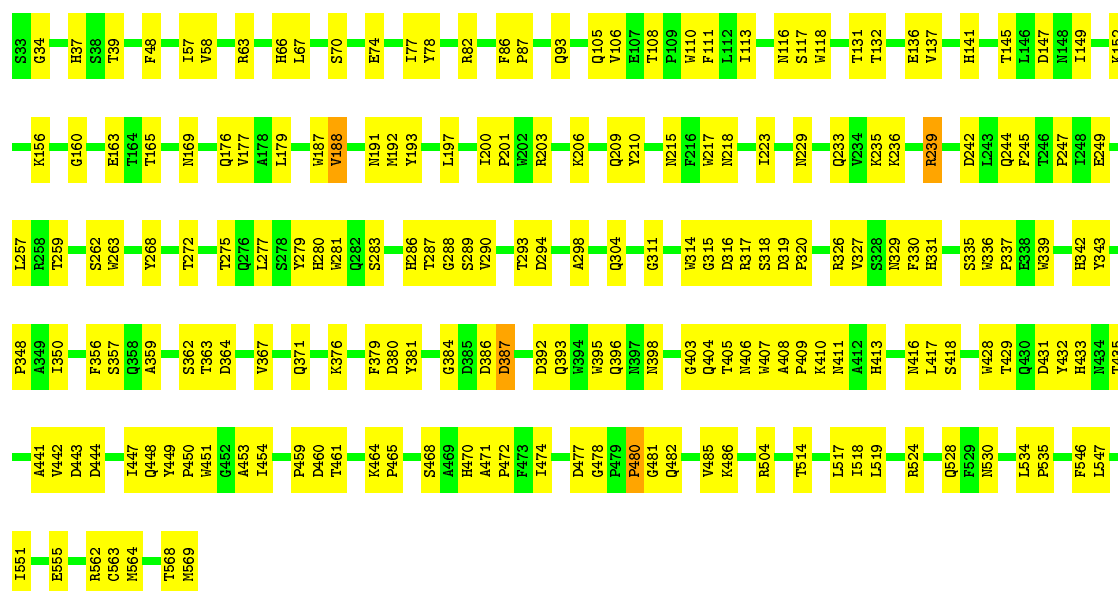
Chain N: •





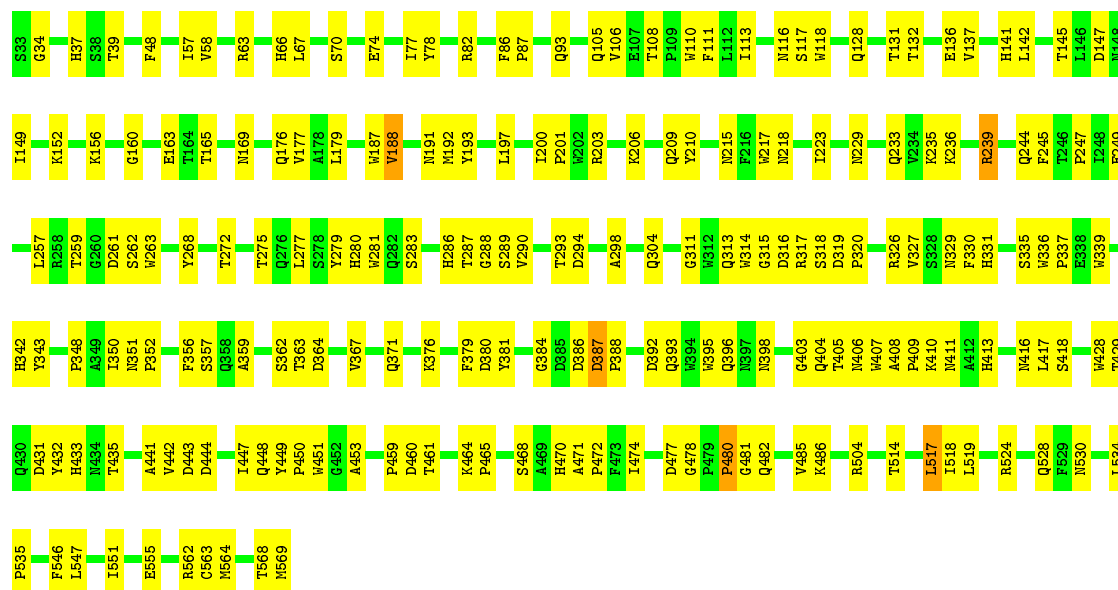
• Molecule 1: VP2

Chain O: 63% 36%



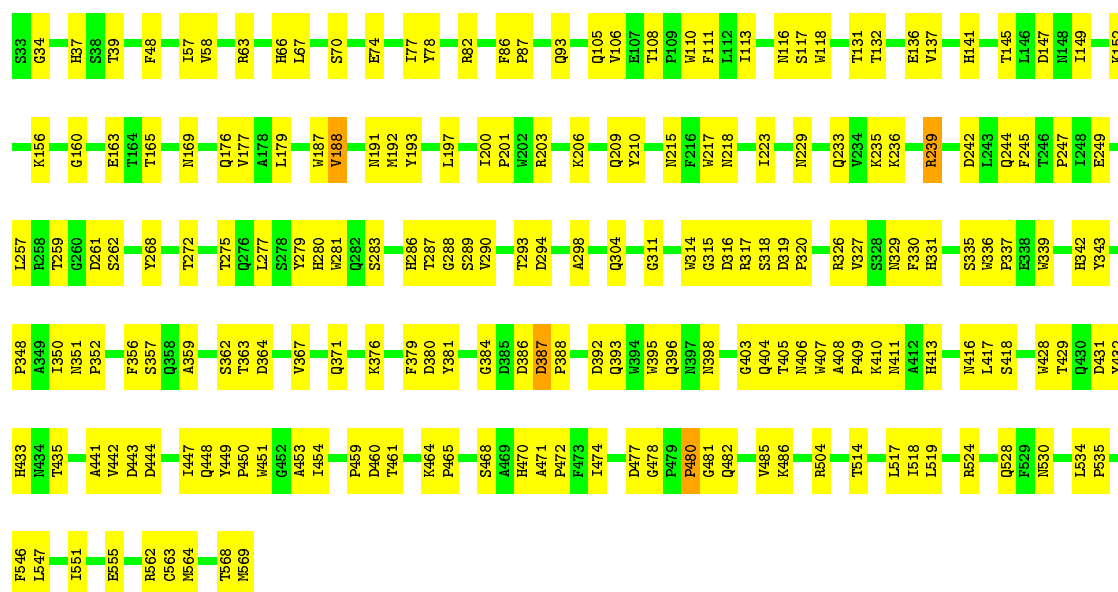
• Molecule 1: VP2

Chain P: 62% 37%



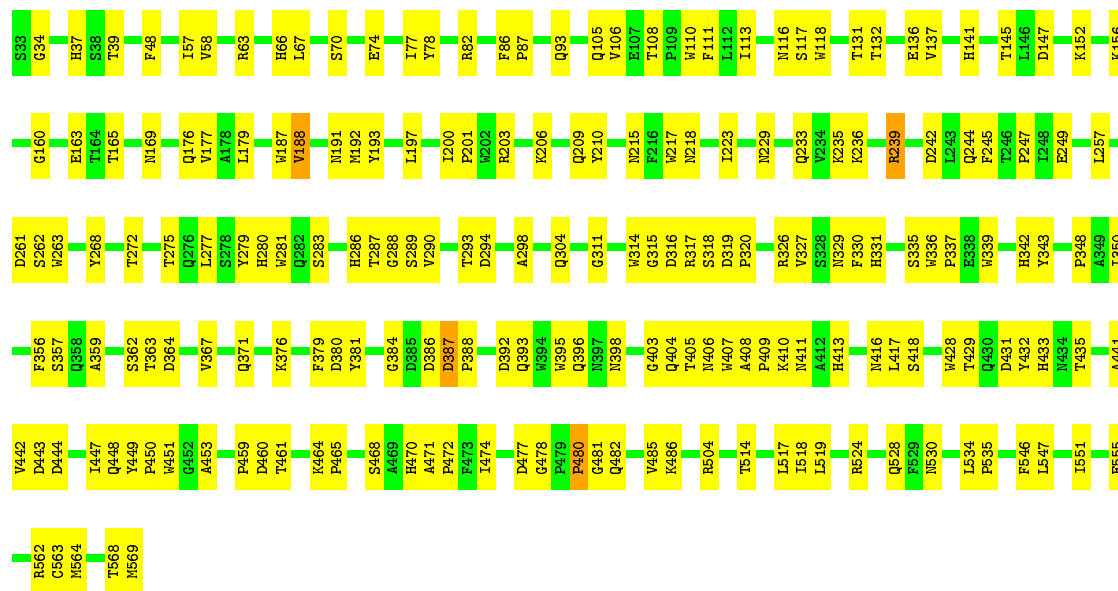
• Molecule 1: VP2

Chain Q:  63% 36%



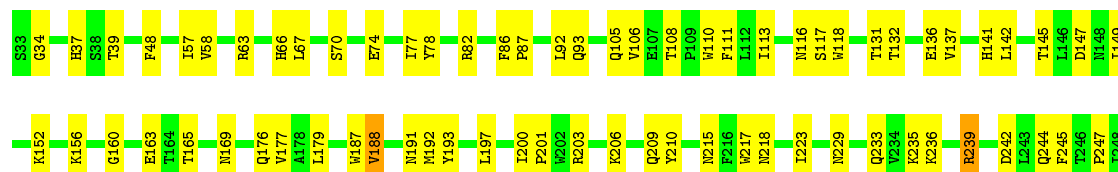
• Molecule 1: VP2

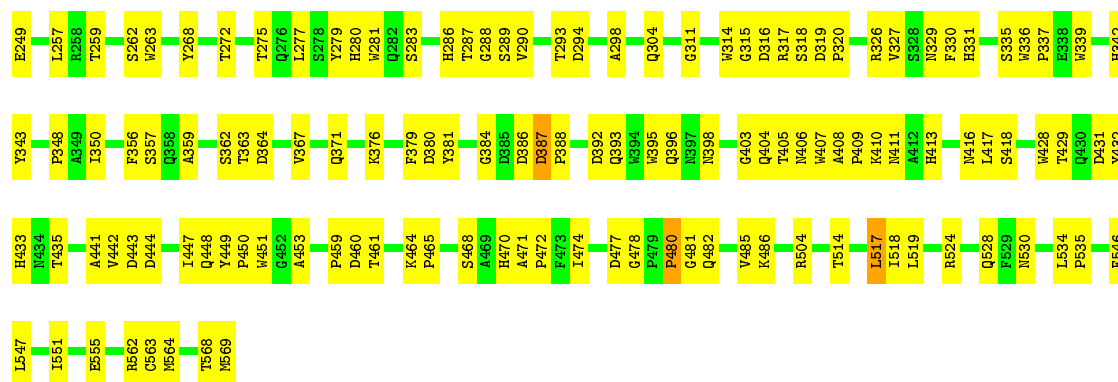
Chain R:  64% 36%



• Molecule 1: VP2

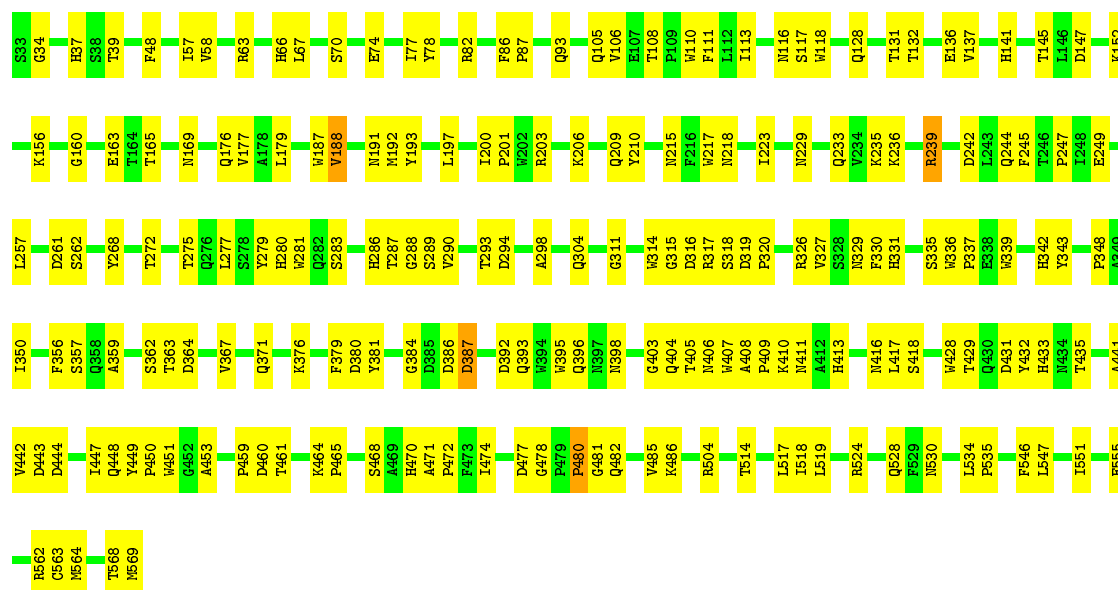
Chain S:  63% 36%





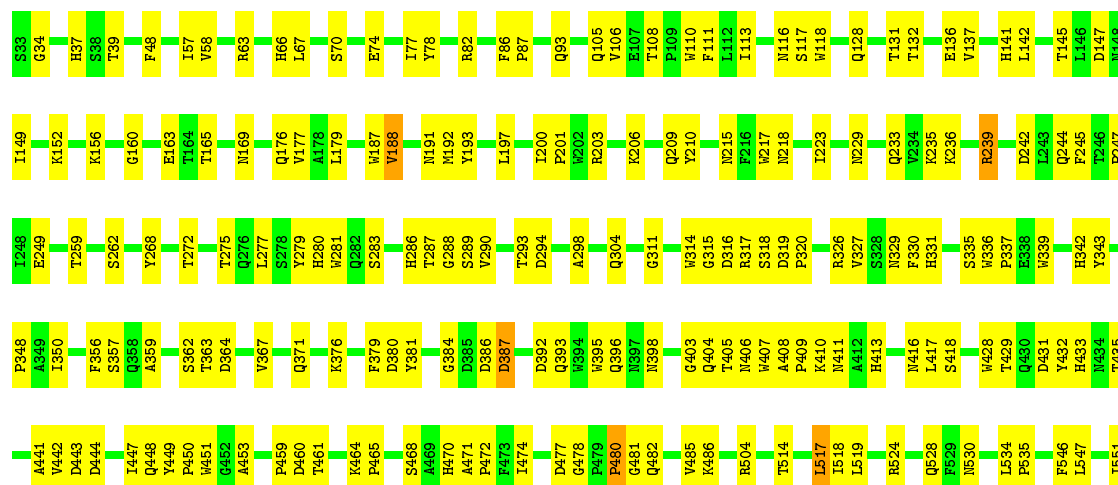
• Molecule 1: VP2

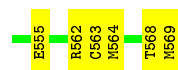
Chain T: 64% 36%



• Molecule 1: VP2

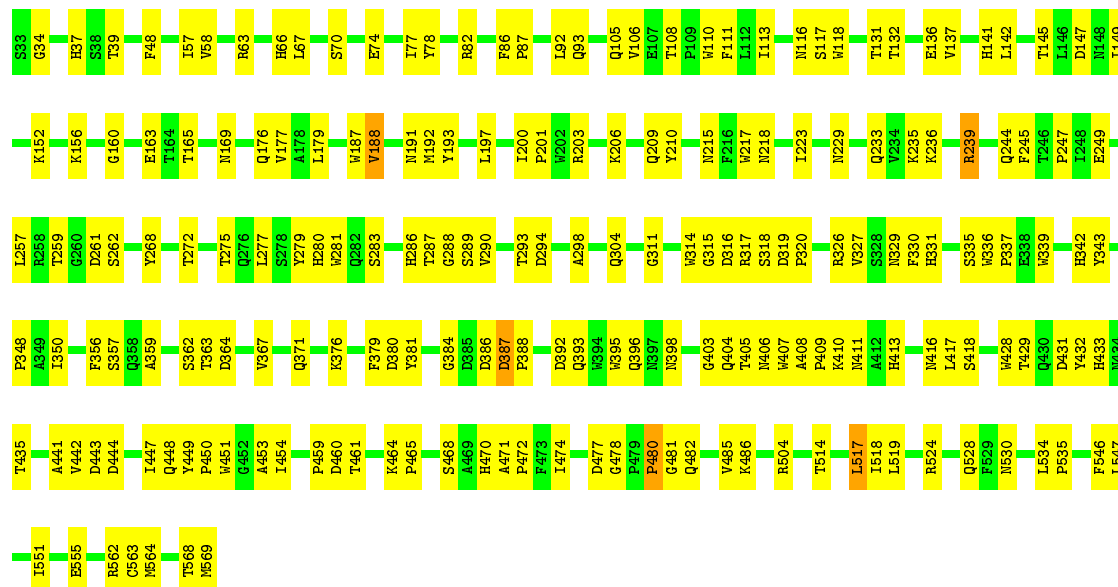
Chain U: 64% 36%





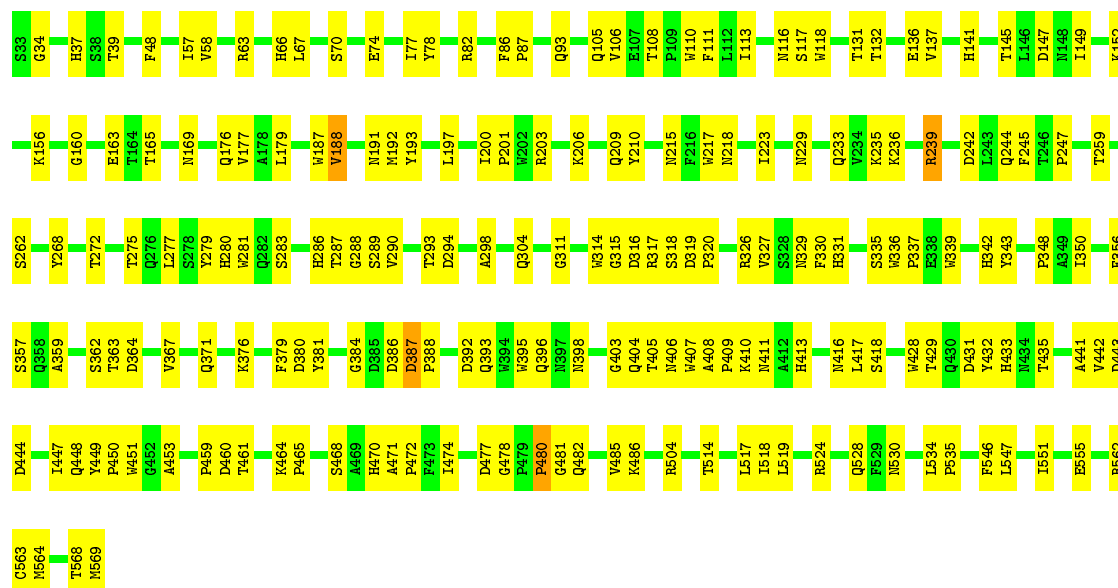
• Molecule 1: VP2

Chain V: 63% 36%



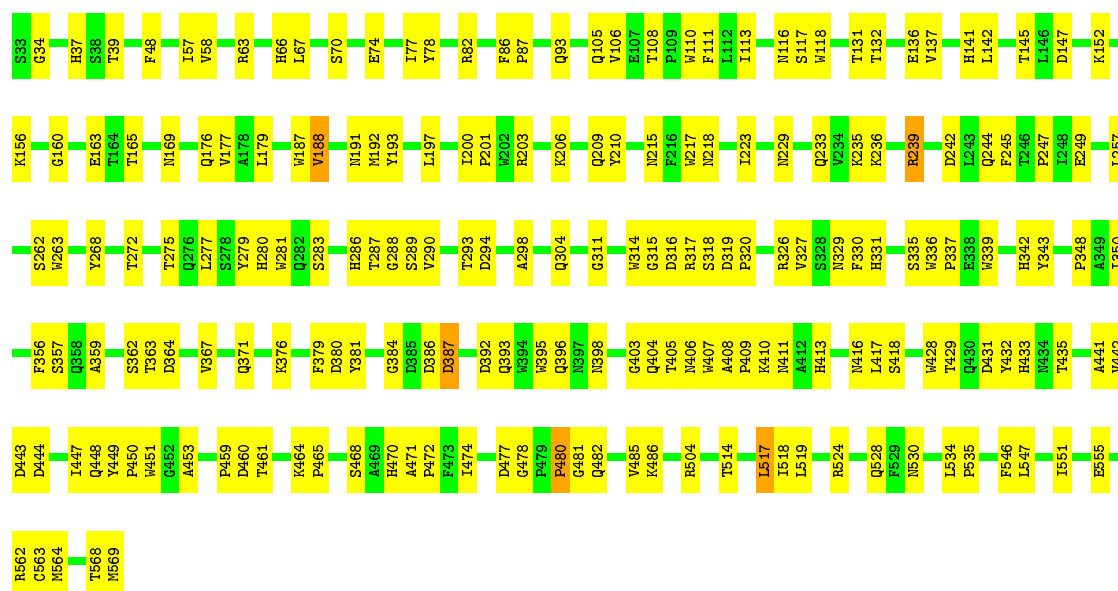
• Molecule 1: VP2

Chain W: 64% 35%



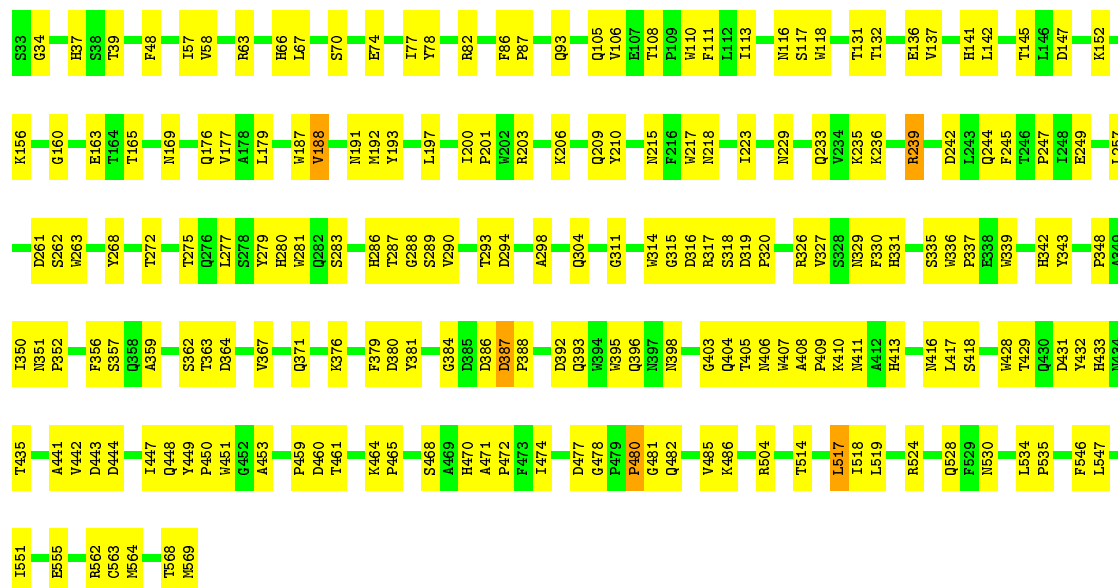
• Molecule 1: VP2

Chain X: 64% 35%



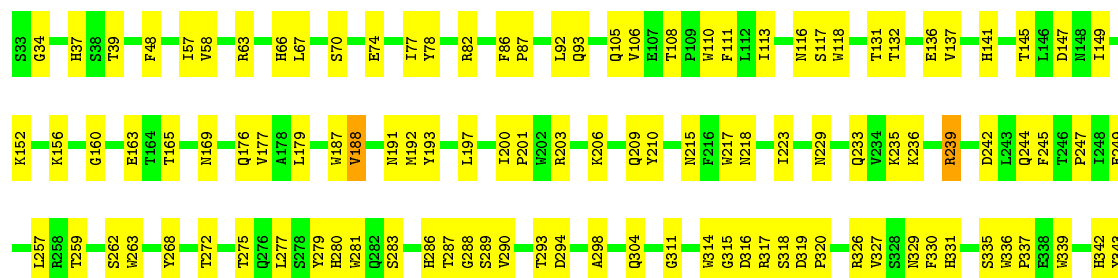
• Molecule 1: VP2

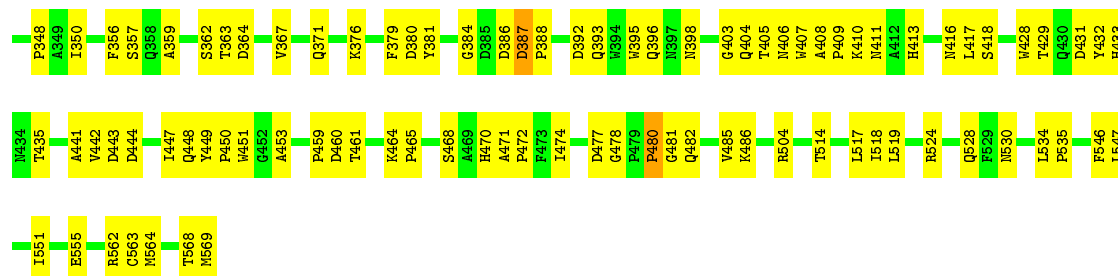
Chain Y: 63% 36% .



• Molecule 1: VP2

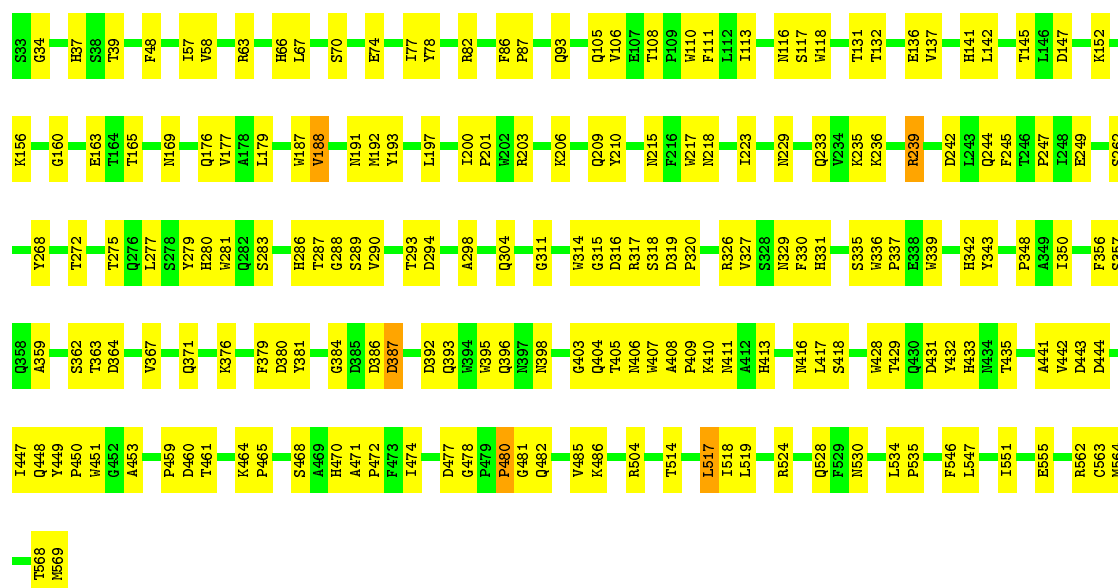
Chain Z: 63% 36% .





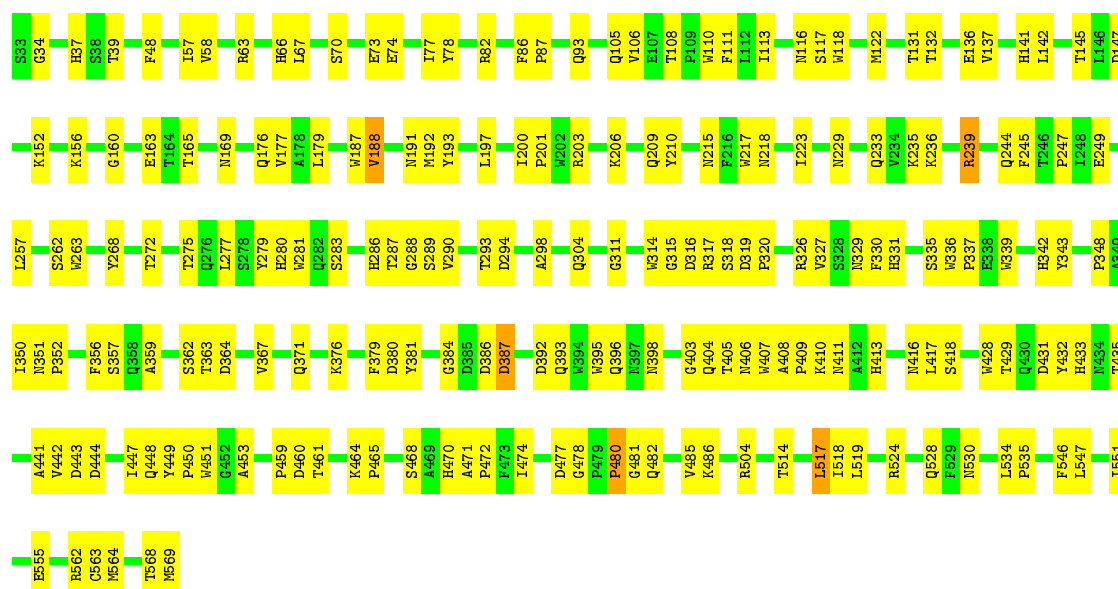
• Molecule 1: VP2

Chain 1: 64% 35%

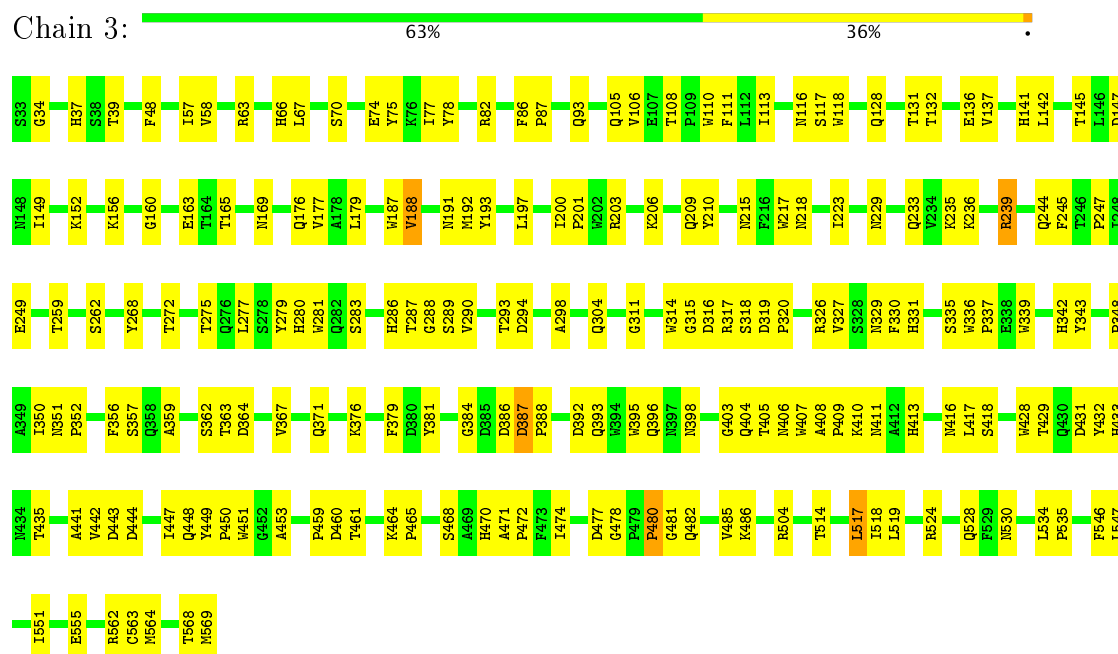


• Molecule 1: VP2

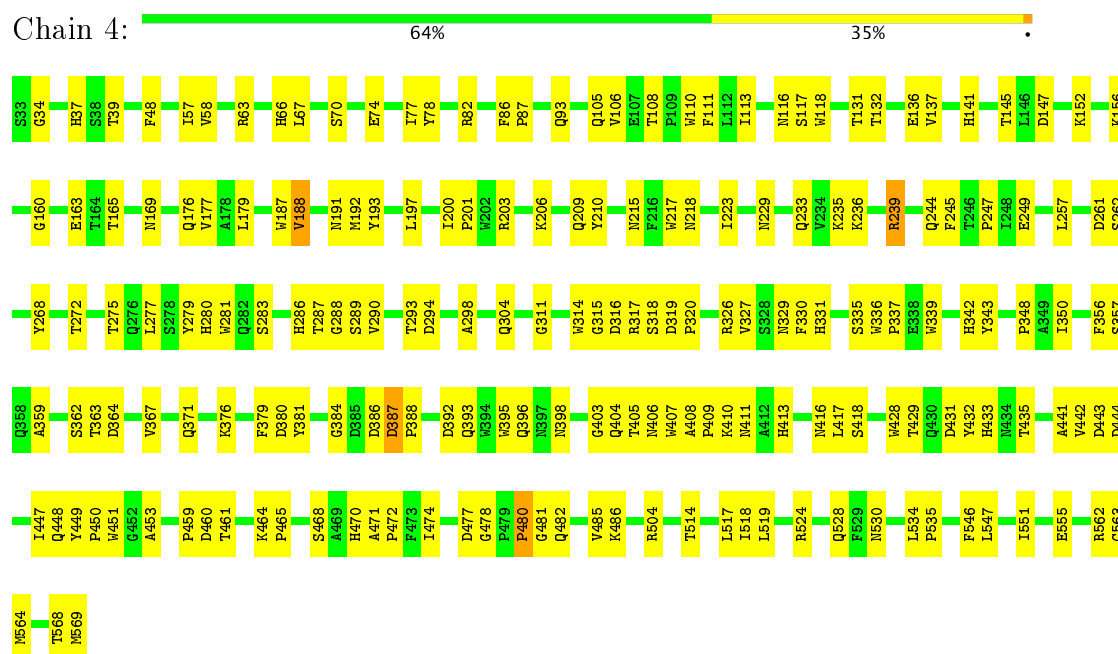
Chain 2: 63% 36%



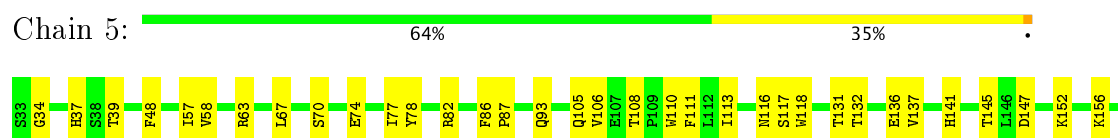
- Molecule 1: VP2

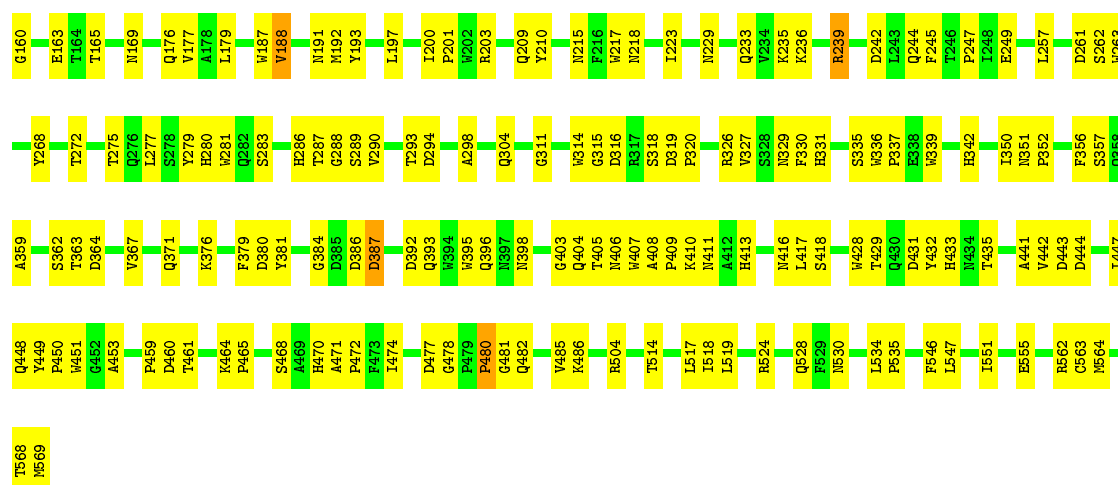


- Molecule 1: VP2



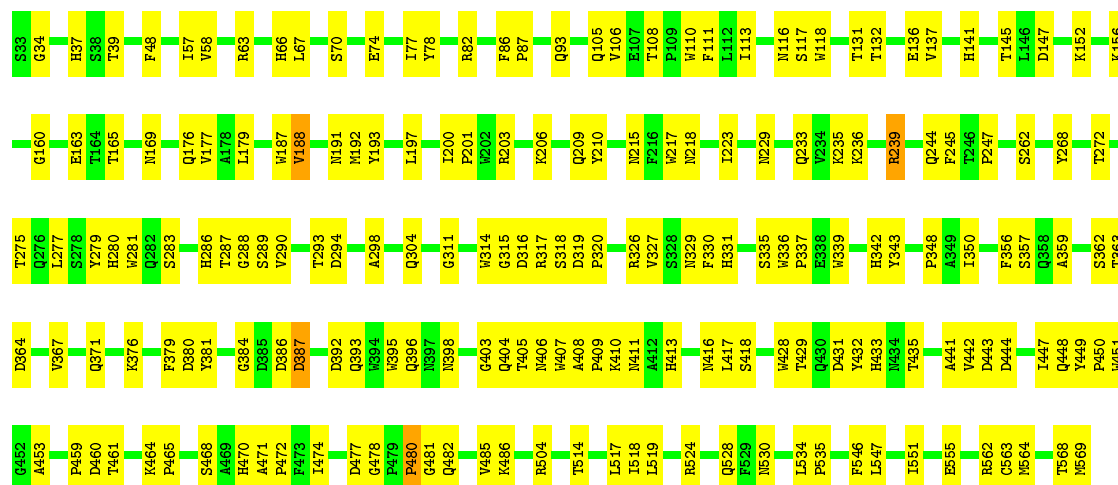
- Molecule 1: VP2





• Molecule 1: VP2

Chain 6: 65% 35% .



• Molecule 1: VP2

Chain a: 98% .



• Molecule 1: VP2

Chain b: 98% .



• Molecule 1: VP2

Chain c: 98% .



- Molecule 1: VP2

Chain d:  98%



- Molecule 1: VP2

Chain e:  98%



- Molecule 1: VP2

Chain f:  98%



- Molecule 1: VP2

Chain g:  98%



- Molecule 1: VP2

Chain h:  98%



- Molecule 1: VP2

Chain i:  98%



- Molecule 1: VP2

Chain j:  98%



• Molecule 1: VP2

Chain k:  98%

• Molecule 1: VP2

Chain l:  98%

• Molecule 1: VP2

Chain m:  98%

• Molecule 1: VP2

Chain n:  98%

• Molecule 1: VP2

Chain o:  98%

• Molecule 1: VP2

Chain p:  98%

• Molecule 1: VP2

Chain q:  98%

• Molecule 1: VP2

Chain r:  98%



- Molecule 1: VP2

Chain s:  98%



- Molecule 1: VP2

Chain t:  98%



- Molecule 1: VP2

Chain u:  98%



- Molecule 1: VP2

Chain v:  98%



- Molecule 1: VP2

Chain w:  98%



- Molecule 1: VP2

Chain x:  98%



- Molecule 1: VP2

Chain y:  98%



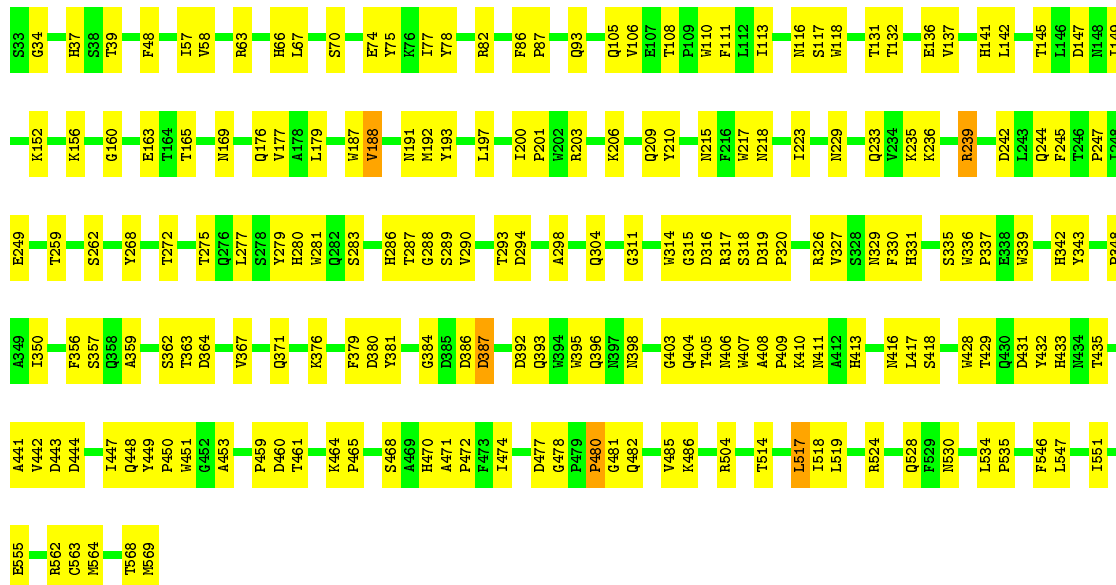
- Molecule 1: VP2

Chain z:  98%



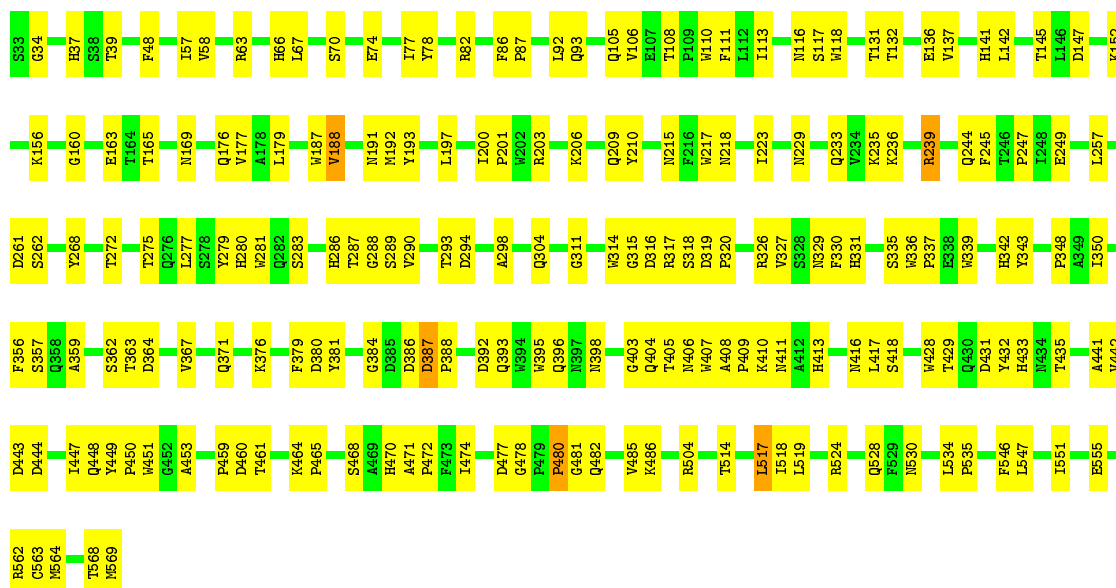
- Molecule 1: VP2

Chain 7:  64%  36%



- Molecule 1: VP2

Chain 0:  64%  36%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	29596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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 >2	RMSZ	# Z >2
1	0	0.49	0/4500	0.60	4/6156 (0.1%)
1	1	0.49	0/4500	0.60	4/6156 (0.1%)
1	2	0.49	0/4500	0.60	4/6156 (0.1%)
1	3	0.49	0/4500	0.60	4/6156 (0.1%)
1	4	0.49	0/4500	0.60	4/6156 (0.1%)
1	5	0.49	0/4500	0.60	4/6156 (0.1%)
1	6	0.49	0/4500	0.60	4/6156 (0.1%)
1	7	0.49	0/4500	0.60	4/6156 (0.1%)
1	A	0.49	0/4500	0.60	4/6156 (0.1%)
1	B	0.49	0/4500	0.60	4/6156 (0.1%)
1	C	0.49	0/4500	0.60	4/6156 (0.1%)
1	D	0.49	0/4500	0.60	4/6156 (0.1%)
1	E	0.49	0/4500	0.60	4/6156 (0.1%)
1	F	0.49	0/4500	0.60	4/6156 (0.1%)
1	G	0.49	0/4500	0.60	4/6156 (0.1%)
1	H	0.49	0/4500	0.60	4/6156 (0.1%)
1	I	0.49	0/4500	0.60	4/6156 (0.1%)
1	J	0.49	0/4500	0.60	4/6156 (0.1%)
1	K	0.49	0/4500	0.60	4/6156 (0.1%)
1	L	0.49	0/4500	0.60	4/6156 (0.1%)
1	M	0.49	0/4500	0.60	4/6156 (0.1%)
1	N	0.49	0/4500	0.60	4/6156 (0.1%)
1	O	0.49	0/4500	0.60	4/6156 (0.1%)
1	P	0.49	0/4500	0.60	4/6156 (0.1%)
1	Q	0.49	0/4500	0.60	4/6156 (0.1%)
1	R	0.49	0/4500	0.60	4/6156 (0.1%)
1	S	0.49	0/4500	0.60	4/6156 (0.1%)
1	T	0.49	0/4500	0.60	4/6156 (0.1%)
1	U	0.49	0/4500	0.60	4/6156 (0.1%)
1	V	0.49	0/4500	0.60	4/6156 (0.1%)
1	W	0.49	0/4500	0.60	4/6156 (0.1%)
1	X	0.49	0/4500	0.60	4/6156 (0.1%)
1	Y	0.49	0/4500	0.60	4/6156 (0.1%)
1	Z	0.49	0/4500	0.60	4/6156 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.49	0/4500	0.60	4/6156 (0.1%)
1	b	0.49	0/4500	0.60	4/6156 (0.1%)
1	c	0.49	0/4500	0.60	4/6156 (0.1%)
1	d	0.49	0/4500	0.60	4/6156 (0.1%)
1	e	0.49	0/4500	0.60	4/6156 (0.1%)
1	f	0.49	0/4500	0.60	4/6156 (0.1%)
1	g	0.49	0/4500	0.60	4/6156 (0.1%)
1	h	0.49	0/4500	0.60	4/6156 (0.1%)
1	i	0.49	0/4500	0.60	4/6156 (0.1%)
1	j	0.49	0/4500	0.60	4/6156 (0.1%)
1	k	0.49	0/4500	0.60	4/6156 (0.1%)
1	l	0.49	0/4500	0.60	4/6156 (0.1%)
1	m	0.49	0/4500	0.60	4/6156 (0.1%)
1	n	0.49	0/4500	0.60	4/6156 (0.1%)
1	o	0.49	0/4500	0.60	4/6156 (0.1%)
1	p	0.49	0/4500	0.60	4/6156 (0.1%)
1	q	0.49	0/4500	0.60	4/6156 (0.1%)
1	r	0.49	0/4500	0.60	4/6156 (0.1%)
1	s	0.49	0/4500	0.60	4/6156 (0.1%)
1	t	0.49	0/4500	0.60	4/6156 (0.1%)
1	u	0.49	0/4500	0.60	4/6156 (0.1%)
1	v	0.49	0/4500	0.60	4/6156 (0.1%)
1	w	0.49	0/4500	0.60	4/6156 (0.1%)
1	x	0.49	0/4500	0.60	4/6156 (0.1%)
1	y	0.49	0/4500	0.60	4/6156 (0.1%)
1	z	0.49	0/4500	0.60	4/6156 (0.1%)
All	All	0.49	0/270000	0.60	240/369360 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1
1	1	0	1
1	2	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	R	0	1
1	S	0	1
1	T	0	1
1	U	0	1
1	V	0	1
1	W	0	1
1	X	0	1
1	Y	0	1
1	Z	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	d	0	1
1	e	0	1
1	f	0	1
1	g	0	1
1	h	0	1
1	i	0	1
1	j	0	1
1	k	0	1
1	l	0	1
1	m	0	1
1	n	0	1
1	o	0	1
1	p	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	1
1	r	0	1
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	1
1	x	0	1
1	y	0	1
1	z	0	1
All	All	0	60

There are no bond length outliers.

The worst 5 of 240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	293	THR	C-N-CA	-6.01	106.68	121.70
1	0	293	THR	C-N-CA	-6.01	106.68	121.70
1	D	293	THR	C-N-CA	-6.00	106.69	121.70
1	Y	293	THR	C-N-CA	-6.00	106.70	121.70
1	g	293	THR	C-N-CA	-6.00	106.70	121.70

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	PRO	Peptide
1	B	480	PRO	Peptide
1	C	480	PRO	Peptide
1	D	480	PRO	Peptide
1	E	480	PRO	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4353	0	4079	223	0
1	1	4353	0	4079	216	0
1	2	4353	0	4079	221	0
1	3	4353	0	4079	218	0
1	4	4353	0	4079	215	0
1	5	4353	0	4079	218	0
1	6	4353	0	4079	216	0
1	7	4353	0	4079	221	0
1	A	4353	0	4079	297	0
1	B	4353	0	4079	307	0
1	C	4353	0	4079	310	0
1	D	4353	0	4079	307	0
1	E	4353	0	4079	307	0
1	F	4353	0	4079	304	0
1	G	4353	0	4079	309	0
1	H	4353	0	4079	305	0
1	I	4353	0	4079	306	0
1	J	4353	0	4079	305	0
1	K	4353	0	4079	314	0
1	L	4353	0	4079	309	0
1	M	4353	0	4079	306	0
1	N	4353	0	4079	308	0
1	O	4353	0	4079	309	0
1	P	4353	0	4079	306	0
1	Q	4353	0	4079	302	0
1	R	4353	0	4079	270	0
1	S	4353	0	4079	274	0
1	T	4353	0	4079	304	0
1	U	4353	0	4079	303	0
1	V	4353	0	4079	312	0
1	W	4353	0	4079	304	0
1	X	4353	0	4079	300	0
1	Y	4353	0	4079	309	0
1	Z	4353	0	4079	307	0
1	a	4353	0	4079	0	0
1	b	4353	0	4079	0	0
1	c	4353	0	4079	0	0
1	d	4353	0	4079	0	0
1	e	4353	0	4079	0	0
1	f	4353	0	4079	0	0
1	g	4353	0	4079	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	4353	0	4079	0	0
1	i	4353	0	4079	0	0
1	j	4353	0	4079	0	0
1	k	4353	0	4079	0	0
1	l	4353	0	4079	0	0
1	m	4353	0	4079	0	0
1	n	4353	0	4079	0	0
1	o	4353	0	4079	0	0
1	p	4353	0	4079	0	0
1	q	4353	0	4079	0	0
1	r	4353	0	4079	0	0
1	s	4353	0	4079	0	0
1	t	4353	0	4079	0	0
1	u	4353	0	4079	0	0
1	v	4353	0	4079	0	0
1	w	4353	0	4079	0	0
1	x	4353	0	4079	0	0
1	y	4353	0	4079	0	0
1	z	4353	0	4079	0	0
All	All	261180	0	244740	7092	0

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 14.

The worst 5 of 7092 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)
1:3:272:THR:HG22	1:3:474:ILE:O	1.39	1.23
1:S:272:THR:HG22	1:S:474:ILE:O	1.39	1.23
1:F:272:THR:HG22	1:F:474:ILE:O	1.40	1.22
1:Z:272:THR:HG22	1:Z:474:ILE:O	1.39	1.22
1:W:272:THR:HG22	1:W:474:ILE:O	1.39	1.22

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	1	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	2	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	3	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	4	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	5	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	6	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	7	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	A	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	B	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	C	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	D	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	E	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	F	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	G	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	H	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	I	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	J	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	K	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	L	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	M	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	N	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	O	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	P	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	Q	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	S	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	T	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	U	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	V	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	W	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	X	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	Y	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	Z	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	a	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	b	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	c	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	d	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	e	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	f	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	g	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	h	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	i	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	j	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	k	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	l	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	m	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	n	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	o	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	p	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	q	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	r	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	s	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	t	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	u	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	v	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	x	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	y	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
1	z	535/537 (100%)	513 (96%)	21 (4%)	1 (0%)	51	81
All	All	32100/32220 (100%)	30780 (96%)	1260 (4%)	60 (0%)	54	81

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	VAL
1	B	188	VAL
1	C	188	VAL
1	D	188	VAL
1	E	188	VAL

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 PDB entries followed by that with respect to all EM entries.

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	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	1	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	2	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	3	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	4	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	5	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	6	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	7	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	A	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	B	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	C	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	D	473/473 (100%)	470 (99%)	3 (1%)	89	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	F	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	G	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	H	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	I	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	J	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	K	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	L	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	M	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	N	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	O	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	P	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	Q	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	R	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	S	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	T	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	U	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	V	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	W	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	X	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	Y	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	Z	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	a	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	b	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	c	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	d	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	e	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	f	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	g	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	h	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	i	473/473 (100%)	470 (99%)	3 (1%)	89	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	k	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	l	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	m	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	n	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	o	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	p	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	q	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	r	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	s	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	t	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	u	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	v	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	w	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	x	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	y	473/473 (100%)	470 (99%)	3 (1%)	89	96
1	z	473/473 (100%)	470 (99%)	3 (1%)	89	96
All	All	28380/28380 (100%)	28200 (99%)	180 (1%)	89	96

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	239	ARG
1	b	363	THR
1	x	363	THR
1	2	387	ASP
1	5	363	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 998 such sidechains are listed below:

Mol	Chain	Res	Type
1	2	93	GLN
1	b	280	HIS
1	x	244	GLN
1	2	393	GLN

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Mol	Chain	Res	Type
1	5	244	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 ⓘ

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.