



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 3, 2019 – 08:20 PM EST

PDB ID : 6V1G
EMDB ID: : EMD-21011
Title : Genome-containing AAVrh.10
Authors : Mietzsch, M.; Agbandje-McKenna, M.
Deposited on : 2019-11-20
Resolution : 2.98 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

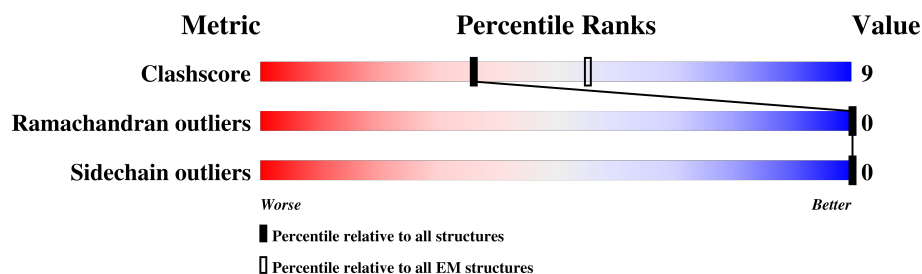
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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.



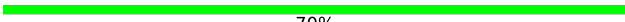
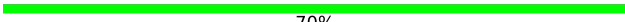
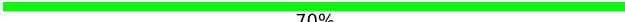
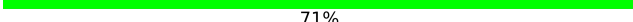
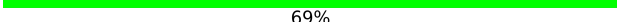
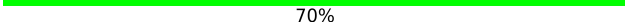
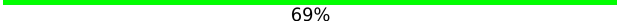
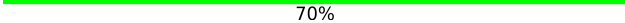
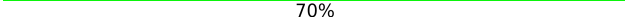
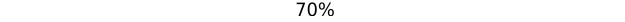
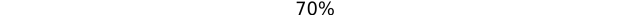
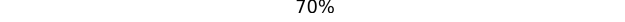
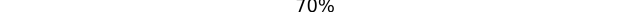
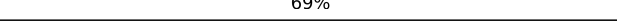
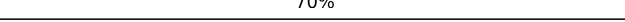
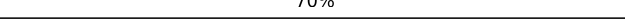
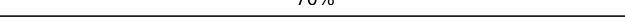
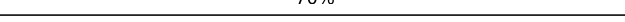
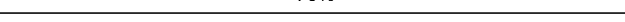






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	1	520	70%	30%
1	2	520	70%	30%
1	3	520	70%	30%
1	4	520	71%	29%
1	5	520	71%	29%
1	6	520	71%	29%
1	7	520	71%	29%
1	8	520	71%	29%
1	A	520	70%	30%
















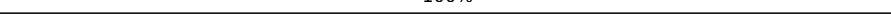
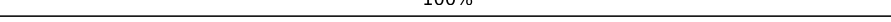
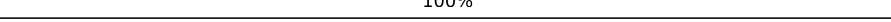

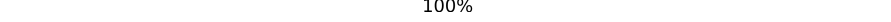
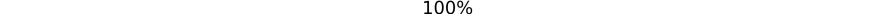
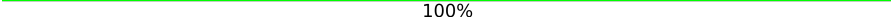
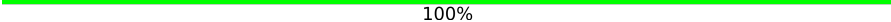


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Mol	Chain	Length	Quality of chain	
1	B	520		30%
1	C	520		30%
1	D	520		30%
1	E	520		29%
1	F	520		31%
1	G	520		30%
1	H	520		31%
1	I	520		30%
1	J	520		30%
1	K	520		30%
1	L	520		30%
1	M	520		30%
1	N	520		30%
1	O	520		31%
1	P	520		30%
1	Q	520		30%
1	R	520		30%
1	S	520		30%
1	T	520		30%
1	U	520		29%
1	V	520		30%
1	W	520		30%
1	X	520		30%
1	Y	520		30%
1	Z	520		31%


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Mol	Chain	Length	Quality of chain
1	a	520	 100%
1	b	520	 100%
1	c	520	 100%
1	d	520	 100%
1	e	520	 100%
1	f	520	 100%
1	g	520	 100%
1	h	520	 100%
1	i	520	 100%
1	j	520	 100%
1	k	520	 100%
1	l	520	 100%
1	m	520	 100%
1	n	520	 100%
1	o	520	 100%
1	p	520	 100%
1	q	520	 100%
1	r	520	 100%
1	s	520	 100%
1	t	520	 100%
1	u	520	 100%
1	v	520	 100%
1	w	520	 100%
1	x	520	 100%
1	y	520	 100%

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Mol	Chain	Length	Quality of chain
1	z	520	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 249900 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	B	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	C	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	D	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	E	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	F	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	G	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	H	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	I	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	J	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	K	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	L	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	M	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	N	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	O	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	P	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	Q	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	S	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	T	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	U	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	V	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	W	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	X	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	Y	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	Z	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	a	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	b	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	c	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	d	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	e	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	f	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	g	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	h	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	i	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	j	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	k	520	Total 4128	C 2608	N 712	O 794	S 14	0	0
1	l	520	Total 4128	C 2608	N 712	O 794	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	n	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	o	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	p	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	q	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	r	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	s	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	t	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	u	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	v	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	w	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	x	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	y	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	z	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	1	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	2	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	3	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	4	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	5	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	6	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		
1	7	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	520	Total	C	N	O	S	0	0
			4128	2608	712	794	14		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LEU	PRO	conflict	UNP Q6JC62
A	406	LEU	ARG	conflict	UNP Q6JC62
A	720	ASP	GLU	conflict	UNP Q6JC62
B	365	LEU	PRO	conflict	UNP Q6JC62
B	406	LEU	ARG	conflict	UNP Q6JC62
B	720	ASP	GLU	conflict	UNP Q6JC62
C	365	LEU	PRO	conflict	UNP Q6JC62
C	406	LEU	ARG	conflict	UNP Q6JC62
C	720	ASP	GLU	conflict	UNP Q6JC62
D	365	LEU	PRO	conflict	UNP Q6JC62
D	406	LEU	ARG	conflict	UNP Q6JC62
D	720	ASP	GLU	conflict	UNP Q6JC62
E	365	LEU	PRO	conflict	UNP Q6JC62
E	406	LEU	ARG	conflict	UNP Q6JC62
E	720	ASP	GLU	conflict	UNP Q6JC62
F	365	LEU	PRO	conflict	UNP Q6JC62
F	406	LEU	ARG	conflict	UNP Q6JC62
F	720	ASP	GLU	conflict	UNP Q6JC62
G	365	LEU	PRO	conflict	UNP Q6JC62
G	406	LEU	ARG	conflict	UNP Q6JC62
G	720	ASP	GLU	conflict	UNP Q6JC62
H	365	LEU	PRO	conflict	UNP Q6JC62
H	406	LEU	ARG	conflict	UNP Q6JC62
H	720	ASP	GLU	conflict	UNP Q6JC62
I	365	LEU	PRO	conflict	UNP Q6JC62
I	406	LEU	ARG	conflict	UNP Q6JC62
I	720	ASP	GLU	conflict	UNP Q6JC62
J	365	LEU	PRO	conflict	UNP Q6JC62
J	406	LEU	ARG	conflict	UNP Q6JC62
J	720	ASP	GLU	conflict	UNP Q6JC62
K	365	LEU	PRO	conflict	UNP Q6JC62
K	406	LEU	ARG	conflict	UNP Q6JC62
K	720	ASP	GLU	conflict	UNP Q6JC62
L	365	LEU	PRO	conflict	UNP Q6JC62
L	406	LEU	ARG	conflict	UNP Q6JC62
L	720	ASP	GLU	conflict	UNP Q6JC62

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Chain	Residue	Modelled	Actual	Comment	Reference
M	365	LEU	PRO	conflict	UNP Q6JC62
M	406	LEU	ARG	conflict	UNP Q6JC62
M	720	ASP	GLU	conflict	UNP Q6JC62
N	365	LEU	PRO	conflict	UNP Q6JC62
N	406	LEU	ARG	conflict	UNP Q6JC62
N	720	ASP	GLU	conflict	UNP Q6JC62
O	365	LEU	PRO	conflict	UNP Q6JC62
O	406	LEU	ARG	conflict	UNP Q6JC62
O	720	ASP	GLU	conflict	UNP Q6JC62
P	365	LEU	PRO	conflict	UNP Q6JC62
P	406	LEU	ARG	conflict	UNP Q6JC62
P	720	ASP	GLU	conflict	UNP Q6JC62
Q	365	LEU	PRO	conflict	UNP Q6JC62
Q	406	LEU	ARG	conflict	UNP Q6JC62
Q	720	ASP	GLU	conflict	UNP Q6JC62
R	365	LEU	PRO	conflict	UNP Q6JC62
R	406	LEU	ARG	conflict	UNP Q6JC62
R	720	ASP	GLU	conflict	UNP Q6JC62
S	365	LEU	PRO	conflict	UNP Q6JC62
S	406	LEU	ARG	conflict	UNP Q6JC62
S	720	ASP	GLU	conflict	UNP Q6JC62
T	365	LEU	PRO	conflict	UNP Q6JC62
T	406	LEU	ARG	conflict	UNP Q6JC62
T	720	ASP	GLU	conflict	UNP Q6JC62
U	365	LEU	PRO	conflict	UNP Q6JC62
U	406	LEU	ARG	conflict	UNP Q6JC62
U	720	ASP	GLU	conflict	UNP Q6JC62
V	365	LEU	PRO	conflict	UNP Q6JC62
V	406	LEU	ARG	conflict	UNP Q6JC62
V	720	ASP	GLU	conflict	UNP Q6JC62
W	365	LEU	PRO	conflict	UNP Q6JC62
W	406	LEU	ARG	conflict	UNP Q6JC62
W	720	ASP	GLU	conflict	UNP Q6JC62
X	365	LEU	PRO	conflict	UNP Q6JC62
X	406	LEU	ARG	conflict	UNP Q6JC62
X	720	ASP	GLU	conflict	UNP Q6JC62
Y	365	LEU	PRO	conflict	UNP Q6JC62
Y	406	LEU	ARG	conflict	UNP Q6JC62
Y	720	ASP	GLU	conflict	UNP Q6JC62
Z	365	LEU	PRO	conflict	UNP Q6JC62
Z	406	LEU	ARG	conflict	UNP Q6JC62
Z	720	ASP	GLU	conflict	UNP Q6JC62

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Chain	Residue	Modelled	Actual	Comment	Reference
a	365	LEU	PRO	conflict	UNP Q6JC62
a	406	LEU	ARG	conflict	UNP Q6JC62
a	720	ASP	GLU	conflict	UNP Q6JC62
b	365	LEU	PRO	conflict	UNP Q6JC62
b	406	LEU	ARG	conflict	UNP Q6JC62
b	720	ASP	GLU	conflict	UNP Q6JC62
c	365	LEU	PRO	conflict	UNP Q6JC62
c	406	LEU	ARG	conflict	UNP Q6JC62
c	720	ASP	GLU	conflict	UNP Q6JC62
d	365	LEU	PRO	conflict	UNP Q6JC62
d	406	LEU	ARG	conflict	UNP Q6JC62
d	720	ASP	GLU	conflict	UNP Q6JC62
e	365	LEU	PRO	conflict	UNP Q6JC62
e	406	LEU	ARG	conflict	UNP Q6JC62
e	720	ASP	GLU	conflict	UNP Q6JC62
f	365	LEU	PRO	conflict	UNP Q6JC62
f	406	LEU	ARG	conflict	UNP Q6JC62
f	720	ASP	GLU	conflict	UNP Q6JC62
g	365	LEU	PRO	conflict	UNP Q6JC62
g	406	LEU	ARG	conflict	UNP Q6JC62
g	720	ASP	GLU	conflict	UNP Q6JC62
h	365	LEU	PRO	conflict	UNP Q6JC62
h	406	LEU	ARG	conflict	UNP Q6JC62
h	720	ASP	GLU	conflict	UNP Q6JC62
i	365	LEU	PRO	conflict	UNP Q6JC62
i	406	LEU	ARG	conflict	UNP Q6JC62
i	720	ASP	GLU	conflict	UNP Q6JC62
j	365	LEU	PRO	conflict	UNP Q6JC62
j	406	LEU	ARG	conflict	UNP Q6JC62
j	720	ASP	GLU	conflict	UNP Q6JC62
k	365	LEU	PRO	conflict	UNP Q6JC62
k	406	LEU	ARG	conflict	UNP Q6JC62
k	720	ASP	GLU	conflict	UNP Q6JC62
l	365	LEU	PRO	conflict	UNP Q6JC62
l	406	LEU	ARG	conflict	UNP Q6JC62
l	720	ASP	GLU	conflict	UNP Q6JC62
m	365	LEU	PRO	conflict	UNP Q6JC62
m	406	LEU	ARG	conflict	UNP Q6JC62
m	720	ASP	GLU	conflict	UNP Q6JC62
n	365	LEU	PRO	conflict	UNP Q6JC62
n	406	LEU	ARG	conflict	UNP Q6JC62
n	720	ASP	GLU	conflict	UNP Q6JC62

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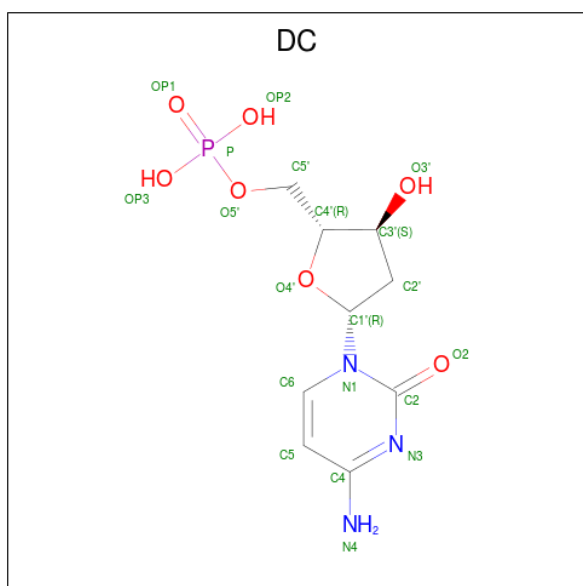
Chain	Residue	Modelled	Actual	Comment	Reference
o	365	LEU	PRO	conflict	UNP Q6JC62
o	406	LEU	ARG	conflict	UNP Q6JC62
o	720	ASP	GLU	conflict	UNP Q6JC62
p	365	LEU	PRO	conflict	UNP Q6JC62
p	406	LEU	ARG	conflict	UNP Q6JC62
p	720	ASP	GLU	conflict	UNP Q6JC62
q	365	LEU	PRO	conflict	UNP Q6JC62
q	406	LEU	ARG	conflict	UNP Q6JC62
q	720	ASP	GLU	conflict	UNP Q6JC62
r	365	LEU	PRO	conflict	UNP Q6JC62
r	406	LEU	ARG	conflict	UNP Q6JC62
r	720	ASP	GLU	conflict	UNP Q6JC62
s	365	LEU	PRO	conflict	UNP Q6JC62
s	406	LEU	ARG	conflict	UNP Q6JC62
s	720	ASP	GLU	conflict	UNP Q6JC62
t	365	LEU	PRO	conflict	UNP Q6JC62
t	406	LEU	ARG	conflict	UNP Q6JC62
t	720	ASP	GLU	conflict	UNP Q6JC62
u	365	LEU	PRO	conflict	UNP Q6JC62
u	406	LEU	ARG	conflict	UNP Q6JC62
u	720	ASP	GLU	conflict	UNP Q6JC62
v	365	LEU	PRO	conflict	UNP Q6JC62
v	406	LEU	ARG	conflict	UNP Q6JC62
v	720	ASP	GLU	conflict	UNP Q6JC62
w	365	LEU	PRO	conflict	UNP Q6JC62
w	406	LEU	ARG	conflict	UNP Q6JC62
w	720	ASP	GLU	conflict	UNP Q6JC62
x	365	LEU	PRO	conflict	UNP Q6JC62
x	406	LEU	ARG	conflict	UNP Q6JC62
x	720	ASP	GLU	conflict	UNP Q6JC62
y	365	LEU	PRO	conflict	UNP Q6JC62
y	406	LEU	ARG	conflict	UNP Q6JC62
y	720	ASP	GLU	conflict	UNP Q6JC62
z	365	LEU	PRO	conflict	UNP Q6JC62
z	406	LEU	ARG	conflict	UNP Q6JC62
z	720	ASP	GLU	conflict	UNP Q6JC62
1	365	LEU	PRO	conflict	UNP Q6JC62
1	406	LEU	ARG	conflict	UNP Q6JC62
1	720	ASP	GLU	conflict	UNP Q6JC62
2	365	LEU	PRO	conflict	UNP Q6JC62
2	406	LEU	ARG	conflict	UNP Q6JC62
2	720	ASP	GLU	conflict	UNP Q6JC62

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Chain	Residue	Modelled	Actual	Comment	Reference
3	365	LEU	PRO	conflict	UNP Q6JC62
3	406	LEU	ARG	conflict	UNP Q6JC62
3	720	ASP	GLU	conflict	UNP Q6JC62
4	365	LEU	PRO	conflict	UNP Q6JC62
4	406	LEU	ARG	conflict	UNP Q6JC62
4	720	ASP	GLU	conflict	UNP Q6JC62
5	365	LEU	PRO	conflict	UNP Q6JC62
5	406	LEU	ARG	conflict	UNP Q6JC62
5	720	ASP	GLU	conflict	UNP Q6JC62
6	365	LEU	PRO	conflict	UNP Q6JC62
6	406	LEU	ARG	conflict	UNP Q6JC62
6	720	ASP	GLU	conflict	UNP Q6JC62
7	365	LEU	PRO	conflict	UNP Q6JC62
7	406	LEU	ARG	conflict	UNP Q6JC62
7	720	ASP	GLU	conflict	UNP Q6JC62
8	365	LEU	PRO	conflict	UNP Q6JC62
8	406	LEU	ARG	conflict	UNP Q6JC62
8	720	ASP	GLU	conflict	UNP Q6JC62

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DC) (formula: $C_9H_{14}N_3O_7P$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			16	9	3	4	
2	B	1	Total	C	N	O	0
			16	9	3	4	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total 16	C 9	N 3	O 4	0
2	D	1	Total 16	C 9	N 3	O 4	0
2	E	1	Total 16	C 9	N 3	O 4	0
2	F	1	Total 16	C 9	N 3	O 4	0
2	G	1	Total 16	C 9	N 3	O 4	0
2	H	1	Total 16	C 9	N 3	O 4	0
2	I	1	Total 16	C 9	N 3	O 4	0
2	J	1	Total 16	C 9	N 3	O 4	0
2	K	1	Total 16	C 9	N 3	O 4	0
2	L	1	Total 16	C 9	N 3	O 4	0
2	M	1	Total 16	C 9	N 3	O 4	0
2	N	1	Total 16	C 9	N 3	O 4	0
2	O	1	Total 16	C 9	N 3	O 4	0
2	P	1	Total 16	C 9	N 3	O 4	0
2	Q	1	Total 16	C 9	N 3	O 4	0
2	R	1	Total 16	C 9	N 3	O 4	0
2	S	1	Total 16	C 9	N 3	O 4	0
2	T	1	Total 16	C 9	N 3	O 4	0
2	U	1	Total 16	C 9	N 3	O 4	0
2	V	1	Total 16	C 9	N 3	O 4	0
2	W	1	Total 16	C 9	N 3	O 4	0

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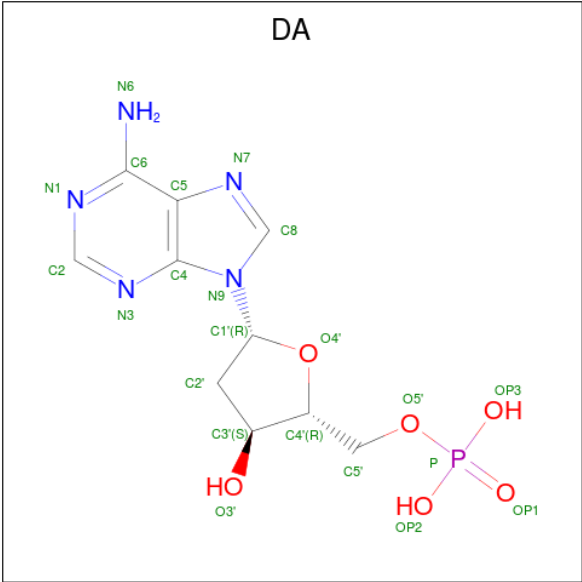
Mol	Chain	Residues	Atoms				AltConf
2	X	1	Total	C	N	O	0
			16	9	3	4	
2	Y	1	Total	C	N	O	0
			16	9	3	4	
2	Z	1	Total	C	N	O	0
			16	9	3	4	
2	a	1	Total	C	N	O	0
			16	9	3	4	
2	b	1	Total	C	N	O	0
			16	9	3	4	
2	c	1	Total	C	N	O	0
			16	9	3	4	
2	d	1	Total	C	N	O	0
			16	9	3	4	
2	e	1	Total	C	N	O	0
			16	9	3	4	
2	f	1	Total	C	N	O	0
			16	9	3	4	
2	g	1	Total	C	N	O	0
			16	9	3	4	
2	h	1	Total	C	N	O	0
			16	9	3	4	
2	i	1	Total	C	N	O	0
			16	9	3	4	
2	j	1	Total	C	N	O	0
			16	9	3	4	
2	k	1	Total	C	N	O	0
			16	9	3	4	
2	l	1	Total	C	N	O	0
			16	9	3	4	
2	m	1	Total	C	N	O	0
			16	9	3	4	
2	n	1	Total	C	N	O	0
			16	9	3	4	
2	o	1	Total	C	N	O	0
			16	9	3	4	
2	p	1	Total	C	N	O	0
			16	9	3	4	
2	q	1	Total	C	N	O	0
			16	9	3	4	
2	r	1	Total	C	N	O	0
			16	9	3	4	

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Mol	Chain	Residues	Atoms				AltConf
2	s	1	Total	C	N	O	0
			16	9	3	4	
2	t	1	Total	C	N	O	0
			16	9	3	4	
2	u	1	Total	C	N	O	0
			16	9	3	4	
2	v	1	Total	C	N	O	0
			16	9	3	4	
2	w	1	Total	C	N	O	0
			16	9	3	4	
2	x	1	Total	C	N	O	0
			16	9	3	4	
2	y	1	Total	C	N	O	0
			16	9	3	4	
2	z	1	Total	C	N	O	0
			16	9	3	4	
2	1	1	Total	C	N	O	0
			16	9	3	4	
2	2	1	Total	C	N	O	0
			16	9	3	4	
2	3	1	Total	C	N	O	0
			16	9	3	4	
2	4	1	Total	C	N	O	0
			16	9	3	4	
2	5	1	Total	C	N	O	0
			16	9	3	4	
2	6	1	Total	C	N	O	0
			16	9	3	4	
2	7	1	Total	C	N	O	0
			16	9	3	4	
2	8	1	Total	C	N	O	0
			16	9	3	4	

- Molecule 3 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: DA) (formula: C₁₀H₁₄N₅O₆P).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	B	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	C	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	D	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	E	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	F	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	G	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	H	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	I	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	J	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	K	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	L	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	M	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	N	1	Total	C	N	O	P	0
			21	10	5	5	1	

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Mol	Chain	Residues	Atoms					AltConf
3	O	1	Total 21	C 10	N 5	O 5	P 1	0
3	P	1	Total 21	C 10	N 5	O 5	P 1	0
3	Q	1	Total 21	C 10	N 5	O 5	P 1	0
3	R	1	Total 21	C 10	N 5	O 5	P 1	0
3	S	1	Total 21	C 10	N 5	O 5	P 1	0
3	T	1	Total 21	C 10	N 5	O 5	P 1	0
3	U	1	Total 21	C 10	N 5	O 5	P 1	0
3	V	1	Total 21	C 10	N 5	O 5	P 1	0
3	W	1	Total 21	C 10	N 5	O 5	P 1	0
3	X	1	Total 21	C 10	N 5	O 5	P 1	0
3	Y	1	Total 21	C 10	N 5	O 5	P 1	0
3	Z	1	Total 21	C 10	N 5	O 5	P 1	0
3	a	1	Total 21	C 10	N 5	O 5	P 1	0
3	b	1	Total 21	C 10	N 5	O 5	P 1	0
3	c	1	Total 21	C 10	N 5	O 5	P 1	0
3	d	1	Total 21	C 10	N 5	O 5	P 1	0
3	e	1	Total 21	C 10	N 5	O 5	P 1	0
3	f	1	Total 21	C 10	N 5	O 5	P 1	0
3	g	1	Total 21	C 10	N 5	O 5	P 1	0
3	h	1	Total 21	C 10	N 5	O 5	P 1	0
3	i	1	Total 21	C 10	N 5	O 5	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
3	j	1	Total 21	C 10	N 5	O 5	P 1	0
3	k	1	Total 21	C 10	N 5	O 5	P 1	0
3	l	1	Total 21	C 10	N 5	O 5	P 1	0
3	m	1	Total 21	C 10	N 5	O 5	P 1	0
3	n	1	Total 21	C 10	N 5	O 5	P 1	0
3	o	1	Total 21	C 10	N 5	O 5	P 1	0
3	p	1	Total 21	C 10	N 5	O 5	P 1	0
3	q	1	Total 21	C 10	N 5	O 5	P 1	0
3	r	1	Total 21	C 10	N 5	O 5	P 1	0
3	s	1	Total 21	C 10	N 5	O 5	P 1	0
3	t	1	Total 21	C 10	N 5	O 5	P 1	0
3	u	1	Total 21	C 10	N 5	O 5	P 1	0
3	v	1	Total 21	C 10	N 5	O 5	P 1	0
3	w	1	Total 21	C 10	N 5	O 5	P 1	0
3	x	1	Total 21	C 10	N 5	O 5	P 1	0
3	y	1	Total 21	C 10	N 5	O 5	P 1	0
3	z	1	Total 21	C 10	N 5	O 5	P 1	0
3	1	1	Total 21	C 10	N 5	O 5	P 1	0
3	2	1	Total 21	C 10	N 5	O 5	P 1	0
3	3	1	Total 21	C 10	N 5	O 5	P 1	0
3	4	1	Total 21	C 10	N 5	O 5	P 1	0

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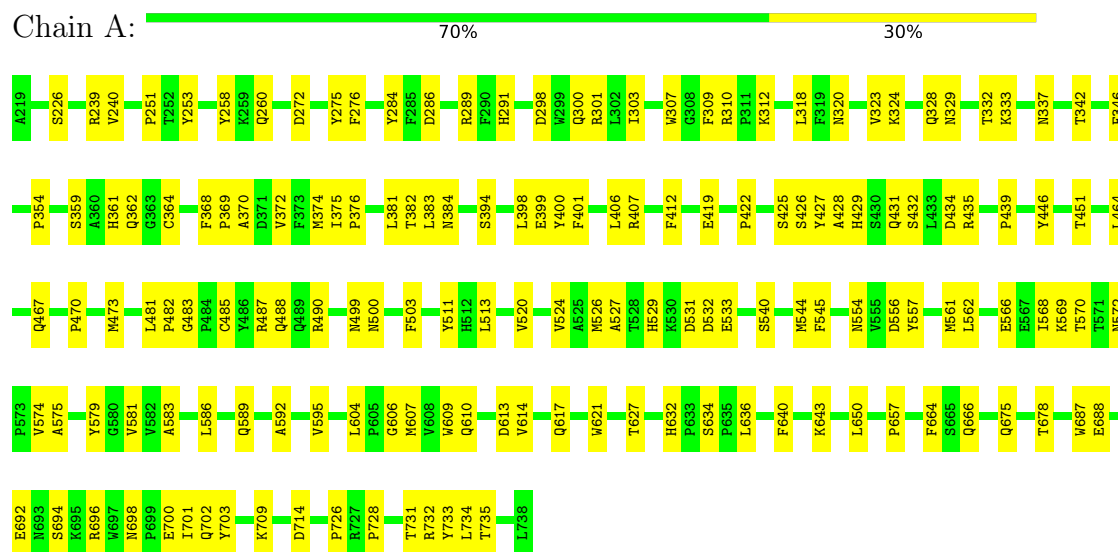
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Mol	Chain	Residues	Atoms					AltConf
3	5	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	6	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	7	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	8	1	Total	C	N	O	P	0
			21	10	5	5	1	

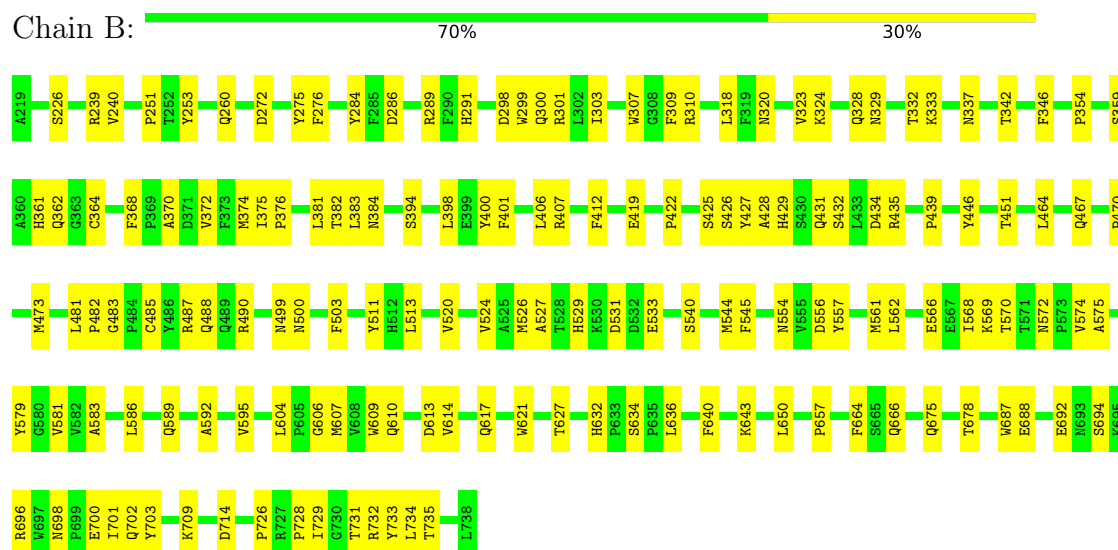
3 Residue-property plots

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.

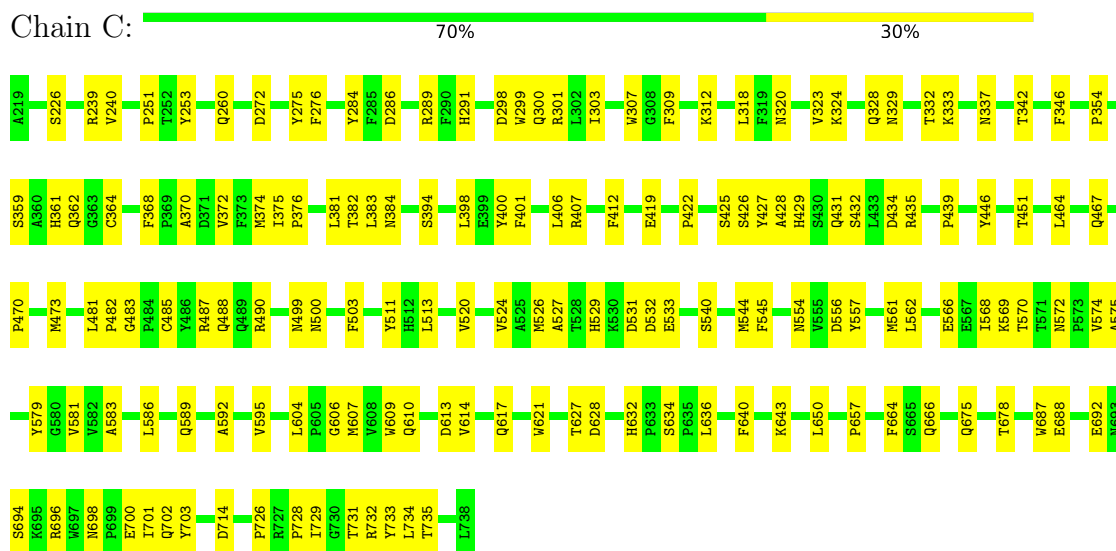
• Molecule 1: Capsid protein VP1



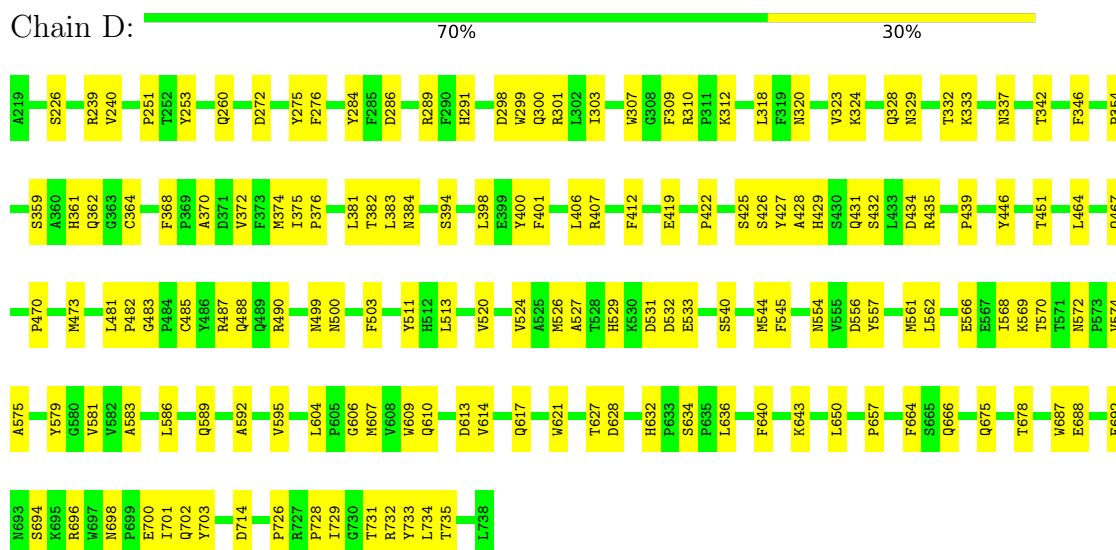
• Molecule 1: Capsid protein VP1



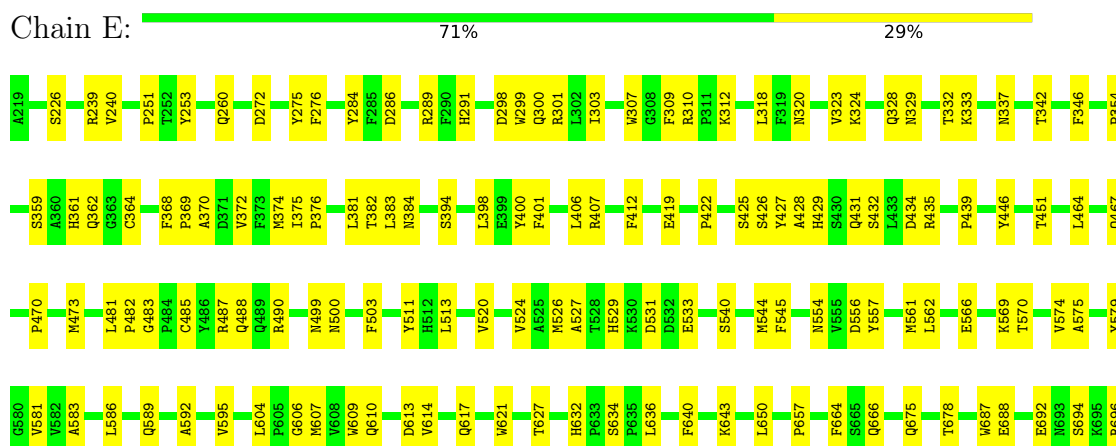
• Molecule 1: Capsid protein VP1

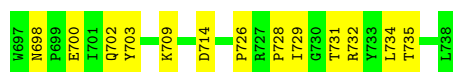


• Molecule 1: Capsid protein VP1



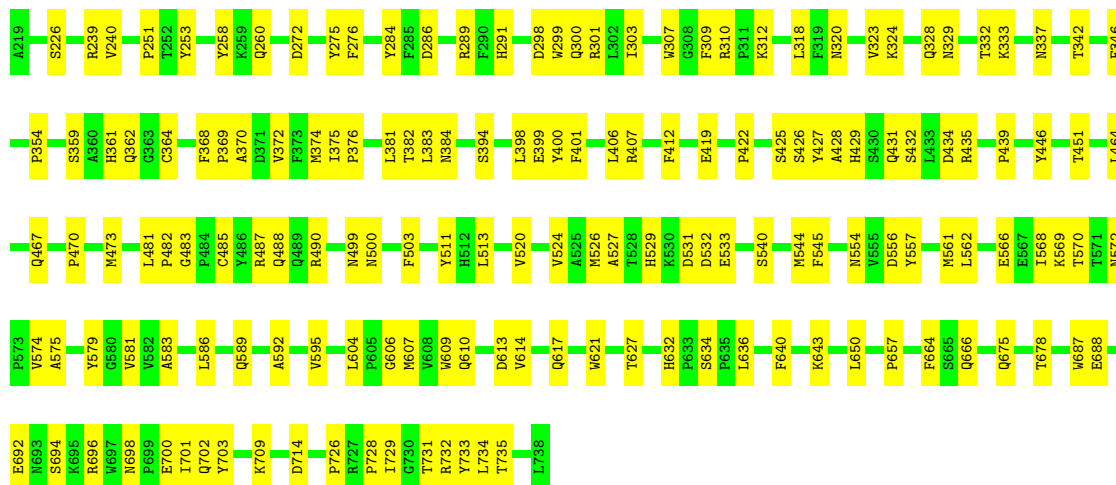
• Molecule 1: Capsid protein VP1





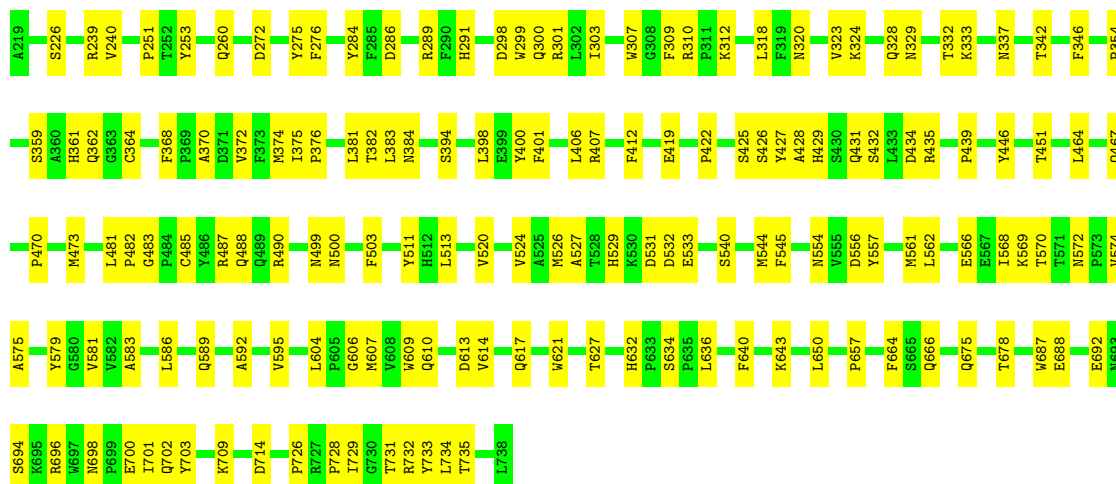
- Molecule 1: Capsid protein VP1

Chain F:



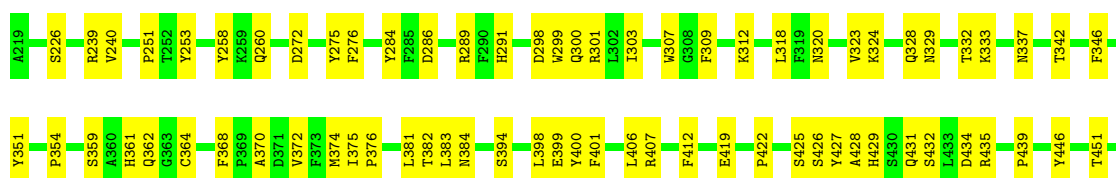
- Molecule 1: Capsid protein VP1

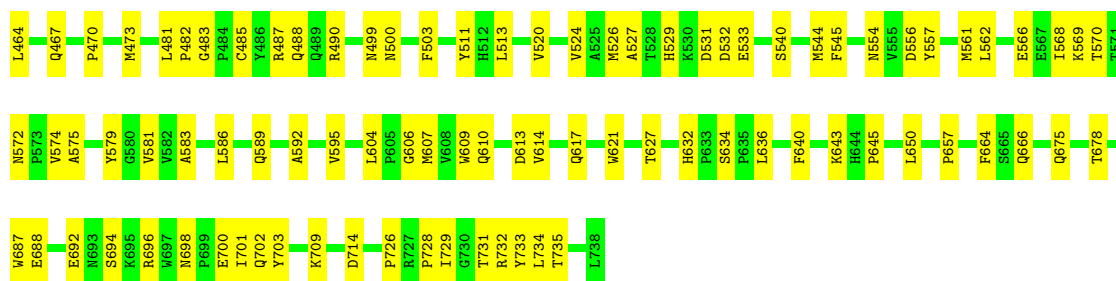
Chain G:



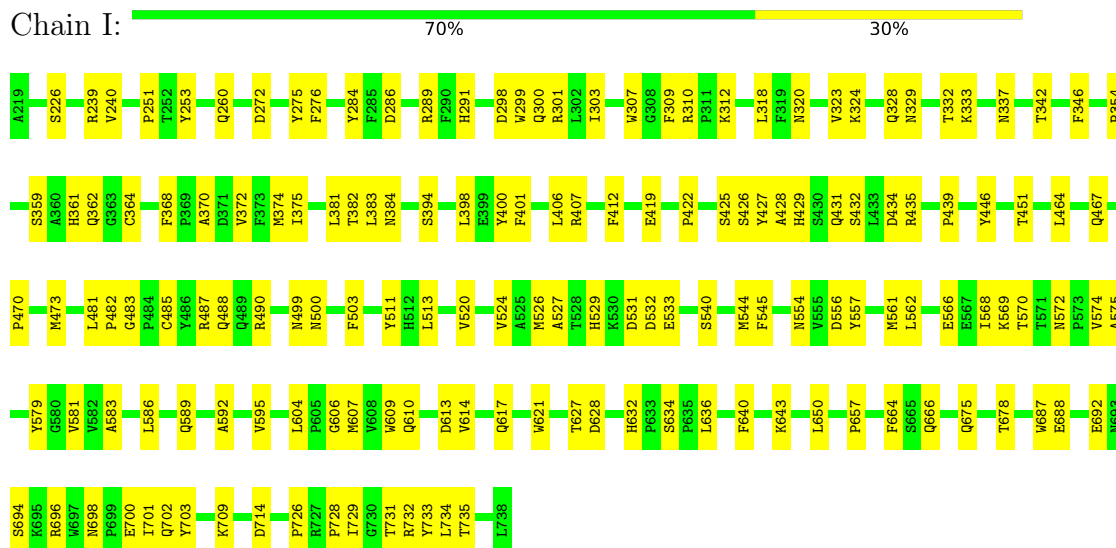
- Molecule 1: Capsid protein VP1

Chain H:

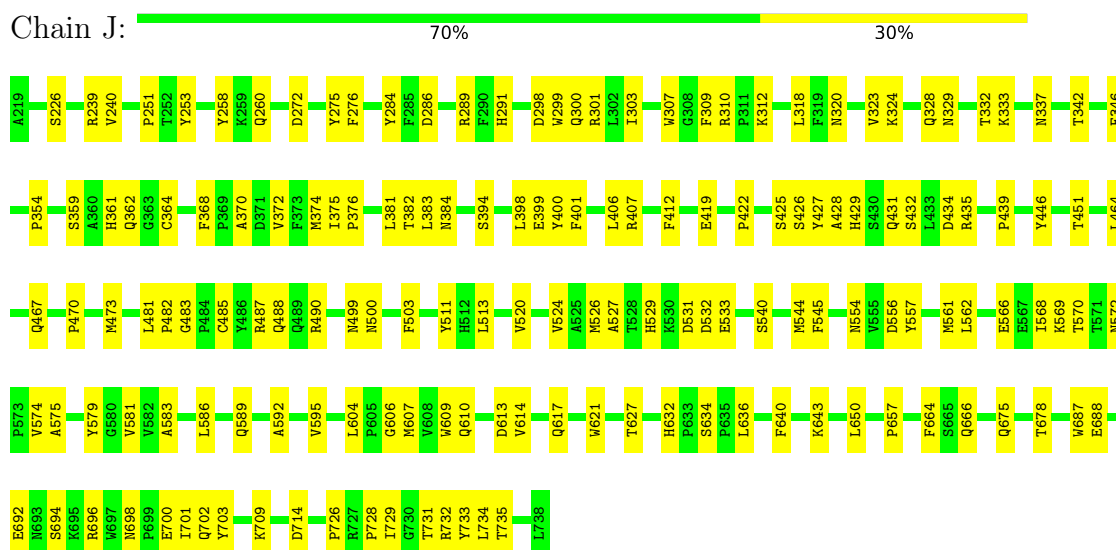




• Molecule 1: Capsid protein VP1

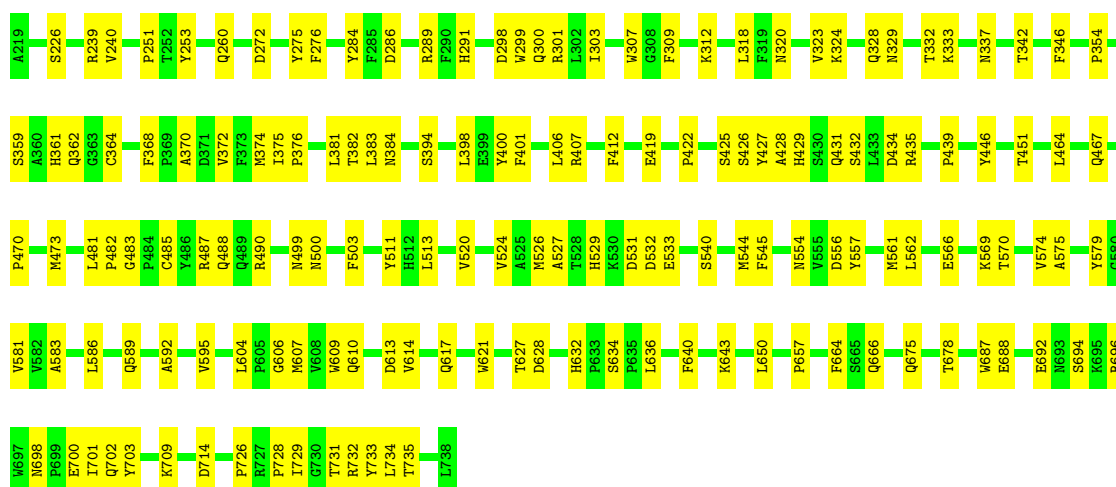


• Molecule 1: Capsid protein VP1



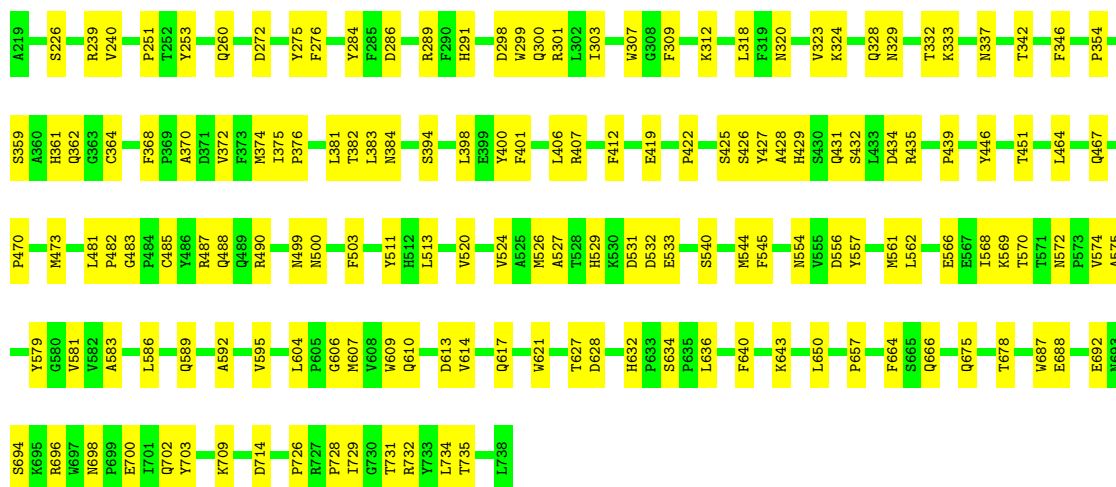
• Molecule 1: Capsid protein VP1





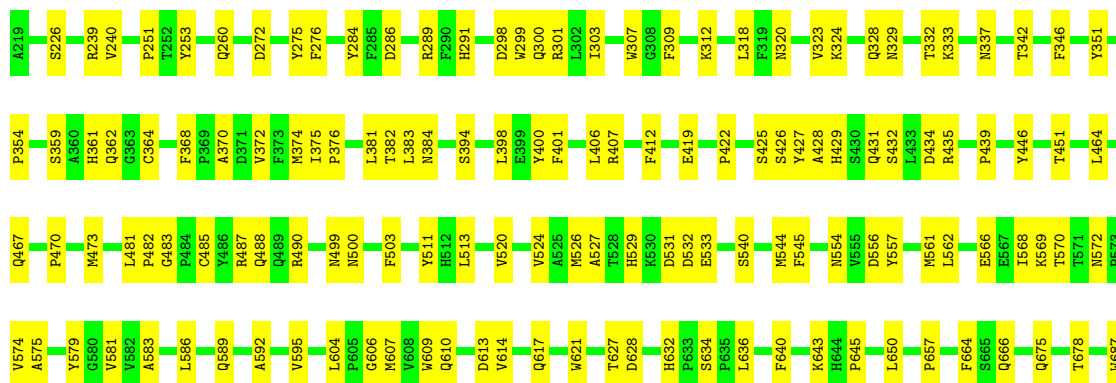
• Molecule 1: Capsid protein VP1

Chain L: 70% 30%



• Molecule 1: Capsid protein VP1

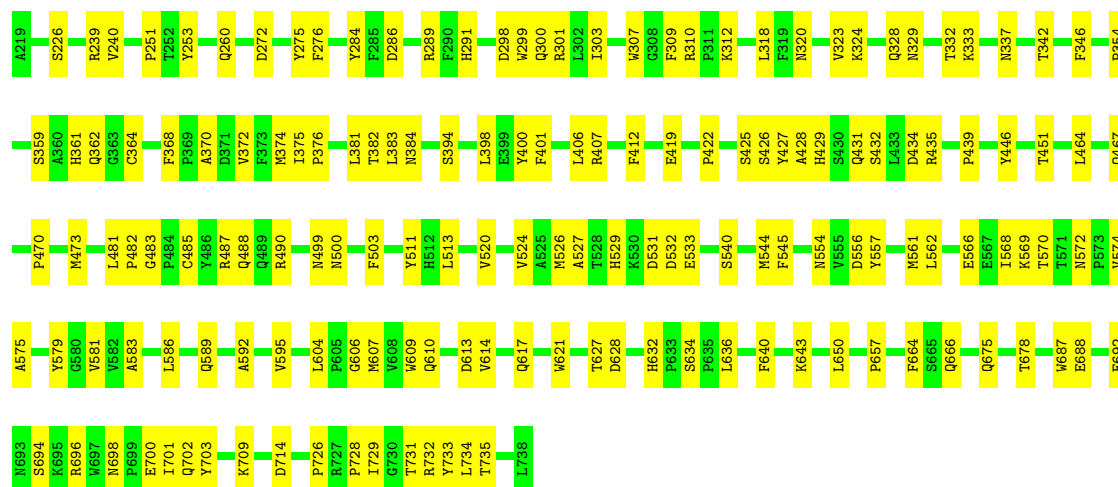
Chain M: 70% 30%





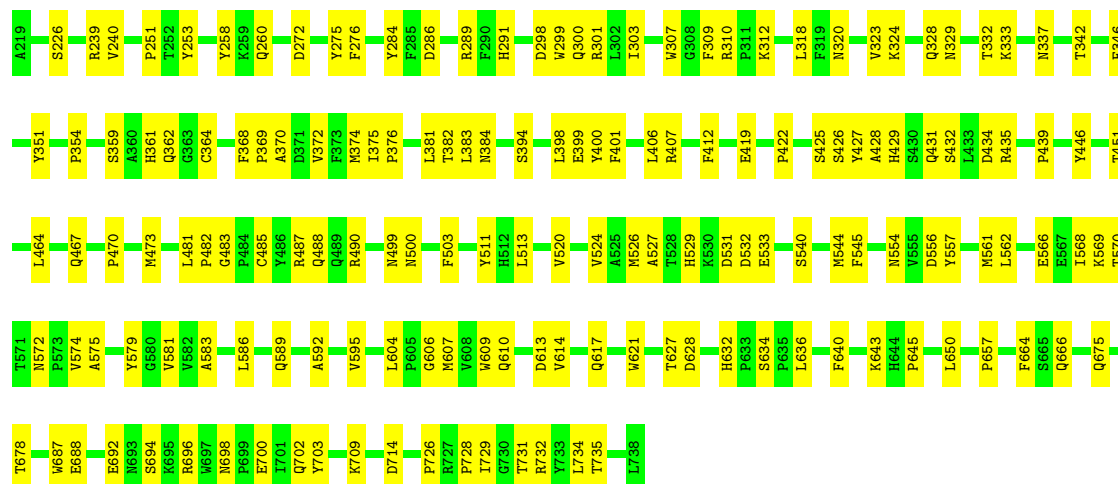
● Molecule 1: Capsid protein VP1

Chain N: 70% 30%



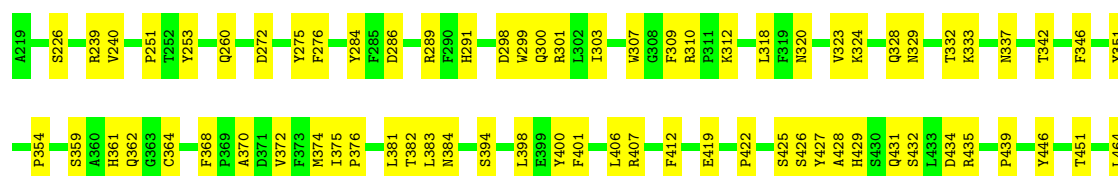
● Molecule 1: Capsid protein VP1

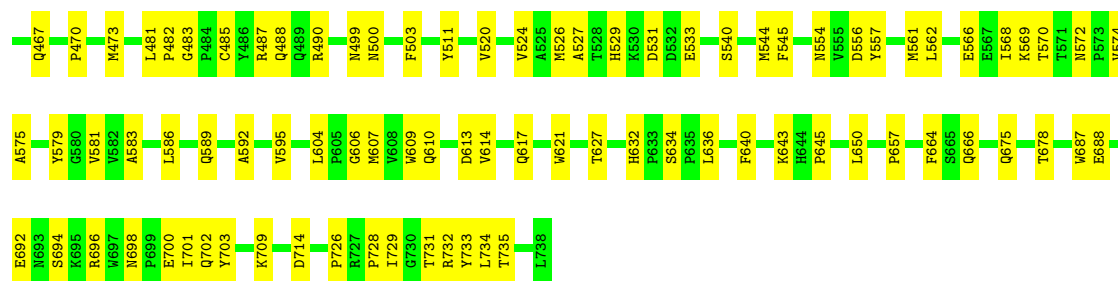
Chain O: 69% 31%



● Molecule 1: Capsid protein VP1

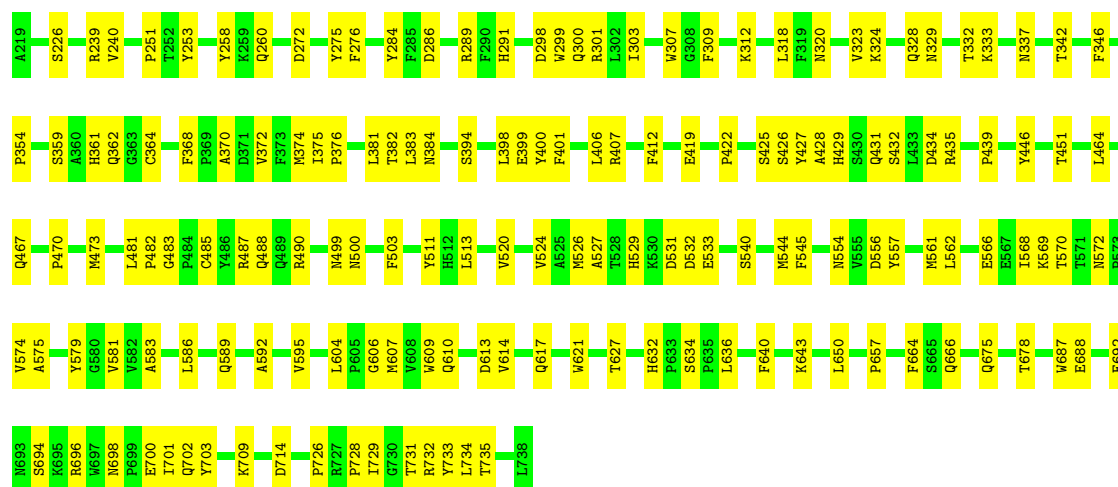
Chain P: 70% 30%





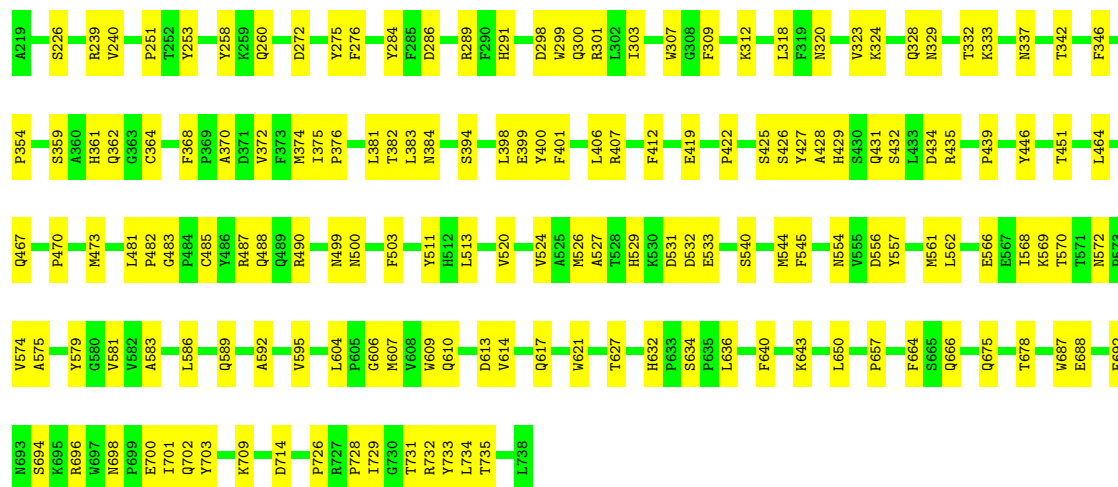
• Molecule 1: Capsid protein VP1

Chain Q: 70% 30%



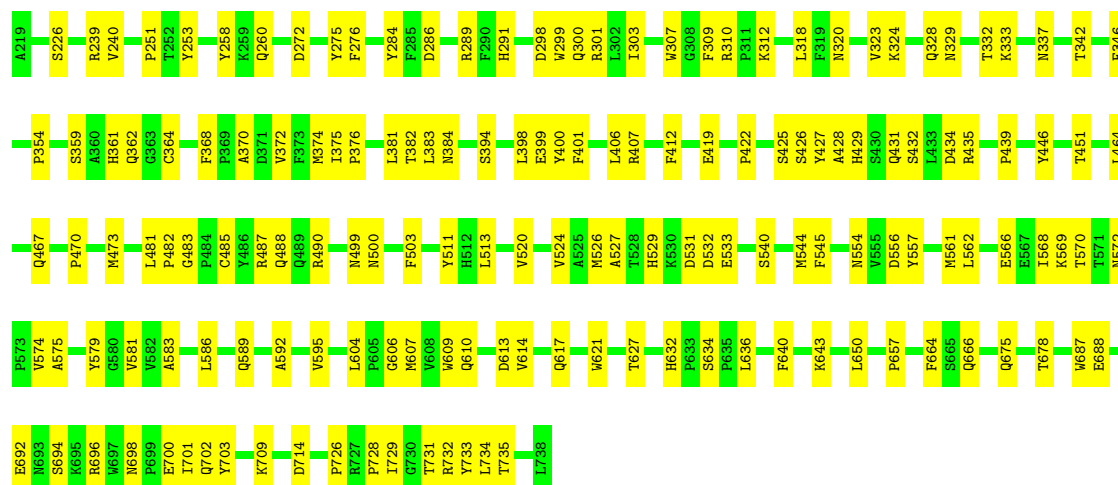
• Molecule 1: Capsid protein VP1

Chain R: 70% 30%

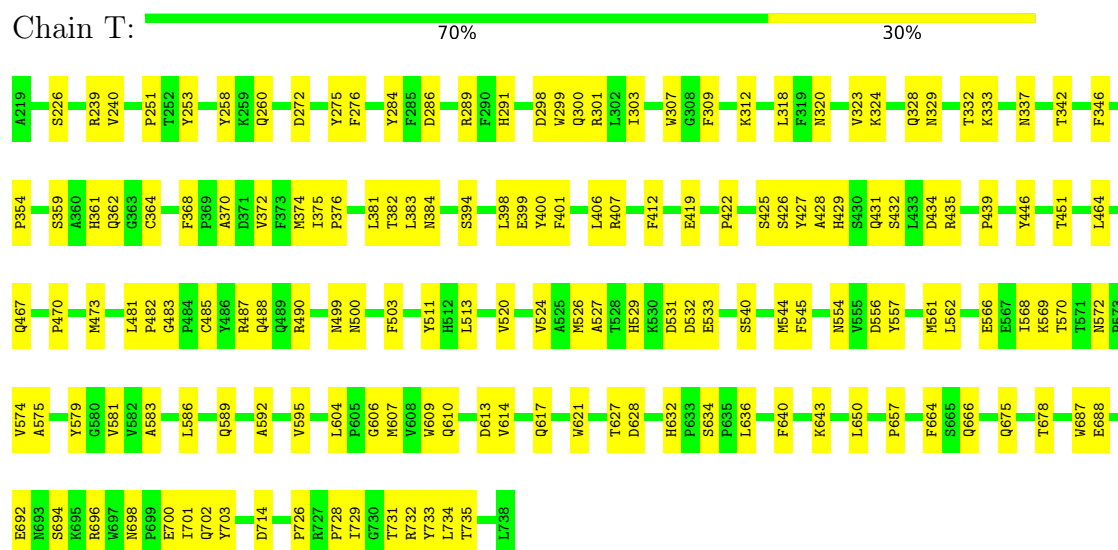


• Molecule 1: Capsid protein VP1

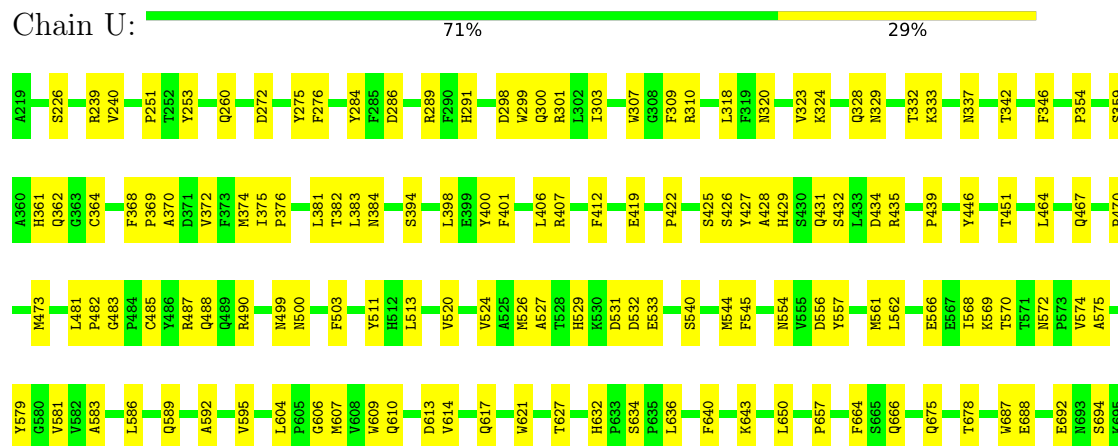
Chain S: 70% 30%



- Molecule 1: Capsid protein VP1



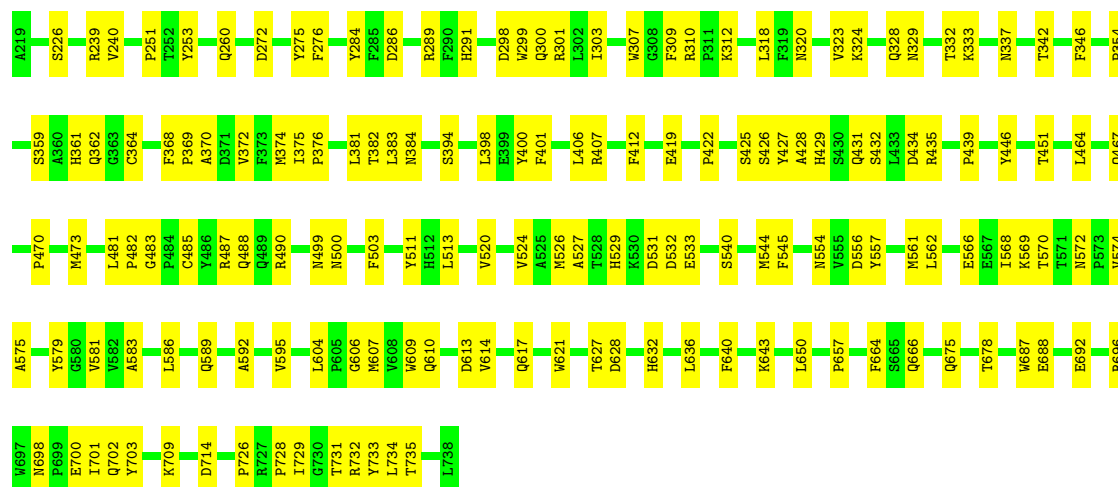
- Molecule 1: Capsid protein VP1





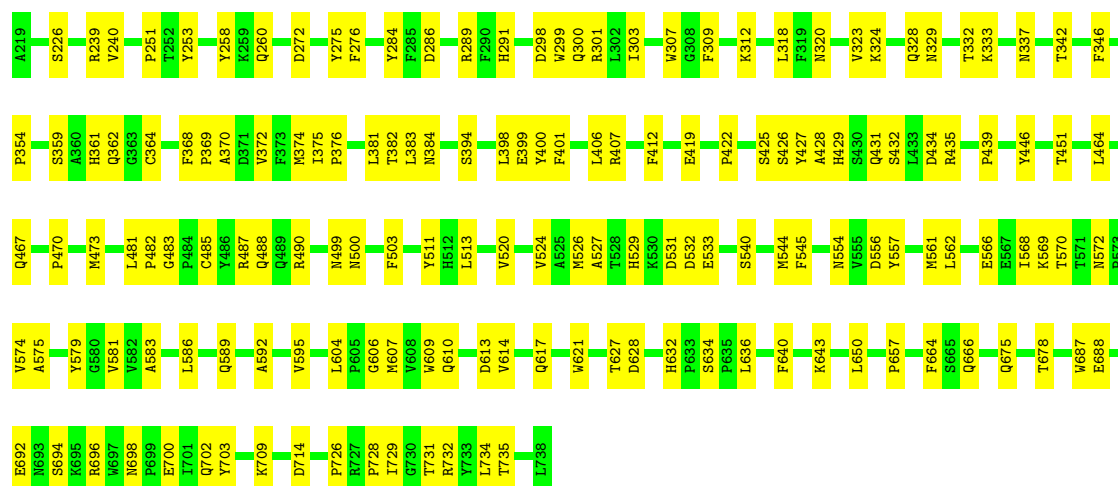
• Molecule 1: Capsid protein VP1

Chain V: 70% 30%



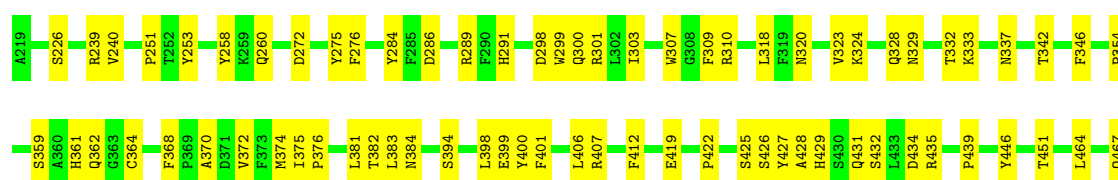
• Molecule 1: Capsid protein VP1

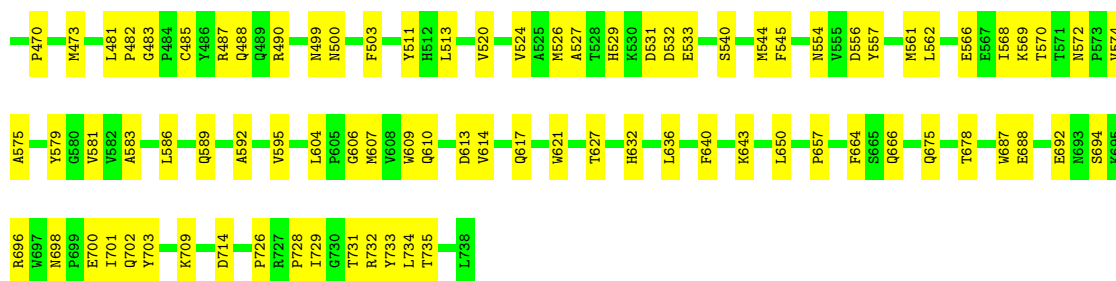
Chain W: 70% 30%



• Molecule 1: Capsid protein VP1

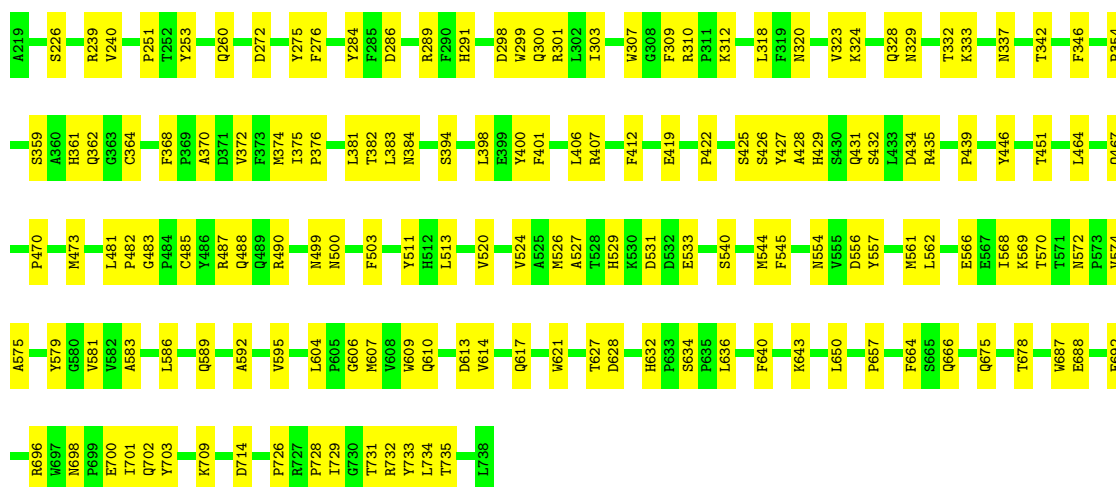
Chain X: 70% 30%





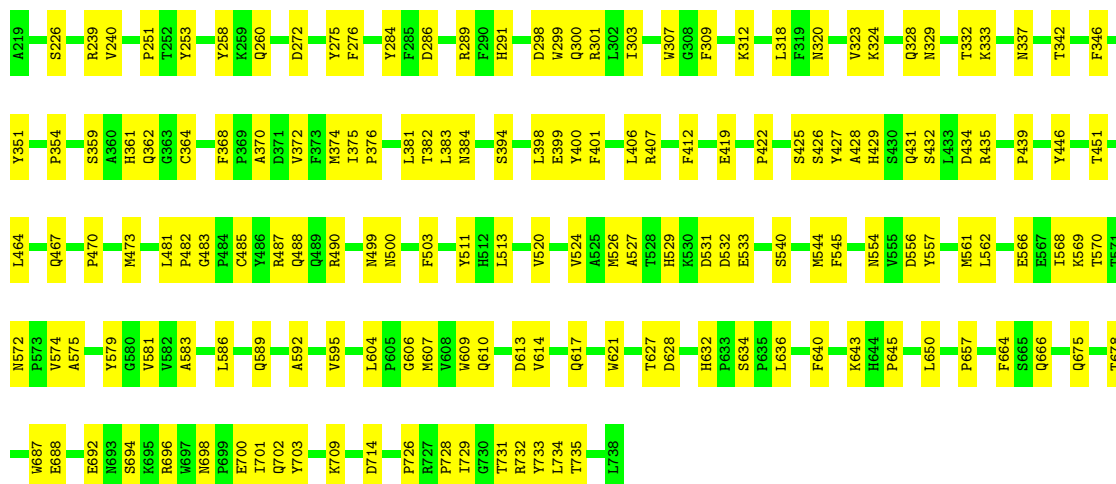
• Molecule 1: Capsid protein VP1

Chain Y: 70% 30%



• Molecule 1: Capsid protein VP1

Chain Z: 69% 31%



• Molecule 1: Capsid protein VP1

Chain a: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Capsid protein VP1

Chain y:  100%

There are no outlier residues recorded for this chain.

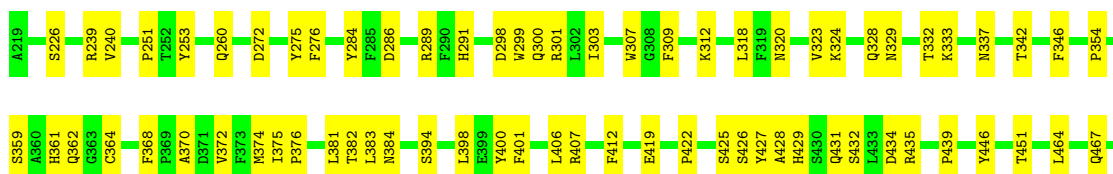
- Molecule 1: Capsid protein VP1

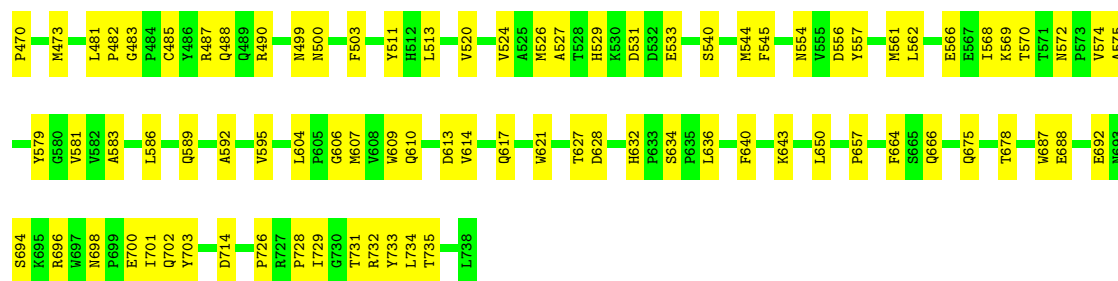
Chain z:  100%

There are no outlier residues recorded for this chain.

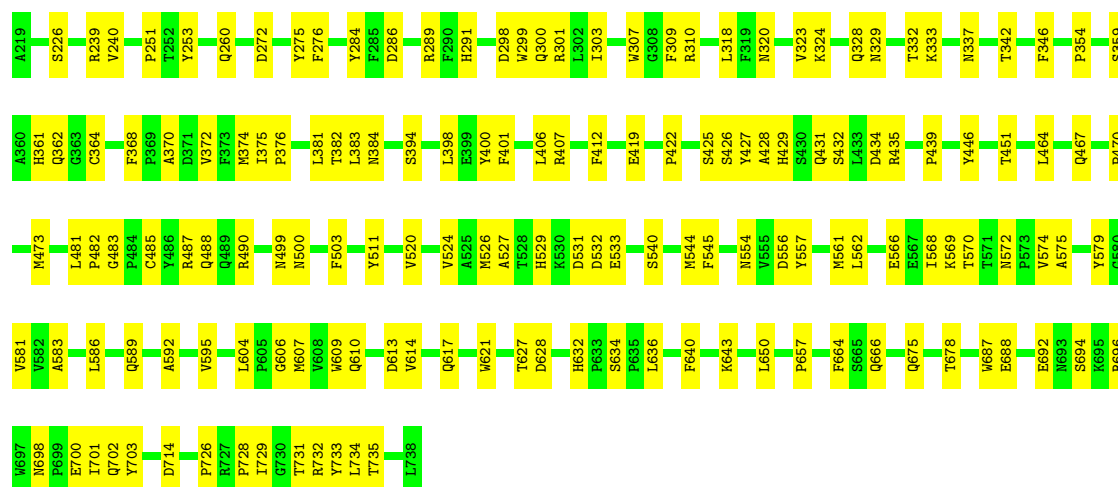
- Molecule 1: Capsid protein VP1

Chain 1:  70% 30%

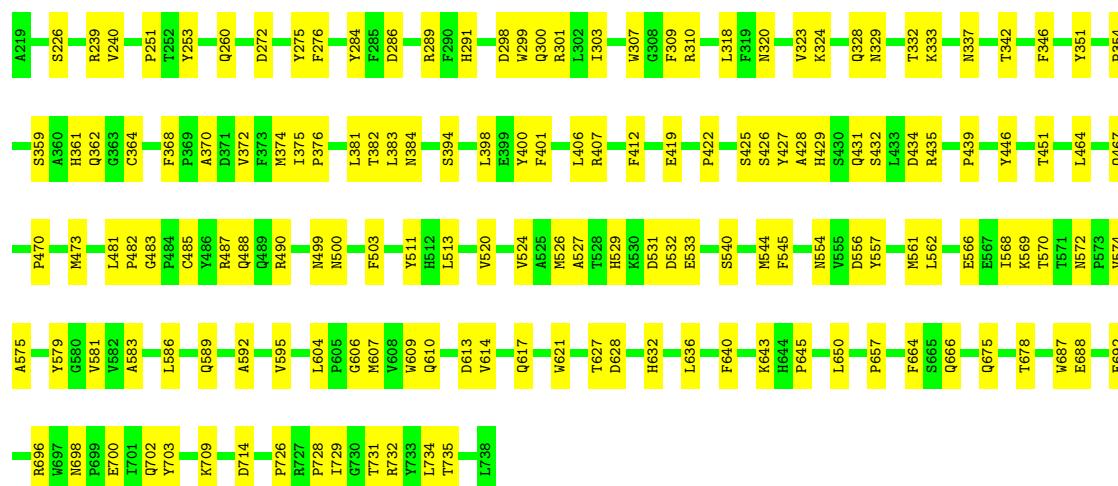




- Molecule 1: Capsid protein VP1

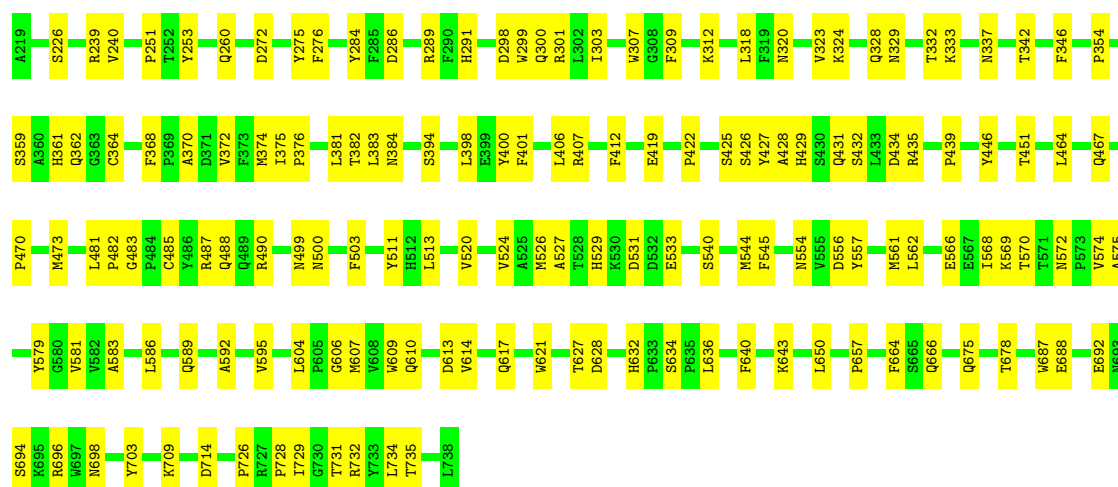


- Molecule 1: Capsid protein VP1



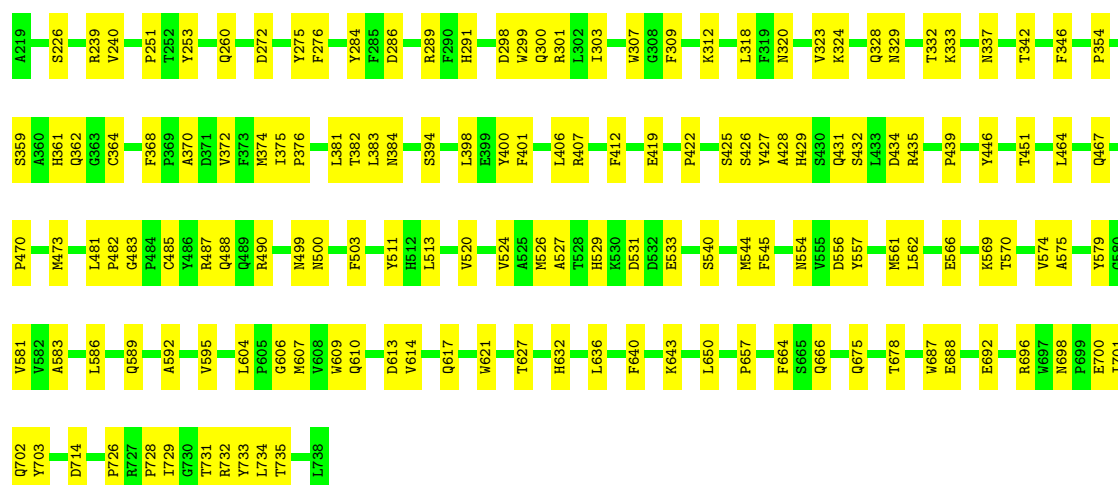
- Molecule 1: Capsid protein VP1





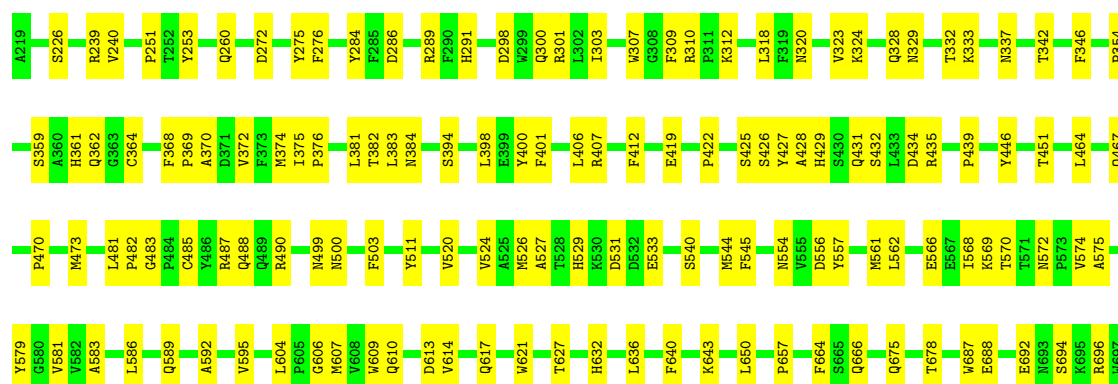
• Molecule 1: Capsid protein VP1

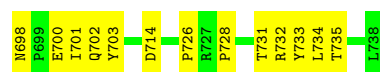
Chain 5: 71% 29%



• Molecule 1: Capsid protein VP1

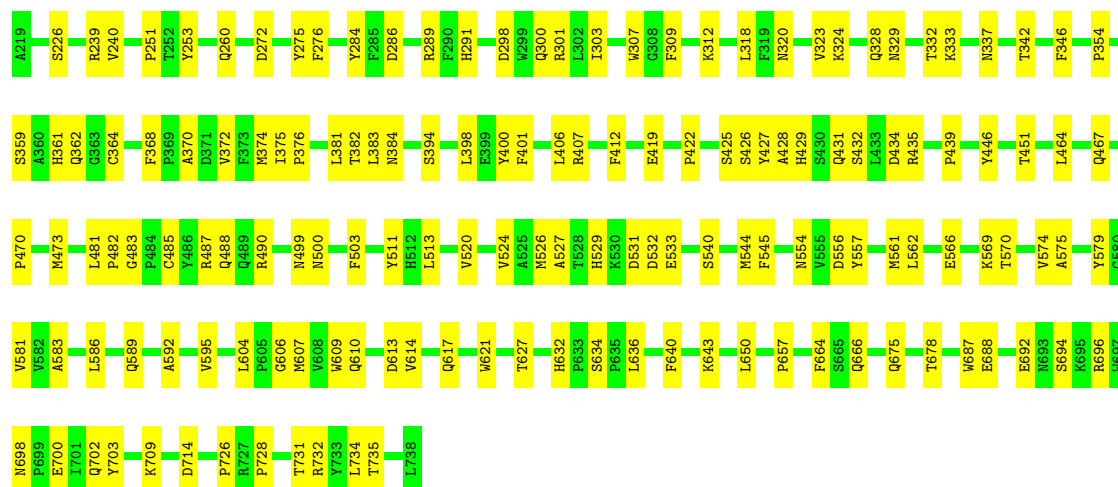
Chain 6: 71% 29%





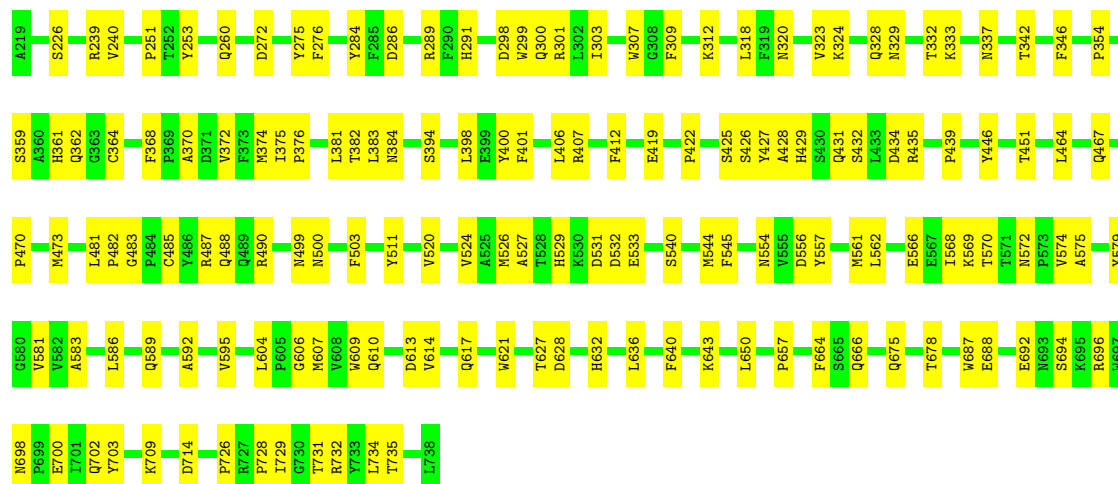
● Molecule 1: Capsid protein VP1

Chain 7: 71% 29%



● Molecule 1: Capsid protein VP1

Chain 8: 71% 29%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	82463	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	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.56	0/4251	0.54	0/5797
1	2	0.56	0/4251	0.54	0/5797
1	3	0.56	0/4251	0.54	0/5797
1	4	0.56	0/4251	0.54	0/5797
1	5	0.56	0/4251	0.54	0/5797
1	6	0.56	0/4251	0.54	0/5797
1	7	0.56	0/4251	0.54	0/5797
1	8	0.56	0/4251	0.54	0/5797
1	A	0.56	0/4251	0.54	0/5797
1	B	0.56	0/4251	0.54	0/5797
1	C	0.56	0/4251	0.54	0/5797
1	D	0.56	0/4251	0.54	0/5797
1	E	0.56	0/4251	0.54	0/5797
1	F	0.56	0/4251	0.54	0/5797
1	G	0.56	0/4251	0.54	0/5797
1	H	0.56	0/4251	0.54	0/5797
1	I	0.56	0/4251	0.54	0/5797
1	J	0.56	0/4251	0.54	0/5797
1	K	0.56	0/4251	0.54	0/5797
1	L	0.56	0/4251	0.54	0/5797
1	M	0.56	0/4251	0.54	0/5797
1	N	0.56	0/4251	0.54	0/5797
1	O	0.56	0/4251	0.54	0/5797
1	P	0.56	0/4251	0.54	0/5797
1	Q	0.56	0/4251	0.54	0/5797
1	R	0.56	0/4251	0.54	0/5797
1	S	0.56	0/4251	0.54	0/5797
1	T	0.56	0/4251	0.54	0/5797
1	U	0.56	0/4251	0.54	0/5797
1	V	0.56	0/4251	0.54	0/5797
1	W	0.56	0/4251	0.54	0/5797
1	X	0.56	0/4251	0.54	0/5797
1	Y	0.56	0/4251	0.54	0/5797
1	Z	0.56	0/4251	0.54	0/5797

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.56	0/4251	0.54	0/5797
1	b	0.56	0/4251	0.54	0/5797
1	c	0.56	0/4251	0.54	0/5797
1	d	0.56	0/4251	0.54	0/5797
1	e	0.56	0/4251	0.54	0/5797
1	f	0.56	0/4251	0.54	0/5797
1	g	0.56	0/4251	0.54	0/5797
1	h	0.56	0/4251	0.54	0/5797
1	i	0.56	0/4251	0.54	0/5797
1	j	0.56	0/4251	0.54	0/5797
1	k	0.56	0/4251	0.54	0/5797
1	l	0.56	0/4251	0.54	0/5797
1	m	0.56	0/4251	0.54	0/5797
1	n	0.56	0/4251	0.54	0/5797
1	o	0.56	0/4251	0.54	0/5797
1	p	0.56	0/4251	0.54	0/5797
1	q	0.56	0/4251	0.54	0/5797
1	r	0.56	0/4251	0.54	0/5797
1	s	0.56	0/4251	0.54	0/5797
1	t	0.56	0/4251	0.54	0/5797
1	u	0.56	0/4251	0.54	0/5797
1	v	0.56	0/4251	0.54	0/5797
1	w	0.56	0/4251	0.54	0/5797
1	x	0.56	0/4251	0.54	0/5797
1	y	0.56	0/4251	0.54	0/5797
1	z	0.56	0/4251	0.54	0/5797
All	All	0.56	0/255060	0.54	0/347820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4128	0	3893	138	0
1	2	4128	0	3893	139	0
1	3	4128	0	3893	138	0
1	4	4128	0	3893	136	0
1	5	4128	0	3893	133	0
1	6	4128	0	3893	135	0
1	7	4128	0	3893	134	0
1	8	4128	0	3893	135	0
1	A	4128	0	3893	194	0
1	B	4128	0	3893	188	0
1	C	4128	0	3893	192	0
1	D	4128	0	3893	198	0
1	E	4128	0	3893	193	0
1	F	4128	0	3893	197	0
1	G	4128	0	3893	193	0
1	H	4128	0	3893	194	0
1	I	4128	0	3893	185	0
1	J	4128	0	3893	197	0
1	K	4128	0	3893	196	0
1	L	4128	0	3893	195	0
1	M	4128	0	3893	194	0
1	N	4128	0	3893	195	0
1	O	4128	0	3893	196	0
1	P	4128	0	3893	186	0
1	Q	4128	0	3893	188	0
1	R	4128	0	3893	171	0
1	S	4128	0	3893	175	0
1	T	4128	0	3893	190	0
1	U	4128	0	3893	188	0
1	V	4128	0	3893	191	0
1	W	4128	0	3893	194	0
1	X	4128	0	3893	192	0
1	Y	4128	0	3893	193	0
1	Z	4128	0	3893	196	0
1	a	4128	0	3893	0	0
1	b	4128	0	3893	0	0
1	c	4128	0	3893	0	0
1	d	4128	0	3893	0	0
1	e	4128	0	3893	0	0
1	f	4128	0	3893	0	0
1	g	4128	0	3893	0	0
1	h	4128	0	3893	0	0
1	i	4128	0	3893	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4128	0	3893	0	0
1	k	4128	0	3893	0	0
1	l	4128	0	3893	0	0
1	m	4128	0	3893	0	0
1	n	4128	0	3893	0	0
1	o	4128	0	3893	0	0
1	p	4128	0	3893	0	0
1	q	4128	0	3893	0	0
1	r	4128	0	3893	0	0
1	s	4128	0	3893	0	0
1	t	4128	0	3893	0	0
1	u	4128	0	3893	0	0
1	v	4128	0	3893	0	0
1	w	4128	0	3893	0	0
1	x	4128	0	3893	0	0
1	y	4128	0	3893	0	0
1	z	4128	0	3893	0	0
2	1	16	0	12	1	0
2	2	16	0	12	1	0
2	3	16	0	12	1	0
2	4	16	0	12	1	0
2	5	16	0	12	1	0
2	6	16	0	12	1	0
2	7	16	0	12	1	0
2	8	16	0	12	1	0
2	A	16	0	12	1	0
2	B	16	0	12	1	0
2	C	16	0	12	1	0
2	D	16	0	12	1	0
2	E	16	0	12	1	0
2	F	16	0	12	1	0
2	G	16	0	12	1	0
2	H	16	0	12	1	0
2	I	16	0	12	1	0
2	J	16	0	12	1	0
2	K	16	0	12	1	0
2	L	16	0	12	1	0
2	M	16	0	12	1	0
2	N	16	0	12	1	0
2	O	16	0	12	1	0
2	P	16	0	12	1	0
2	Q	16	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	16	0	12	1	0
2	S	16	0	12	1	0
2	T	16	0	12	1	0
2	U	16	0	12	1	0
2	V	16	0	12	1	0
2	W	16	0	12	1	0
2	X	16	0	12	1	0
2	Y	16	0	12	1	0
2	Z	16	0	12	1	0
2	a	16	0	12	0	0
2	b	16	0	12	0	0
2	c	16	0	12	0	0
2	d	16	0	12	0	0
2	e	16	0	12	0	0
2	f	16	0	12	0	0
2	g	16	0	12	0	0
2	h	16	0	12	0	0
2	i	16	0	12	0	0
2	j	16	0	12	0	0
2	k	16	0	12	0	0
2	l	16	0	12	0	0
2	m	16	0	12	0	0
2	n	16	0	12	0	0
2	o	16	0	12	0	0
2	p	16	0	12	0	0
2	q	16	0	12	0	0
2	r	16	0	12	0	0
2	s	16	0	12	0	0
2	t	16	0	12	0	0
2	u	16	0	12	0	0
2	v	16	0	12	0	0
2	w	16	0	12	0	0
2	x	16	0	12	0	0
2	y	16	0	12	0	0
2	z	16	0	12	0	0
3	1	21	0	12	4	0
3	2	21	0	12	4	0
3	3	21	0	12	3	0
3	4	21	0	12	4	0
3	5	21	0	12	3	0
3	6	21	0	12	3	0
3	7	21	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8	21	0	12	3	0
3	A	21	0	12	4	0
3	B	21	0	12	4	0
3	C	21	0	12	4	0
3	D	21	0	12	4	0
3	E	21	0	12	4	0
3	F	21	0	12	4	0
3	G	21	0	12	4	0
3	H	21	0	12	4	0
3	I	21	0	12	4	0
3	J	21	0	12	4	0
3	K	21	0	12	4	0
3	L	21	0	12	3	0
3	M	21	0	12	4	0
3	N	21	0	12	4	0
3	O	21	0	12	4	0
3	P	21	0	12	3	0
3	Q	21	0	12	4	0
3	R	21	0	12	4	0
3	S	21	0	12	4	0
3	T	21	0	12	4	0
3	U	21	0	12	4	0
3	V	21	0	12	3	0
3	W	21	0	12	4	0
3	X	21	0	12	3	0
3	Y	21	0	12	4	0
3	Z	21	0	12	4	0
3	a	21	0	12	0	0
3	b	21	0	12	0	0
3	c	21	0	12	0	0
3	d	21	0	12	0	0
3	e	21	0	12	0	0
3	f	21	0	12	0	0
3	g	21	0	12	0	0
3	h	21	0	12	0	0
3	i	21	0	12	0	0
3	j	21	0	12	0	0
3	k	21	0	12	0	0
3	l	21	0	12	0	0
3	m	21	0	12	0	0
3	n	21	0	12	0	0
3	o	21	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	p	21	0	12	0	0
3	q	21	0	12	0	0
3	r	21	0	12	0	0
3	s	21	0	12	0	0
3	t	21	0	12	0	0
3	u	21	0	12	0	0
3	v	21	0	12	0	0
3	w	21	0	12	0	0
3	x	21	0	12	0	0
3	y	21	0	12	0	0
3	z	21	0	12	0	0
All	All	249900	0	235020	4470	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 9.

The worst 5 of 4470 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:253:TYR:OH	1:C:375:ILE:O	2.05	0.76
1:L:253:TYR:OH	1:L:375:ILE:O	2.05	0.76
1:R:253:TYR:OH	1:R:375:ILE:O	2.04	0.76
1:T:253:TYR:OH	1:T:375:ILE:O	2.05	0.76
1:V:253:TYR:OH	1:V:375:ILE:O	2.04	0.76

There are no symmetry-related clashes.

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 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	1	518/520 (100%)	507 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	3	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	4	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	5	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	6	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	7	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	8	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	A	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	B	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	C	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	D	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	E	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	F	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	G	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	H	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	I	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	J	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	K	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	L	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	M	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	N	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	O	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	P	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	Q	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	R	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	S	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	T	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	U	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	V	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	W	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	X	518/520 (100%)	507 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	Z	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	a	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	b	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	c	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	d	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	e	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	f	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	g	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	h	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	i	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	j	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	k	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	l	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	m	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	n	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	o	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	p	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	q	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	r	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	s	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	t	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	u	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	v	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	w	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	x	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	y	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
1	z	518/520 (100%)	507 (98%)	11 (2%)	0	100	100
All	All	31080/31200 (100%)	30420 (98%)	660 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1	452/452 (100%)	452 (100%)	0	100	100
1	2	452/452 (100%)	452 (100%)	0	100	100
1	3	452/452 (100%)	452 (100%)	0	100	100
1	4	452/452 (100%)	452 (100%)	0	100	100
1	5	452/452 (100%)	452 (100%)	0	100	100
1	6	452/452 (100%)	452 (100%)	0	100	100
1	7	452/452 (100%)	452 (100%)	0	100	100
1	8	452/452 (100%)	452 (100%)	0	100	100
1	A	452/452 (100%)	452 (100%)	0	100	100
1	B	452/452 (100%)	452 (100%)	0	100	100
1	C	452/452 (100%)	452 (100%)	0	100	100
1	D	452/452 (100%)	452 (100%)	0	100	100
1	E	452/452 (100%)	452 (100%)	0	100	100
1	F	452/452 (100%)	452 (100%)	0	100	100
1	G	452/452 (100%)	452 (100%)	0	100	100
1	H	452/452 (100%)	452 (100%)	0	100	100
1	I	452/452 (100%)	452 (100%)	0	100	100
1	J	452/452 (100%)	452 (100%)	0	100	100
1	K	452/452 (100%)	452 (100%)	0	100	100
1	L	452/452 (100%)	452 (100%)	0	100	100
1	M	452/452 (100%)	452 (100%)	0	100	100
1	N	452/452 (100%)	452 (100%)	0	100	100
1	O	452/452 (100%)	452 (100%)	0	100	100
1	P	452/452 (100%)	452 (100%)	0	100	100
1	Q	452/452 (100%)	452 (100%)	0	100	100
1	R	452/452 (100%)	452 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	452/452 (100%)	452 (100%)	0	100	100
1	T	452/452 (100%)	452 (100%)	0	100	100
1	U	452/452 (100%)	452 (100%)	0	100	100
1	V	452/452 (100%)	452 (100%)	0	100	100
1	W	452/452 (100%)	452 (100%)	0	100	100
1	X	452/452 (100%)	452 (100%)	0	100	100
1	Y	452/452 (100%)	452 (100%)	0	100	100
1	Z	452/452 (100%)	452 (100%)	0	100	100
1	a	452/452 (100%)	452 (100%)	0	100	100
1	b	452/452 (100%)	452 (100%)	0	100	100
1	c	452/452 (100%)	452 (100%)	0	100	100
1	d	452/452 (100%)	452 (100%)	0	100	100
1	e	452/452 (100%)	452 (100%)	0	100	100
1	f	452/452 (100%)	452 (100%)	0	100	100
1	g	452/452 (100%)	452 (100%)	0	100	100
1	h	452/452 (100%)	452 (100%)	0	100	100
1	i	452/452 (100%)	452 (100%)	0	100	100
1	j	452/452 (100%)	452 (100%)	0	100	100
1	k	452/452 (100%)	452 (100%)	0	100	100
1	l	452/452 (100%)	452 (100%)	0	100	100
1	m	452/452 (100%)	452 (100%)	0	100	100
1	n	452/452 (100%)	452 (100%)	0	100	100
1	o	452/452 (100%)	452 (100%)	0	100	100
1	p	452/452 (100%)	452 (100%)	0	100	100
1	q	452/452 (100%)	452 (100%)	0	100	100
1	r	452/452 (100%)	452 (100%)	0	100	100
1	s	452/452 (100%)	452 (100%)	0	100	100
1	t	452/452 (100%)	452 (100%)	0	100	100
1	u	452/452 (100%)	452 (100%)	0	100	100
1	v	452/452 (100%)	452 (100%)	0	100	100
1	w	452/452 (100%)	452 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	452/452 (100%)	452 (100%)	0	100	100
1	y	452/452 (100%)	452 (100%)	0	100	100
1	z	452/452 (100%)	452 (100%)	0	100	100
All	All	27120/27120 (100%)	27120 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 539 such sidechains are listed below:

Mol	Chain	Res	Type
1	b	362	GLN
1	h	610	GLN
1	4	587	GLN
1	b	737	ASN
1	e	587	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 ⓘ

120 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.