



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 4, 2019 – 01:47 PM EST

PDB ID : 6V1Z
EMDB ID: : EMD-21020
Title : genome-containing AAVrh.39 particles
Authors : Mietzsch, M.; Agbandje-McKenna, M.
Deposited on : 2019-11-21
Resolution : 3.58 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

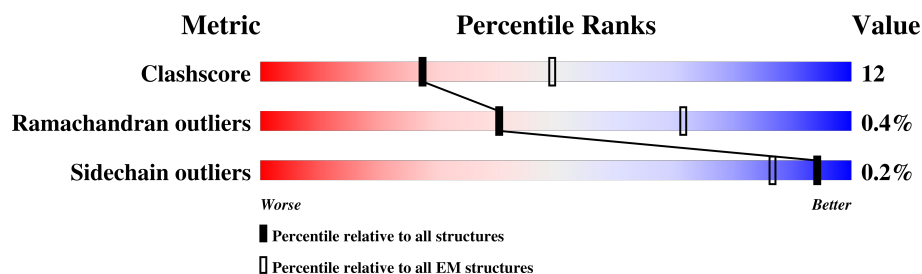
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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	521	63%	37%
1	2	521	62%	37%
1	3	521	62%	38%
1	4	521	62%	38%
1	5	521	63%	37%
1	6	521	62%	38%
1	7	521	62%	38%
1	8	521	62%	38%
1	A	521	61%	38%

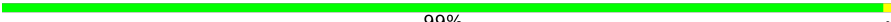














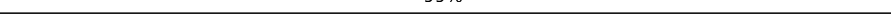
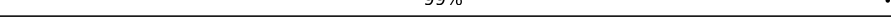
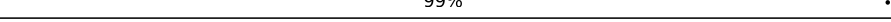
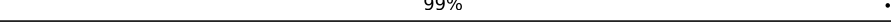
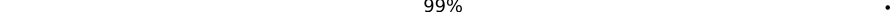
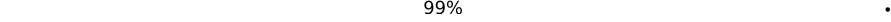
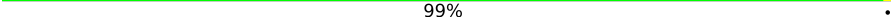
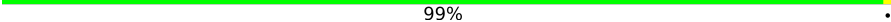

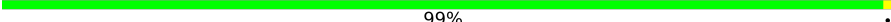
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Mol	Chain	Length	Quality of chain	
1	B	521		38%
1	C	521		38%
1	D	521		38%
1	E	521		39%
1	F	521		38%
1	G	521		39%
1	H	521		39%
1	I	521		38%
1	J	521		37%
1	K	521		38%
1	L	521		39%
1	M	521		39%
1	N	521		39%
1	O	521		39%
1	P	521		38%
1	Q	521		39%
1	R	521		38%
1	S	521		39%
1	T	521		38%
1	U	521		39%
1	V	521		38%
1	W	521		39%
1	X	521		38%
1	Y	521		39%
1	Z	521		38%

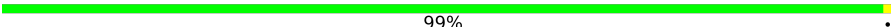
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Mol	Chain	Length	Quality of chain
1	a	521	 99% .
1	b	521	 99% .
1	c	521	 99% .
1	d	521	 99% .
1	e	521	 99% .
1	f	521	 99% .
1	g	521	 99% .
1	h	521	 99% .
1	i	521	 99% .
1	j	521	 99% .
1	k	521	 99% .
1	l	521	 99% .
1	m	521	 99% .
1	n	521	 99% .
1	o	521	 99% .
1	p	521	 99% .
1	q	521	 99% .
1	r	521	 99% .
1	s	521	 99% .
1	t	521	 99% .
1	u	521	 99% .
1	v	521	 99% .
1	w	521	 99% .
1	x	521	 99% .
1	y	521	 99% .

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Mol	Chain	Length	Quality of chain
1	z	521	 99%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 250920 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	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	B	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	C	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	D	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	E	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	F	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	G	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	H	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	I	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	J	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	K	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	L	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	M	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	N	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	O	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	P	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		
1	Q	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	S	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	T	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	U	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	V	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	W	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	X	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	Y	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	Z	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	a	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	b	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	c	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	d	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	e	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	f	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	g	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	h	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	i	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	j	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	k	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	l	521	Total 4145	C 2617	N 717	O 797	S 14	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	n	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	o	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	p	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	q	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	r	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	s	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	t	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	u	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	v	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	w	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	x	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	y	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	z	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	1	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	2	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	3	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	4	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	5	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	6	521	Total 4145	C 2617	N 717	O 797	S 14	1	0
1	7	521	Total 4145	C 2617	N 717	O 797	S 14	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	521	Total	C	N	O	S	1	0
			4145	2617	717	797	14		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ASN	SER	conflict	UNP B4Y886
A	417	GLN	THR	conflict	UNP B4Y886
B	315	ASN	SER	conflict	UNP B4Y886
B	417	GLN	THR	conflict	UNP B4Y886
C	315	ASN	SER	conflict	UNP B4Y886
C	417	GLN	THR	conflict	UNP B4Y886
D	315	ASN	SER	conflict	UNP B4Y886
D	417	GLN	THR	conflict	UNP B4Y886
E	315	ASN	SER	conflict	UNP B4Y886
E	417	GLN	THR	conflict	UNP B4Y886
F	315	ASN	SER	conflict	UNP B4Y886
F	417	GLN	THR	conflict	UNP B4Y886
G	315	ASN	SER	conflict	UNP B4Y886
G	417	GLN	THR	conflict	UNP B4Y886
H	315	ASN	SER	conflict	UNP B4Y886
H	417	GLN	THR	conflict	UNP B4Y886
I	315	ASN	SER	conflict	UNP B4Y886
I	417	GLN	THR	conflict	UNP B4Y886
J	315	ASN	SER	conflict	UNP B4Y886
J	417	GLN	THR	conflict	UNP B4Y886
K	315	ASN	SER	conflict	UNP B4Y886
K	417	GLN	THR	conflict	UNP B4Y886
L	315	ASN	SER	conflict	UNP B4Y886
L	417	GLN	THR	conflict	UNP B4Y886
M	315	ASN	SER	conflict	UNP B4Y886
M	417	GLN	THR	conflict	UNP B4Y886
N	315	ASN	SER	conflict	UNP B4Y886
N	417	GLN	THR	conflict	UNP B4Y886
O	315	ASN	SER	conflict	UNP B4Y886
O	417	GLN	THR	conflict	UNP B4Y886
P	315	ASN	SER	conflict	UNP B4Y886
P	417	GLN	THR	conflict	UNP B4Y886
Q	315	ASN	SER	conflict	UNP B4Y886
Q	417	GLN	THR	conflict	UNP B4Y886
R	315	ASN	SER	conflict	UNP B4Y886
R	417	GLN	THR	conflict	UNP B4Y886

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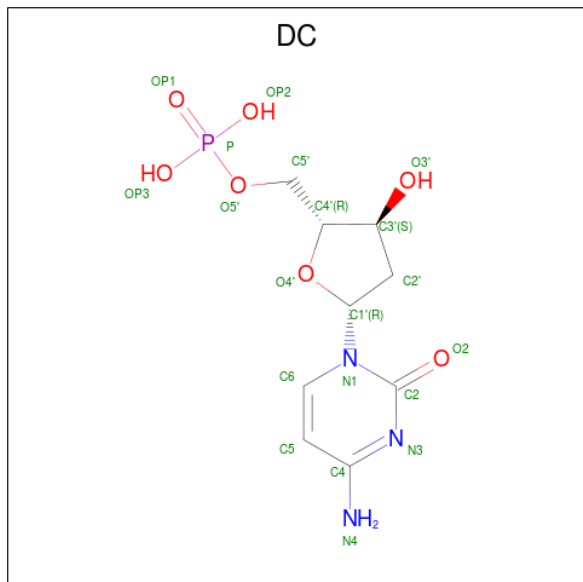
Chain	Residue	Modelled	Actual	Comment	Reference
S	315	ASN	SER	conflict	UNP B4Y886
S	417	GLN	THR	conflict	UNP B4Y886
T	315	ASN	SER	conflict	UNP B4Y886
T	417	GLN	THR	conflict	UNP B4Y886
U	315	ASN	SER	conflict	UNP B4Y886
U	417	GLN	THR	conflict	UNP B4Y886
V	315	ASN	SER	conflict	UNP B4Y886
V	417	GLN	THR	conflict	UNP B4Y886
W	315	ASN	SER	conflict	UNP B4Y886
W	417	GLN	THR	conflict	UNP B4Y886
X	315	ASN	SER	conflict	UNP B4Y886
X	417	GLN	THR	conflict	UNP B4Y886
Y	315	ASN	SER	conflict	UNP B4Y886
Y	417	GLN	THR	conflict	UNP B4Y886
Z	315	ASN	SER	conflict	UNP B4Y886
Z	417	GLN	THR	conflict	UNP B4Y886
a	315	ASN	SER	conflict	UNP B4Y886
a	417	GLN	THR	conflict	UNP B4Y886
b	315	ASN	SER	conflict	UNP B4Y886
b	417	GLN	THR	conflict	UNP B4Y886
c	315	ASN	SER	conflict	UNP B4Y886
c	417	GLN	THR	conflict	UNP B4Y886
d	315	ASN	SER	conflict	UNP B4Y886
d	417	GLN	THR	conflict	UNP B4Y886
e	315	ASN	SER	conflict	UNP B4Y886
e	417	GLN	THR	conflict	UNP B4Y886
f	315	ASN	SER	conflict	UNP B4Y886
f	417	GLN	THR	conflict	UNP B4Y886
g	315	ASN	SER	conflict	UNP B4Y886
g	417	GLN	THR	conflict	UNP B4Y886
h	315	ASN	SER	conflict	UNP B4Y886
h	417	GLN	THR	conflict	UNP B4Y886
i	315	ASN	SER	conflict	UNP B4Y886
i	417	GLN	THR	conflict	UNP B4Y886
j	315	ASN	SER	conflict	UNP B4Y886
j	417	GLN	THR	conflict	UNP B4Y886
k	315	ASN	SER	conflict	UNP B4Y886
k	417	GLN	THR	conflict	UNP B4Y886
l	315	ASN	SER	conflict	UNP B4Y886
l	417	GLN	THR	conflict	UNP B4Y886
m	315	ASN	SER	conflict	UNP B4Y886
m	417	GLN	THR	conflict	UNP B4Y886

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Chain	Residue	Modelled	Actual	Comment	Reference
n	315	ASN	SER	conflict	UNP B4Y886
n	417	GLN	THR	conflict	UNP B4Y886
o	315	ASN	SER	conflict	UNP B4Y886
o	417	GLN	THR	conflict	UNP B4Y886
p	315	ASN	SER	conflict	UNP B4Y886
p	417	GLN	THR	conflict	UNP B4Y886
q	315	ASN	SER	conflict	UNP B4Y886
q	417	GLN	THR	conflict	UNP B4Y886
r	315	ASN	SER	conflict	UNP B4Y886
r	417	GLN	THR	conflict	UNP B4Y886
s	315	ASN	SER	conflict	UNP B4Y886
s	417	GLN	THR	conflict	UNP B4Y886
t	315	ASN	SER	conflict	UNP B4Y886
t	417	GLN	THR	conflict	UNP B4Y886
u	315	ASN	SER	conflict	UNP B4Y886
u	417	GLN	THR	conflict	UNP B4Y886
v	315	ASN	SER	conflict	UNP B4Y886
v	417	GLN	THR	conflict	UNP B4Y886
w	315	ASN	SER	conflict	UNP B4Y886
w	417	GLN	THR	conflict	UNP B4Y886
x	315	ASN	SER	conflict	UNP B4Y886
x	417	GLN	THR	conflict	UNP B4Y886
y	315	ASN	SER	conflict	UNP B4Y886
y	417	GLN	THR	conflict	UNP B4Y886
z	315	ASN	SER	conflict	UNP B4Y886
z	417	GLN	THR	conflict	UNP B4Y886
1	315	ASN	SER	conflict	UNP B4Y886
1	417	GLN	THR	conflict	UNP B4Y886
2	315	ASN	SER	conflict	UNP B4Y886
2	417	GLN	THR	conflict	UNP B4Y886
3	315	ASN	SER	conflict	UNP B4Y886
3	417	GLN	THR	conflict	UNP B4Y886
4	315	ASN	SER	conflict	UNP B4Y886
4	417	GLN	THR	conflict	UNP B4Y886
5	315	ASN	SER	conflict	UNP B4Y886
5	417	GLN	THR	conflict	UNP B4Y886
6	315	ASN	SER	conflict	UNP B4Y886
6	417	GLN	THR	conflict	UNP B4Y886
7	315	ASN	SER	conflict	UNP B4Y886
7	417	GLN	THR	conflict	UNP B4Y886
8	315	ASN	SER	conflict	UNP B4Y886
8	417	GLN	THR	conflict	UNP B4Y886

- 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	
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	

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Mol	Chain	Residues	Atoms				AltConf
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	
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	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	

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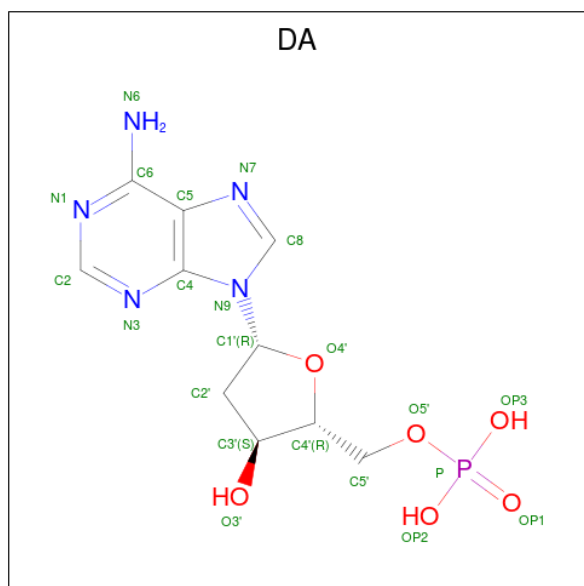
Mol	Chain	Residues	Atoms				AltConf
2	h	1	Total	C	N	O	0
			16	9	3	4	
2	i	1	Total	C	N	O	0
			16	9	3	4	
2	j	1	Total	C	N	O	0
			16	9	3	4	
2	k	1	Total	C	N	O	0
			16	9	3	4	
2	l	1	Total	C	N	O	0
			16	9	3	4	
2	m	1	Total	C	N	O	0
			16	9	3	4	
2	n	1	Total	C	N	O	0
			16	9	3	4	
2	o	1	Total	C	N	O	0
			16	9	3	4	
2	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	
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	

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Mol	Chain	Residues	Atoms				AltConf
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	

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Mol	Chain	Residues	Atoms					AltConf
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
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

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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	
3	o	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	p	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	q	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	r	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	s	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	t	1	Total	C	N	O	P	0
			21	10	5	5	1	
3	u	1	Total	C	N	O	P	0
			21	10	5	5	1	

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

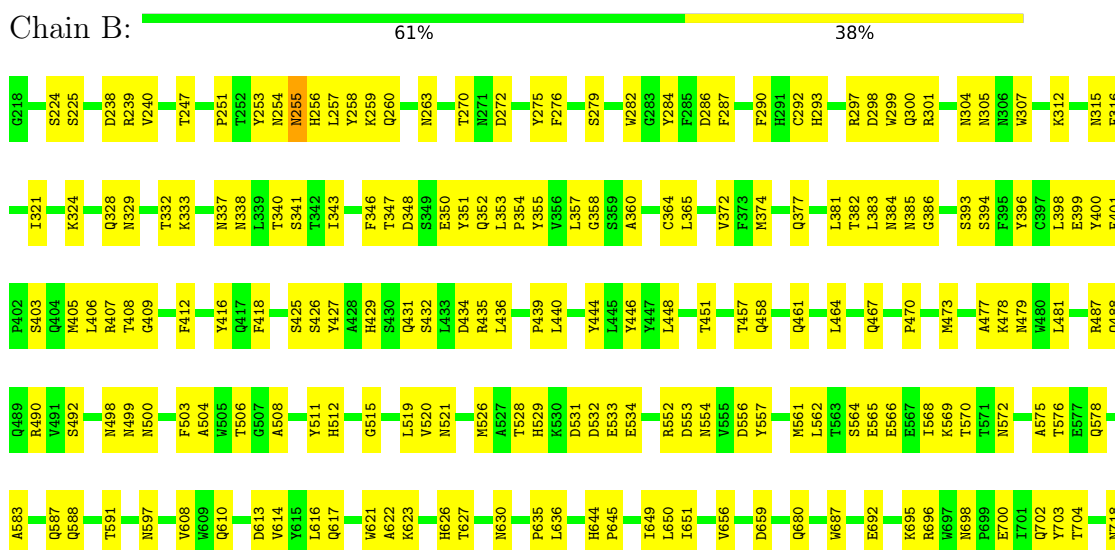
3 Residue-property plots

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.

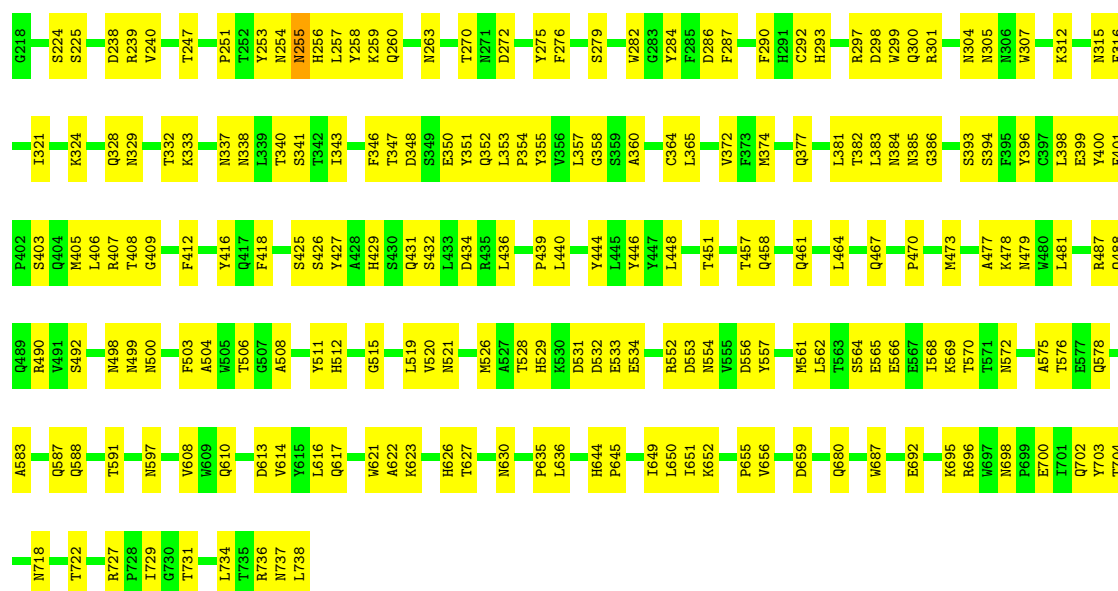
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1

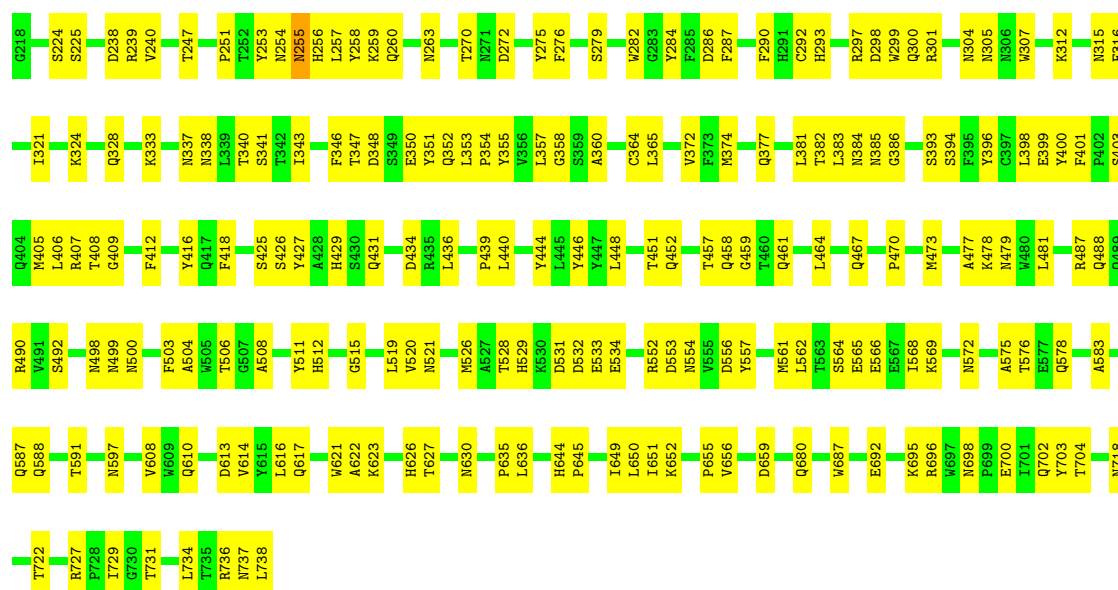






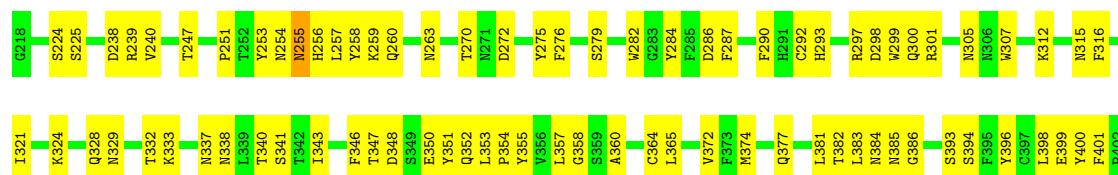
• Molecule 1: Capsid protein VP1

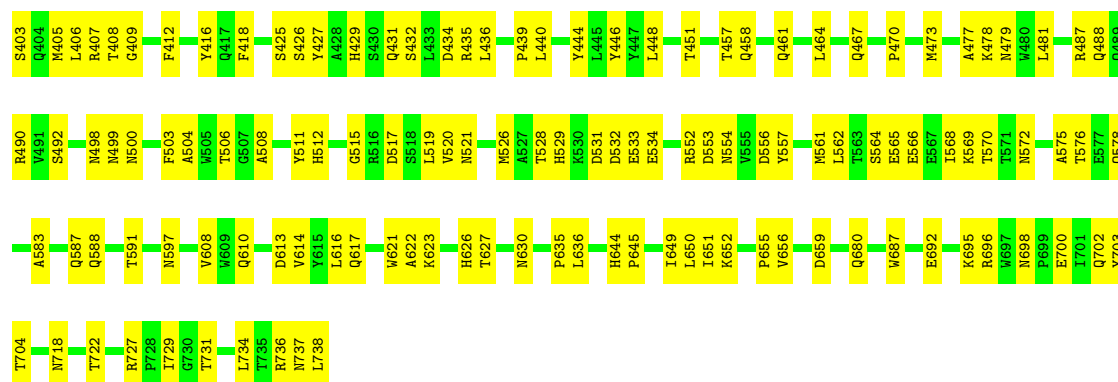
Chain F:



• Molecule 1: Capsid protein VP1

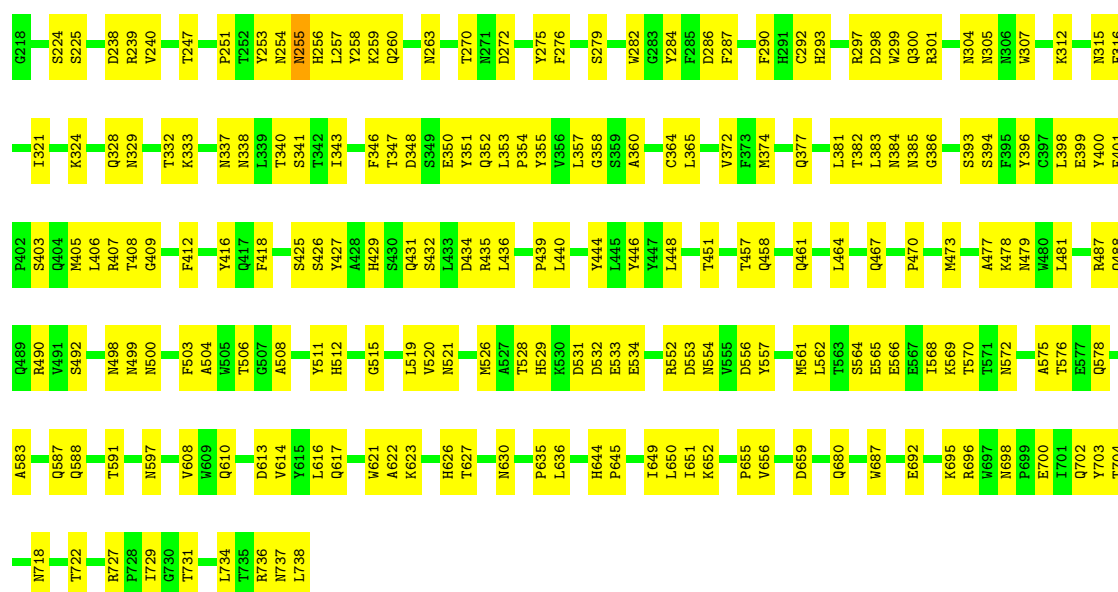
Chain G:





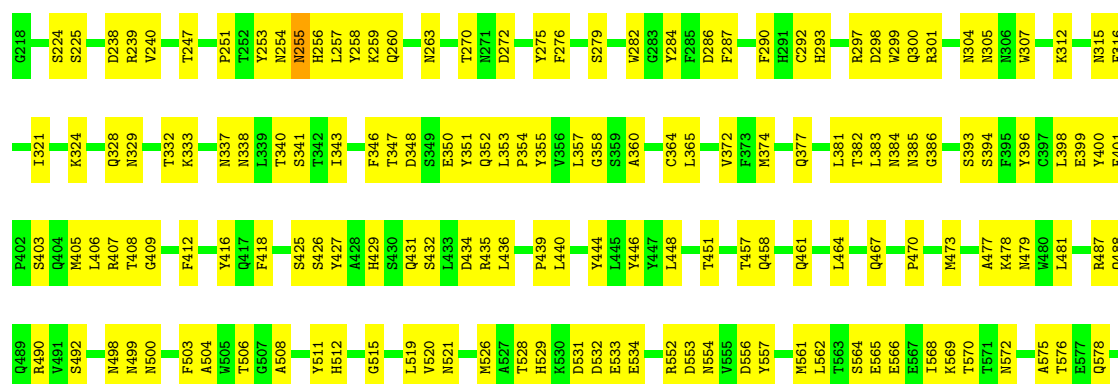
• Molecule 1: Capsid protein VP1

Chain H: 61% 39%



• Molecule 1: Capsid protein VP1

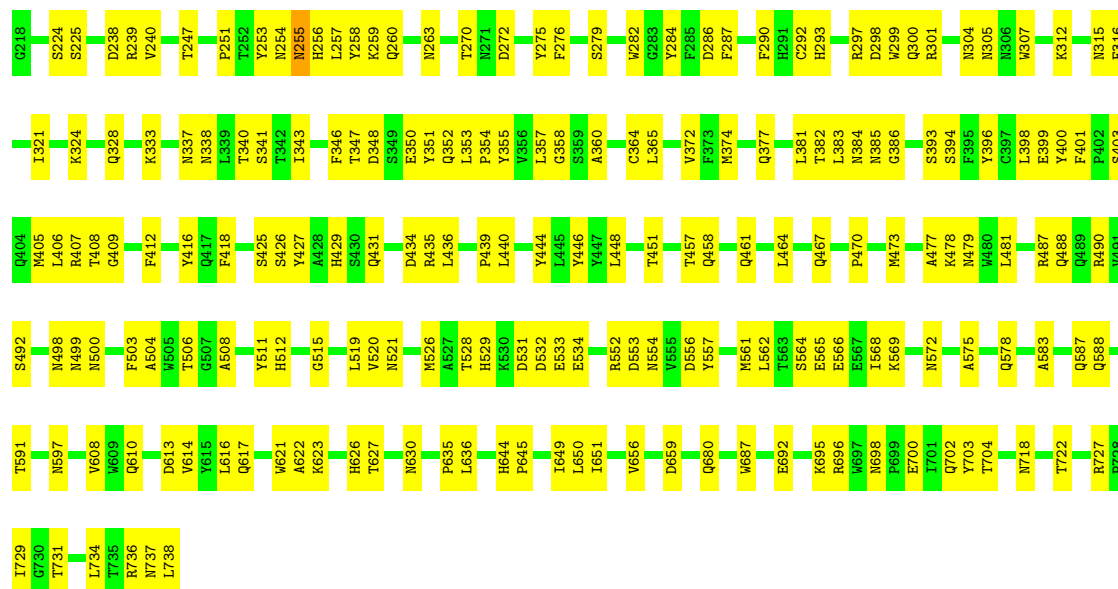
Chain I: 61% 38%





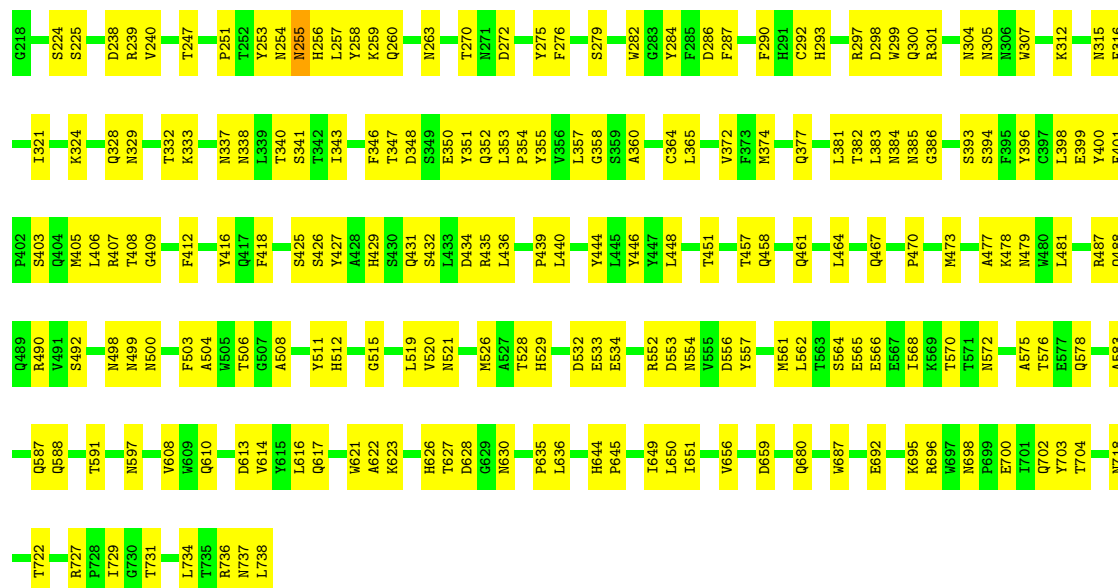
• Molecule 1: Capsid protein VP1

Chain J: 62% 37%



• Molecule 1: Capsid protein VP1

Chain K: 62% 38%



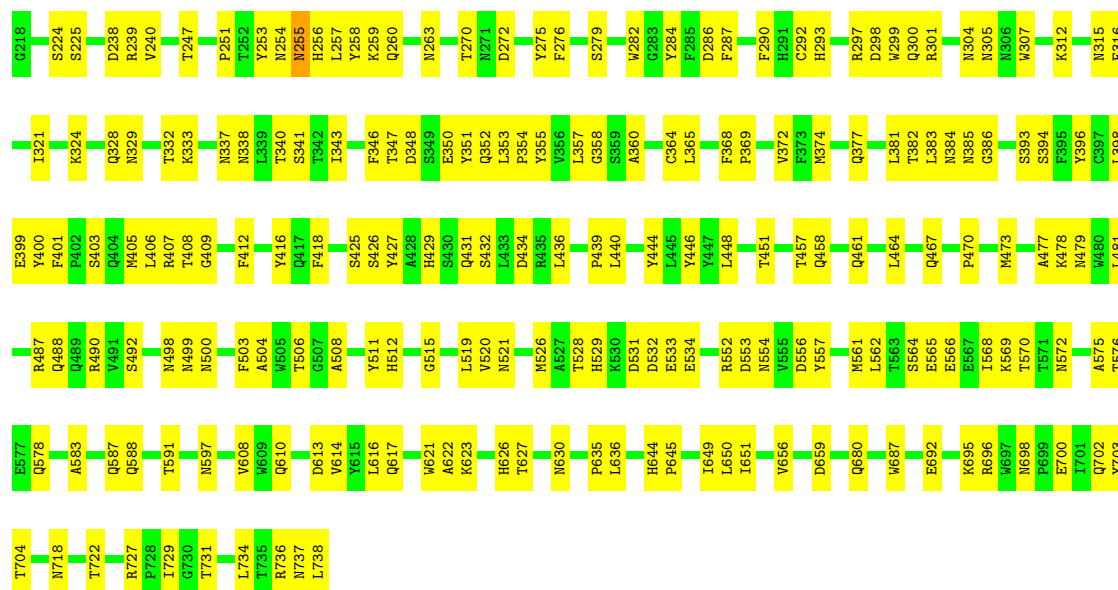
• Molecule 1: Capsid protein VP1

Chain L:



61%

39%



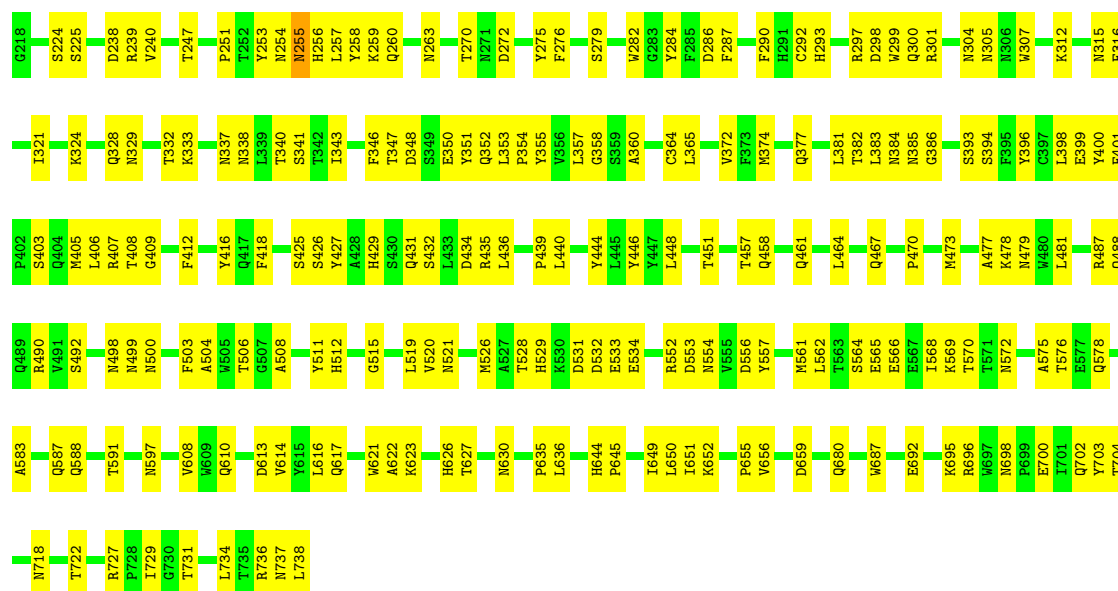
- Molecule 1: Capsid protein VP1

Chain M:



61%

39%



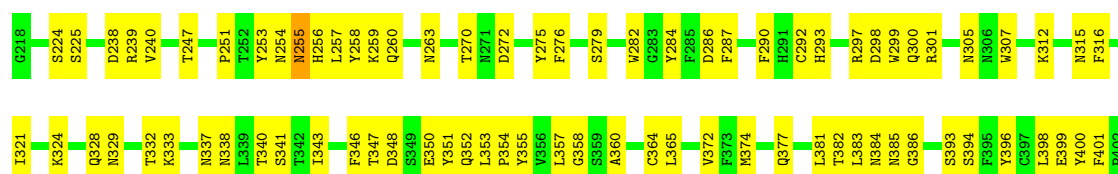
- Molecule 1: Capsid protein VP1

Chain N:



61%

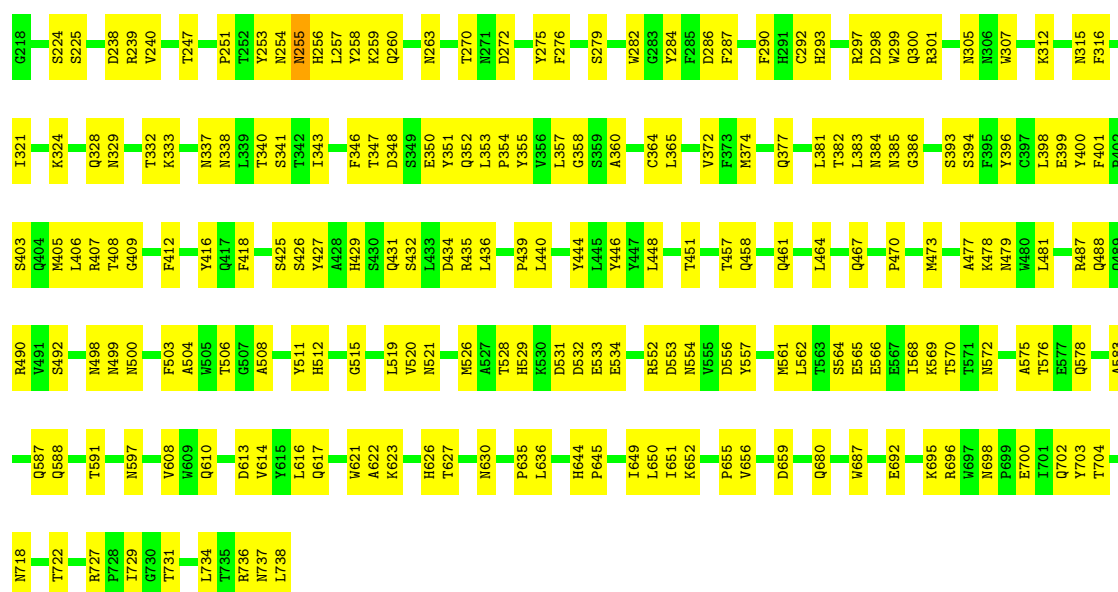
39%





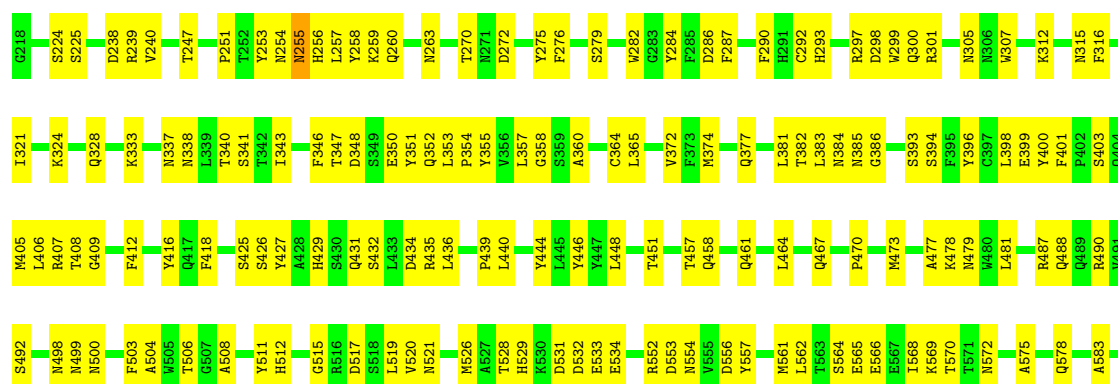
• Molecule 1: Capsid protein VP1

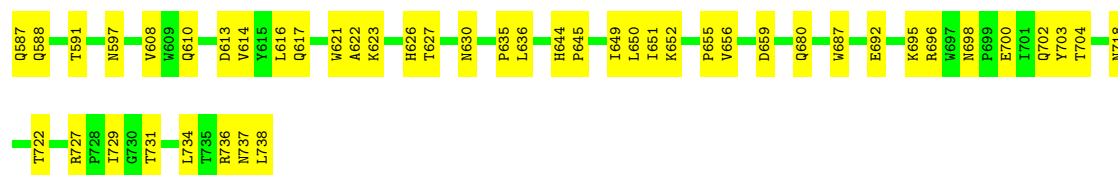
Chain O: 61% 39%



• Molecule 1: Capsid protein VP1

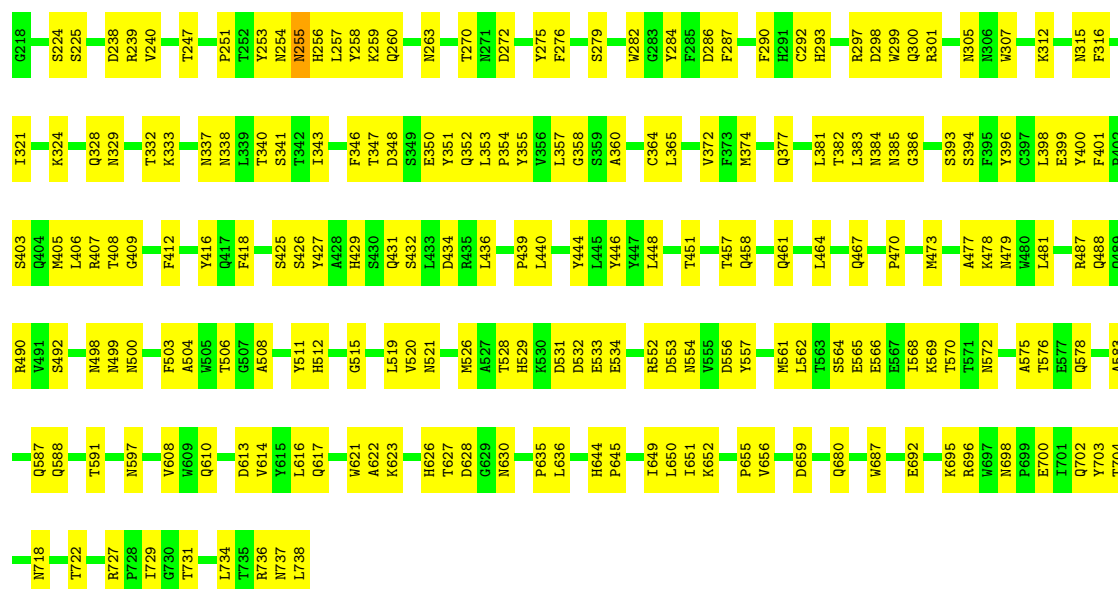
Chain P: 62% 38%





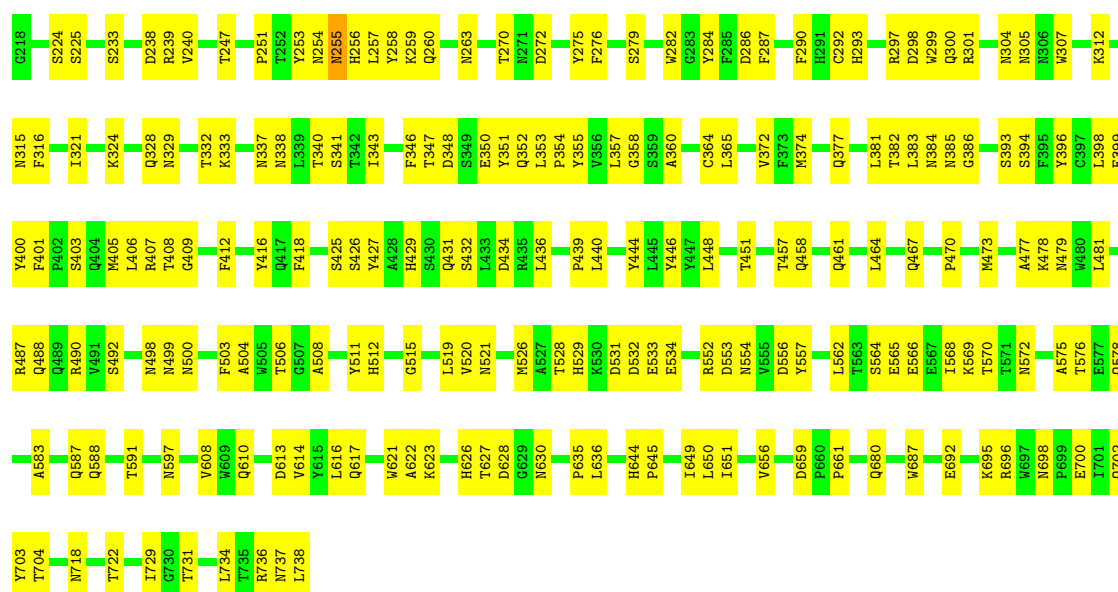
• Molecule 1: Capsid protein VP1

Chain Q: 61% 39%



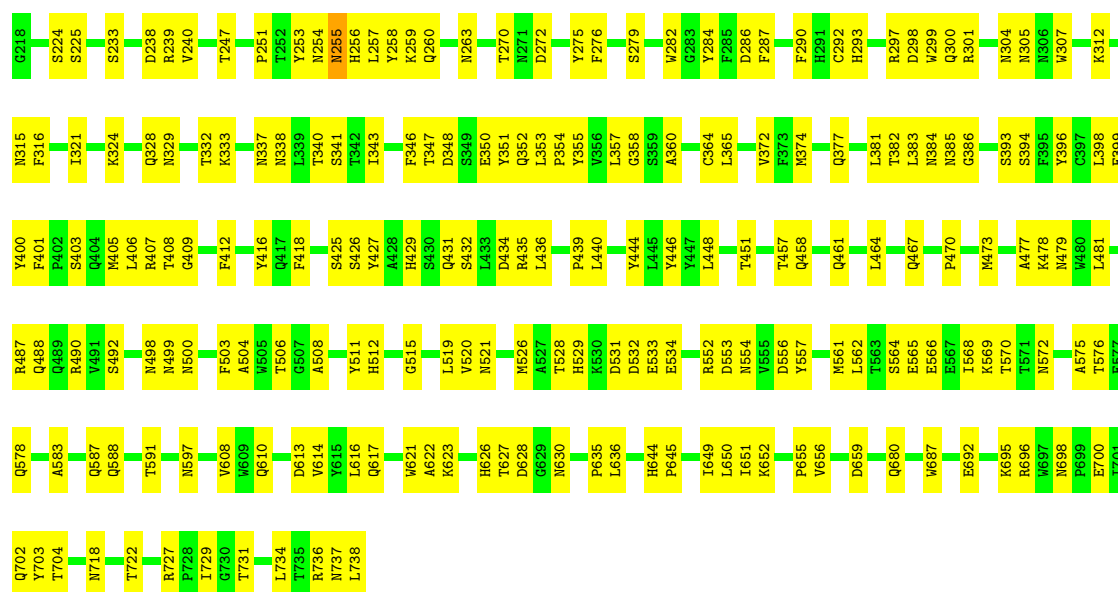
• Molecule 1: Capsid protein VP1

Chain R: 61% 38%



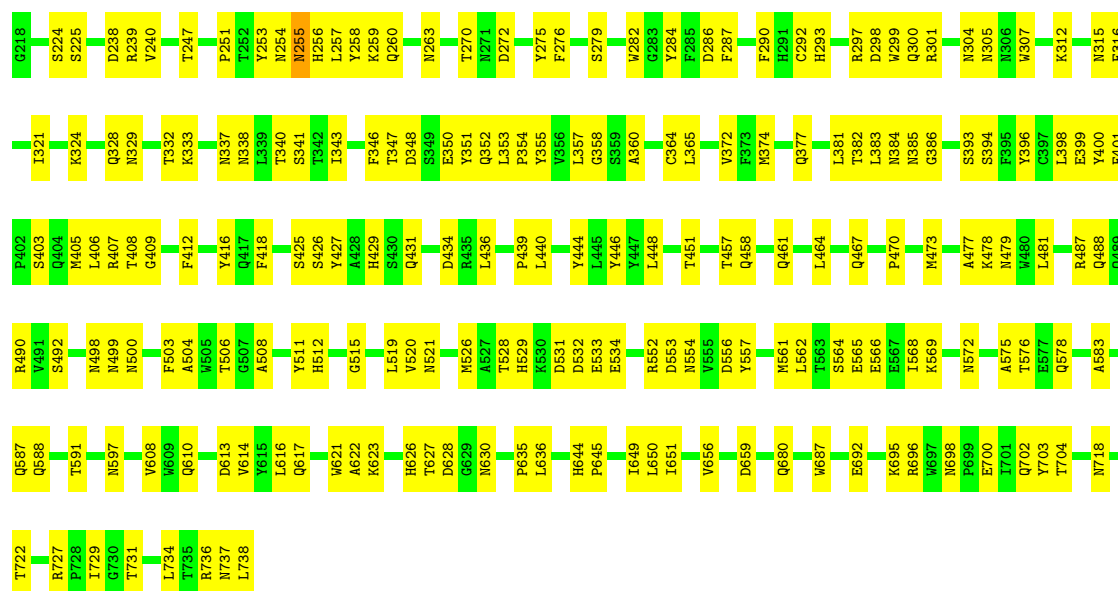
• Molecule 1: Capsid protein VP1

Chain S:



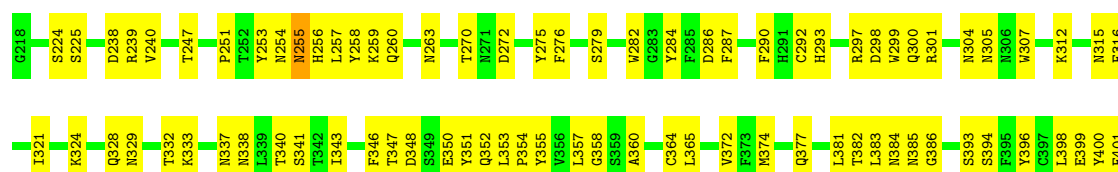
- Molecule 1: Capsid protein VP1

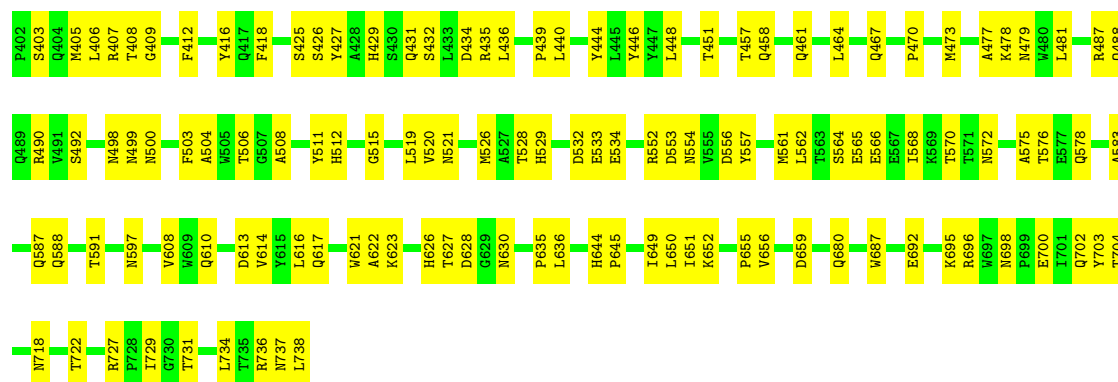
Chain T:



- Molecule 1: Capsid protein VP1

Chain U:

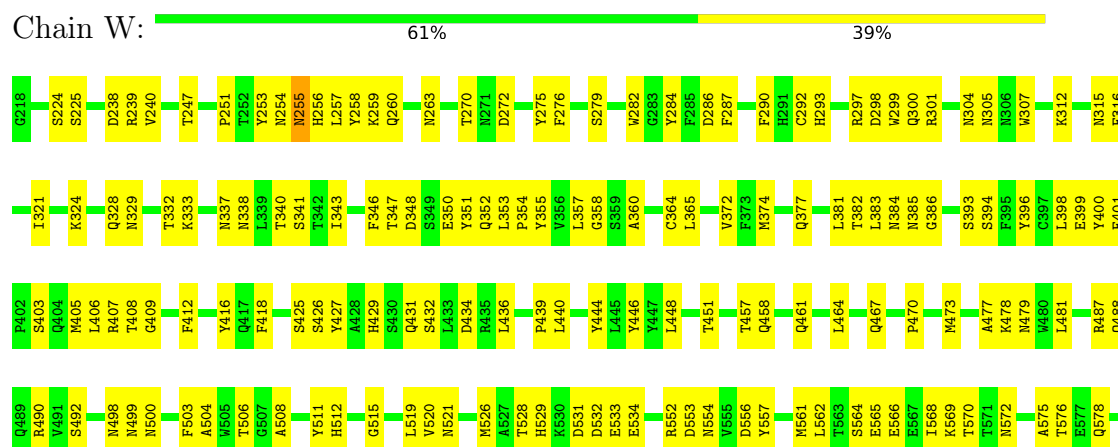




• Molecule 1: Capsid protein VP1



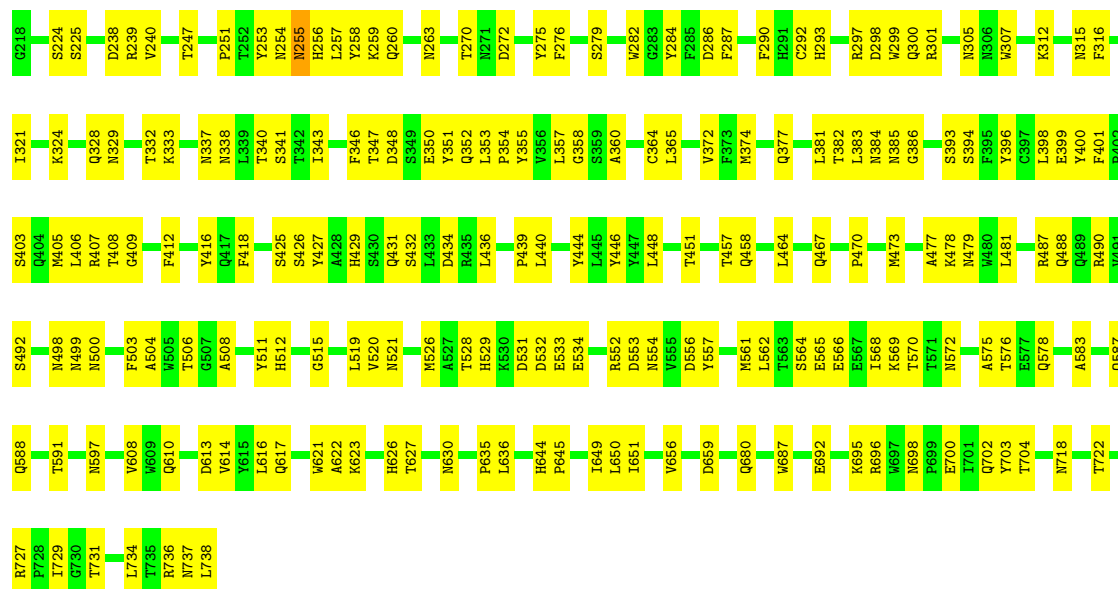
• Molecule 1: Capsid protein VP1





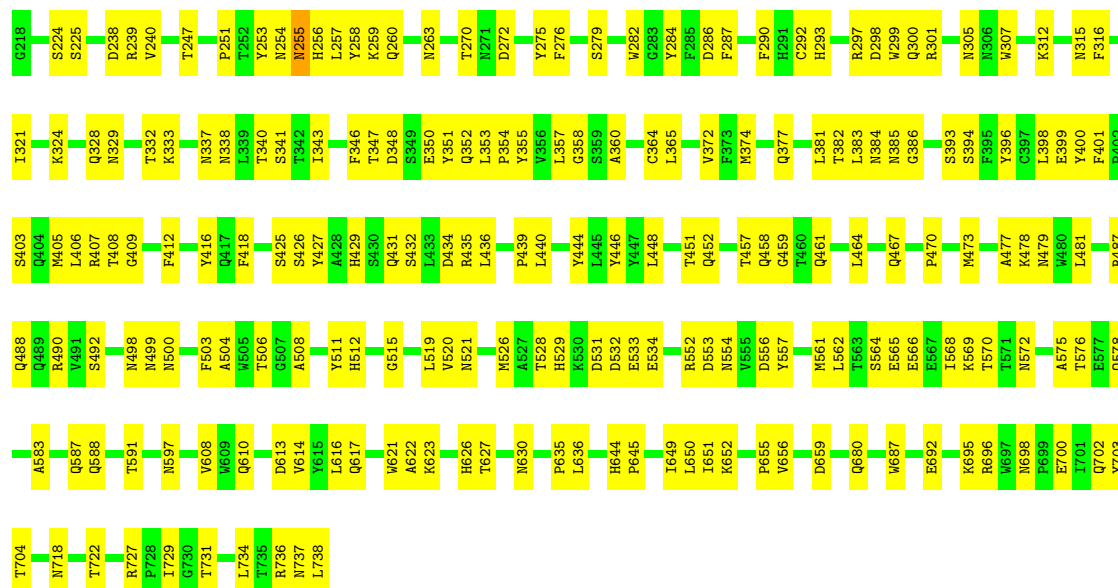
• Molecule 1: Capsid protein VP1

Chain X: 62% 38%

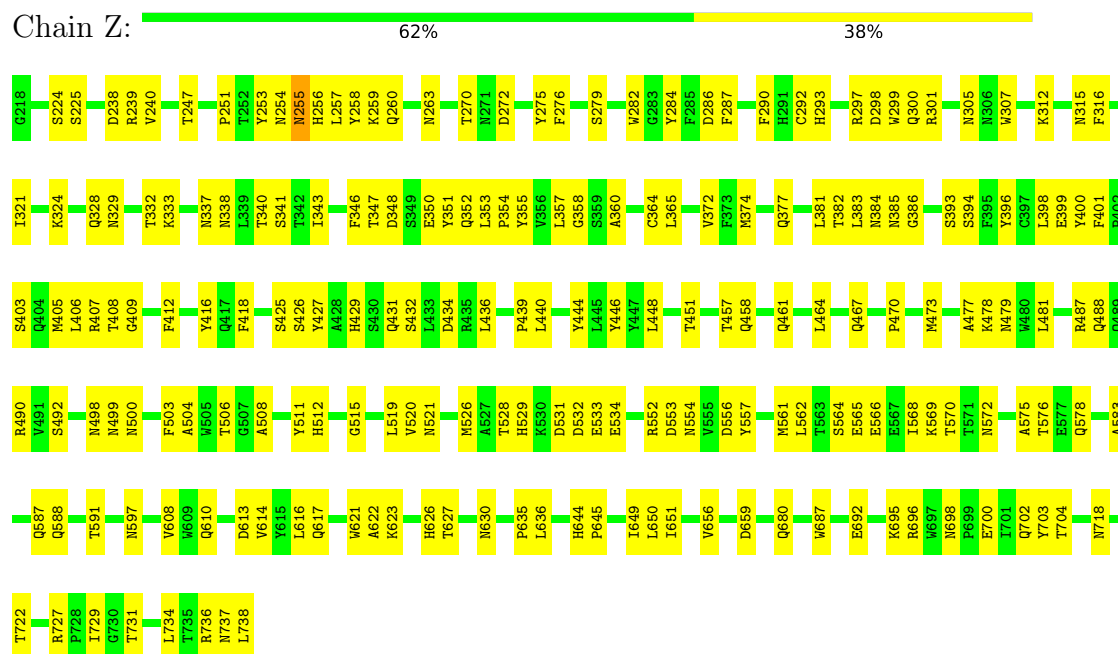


• Molecule 1: Capsid protein VP1

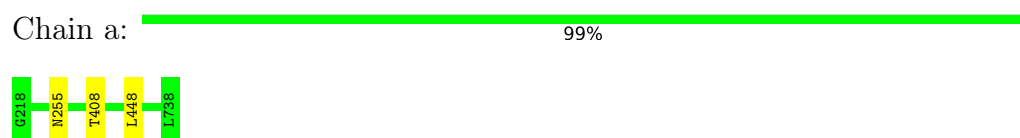
Chain Y: 61% 39%



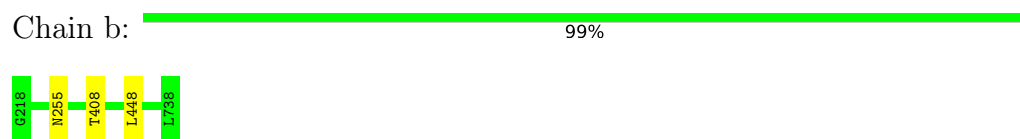
• Molecule 1: Capsid protein VP1



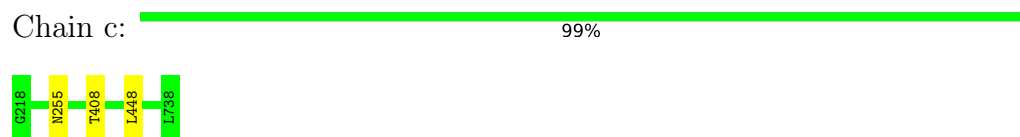
- Molecule 1: Capsid protein VP1



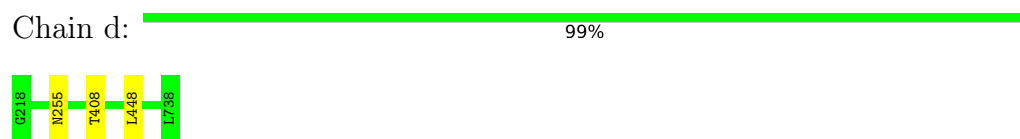
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1





- Molecule 1: Capsid protein VP1

Chain f:  99%



- Molecule 1: Capsid protein VP1

Chain g:  99%



- Molecule 1: Capsid protein VP1

Chain h:  99%



- Molecule 1: Capsid protein VP1

Chain i:  99%



- Molecule 1: Capsid protein VP1

Chain j:  99%



- Molecule 1: Capsid protein VP1

Chain k:  99%



- Molecule 1: Capsid protein VP1

Chain l:  99%



- Molecule 1: Capsid protein VP1

Chain m:  99%



- Molecule 1: Capsid protein VP1

Chain n:  99%



- Molecule 1: Capsid protein VP1

Chain o:  99%



- Molecule 1: Capsid protein VP1

Chain p:  99%



- Molecule 1: Capsid protein VP1

Chain q:  99%



- Molecule 1: Capsid protein VP1

Chain r:  99%



- Molecule 1: Capsid protein VP1

Chain s:  99%



- Molecule 1: Capsid protein VP1

Chain t:  99%



- Molecule 1: Capsid protein VP1

Chain u:  99%



- Molecule 1: Capsid protein VP1

Chain v:  99%



- Molecule 1: Capsid protein VP1

Chain w:  99%



- Molecule 1: Capsid protein VP1

Chain x:  99%



- Molecule 1: Capsid protein VP1

Chain y:  99%



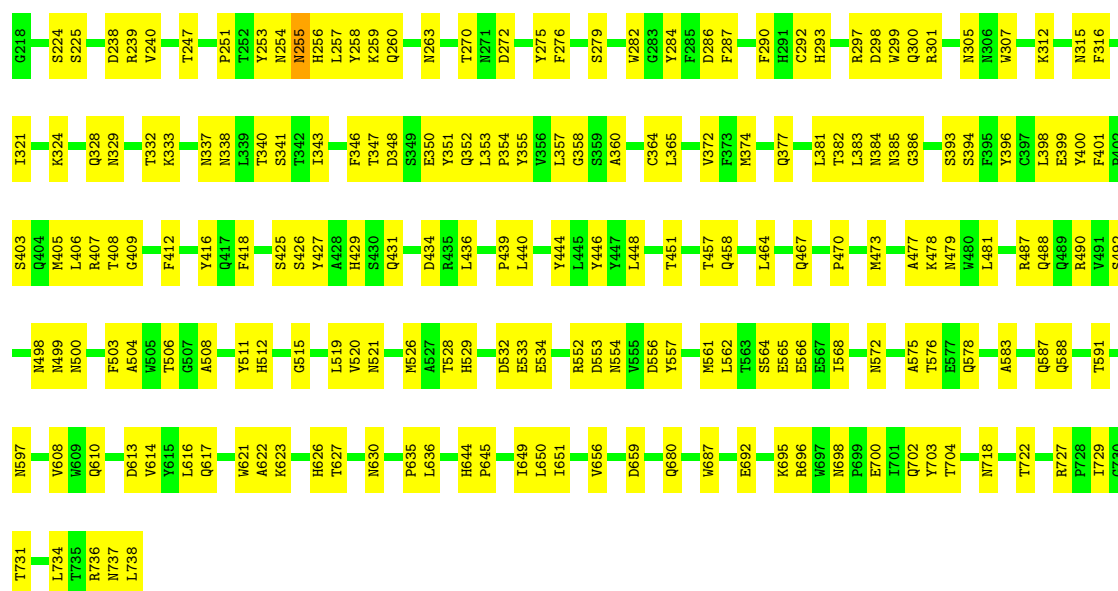
- Molecule 1: Capsid protein VP1

Chain z:  99%



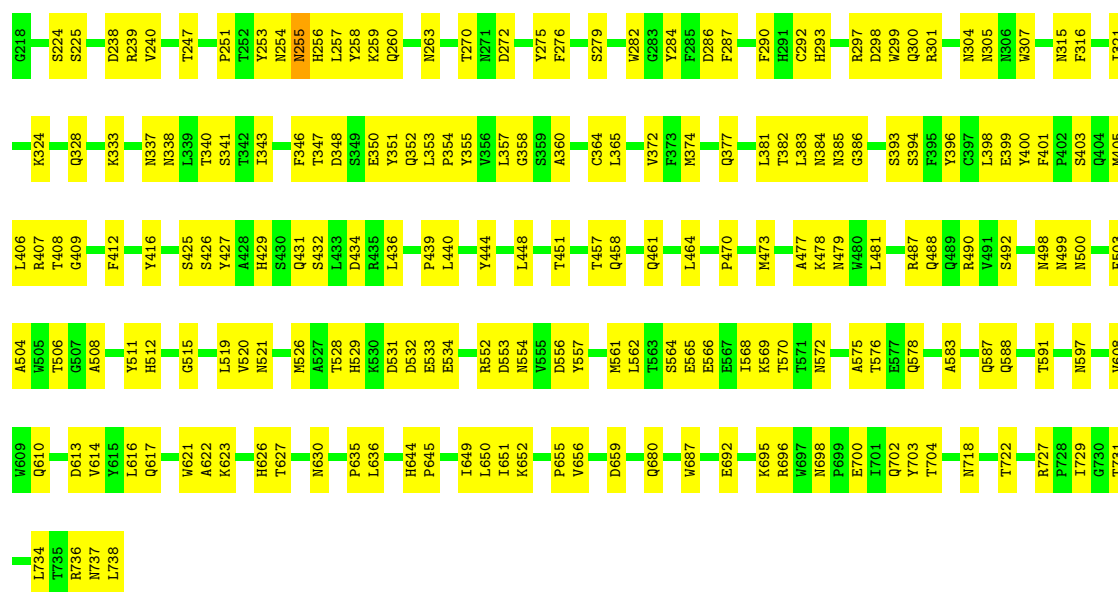
- Molecule 1: Capsid protein VP1

Chain 1:  63%  37%



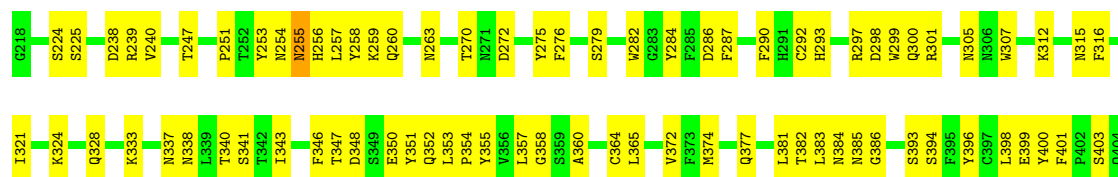
• Molecule 1: Capsid protein VP1

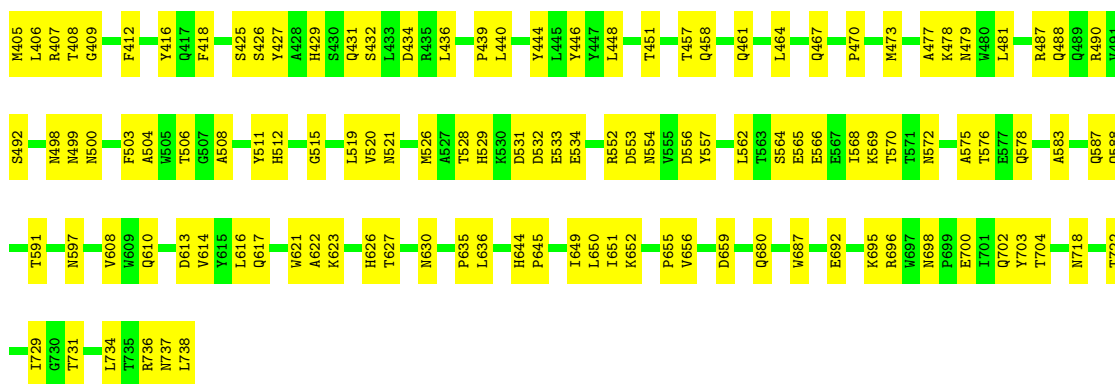
Chain 2: 62% 37%



• Molecule 1: Capsid protein VP1

Chain 3: 62% 38%

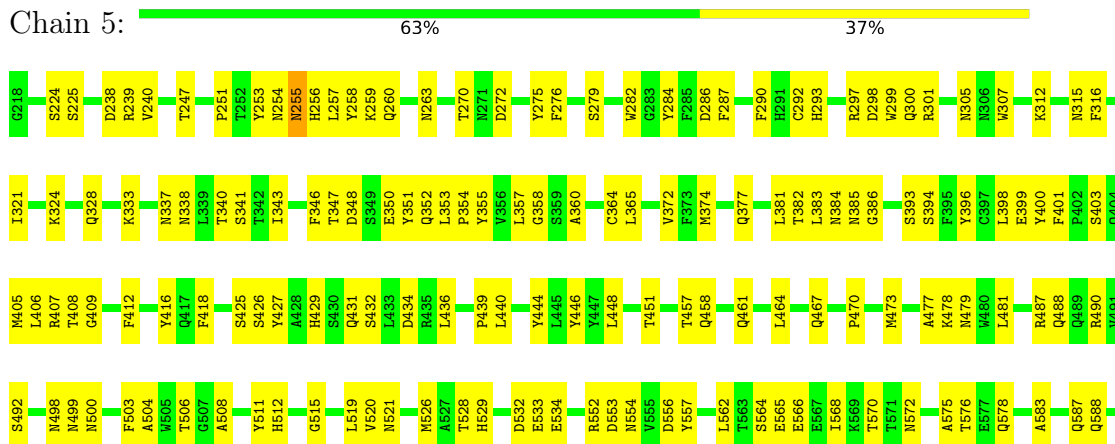


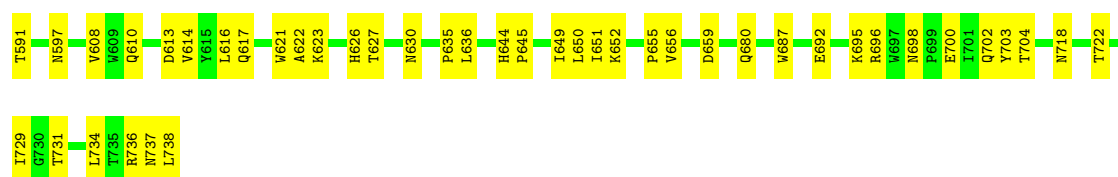


- Molecule 1: Capsid protein VP1



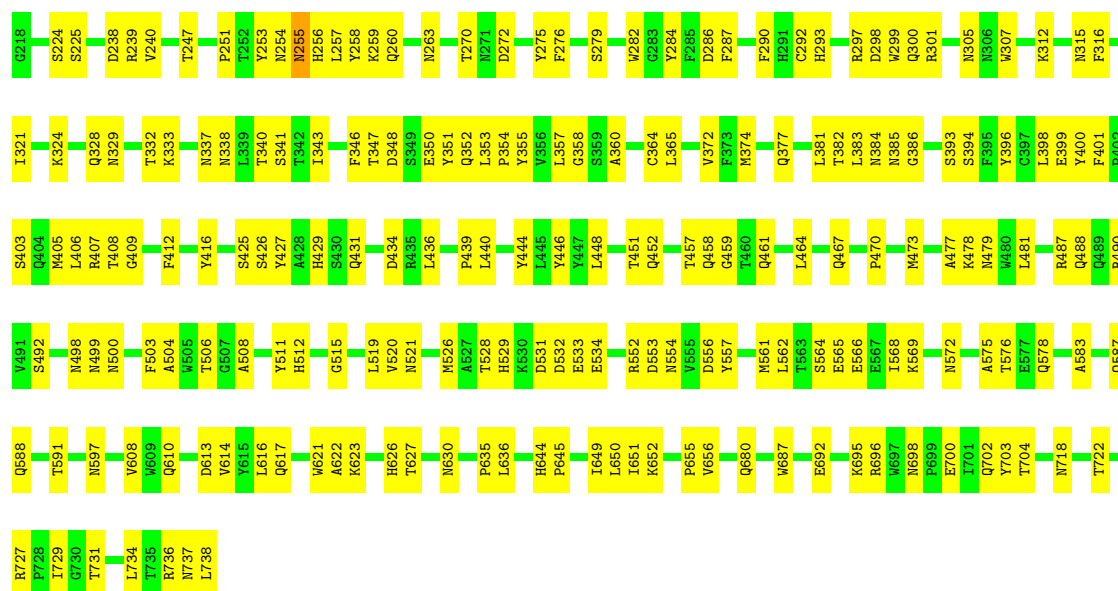
- Molecule 1: Capsid protein VP1





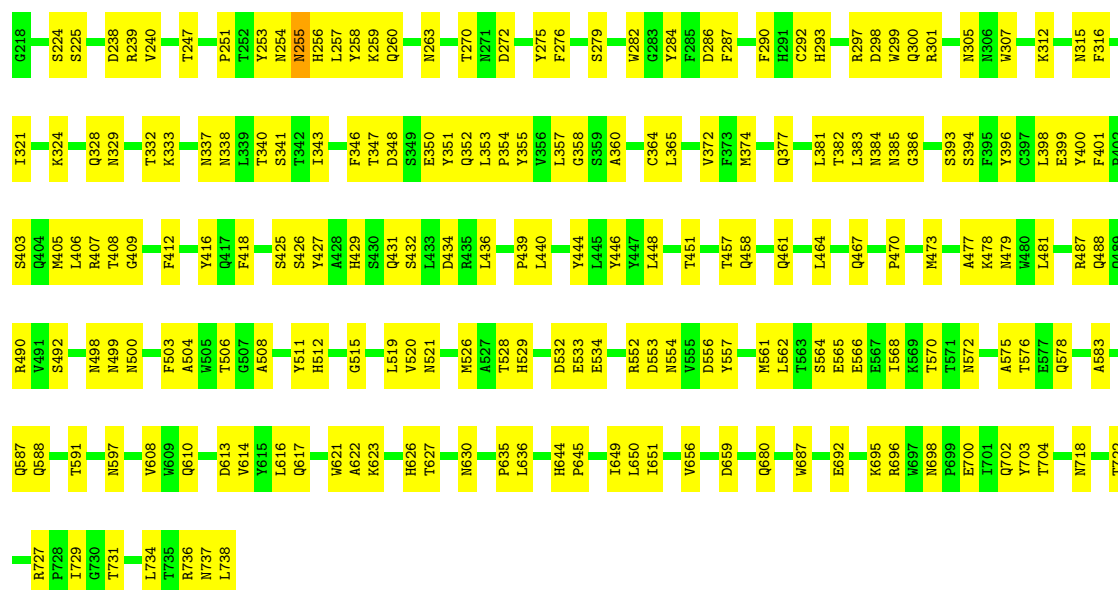
• Molecule 1: Capsid protein VP1

Chain 6: 62% 38%



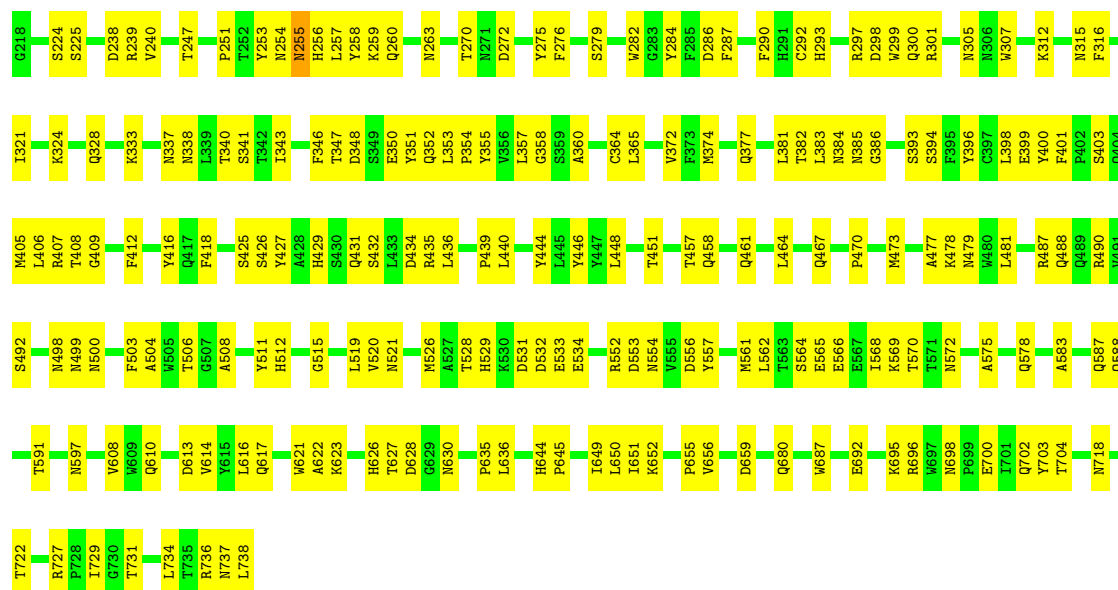
• Molecule 1: Capsid protein VP1

Chain 7: 62% 38%



• Molecule 1: Capsid protein VP1

Chain 8:



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1326	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 ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	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	0.57	0/4272	0.56	0/5826
1	2	0.57	0/4272	0.56	0/5826
1	3	0.57	0/4272	0.56	0/5826
1	4	0.57	0/4272	0.56	0/5826
1	5	0.57	0/4272	0.56	0/5826
1	6	0.57	0/4272	0.56	0/5826
1	7	0.57	0/4272	0.56	0/5826
1	8	0.57	0/4272	0.56	0/5826
1	A	0.57	0/4272	0.56	0/5826
1	B	0.57	0/4272	0.56	0/5826
1	C	0.57	0/4272	0.56	0/5826
1	D	0.57	0/4272	0.56	0/5826
1	E	0.57	0/4272	0.56	0/5826
1	F	0.57	0/4272	0.56	0/5826
1	G	0.57	0/4272	0.56	0/5826
1	H	0.57	0/4272	0.56	0/5826
1	I	0.57	0/4272	0.56	0/5826
1	J	0.57	0/4272	0.56	0/5826
1	K	0.57	0/4272	0.56	0/5826
1	L	0.57	0/4272	0.56	0/5826
1	M	0.57	0/4272	0.56	0/5826
1	N	0.57	0/4272	0.56	0/5826
1	O	0.57	0/4272	0.56	0/5826
1	P	0.57	0/4272	0.56	0/5826
1	Q	0.57	0/4272	0.56	0/5826
1	R	0.57	0/4272	0.56	0/5826
1	S	0.57	0/4272	0.56	0/5826
1	T	0.57	0/4272	0.56	0/5826
1	U	0.57	0/4272	0.56	0/5826
1	V	0.57	0/4272	0.56	0/5826
1	W	0.57	0/4272	0.56	0/5826
1	X	0.57	0/4272	0.56	0/5826
1	Y	0.57	0/4272	0.56	0/5826
1	Z	0.57	0/4272	0.56	0/5826

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	a	0.57	0/4272	0.56	0/5826
1	b	0.57	0/4272	0.56	0/5826
1	c	0.57	0/4272	0.56	0/5826
1	d	0.57	0/4272	0.56	0/5826
1	e	0.57	0/4272	0.56	0/5826
1	f	0.57	0/4272	0.56	0/5826
1	g	0.57	0/4272	0.56	0/5826
1	h	0.57	0/4272	0.56	0/5826
1	i	0.57	0/4272	0.56	0/5826
1	j	0.57	0/4272	0.56	0/5826
1	k	0.57	0/4272	0.56	0/5826
1	l	0.57	0/4272	0.56	0/5826
1	m	0.57	0/4272	0.56	0/5826
1	n	0.57	0/4272	0.56	0/5826
1	o	0.57	0/4272	0.56	0/5826
1	p	0.57	0/4272	0.56	0/5826
1	q	0.57	0/4272	0.56	0/5826
1	r	0.57	0/4272	0.56	0/5826
1	s	0.57	0/4272	0.56	0/5826
1	t	0.57	0/4272	0.56	0/5826
1	u	0.57	0/4272	0.56	0/5826
1	v	0.57	0/4272	0.56	0/5826
1	w	0.57	0/4272	0.56	0/5826
1	x	0.57	0/4272	0.56	0/5826
1	y	0.57	0/4272	0.56	0/5826
1	z	0.57	0/4272	0.56	0/5826
All	All	0.57	0/256320	0.56	0/349560

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	4145	0	3907	173	0
1	2	4145	0	3907	172	0
1	3	4145	0	3907	172	0
1	4	4145	0	3907	174	0
1	5	4145	0	3907	172	0
1	6	4145	0	3907	174	0
1	7	4145	0	3907	171	0
1	8	4145	0	3907	177	0
1	A	4145	0	3907	247	0
1	B	4145	0	3907	246	0
1	C	4145	0	3907	244	0
1	D	4145	0	3907	246	0
1	E	4145	0	3907	247	0
1	F	4145	0	3907	245	0
1	G	4145	0	3907	243	0
1	H	4145	0	3907	240	0
1	I	4145	0	3907	238	0
1	J	4145	0	3907	243	0
1	K	4145	0	3907	245	0
1	L	4145	0	3907	245	0
1	M	4145	0	3907	248	0
1	N	4145	0	3907	247	0
1	O	4145	0	3907	244	0
1	P	4145	0	3907	233	0
1	Q	4145	0	3907	238	0
1	R	4145	0	3907	222	0
1	S	4145	0	3907	227	0
1	T	4145	0	3907	246	0
1	U	4145	0	3907	245	0
1	V	4145	0	3907	249	0
1	W	4145	0	3907	245	0
1	X	4145	0	3907	244	0
1	Y	4145	0	3907	247	0
1	Z	4145	0	3907	246	0
1	a	4145	0	3907	0	0
1	b	4145	0	3907	0	0
1	c	4145	0	3907	0	0
1	d	4145	0	3907	0	0
1	e	4145	0	3907	0	0
1	f	4145	0	3907	0	0
1	g	4145	0	3907	0	0
1	h	4145	0	3907	0	0
1	i	4145	0	3907	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	4145	0	3907	0	0
1	k	4145	0	3907	0	0
1	l	4145	0	3907	0	0
1	m	4145	0	3907	0	0
1	n	4145	0	3907	0	0
1	o	4145	0	3907	0	0
1	p	4145	0	3907	0	0
1	q	4145	0	3907	0	0
1	r	4145	0	3907	0	0
1	s	4145	0	3907	0	0
1	t	4145	0	3907	0	0
1	u	4145	0	3907	0	0
1	v	4145	0	3907	0	0
1	w	4145	0	3907	0	0
1	x	4145	0	3907	0	0
1	y	4145	0	3907	0	0
1	z	4145	0	3907	0	0
2	1	16	0	12	0	0
2	2	16	0	12	0	0
2	3	16	0	12	0	0
2	4	16	0	12	0	0
2	5	16	0	12	0	0
2	6	16	0	12	0	0
2	7	16	0	12	0	0
2	8	16	0	12	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0	0
3	2	21	0	12	0	0
3	3	21	0	12	0	0
3	4	21	0	12	0	0
3	5	21	0	12	0	0
3	6	21	0	12	0	0
3	7	21	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	8	21	0	12	0	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
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
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	250920	0	235860	5698	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 12.

The worst 5 of 5698 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)
1:4:526:MET:HE2	1:4:575:ALA:HA	1.58	0.86
1:N:526:MET:HE2	1:N:575:ALA:HA	1.63	0.85
1:H:526:MET:HE2	1:H:575:ALA:HA	1.59	0.85
1:S:526:MET:HE2	1:S:575:ALA:HA	1.61	0.84
1:C:526:MET:HE2	1:C:575:ALA:HA	1.61	0.84

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	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	3	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	4	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	5	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	6	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	7	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	8	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	A	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	B	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	C	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	D	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	E	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	F	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	G	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	H	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	I	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	J	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	K	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	L	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	M	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	N	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	O	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	P	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	Q	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	R	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	S	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	T	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	U	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	V	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	W	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	X	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	Z	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	a	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	b	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	c	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	d	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	e	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	f	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	g	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	h	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	i	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	j	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	k	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	l	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	m	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	n	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	o	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	p	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	q	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	r	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	s	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	t	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	u	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	v	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	w	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	x	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	y	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
1	z	520/521 (100%)	504 (97%)	14 (3%)	2 (0%)	36	75
All	All	31200/31260 (100%)	30240 (97%)	840 (3%)	120 (0%)	40	75

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	408	THR
1	B	255	ASN
1	B	408	THR
1	C	255	ASN

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	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	2	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	3	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	4	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	5	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	6	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	7	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	8	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	A	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	B	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	C	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	D	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	E	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	F	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	G	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	H	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	I	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	J	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	K	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	L	455/454 (100%)	454 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	N	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	O	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	P	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	Q	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	R	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	S	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	T	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	U	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	V	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	W	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	X	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	Y	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	Z	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	a	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	b	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	c	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	d	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	e	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	f	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	g	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	h	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	i	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	j	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	k	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	l	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	m	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	n	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	o	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	p	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	q	455/454 (100%)	454 (100%)	1 (0%)	94	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	r	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	s	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	t	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	u	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	v	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	w	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	x	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	y	455/454 (100%)	454 (100%)	1 (0%)	94	98
1	z	455/454 (100%)	454 (100%)	1 (0%)	94	98
All	All	27300/27240 (100%)	27240 (100%)	60 (0%)	94	98

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	448	LEU
1	h	448	LEU
1	4	448	LEU
1	e	448	LEU
1	j	448	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 660 such sidechains are listed below:

Mol	Chain	Res	Type
1	b	328	GLN
1	h	610	GLN
1	4	587	GLN
1	b	737	ASN
1	e	597	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.