Full wwPDB EM Validation Report (i)

Mar 3, 2024 – 12:05 PM EST

PDB ID	:	6CBE
EMDB ID	:	EMD-7452
Title	:	Atomic structure of a rationally engineered gene delivery vector, AAV2.5
Authors	:	Burg, M.; Rosebrough, C.; Drouin, L.; Bennett, A.; Mietzsch, M.; Chipman, P.; McKenna, R.; Sousa, D.; Potter, M.; Byrne, B.; Kozyreva, O.G.; Samulski, R.J.; Agbandje-McKenna, M.
Deposited on	:	2018-02-02
Resolution	:	2.78 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

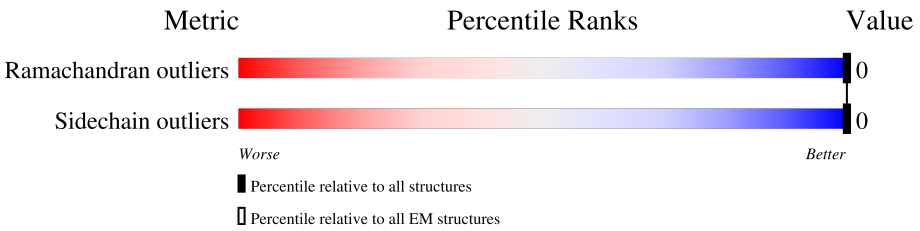
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.78 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	736	24% 70% 30%
1	1	736	24% 70% 30%
1	2	736	23% 70% 30%
1	3	736	24% 70% 30%
1	4	736	26% 70% 30%
1	5	736	24% 70% 30%
1	6	736	25% 70% 30%
1	7	736	25% 70% 30%
1	A	736	24% 70% 30%

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Mol	Chain	Length	Quality of chain
1	B	736	26% 70% 30%
1	C	736	24% 70% 30%
1	D	736	25% 70% 30%
1	E	736	23% 70% 30%
1	F	736	23% 70% 30%
1	G	736	25% 70% 30%
1	H	736	25% 70% 30%
1	I	736	24% 70% 30%
1	J	736	26% 70% 30%
1	K	736	24% 70% 30%
1	L	736	26% 70% 30%
1	M	736	25% 70% 30%
1	N	736	24% 70% 30%
1	O	736	26% 70% 30%
1	P	736	24% 70% 30%
1	Q	736	23% 70% 30%
1	R	736	24% 70% 30%
1	S	736	25% 70% 30%
1	T	736	25% 70% 30%
1	U	736	24% 70% 30%
1	V	736	26% 70% 30%
1	W	736	24% 70% 30%
1	X	736	26% 70% 30%
1	Y	736	24% 70% 30%
1	Z	736	23% 70% 30%

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Mol	Chain	Length	Quality of chain
1	a	736	25% 70% 30%
1	b	736	24% 70% 30%
1	c	736	23% 70% 30%
1	d	736	23% 70% 30%
1	e	736	23% 70% 30%
1	f	736	24% 70% 30%
1	g	736	26% 70% 30%
1	h	736	25% 70% 30%
1	i	736	23% 70% 30%
1	j	736	23% 70% 30%
1	k	736	25% 70% 30%
1	l	736	24% 70% 30%
1	m	736	24% 70% 30%
1	n	736	26% 70% 30%
1	o	736	26% 70% 30%
1	p	736	26% 70% 30%
1	q	736	24% 70% 30%
1	r	736	25% 70% 30%
1	s	736	24% 70% 30%
1	t	736	25% 70% 30%
1	u	736	24% 70% 30%
1	v	736	24% 70% 30%
1	w	736	23% 70% 30%
1	x	736	23% 70% 30%
1	y	736	24% 70% 30%

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Mol	Chain	Length	Quality of chain
1	z	736	24% 70% 30%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 248520 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
			Total	C	N	O	S		
1	A	518	4142	2606	723	800	13	0	0
1	B	518	4142	2606	723	800	13	0	0
1	C	518	4142	2606	723	800	13	0	0
1	D	518	4142	2606	723	800	13	0	0
1	E	518	4142	2606	723	800	13	0	0
1	F	518	4142	2606	723	800	13	0	0
1	G	518	4142	2606	723	800	13	0	0
1	H	518	4142	2606	723	800	13	0	0
1	I	518	4142	2606	723	800	13	0	0
1	J	518	4142	2606	723	800	13	0	0
1	K	518	4142	2606	723	800	13	0	0
1	L	518	4142	2606	723	800	13	0	0
1	M	518	4142	2606	723	800	13	0	0
1	N	518	4142	2606	723	800	13	0	0
1	O	518	4142	2606	723	800	13	0	0
1	P	518	4142	2606	723	800	13	0	0
1	Q	518	4142	2606	723	800	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	S	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	T	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	U	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	V	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	W	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	X	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	Y	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	Z	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	0	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	1	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	2	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	3	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	4	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	5	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	a	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	b	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	c	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	d	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	e	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	f	518	4142	2606	723	800	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	g	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	h	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	i	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	j	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	k	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	l	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	m	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	n	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	o	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	p	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	q	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	r	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	s	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	t	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	u	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	v	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	w	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	x	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	y	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	z	518	4142	2606	723	800	13	0	0
			Total	C	N	O	S		
1	6	518	4142	2606	723	800	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	7	518	4142	2606	723	800	13	0	0

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	ALA	GLN	conflict	UNP P03135
A	265	THR	-	insertion	UNP P03135
A	706	ALA	ASN	conflict	UNP P03135
A	709	ALA	VAL	conflict	UNP P03135
A	717	ASN	THR	conflict	UNP P03135
B	263	ALA	GLN	conflict	UNP P03135
B	265	THR	-	insertion	UNP P03135
B	706	ALA	ASN	conflict	UNP P03135
B	709	ALA	VAL	conflict	UNP P03135
B	717	ASN	THR	conflict	UNP P03135
C	263	ALA	GLN	conflict	UNP P03135
C	265	THR	-	insertion	UNP P03135
C	706	ALA	ASN	conflict	UNP P03135
C	709	ALA	VAL	conflict	UNP P03135
C	717	ASN	THR	conflict	UNP P03135
D	263	ALA	GLN	conflict	UNP P03135
D	265	THR	-	insertion	UNP P03135
D	706	ALA	ASN	conflict	UNP P03135
D	709	ALA	VAL	conflict	UNP P03135
D	717	ASN	THR	conflict	UNP P03135
E	263	ALA	GLN	conflict	UNP P03135
E	265	THR	-	insertion	UNP P03135
E	706	ALA	ASN	conflict	UNP P03135
E	709	ALA	VAL	conflict	UNP P03135
E	717	ASN	THR	conflict	UNP P03135
F	263	ALA	GLN	conflict	UNP P03135
F	265	THR	-	insertion	UNP P03135
F	706	ALA	ASN	conflict	UNP P03135
F	709	ALA	VAL	conflict	UNP P03135
F	717	ASN	THR	conflict	UNP P03135
G	263	ALA	GLN	conflict	UNP P03135
G	265	THR	-	insertion	UNP P03135
G	706	ALA	ASN	conflict	UNP P03135
G	709	ALA	VAL	conflict	UNP P03135
G	717	ASN	THR	conflict	UNP P03135
H	263	ALA	GLN	conflict	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
H	265	THR	-	insertion	UNP P03135
H	706	ALA	ASN	conflict	UNP P03135
H	709	ALA	VAL	conflict	UNP P03135
H	717	ASN	THR	conflict	UNP P03135
I	263	ALA	GLN	conflict	UNP P03135
I	265	THR	-	insertion	UNP P03135
I	706	ALA	ASN	conflict	UNP P03135
I	709	ALA	VAL	conflict	UNP P03135
I	717	ASN	THR	conflict	UNP P03135
J	263	ALA	GLN	conflict	UNP P03135
J	265	THR	-	insertion	UNP P03135
J	706	ALA	ASN	conflict	UNP P03135
J	709	ALA	VAL	conflict	UNP P03135
J	717	ASN	THR	conflict	UNP P03135
K	263	ALA	GLN	conflict	UNP P03135
K	265	THR	-	insertion	UNP P03135
K	706	ALA	ASN	conflict	UNP P03135
K	709	ALA	VAL	conflict	UNP P03135
K	717	ASN	THR	conflict	UNP P03135
L	263	ALA	GLN	conflict	UNP P03135
L	265	THR	-	insertion	UNP P03135
L	706	ALA	ASN	conflict	UNP P03135
L	709	ALA	VAL	conflict	UNP P03135
L	717	ASN	THR	conflict	UNP P03135
M	263	ALA	GLN	conflict	UNP P03135
M	265	THR	-	insertion	UNP P03135
M	706	ALA	ASN	conflict	UNP P03135
M	709	ALA	VAL	conflict	UNP P03135
M	717	ASN	THR	conflict	UNP P03135
N	263	ALA	GLN	conflict	UNP P03135
N	265	THR	-	insertion	UNP P03135
N	706	ALA	ASN	conflict	UNP P03135
N	709	ALA	VAL	conflict	UNP P03135
N	717	ASN	THR	conflict	UNP P03135
O	263	ALA	GLN	conflict	UNP P03135
O	265	THR	-	insertion	UNP P03135
O	706	ALA	ASN	conflict	UNP P03135
O	709	ALA	VAL	conflict	UNP P03135
O	717	ASN	THR	conflict	UNP P03135
P	263	ALA	GLN	conflict	UNP P03135
P	265	THR	-	insertion	UNP P03135
P	706	ALA	ASN	conflict	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
P	709	ALA	VAL	conflict	UNP P03135
P	717	ASN	THR	conflict	UNP P03135
Q	263	ALA	GLN	conflict	UNP P03135
Q	265	THR	-	insertion	UNP P03135
Q	706	ALA	ASN	conflict	UNP P03135
Q	709	ALA	VAL	conflict	UNP P03135
Q	717	ASN	THR	conflict	UNP P03135
R	263	ALA	GLN	conflict	UNP P03135
R	265	THR	-	insertion	UNP P03135
R	706	ALA	ASN	conflict	UNP P03135
R	709	ALA	VAL	conflict	UNP P03135
R	717	ASN	THR	conflict	UNP P03135
S	263	ALA	GLN	conflict	UNP P03135
S	265	THR	-	insertion	UNP P03135
S	706	ALA	ASN	conflict	UNP P03135
S	709	ALA	VAL	conflict	UNP P03135
S	717	ASN	THR	conflict	UNP P03135
T	263	ALA	GLN	conflict	UNP P03135
T	265	THR	-	insertion	UNP P03135
T	706	ALA	ASN	conflict	UNP P03135
T	709	ALA	VAL	conflict	UNP P03135
T	717	ASN	THR	conflict	UNP P03135
U	263	ALA	GLN	conflict	UNP P03135
U	265	THR	-	insertion	UNP P03135
U	706	ALA	ASN	conflict	UNP P03135
U	709	ALA	VAL	conflict	UNP P03135
U	717	ASN	THR	conflict	UNP P03135
V	263	ALA	GLN	conflict	UNP P03135
V	265	THR	-	insertion	UNP P03135
V	706	ALA	ASN	conflict	UNP P03135
V	709	ALA	VAL	conflict	UNP P03135
V	717	ASN	THR	conflict	UNP P03135
W	263	ALA	GLN	conflict	UNP P03135
W	265	THR	-	insertion	UNP P03135
W	706	ALA	ASN	conflict	UNP P03135
W	709	ALA	VAL	conflict	UNP P03135
W	717	ASN	THR	conflict	UNP P03135
X	263	ALA	GLN	conflict	UNP P03135
X	265	THR	-	insertion	UNP P03135
X	706	ALA	ASN	conflict	UNP P03135
X	709	ALA	VAL	conflict	UNP P03135
X	717	ASN	THR	conflict	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	263	ALA	GLN	conflict	UNP P03135
Y	265	THR	-	insertion	UNP P03135
Y	706	ALA	ASN	conflict	UNP P03135
Y	709	ALA	VAL	conflict	UNP P03135
Y	717	ASN	THR	conflict	UNP P03135
Z	263	ALA	GLN	conflict	UNP P03135
Z	265	THR	-	insertion	UNP P03135
Z	706	ALA	ASN	conflict	UNP P03135
Z	709	ALA	VAL	conflict	UNP P03135
Z	717	ASN	THR	conflict	UNP P03135
0	263	ALA	GLN	conflict	UNP P03135
0	265	THR	-	insertion	UNP P03135
0	706	ALA	ASN	conflict	UNP P03135
0	709	ALA	VAL	conflict	UNP P03135
0	717	ASN	THR	conflict	UNP P03135
1	263	ALA	GLN	conflict	UNP P03135
1	265	THR	-	insertion	UNP P03135
1	706	ALA	ASN	conflict	UNP P03135
1	709	ALA	VAL	conflict	UNP P03135
1	717	ASN	THR	conflict	UNP P03135
2	263	ALA	GLN	conflict	UNP P03135
2	265	THR	-	insertion	UNP P03135
2	706	ALA	ASN	conflict	UNP P03135
2	709	ALA	VAL	conflict	UNP P03135
2	717	ASN	THR	conflict	UNP P03135
3	263	ALA	GLN	conflict	UNP P03135
3	265	THR	-	insertion	UNP P03135
3	706	ALA	ASN	conflict	UNP P03135
3	709	ALA	VAL	conflict	UNP P03135
3	717	ASN	THR	conflict	UNP P03135
4	263	ALA	GLN	conflict	UNP P03135
4	265	THR	-	insertion	UNP P03135
4	706	ALA	ASN	conflict	UNP P03135
4	709	ALA	VAL	conflict	UNP P03135
4	717	ASN	THR	conflict	UNP P03135
5	263	ALA	GLN	conflict	UNP P03135
5	265	THR	-	insertion	UNP P03135
5	706	ALA	ASN	conflict	UNP P03135
5	709	ALA	VAL	conflict	UNP P03135
5	717	ASN	THR	conflict	UNP P03135
a	263	ALA	GLN	conflict	UNP P03135
a	265	THR	-	insertion	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
a	706	ALA	ASN	conflict	UNP P03135
a	709	ALA	VAL	conflict	UNP P03135
a	717	ASN	THR	conflict	UNP P03135
b	263	ALA	GLN	conflict	UNP P03135
b	265	THR	-	insertion	UNP P03135
b	706	ALA	ASN	conflict	UNP P03135
b	709	ALA	VAL	conflict	UNP P03135
b	717	ASN	THR	conflict	UNP P03135
c	263	ALA	GLN	conflict	UNP P03135
c	265	THR	-	insertion	UNP P03135
c	706	ALA	ASN	conflict	UNP P03135
c	709	ALA	VAL	conflict	UNP P03135
c	717	ASN	THR	conflict	UNP P03135
d	263	ALA	GLN	conflict	UNP P03135
d	265	THR	-	insertion	UNP P03135
d	706	ALA	ASN	conflict	UNP P03135
d	709	ALA	VAL	conflict	UNP P03135
d	717	ASN	THR	conflict	UNP P03135
e	263	ALA	GLN	conflict	UNP P03135
e	265	THR	-	insertion	UNP P03135
e	706	ALA	ASN	conflict	UNP P03135
e	709	ALA	VAL	conflict	UNP P03135
e	717	ASN	THR	conflict	UNP P03135
f	263	ALA	GLN	conflict	UNP P03135
f	265	THR	-	insertion	UNP P03135
f	706	ALA	ASN	conflict	UNP P03135
f	709	ALA	VAL	conflict	UNP P03135
f	717	ASN	THR	conflict	UNP P03135
g	263	ALA	GLN	conflict	UNP P03135
g	265	THR	-	insertion	UNP P03135
g	706	ALA	ASN	conflict	UNP P03135
g	709	ALA	VAL	conflict	UNP P03135
g	717	ASN	THR	conflict	UNP P03135
h	263	ALA	GLN	conflict	UNP P03135
h	265	THR	-	insertion	UNP P03135
h	706	ALA	ASN	conflict	UNP P03135
h	709	ALA	VAL	conflict	UNP P03135
h	717	ASN	THR	conflict	UNP P03135
i	263	ALA	GLN	conflict	UNP P03135
i	265	THR	-	insertion	UNP P03135
i	706	ALA	ASN	conflict	UNP P03135
i	709	ALA	VAL	conflict	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
i	717	ASN	THR	conflict	UNP P03135
j	263	ALA	GLN	conflict	UNP P03135
j	265	THR	-	insertion	UNP P03135
j	706	ALA	ASN	conflict	UNP P03135
j	709	ALA	VAL	conflict	UNP P03135
j	717	ASN	THR	conflict	UNP P03135
k	263	ALA	GLN	conflict	UNP P03135
k	265	THR	-	insertion	UNP P03135
k	706	ALA	ASN	conflict	UNP P03135
k	709	ALA	VAL	conflict	UNP P03135
k	717	ASN	THR	conflict	UNP P03135
l	263	ALA	GLN	conflict	UNP P03135
l	265	THR	-	insertion	UNP P03135
l	706	ALA	ASN	conflict	UNP P03135
l	709	ALA	VAL	conflict	UNP P03135
l	717	ASN	THR	conflict	UNP P03135
m	263	ALA	GLN	conflict	UNP P03135
m	265	THR	-	insertion	UNP P03135
m	706	ALA	ASN	conflict	UNP P03135
m	709	ALA	VAL	conflict	UNP P03135
m	717	ASN	THR	conflict	UNP P03135
n	263	ALA	GLN	conflict	UNP P03135
n	265	THR	-	insertion	UNP P03135
n	706	ALA	ASN	conflict	UNP P03135
n	709	ALA	VAL	conflict	UNP P03135
n	717	ASN	THR	conflict	UNP P03135
o	263	ALA	GLN	conflict	UNP P03135
o	265	THR	-	insertion	UNP P03135
o	706	ALA	ASN	conflict	UNP P03135
o	709	ALA	VAL	conflict	UNP P03135
o	717	ASN	THR	conflict	UNP P03135
p	263	ALA	GLN	conflict	UNP P03135
p	265	THR	-	insertion	UNP P03135
p	706	ALA	ASN	conflict	UNP P03135
p	709	ALA	VAL	conflict	UNP P03135
p	717	ASN	THR	conflict	UNP P03135
q	263	ALA	GLN	conflict	UNP P03135
q	265	THR	-	insertion	UNP P03135
q	706	ALA	ASN	conflict	UNP P03135
q	709	ALA	VAL	conflict	UNP P03135
q	717	ASN	THR	conflict	UNP P03135
r	263	ALA	GLN	conflict	UNP P03135

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Chain	Residue	Modelled	Actual	Comment	Reference
r	265	THR	-	insertion	UNP P03135
r	706	ALA	ASN	conflict	UNP P03135
r	709	ALA	VAL	conflict	UNP P03135
r	717	ASN	THR	conflict	UNP P03135
s	263	ALA	GLN	conflict	UNP P03135
s	265	THR	-	insertion	UNP P03135
s	706	ALA	ASN	conflict	UNP P03135
s	709	ALA	VAL	conflict	UNP P03135
s	717	ASN	THR	conflict	UNP P03135
t	263	ALA	GLN	conflict	UNP P03135
t	265	THR	-	insertion	UNP P03135
t	706	ALA	ASN	conflict	UNP P03135
t	709	ALA	VAL	conflict	UNP P03135
t	717	ASN	THR	conflict	UNP P03135
u	263	ALA	GLN	conflict	UNP P03135
u	265	THR	-	insertion	UNP P03135
u	706	ALA	ASN	conflict	UNP P03135
u	709	ALA	VAL	conflict	UNP P03135
u	717	ASN	THR	conflict	UNP P03135
v	263	ALA	GLN	conflict	UNP P03135
v	265	THR	-	insertion	UNP P03135
v	706	ALA	ASN	conflict	UNP P03135
v	709	ALA	VAL	conflict	UNP P03135
v	717	ASN	THR	conflict	UNP P03135
w	263	ALA	GLN	conflict	UNP P03135
w	265	THR	-	insertion	UNP P03135
w	706	ALA	ASN	conflict	UNP P03135
w	709	ALA	VAL	conflict	UNP P03135
w	717	ASN	THR	conflict	UNP P03135
x	263	ALA	GLN	conflict	UNP P03135
x	265	THR	-	insertion	UNP P03135
x	706	ALA	ASN	conflict	UNP P03135
x	709	ALA	VAL	conflict	UNP P03135
x	717	ASN	THR	conflict	UNP P03135
y	263	ALA	GLN	conflict	UNP P03135
y	265	THR	-	insertion	UNP P03135
y	706	ALA	ASN	conflict	UNP P03135
y	709	ALA	VAL	conflict	UNP P03135
y	717	ASN	THR	conflict	UNP P03135
z	263	ALA	GLN	conflict	UNP P03135
z	265	THR	-	insertion	UNP P03135
z	706	ALA	ASN	conflict	UNP P03135

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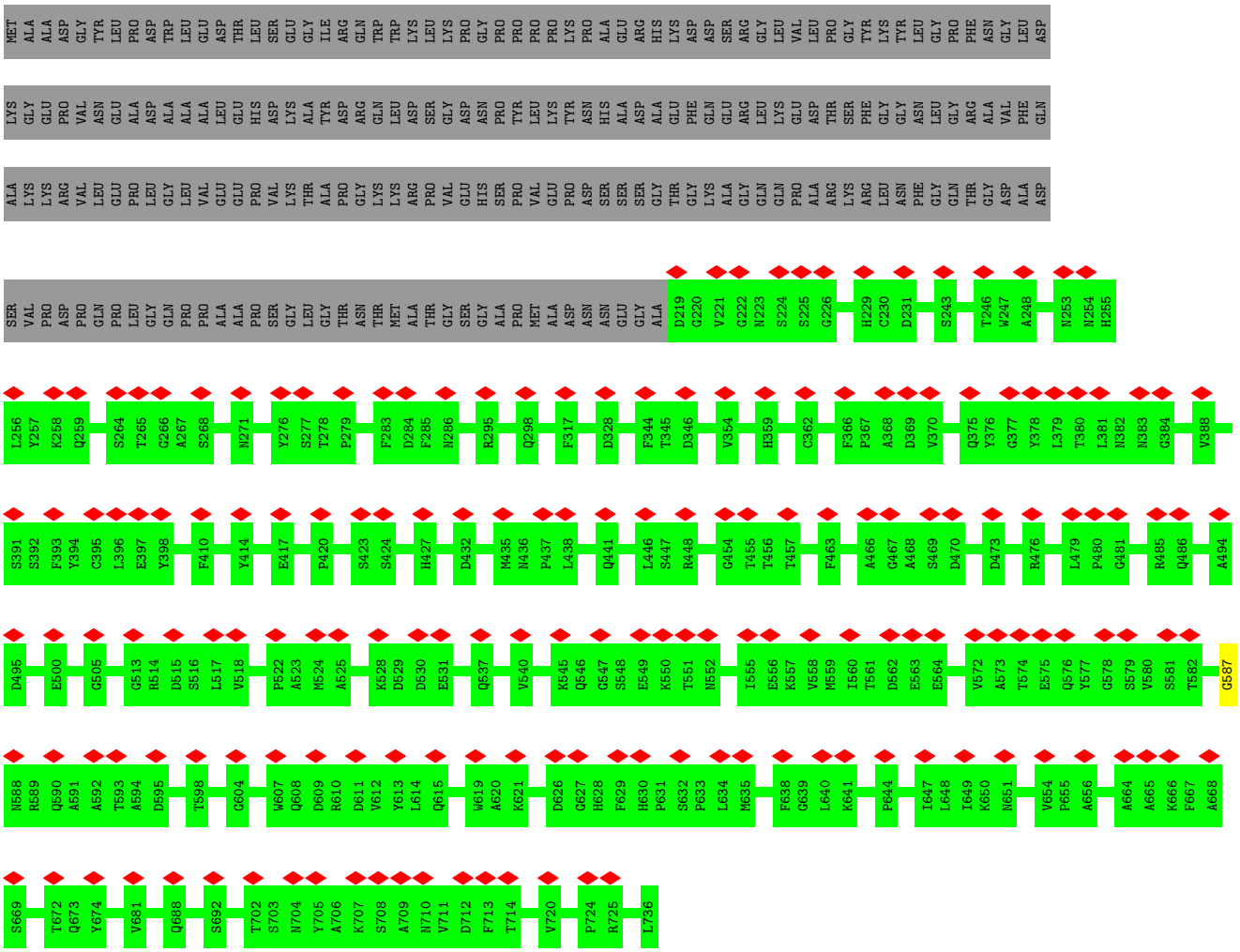
Chain	Residue	Modelled	Actual	Comment	Reference
z	709	ALA	VAL	conflict	UNP P03135
z	717	ASN	THR	conflict	UNP P03135
6	263	ALA	GLN	conflict	UNP P03135
6	265	THR	-	insertion	UNP P03135
6	706	ALA	ASN	conflict	UNP P03135
6	709	ALA	VAL	conflict	UNP P03135
6	717	ASN	THR	conflict	UNP P03135
7	263	ALA	GLN	conflict	UNP P03135
7	265	THR	-	insertion	UNP P03135
7	706	ALA	ASN	conflict	UNP P03135
7	709	ALA	VAL	conflict	UNP P03135
7	717	ASN	THR	conflict	UNP P03135

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

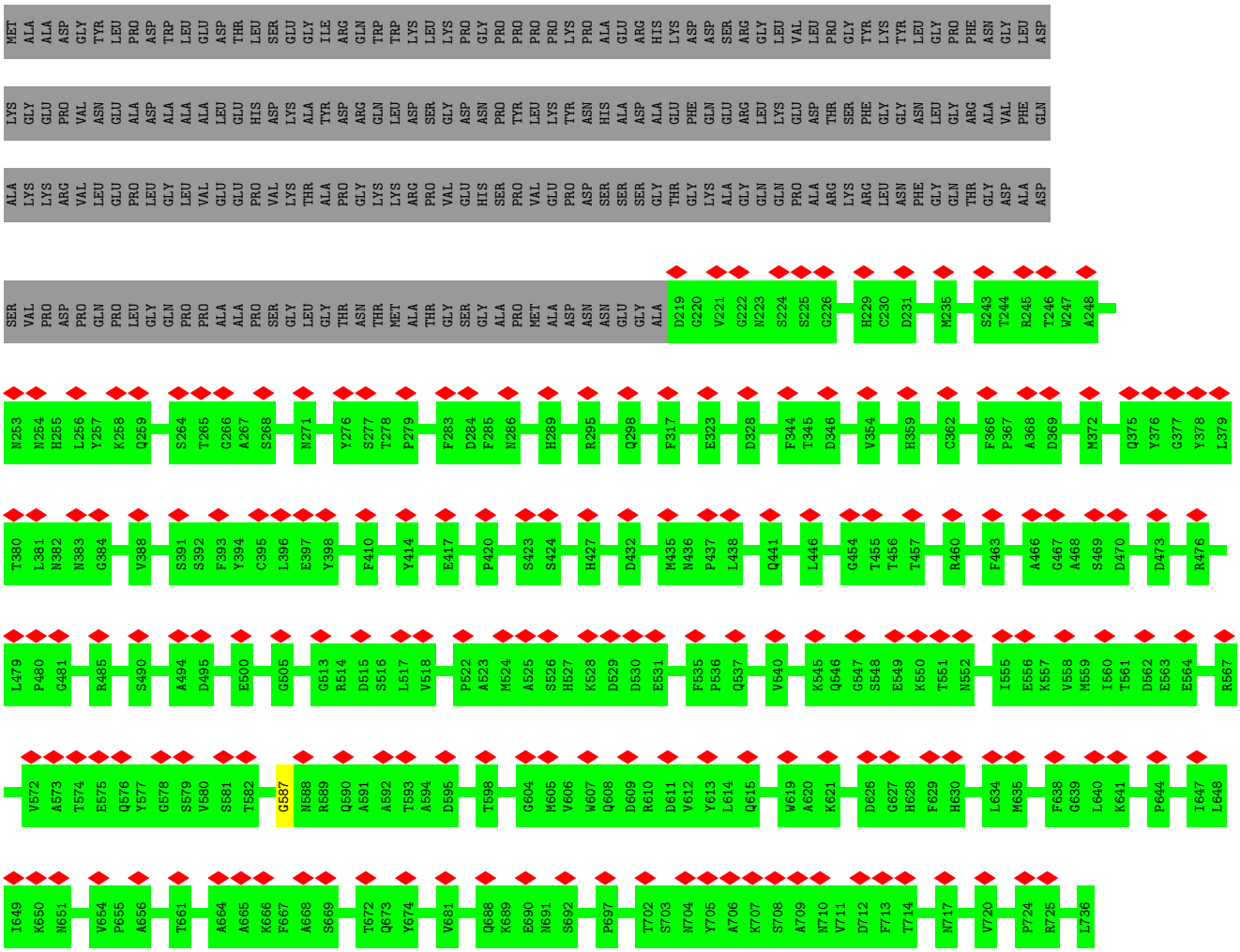
• Molecule 1: Capsid protein VP1

Chain A:



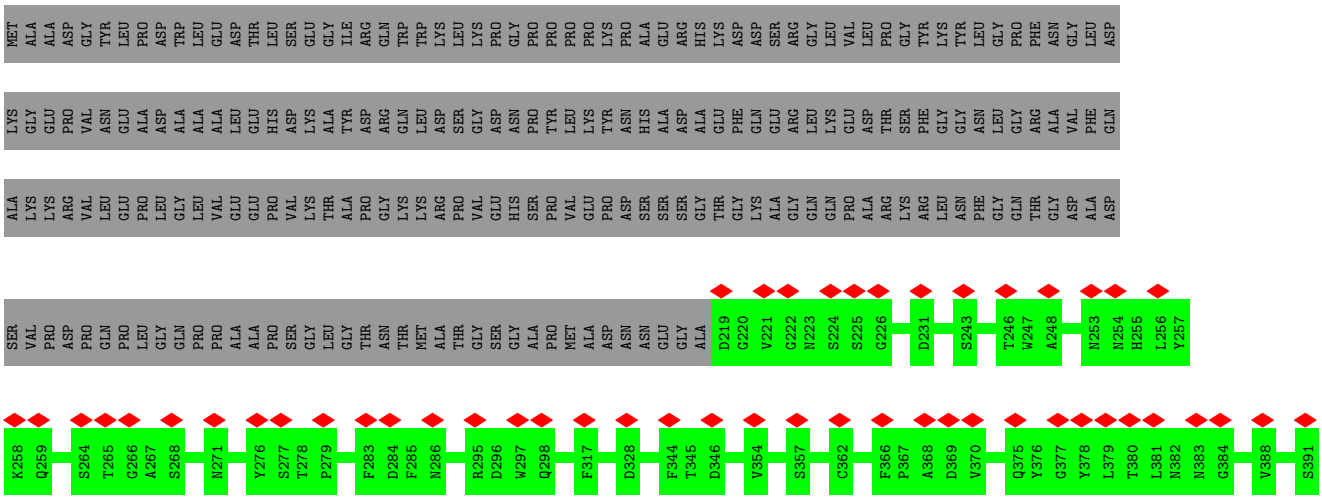
• Molecule 1: Capsid protein VP1

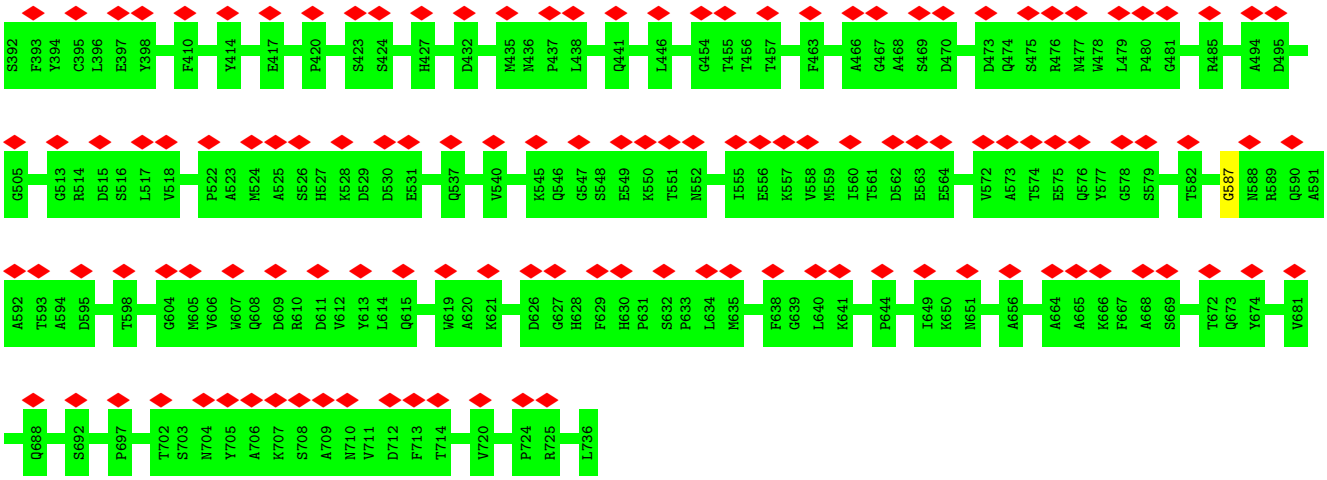
Chain B:



- Molecule 1: Capsid protein VP1

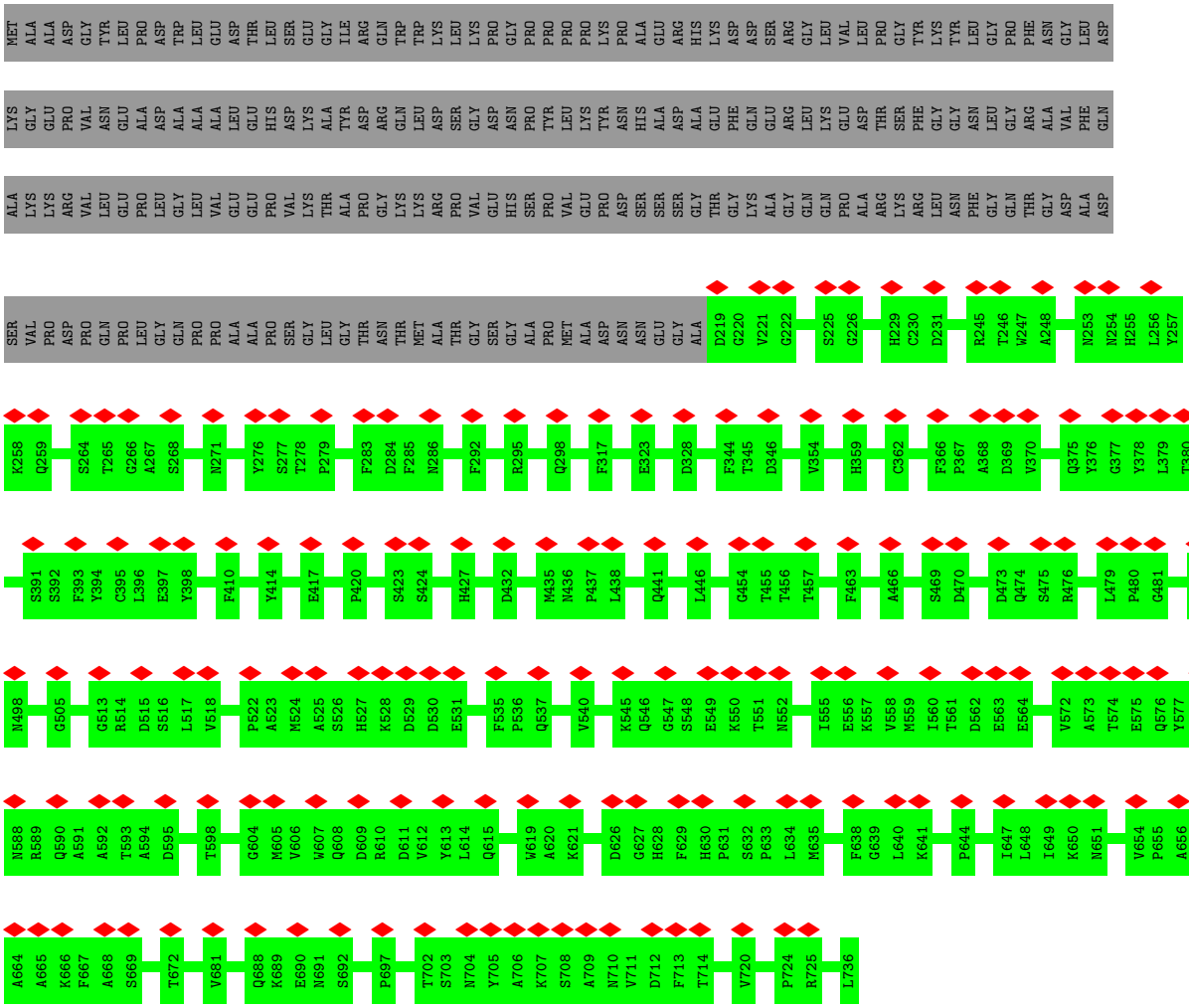
Chain C: 24% 70% 30%





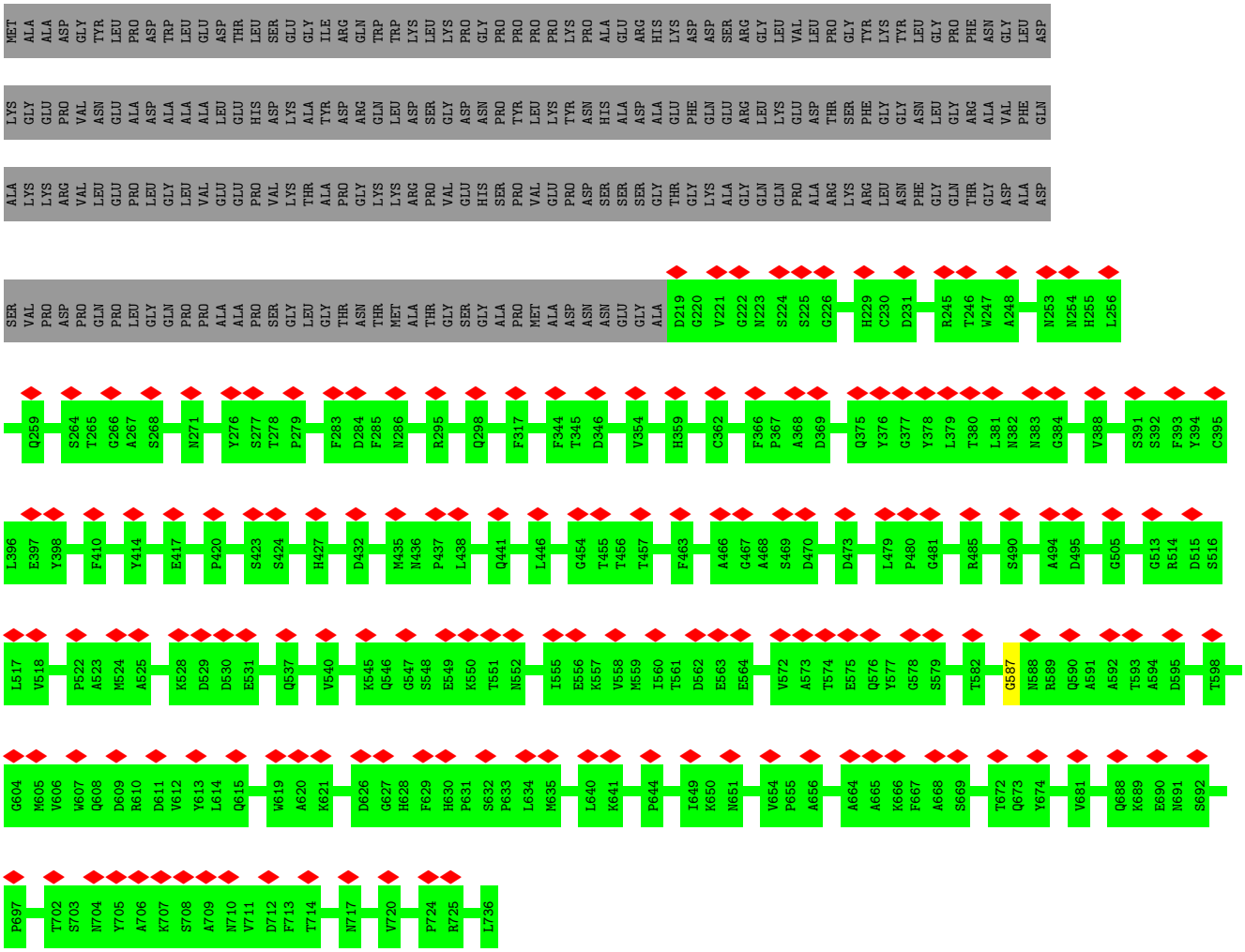
- Molecule 1: Capsid protein VP1

Chain D:



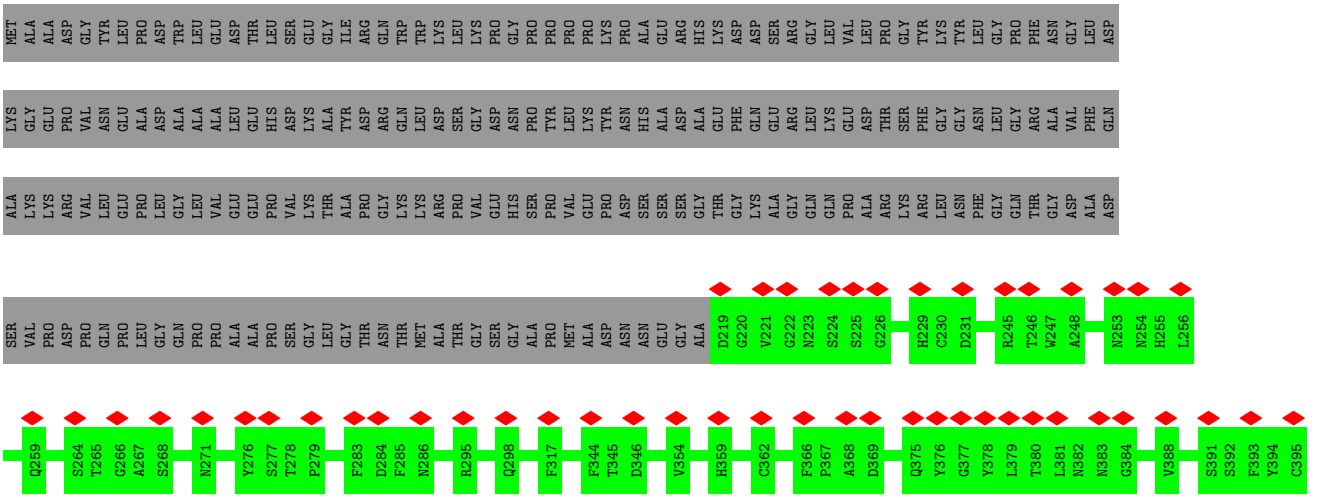
- Molecule 1: Capsid protein VP1

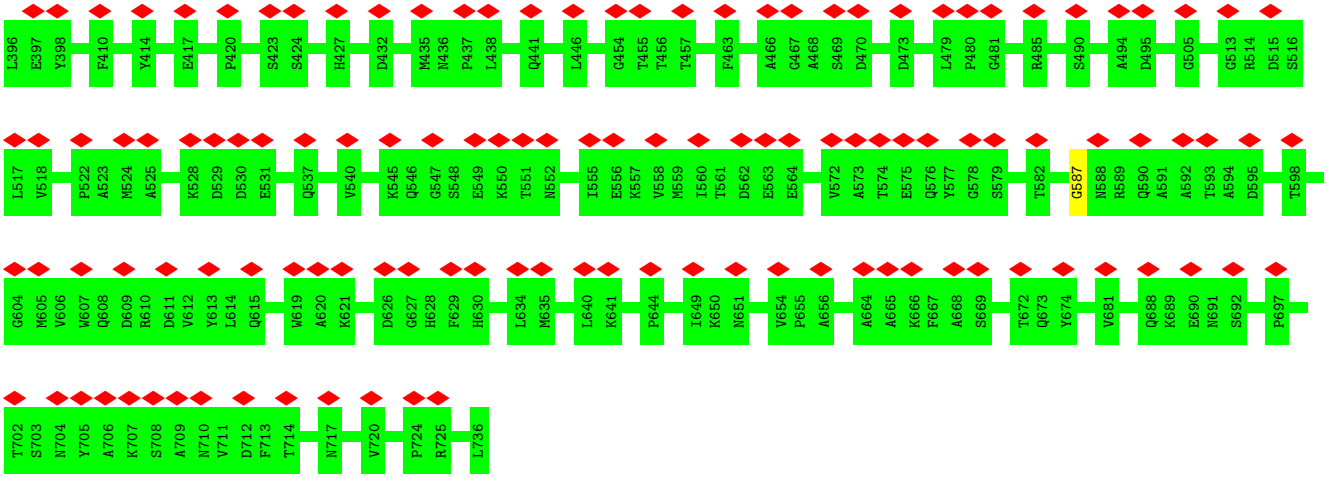
Chain E:



- Molecule 1: Capsid protein VP1

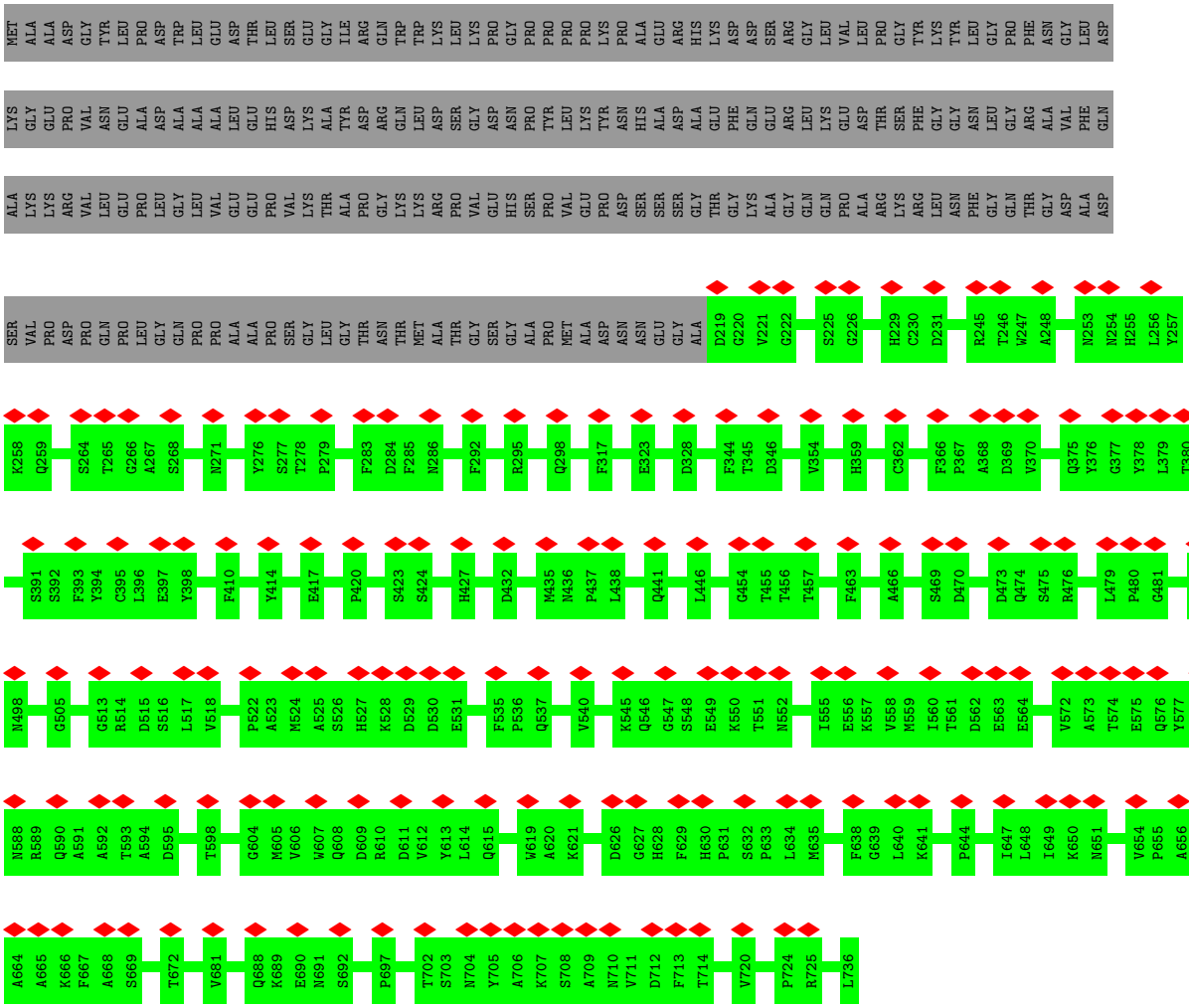
Chain F:





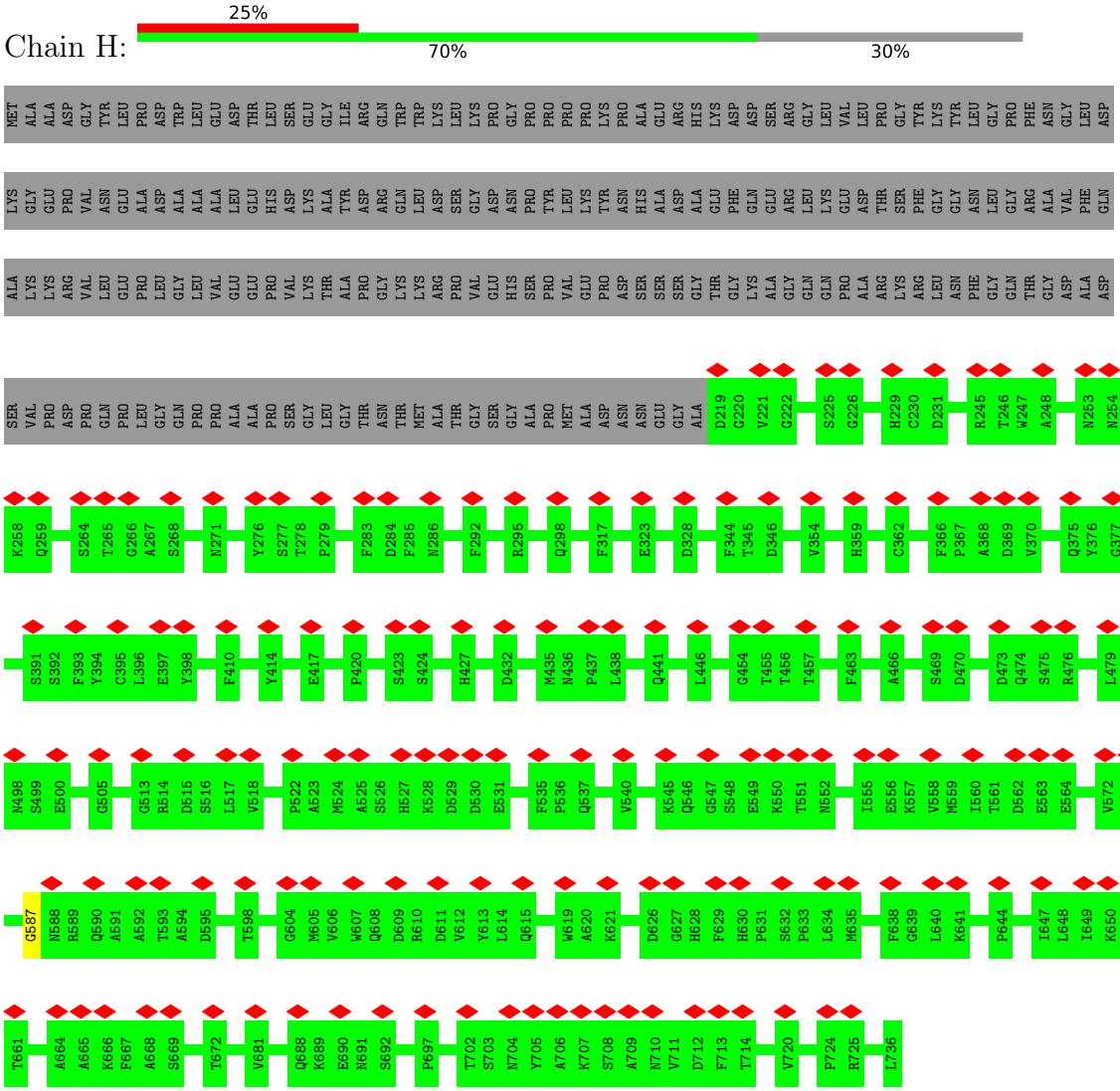
- Molecule 1: Capsid protein VP1

Chain G:



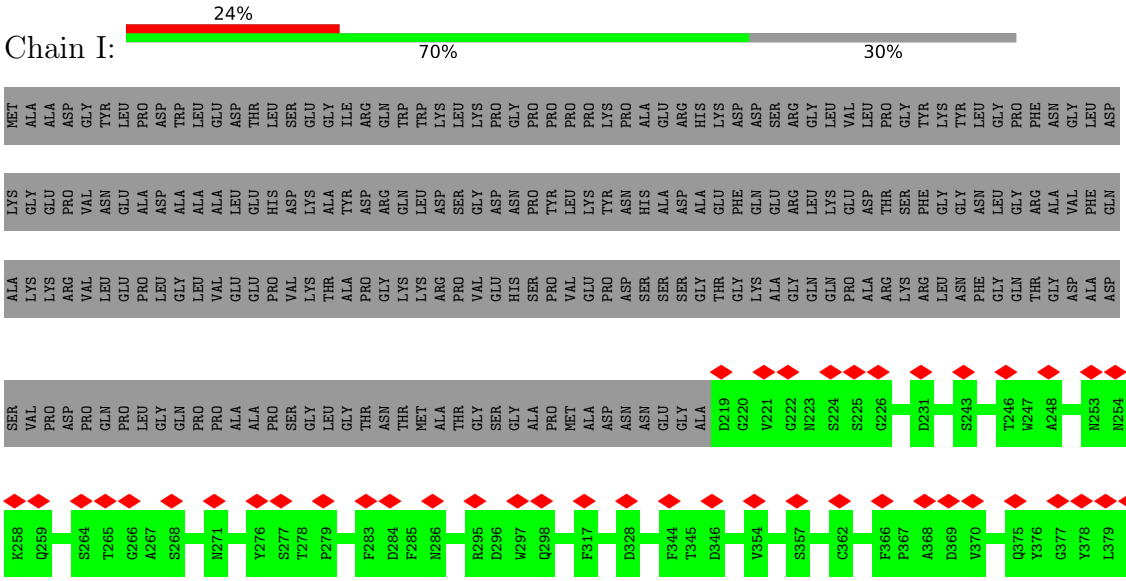
- Molecule 1: Capsid protein VP1

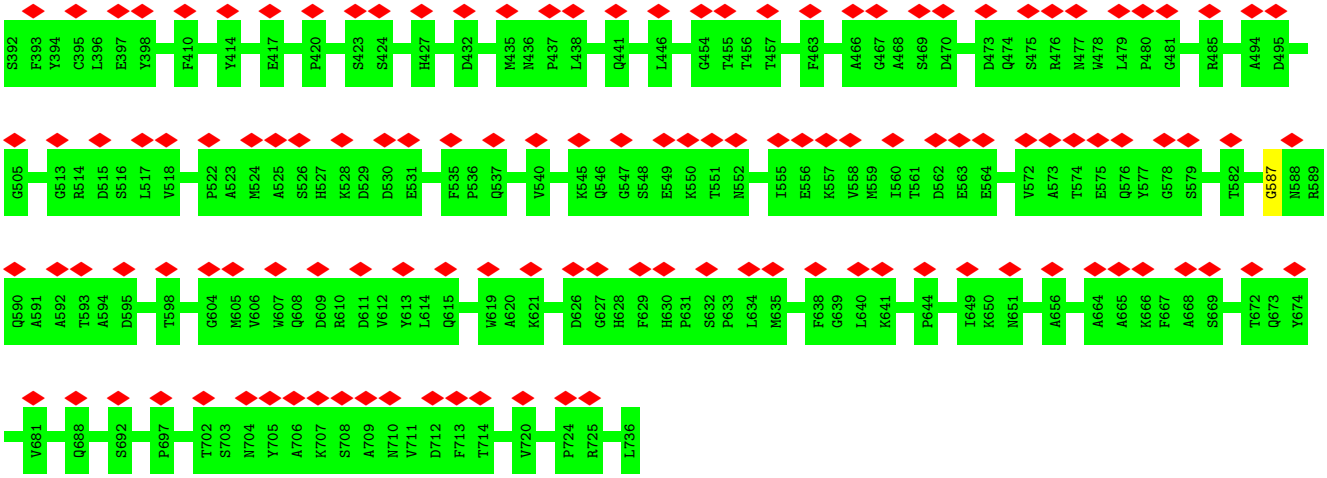
Chain H:



• Molecule 1: Capsid protein VP1

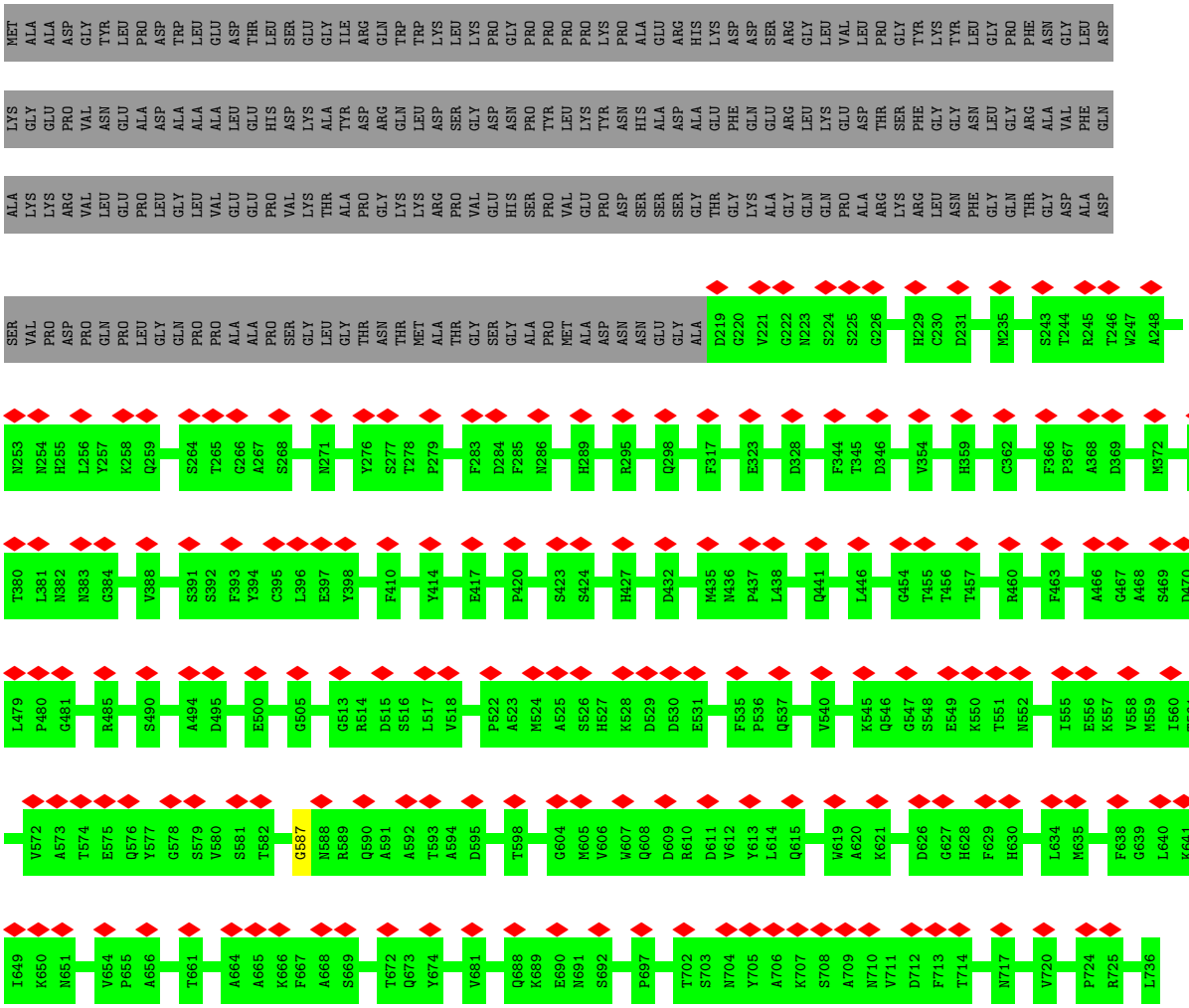
Chain I:





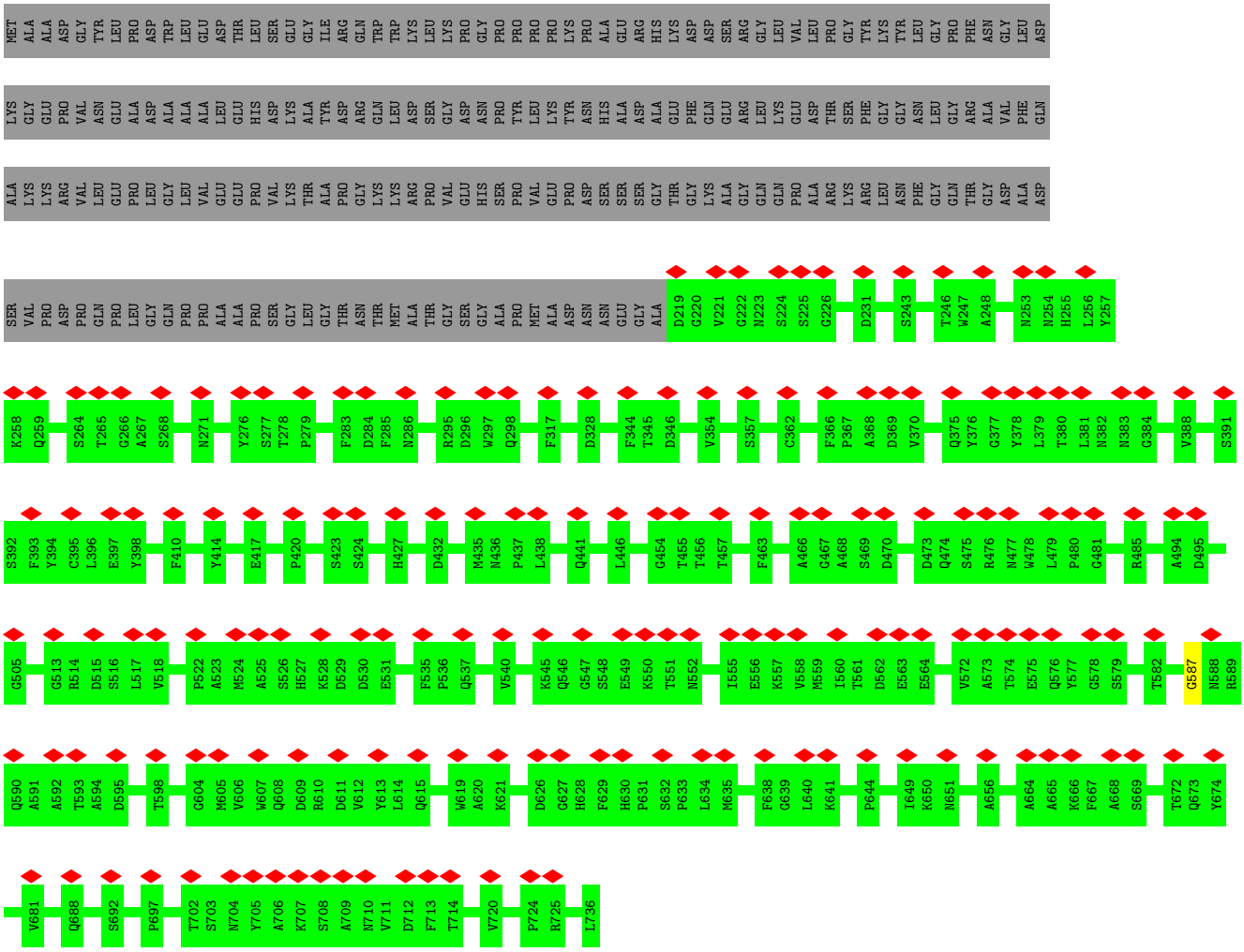
- Molecule 1: Capsid protein VP1

Chain J:



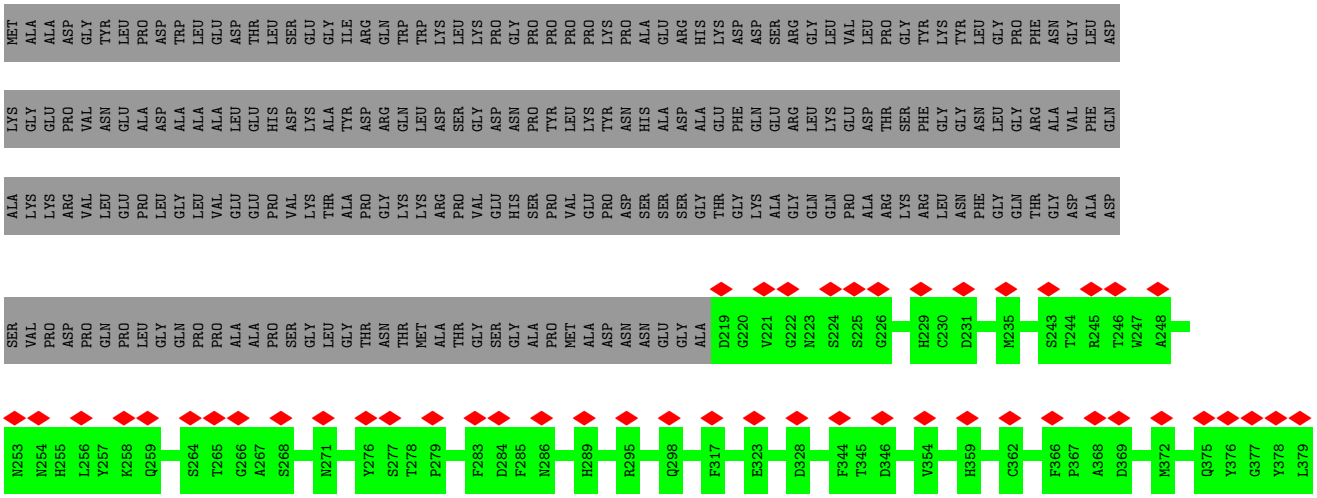
- Molecule 1: Capsid protein VP1

Chain K: 24% 70% 30%



- Molecule 1: Capsid protein VP1

Chain L: 26% 70% 30%



T380 L381 N382 N383 G384 V388 S391 S392 F393 Y394 C395 L396 E397 Y398 F410 Y414 E417 P420 S423 S424 H427 D432 M435 N436 P437 L438 Q441 L446 G454 T455 T456 T457 R460 F463 A466 G467 A468 S469 D470 D473 R476

L479 P480 G481 R485 S490 A494 D495 E500 G505 G513 R514 D515 S516 L517 V518 P522 A523 M524 A525 S526 H527 K528 D529 D530 E531 F535 P536 Q537 V540 K545 Q546 G547 S548 E549 K550 T551 N552 T555 E556 K557 V558 M559 I560 T561 D562 E563 E564 R567

V572 A573 T574 E575 Q576 Y577 G578 S579 V580 S581 T582 G587 N588 R589 Q590 A591 A592 T593 A594 D595 T598 G604 M605 V606 W607 Q608 D609 R610 D611 V612 Y613 L614 Q615 W619 A620 K621 D626 G627 H628 F629 H630 L634 M635 F638 G639 L640 K641 P644 I647 L648

I649 K650 N651 V654 P655 A656 T661 A664 A665 K666 F667 A668 S669 T672 Q673 Y674 V681 Q688 K689 E690 N691 S692 P697 T702 S703 N704 Y705 A706 K707 S708 A709 N710 V711 D712 F713 T714 N717 V720 P724 R725 L736

- Molecule 1: Capsid protein VP1

Chain M: 25% 70% 30%

MET ALA ALA ASP GLY TYR LEU PRO ASP TRP LEU GLU ASP THR LEU SER GLU GLY GLY ILE ARG GLN TRP TRP TRP LYS LEU LYS PRO GLY PRO PRO PRO PRO LYS PRO ALA GLU ARG HIS LYS ASP ASP ASP SER ARG GLY LEU VAL LEU PRO GLY TYR LYS TYR LEU GLY PRO PHE ASN GLY LEU ASP

LYS GLY GLU PRO VAL ASN GLU ALA ASP ALA ALA ALA LEU GLU HIS ASP LYS ALA TYR ASP ARG GLN LEU ASP SER GLY ASP ASN PRO TYR LEU LYS TYR ASN HIS ALA ASP ALA GLU PHE GLN GLU ARG LEU LYS GLU ASP THR SER PHE GLY GLY ASN LEU GLY ARG ALA VAL PHE GLN

ALA LYS LYS ARG VAL LEU GLU PRO LEU GLY LEU VAL GLU GLU PRO VAL LYS THR ALA PRO GLY LYS LYS ARG PRO VAL GLU HIS SER PRO VAL GLU PRO ASP SER SER SER GLY THR GLY LYS ALA GLY GLN GLN PRO ALA ARG LYS ARG LEU ASN PHE GLY GLN THR GLY ASP ALA ASP

SER VAL PRO ASP PRO GLN PRO LEU GLY GLN PRO PRO ALA ALA PRO SER GLY LEU GLY THR ASN THR MET ALA THR GLY SER GLY ALA PRO MET ALA ASP ASN ASN GLU GLY ALA D219 G220 V221 G222 S225 G226 H229 C230 D231 R245 T246 W247 A248 N253 N254 H255 L256 Y257

K258 Q259 S264 T265 G266 A267 S268 N271 Y276 S277 T278 P279 F283 D284 F285 N286 F292 R295 Q298 F317 E323 D328 F344 T345 D346 V354 H359 C362 F366 P367 A368 D369 V370 Q375 Y376 G377 Y378 L379 T380 N383 G384 V388

S391 S392 F393 Y394 C395 L396 E397 Y398 F410 Y414 E417 P420 S423 S424 H427 D432 M435 N436 P437 L438 Q441 L446 G454 T455 T456 T457 F463 A466 S469 D470 D473 Q474 S475 R476 L479 P480 G481 R485 A494 D495

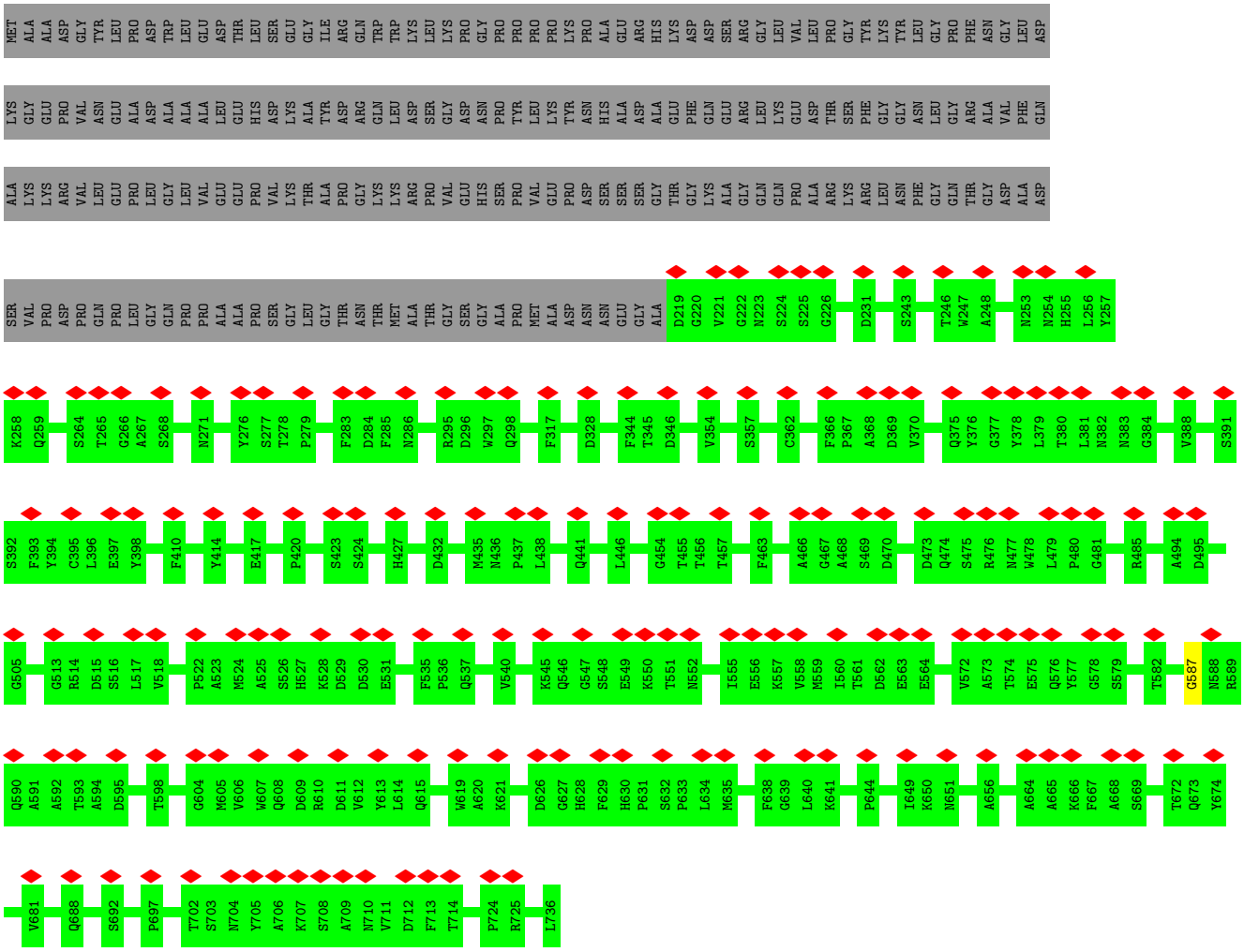
N498 G505 G513 R514 D515 S516 L517 V518 P522 A523 M524 A525 S526 H527 K528 D529 D530 E531 F535 P536 Q537 V540 K545 Q546 G547 S548 E549 K550 T551 N552 I555 E556 K557 V558 M559 I560 T561 D562 E563 E564 V572 A573 T574 E575 Q576 Y577 G578 S579 T582 G587

N588 R589 Q590 A591 A592 T593 A594 D595 T598 G604 M605 V606 W607 Q608 D609 R610 D611 V612 Y613 L614 Q615 W619 A620 K621 D626 G627 H628 F629 H630 P631 S632 P633 L634 M635 F638 G639 L640 K641 P644 I647 L648 I649 K650 N651 V654 P655 A656 M657 T660 T661

A664 A665 K666 F667 A668 S669 T672 V681 Q688 K689 E690 N691 S692 P697 T702 S703 N704 Y705 A706 K707 S708 A709 N710 V711 D712 F713 T714 V720 P724 R725 L736

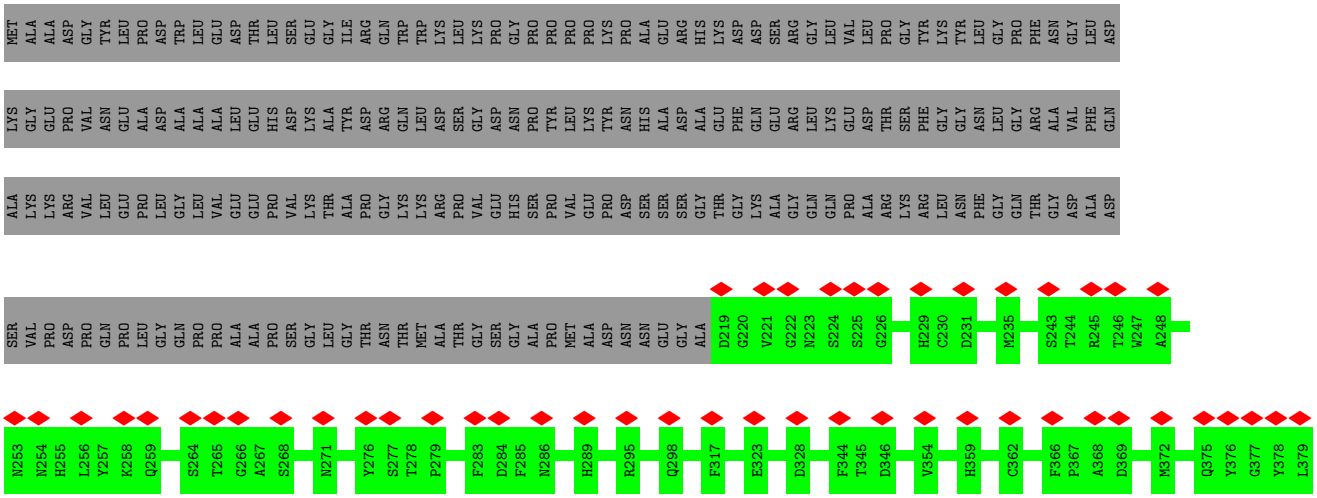
- Molecule 1: Capsid protein VP1

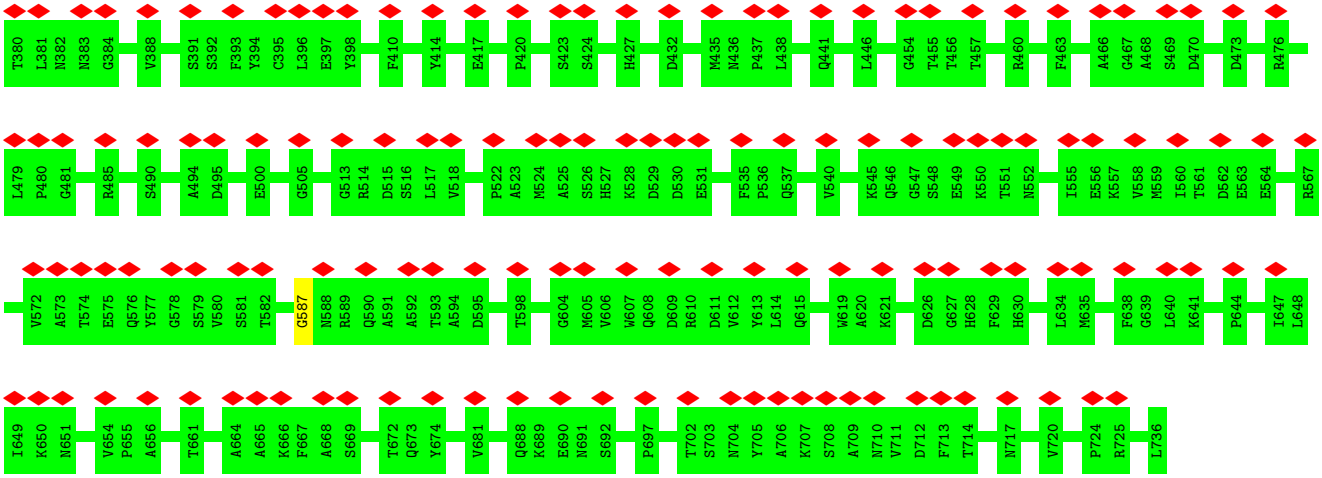
Chain N: 24% 70% 30%



- Molecule 1: Capsid protein VP1

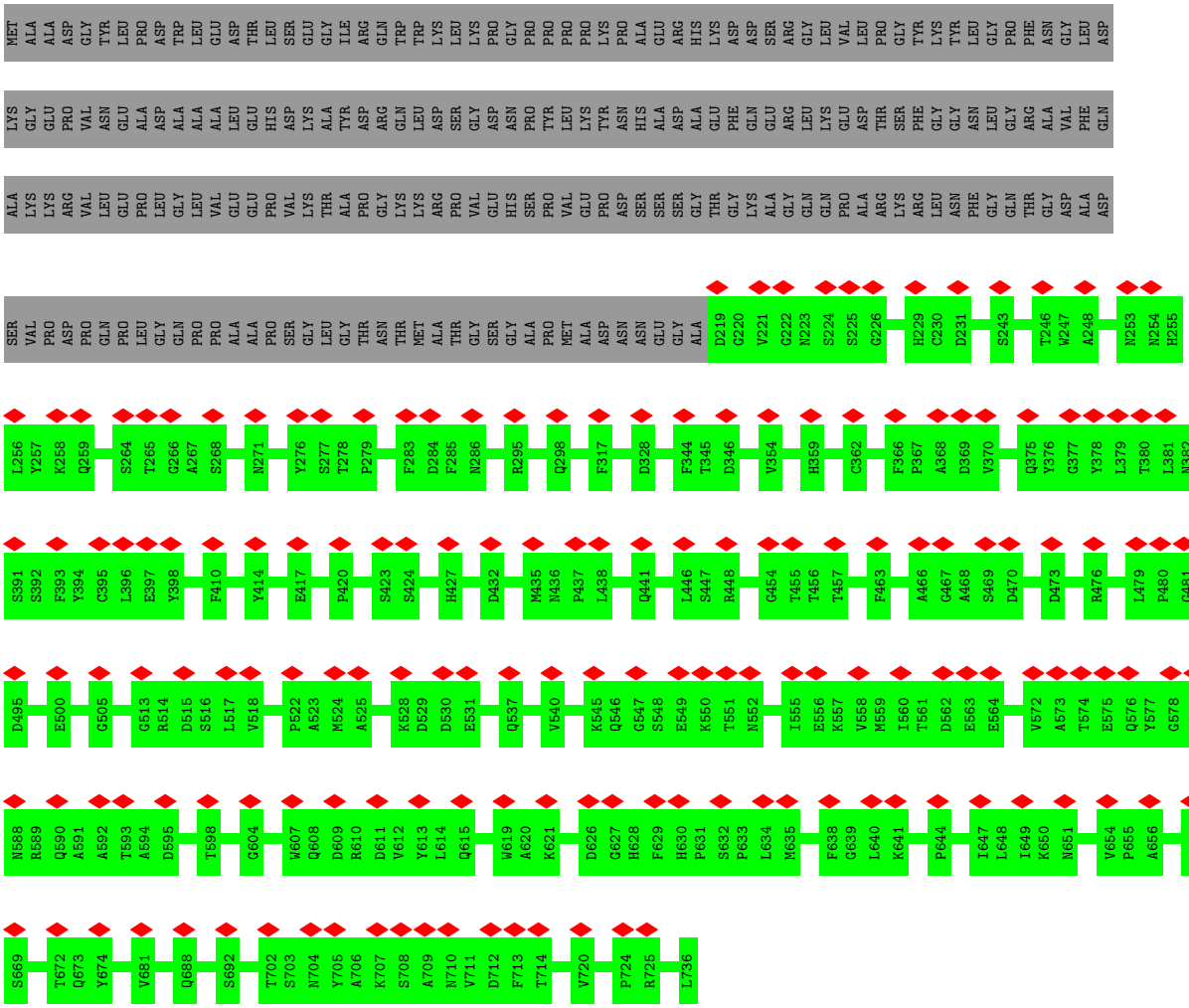
Chain O: 26% 70% 30%





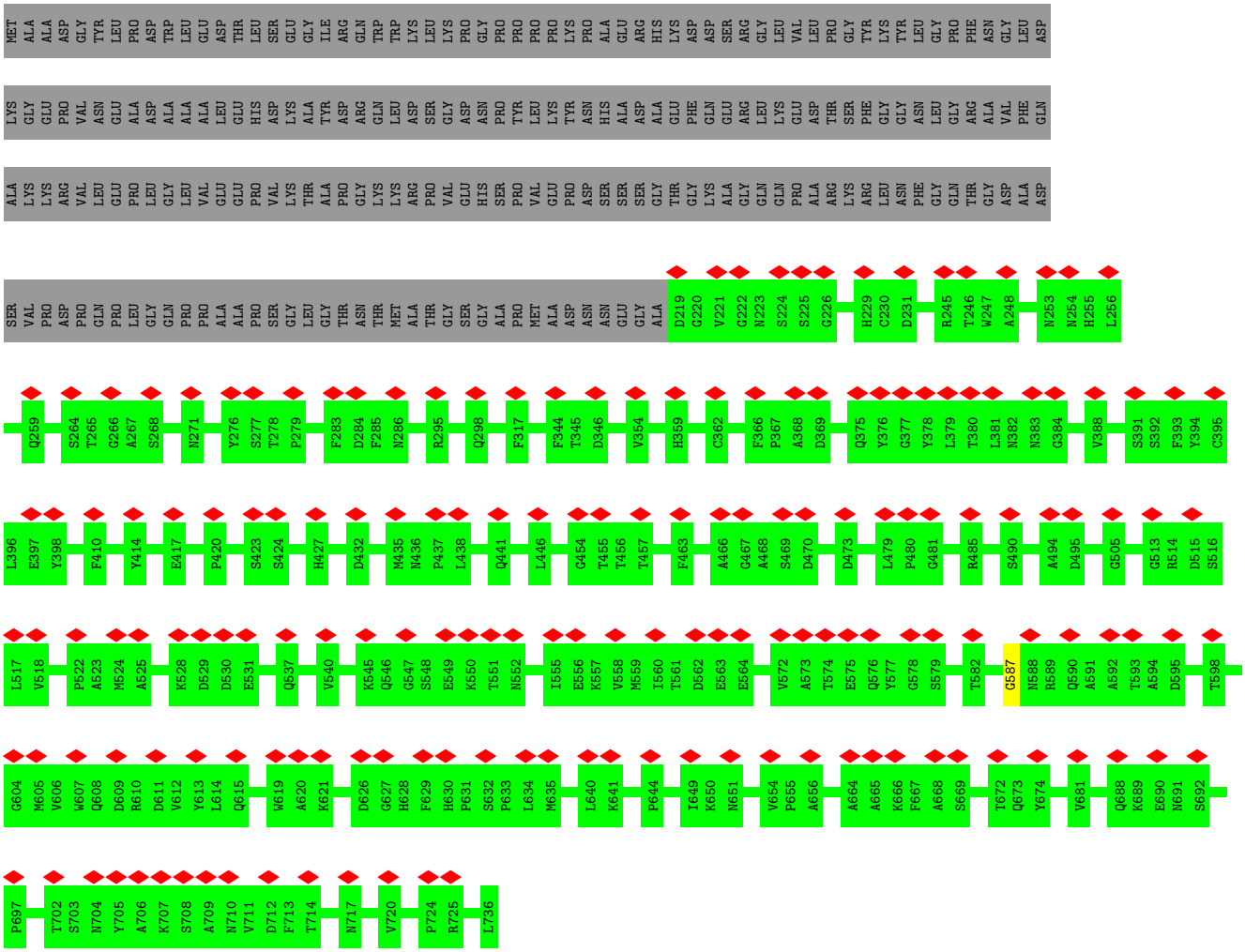
- Molecule 1: Capsid protein VP1

Chain P: 24% 70% 30%



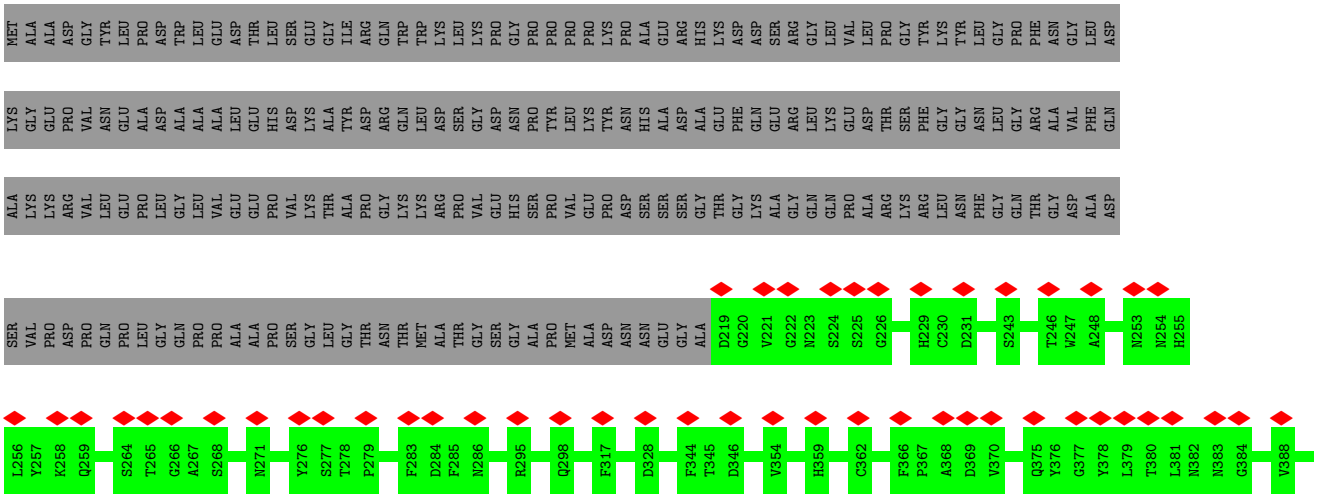
- Molecule 1: Capsid protein VP1

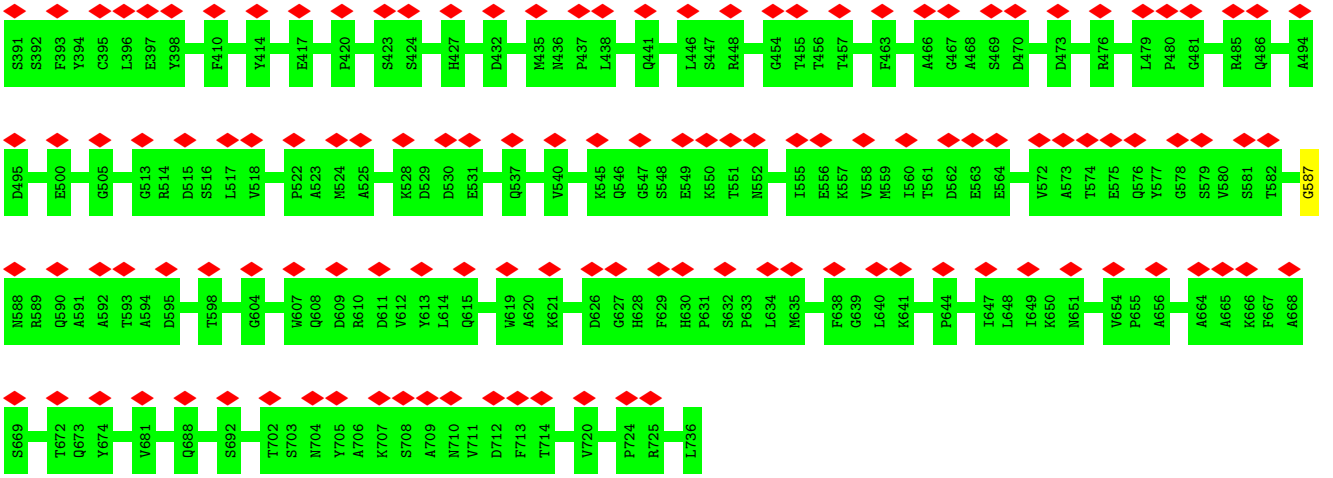
Chain Q:



- Molecule 1: Capsid protein VP1

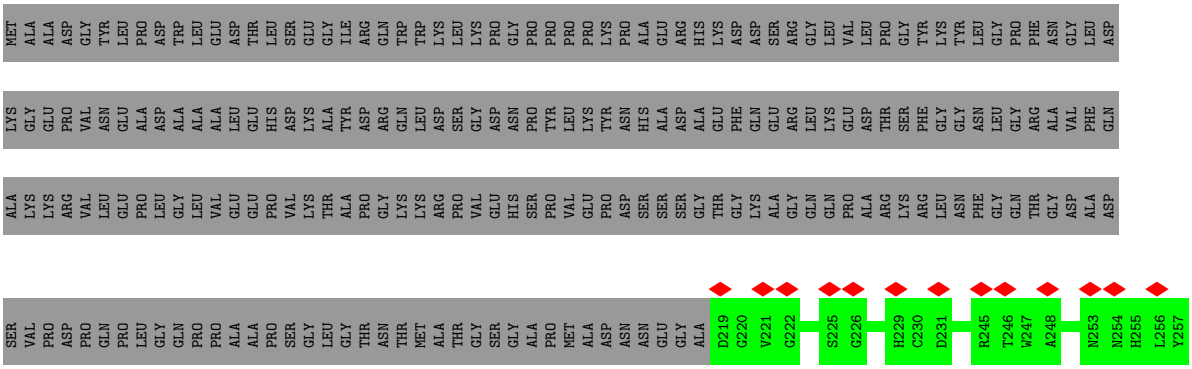
Chain R:





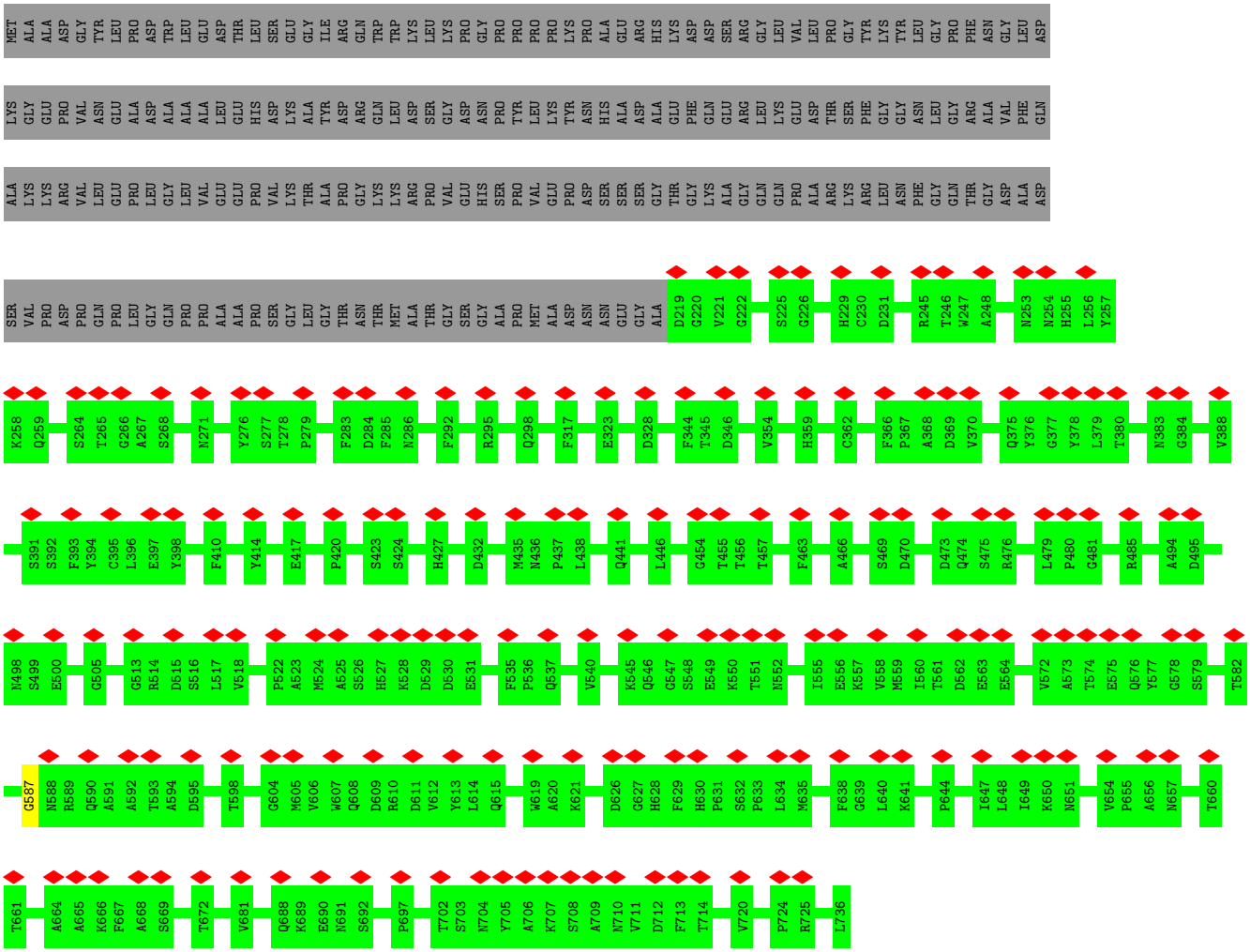
- Molecule 1: Capsid protein VP1

Chain S:



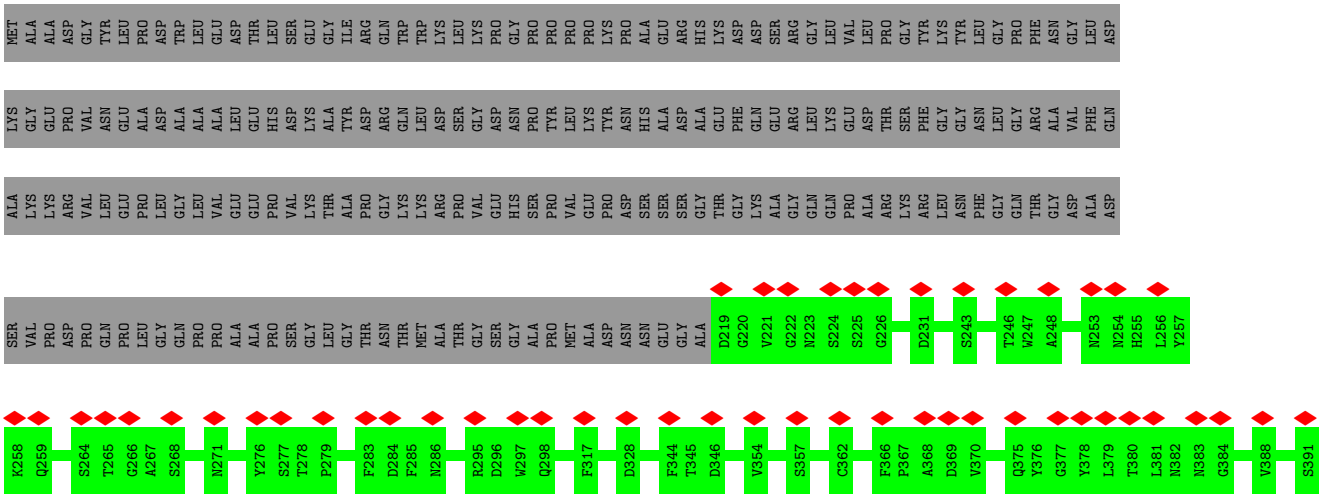
- Molecule 1: Capsid protein VP1

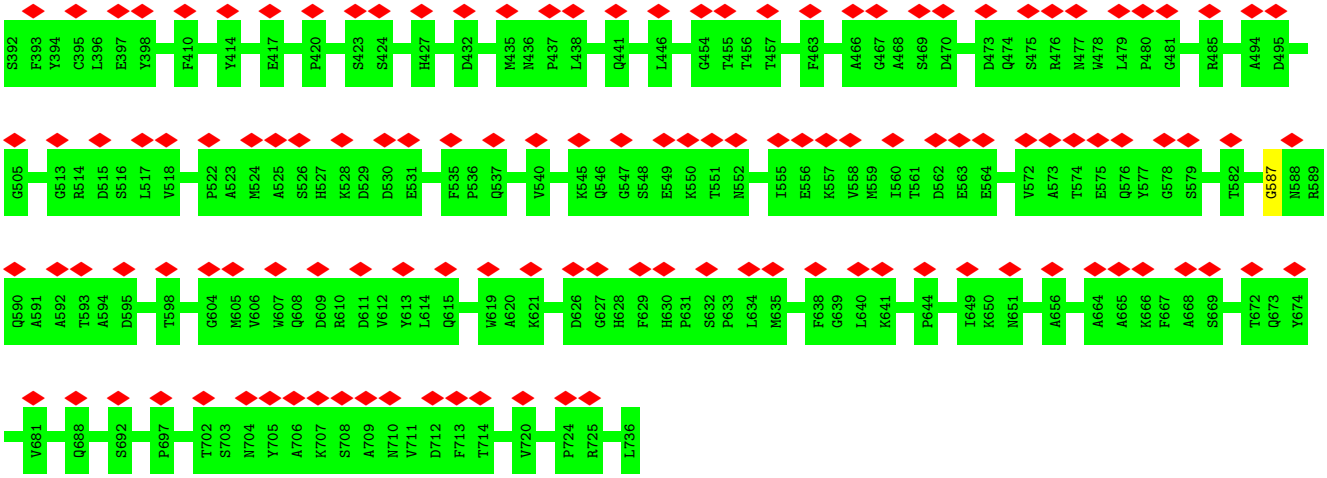
Chain T: 25% 70% 30%



- Molecule 1: Capsid protein VP1

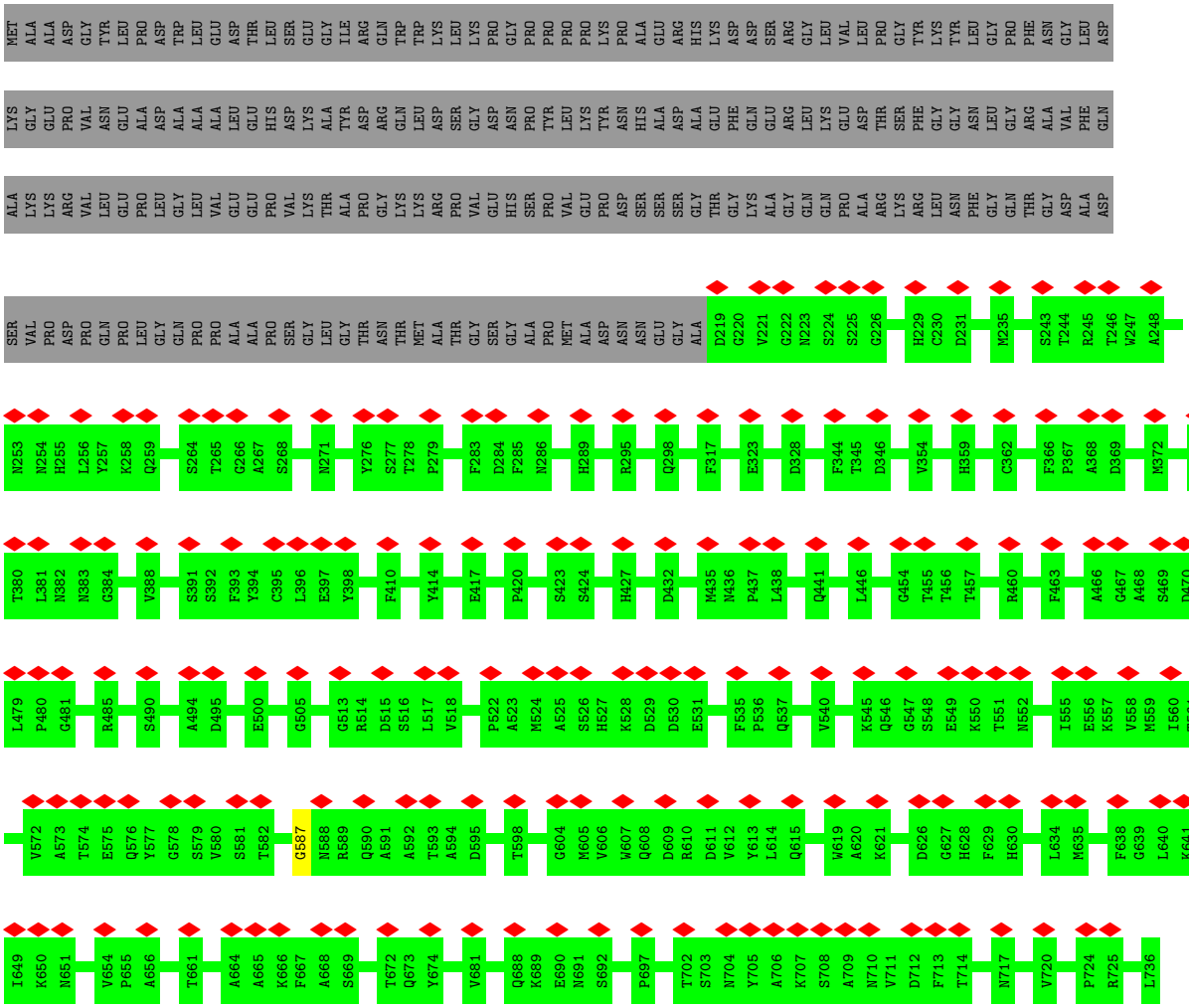
Chain U: 24% 70% 30%





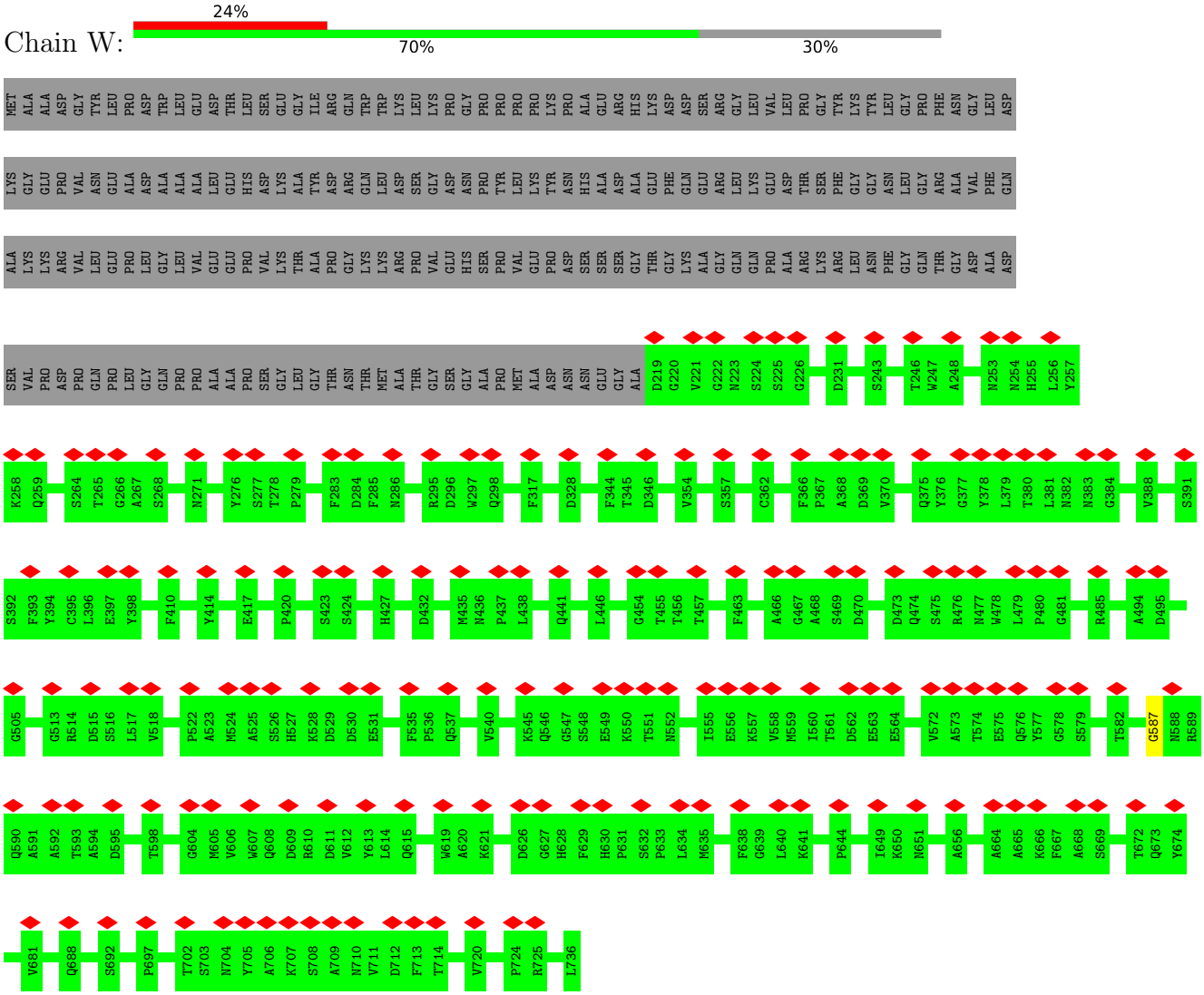
- Molecule 1: Capsid protein VP1

Chain V:



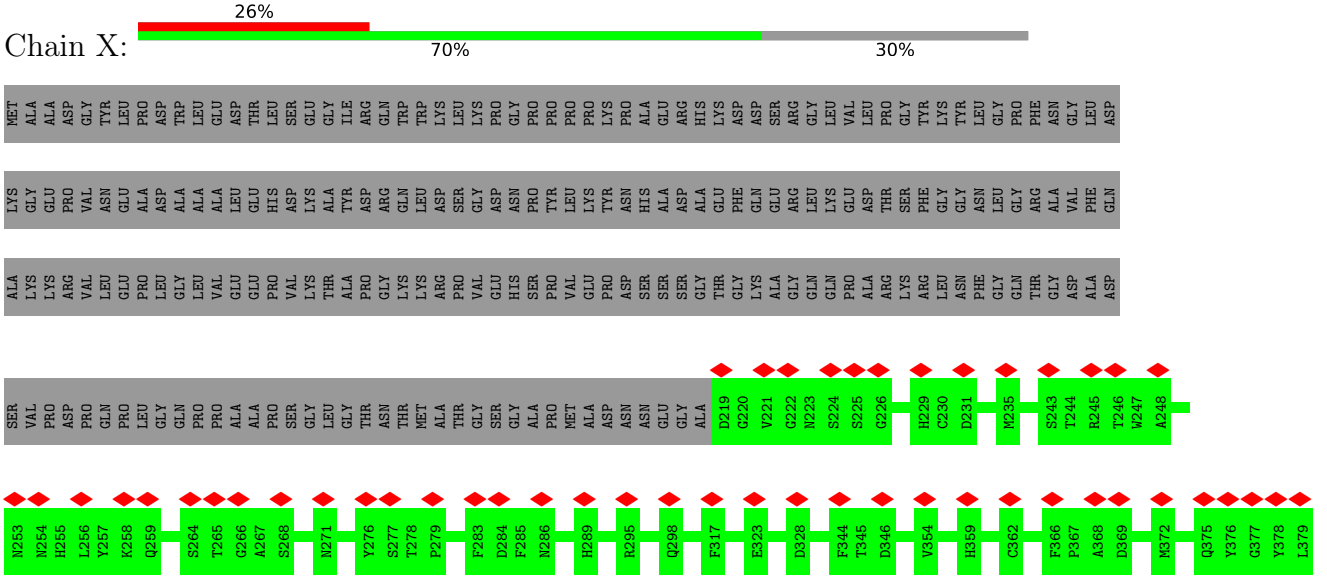
- Molecule 1: Capsid protein VP1

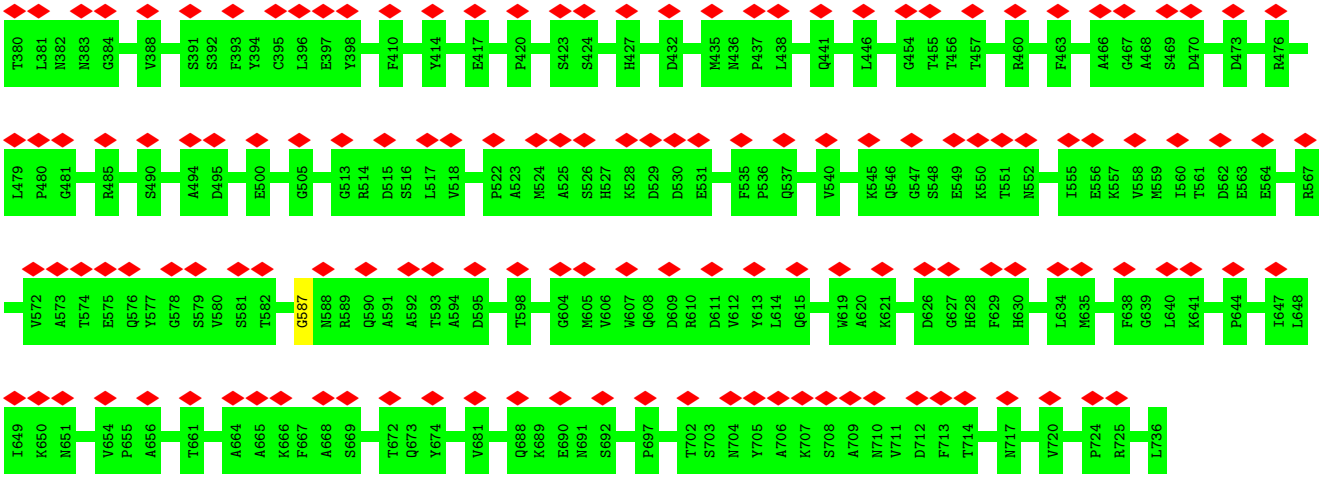
Chain W:



• Molecule 1: Capsid protein VP1

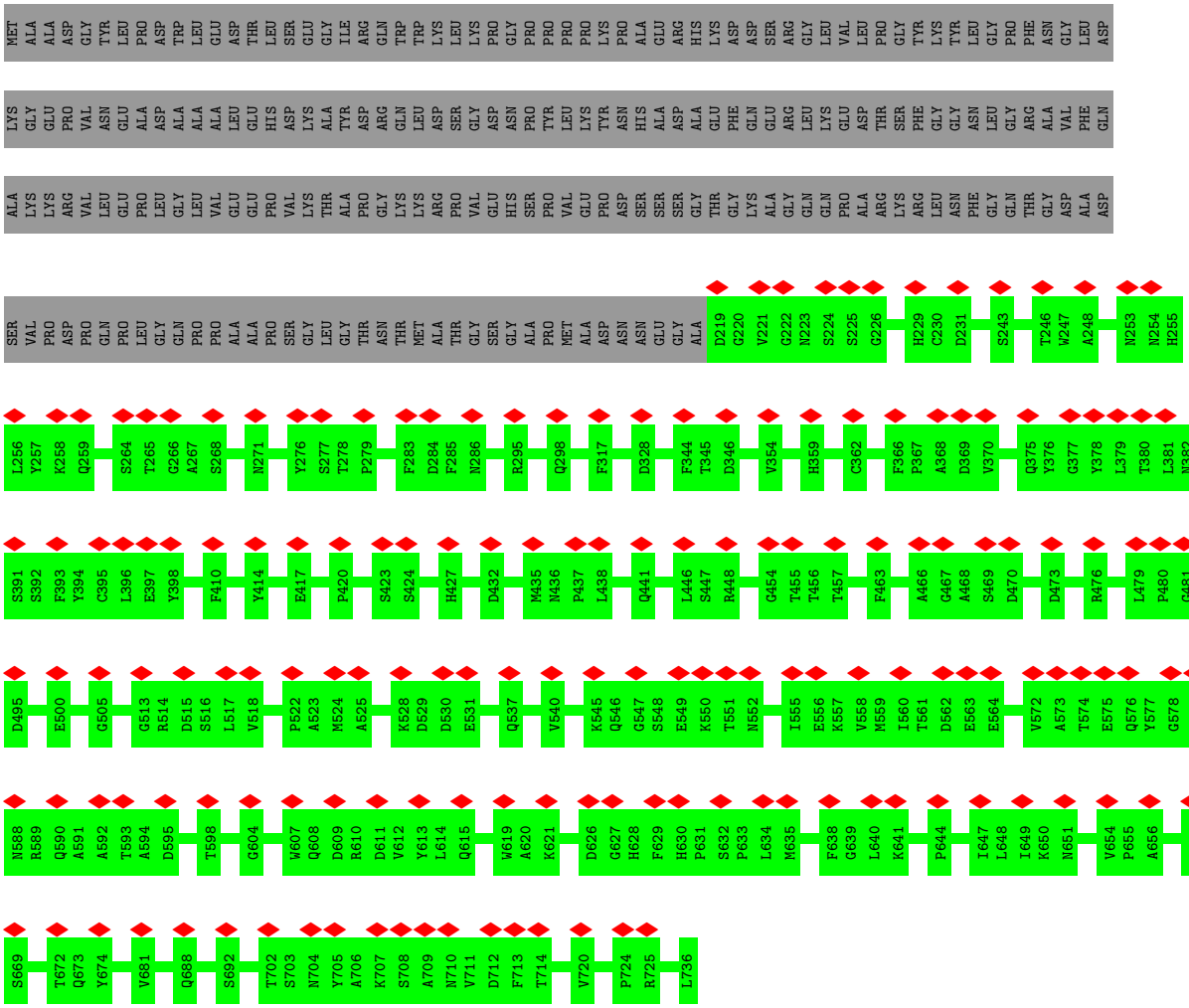
Chain X:





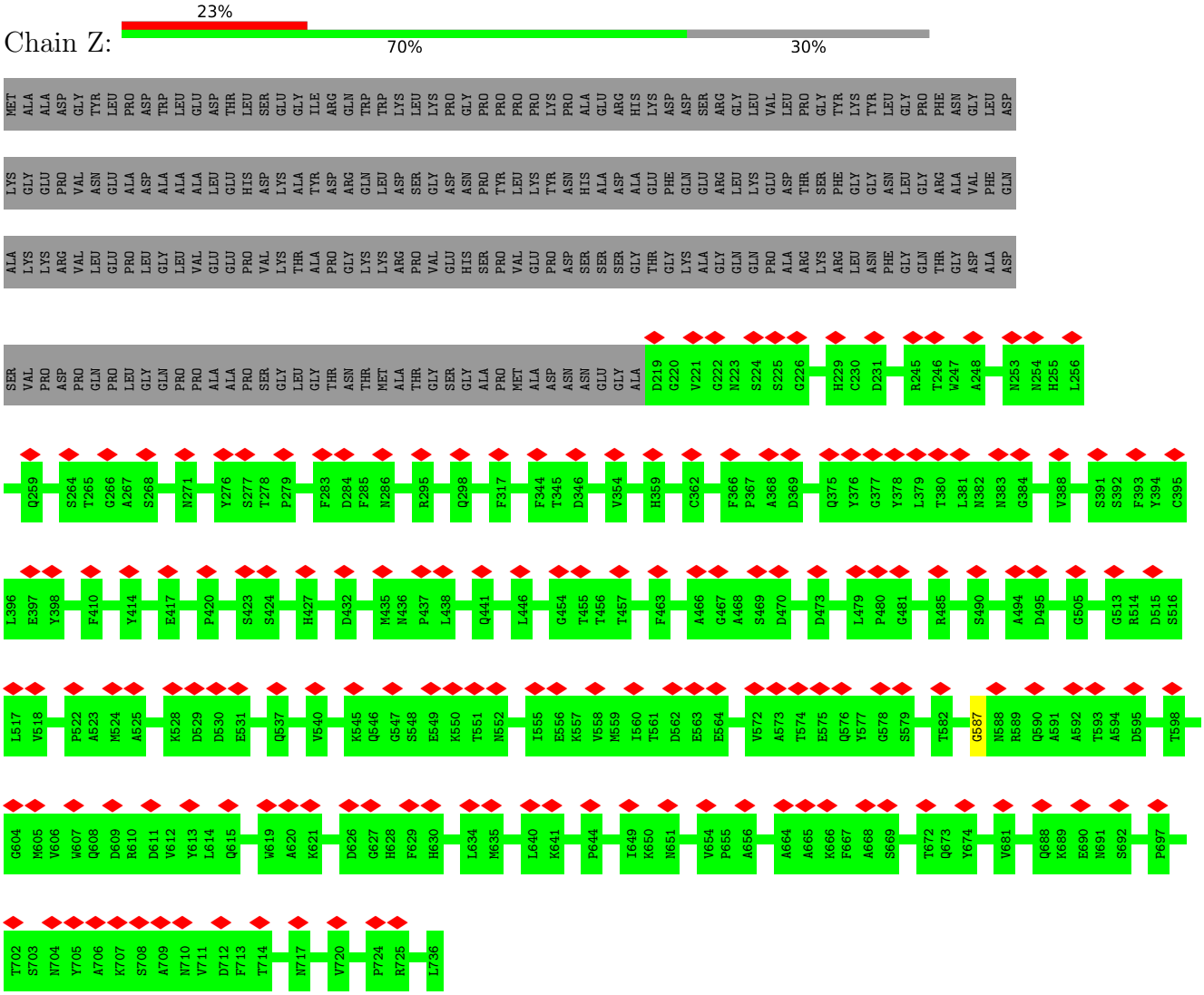
- Molecule 1: Capsid protein VP1

Chain Y:



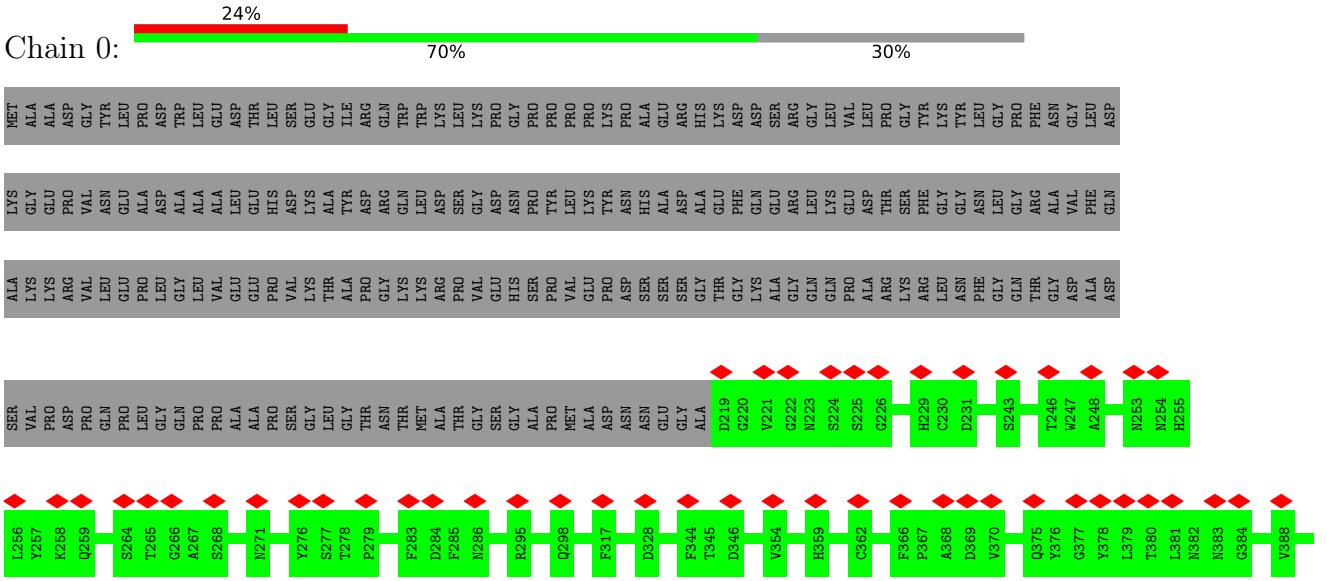
- Molecule 1: Capsid protein VP1

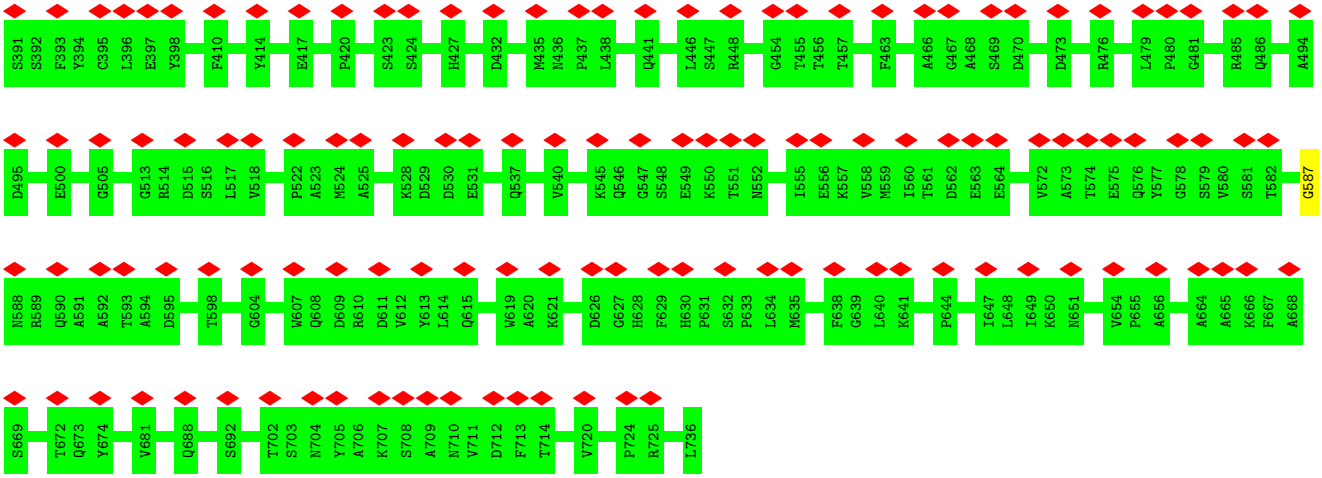
Chain Z:



• Molecule 1: Capsid protein VP1

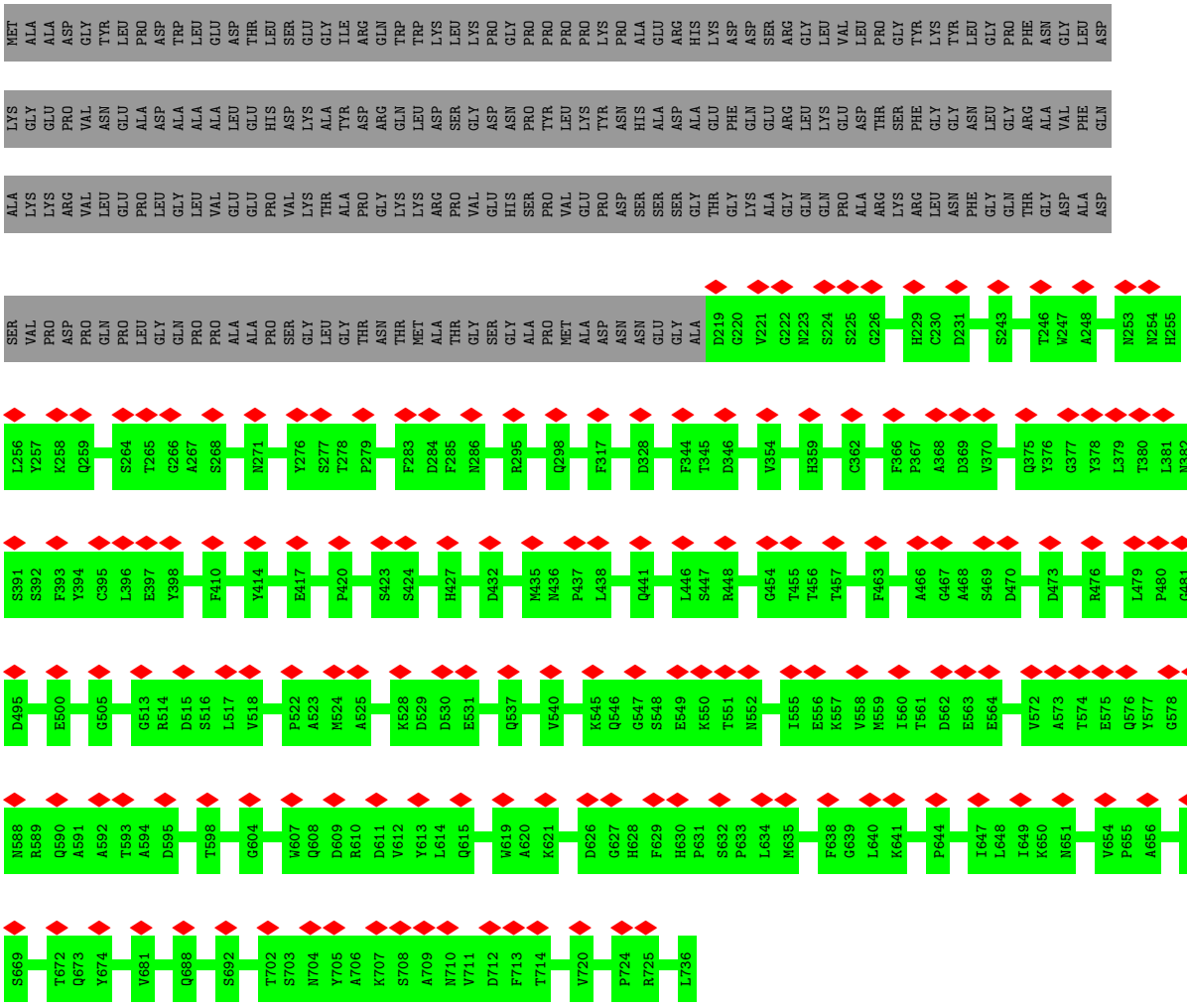
Chain 0:





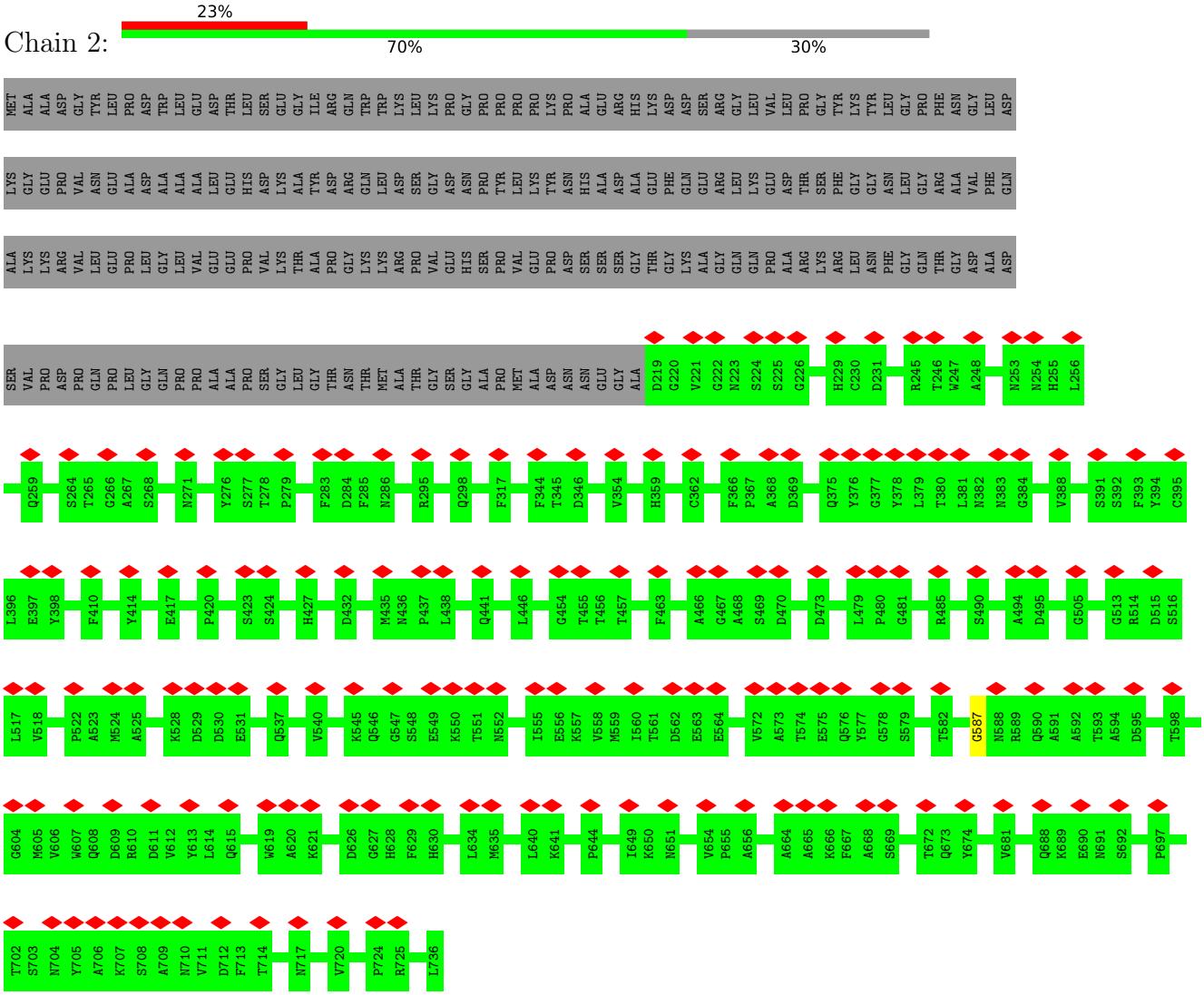
- Molecule 1: Capsid protein VP1

Chain 1:



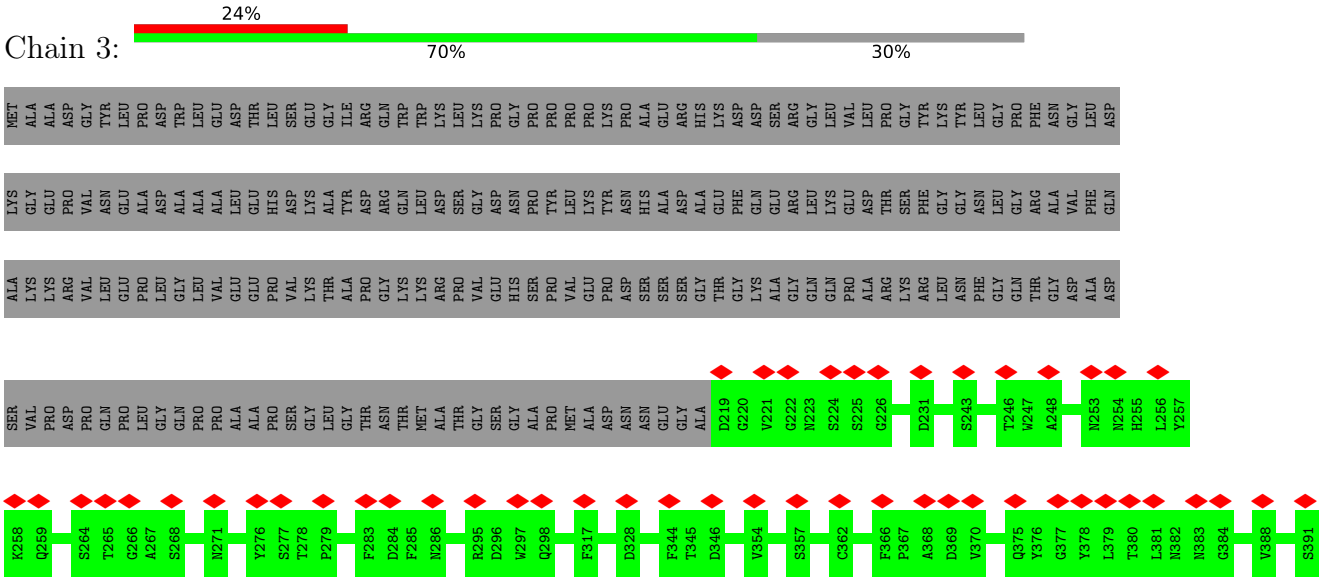
- Molecule 1: Capsid protein VP1

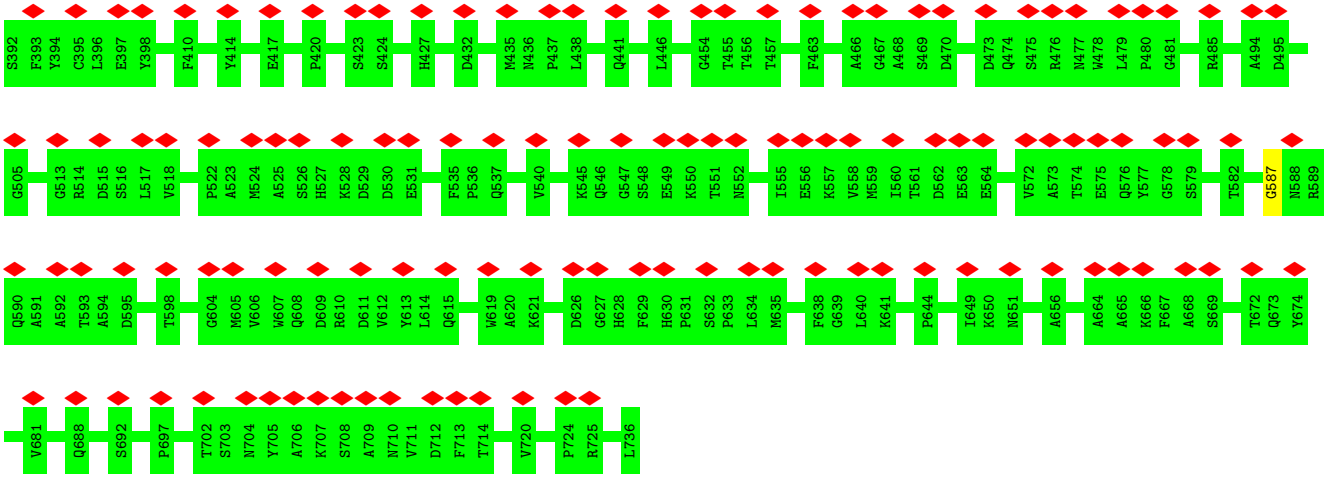
Chain 2:



- Molecule 1: Capsid protein VP1

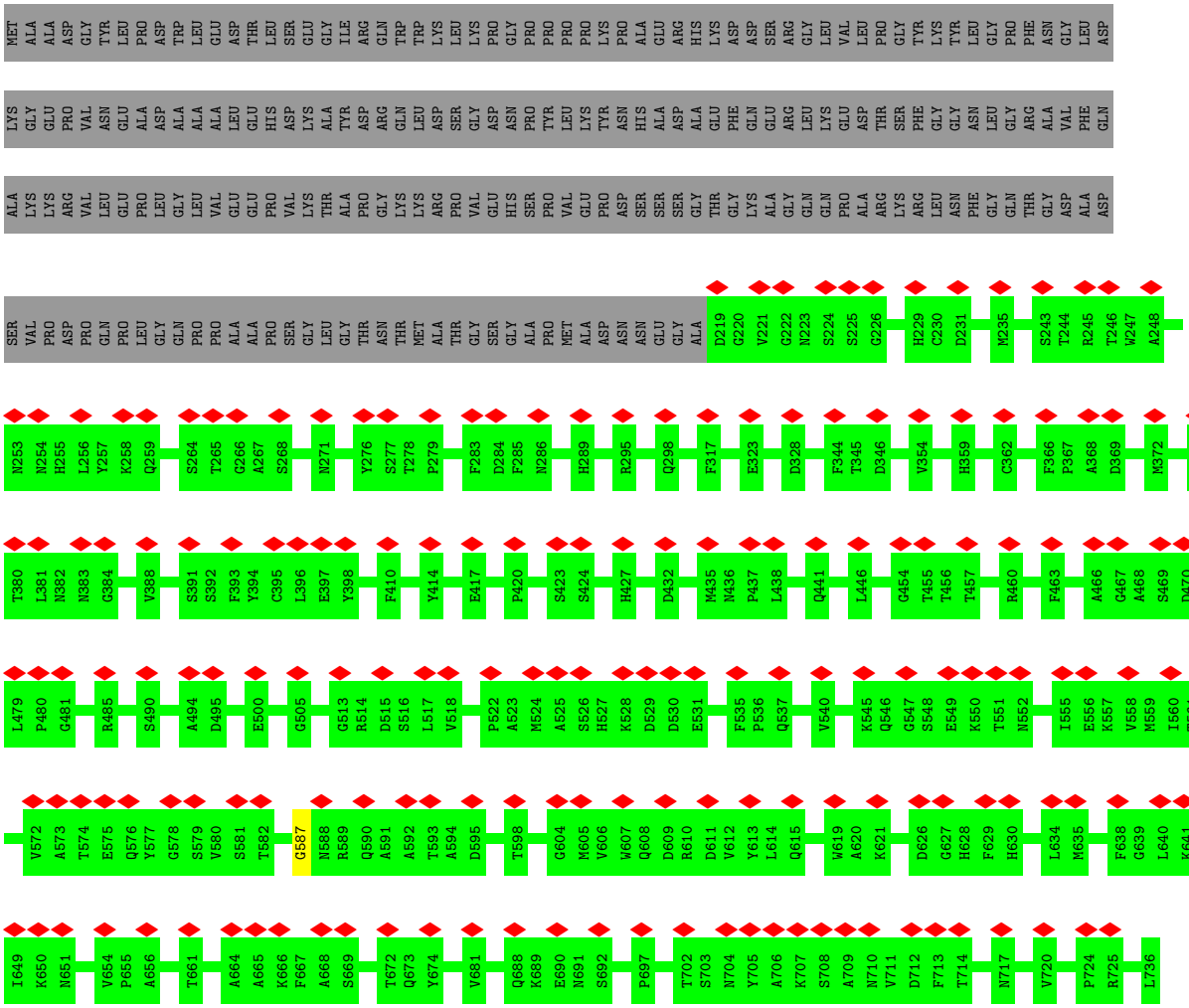
Chain 3:





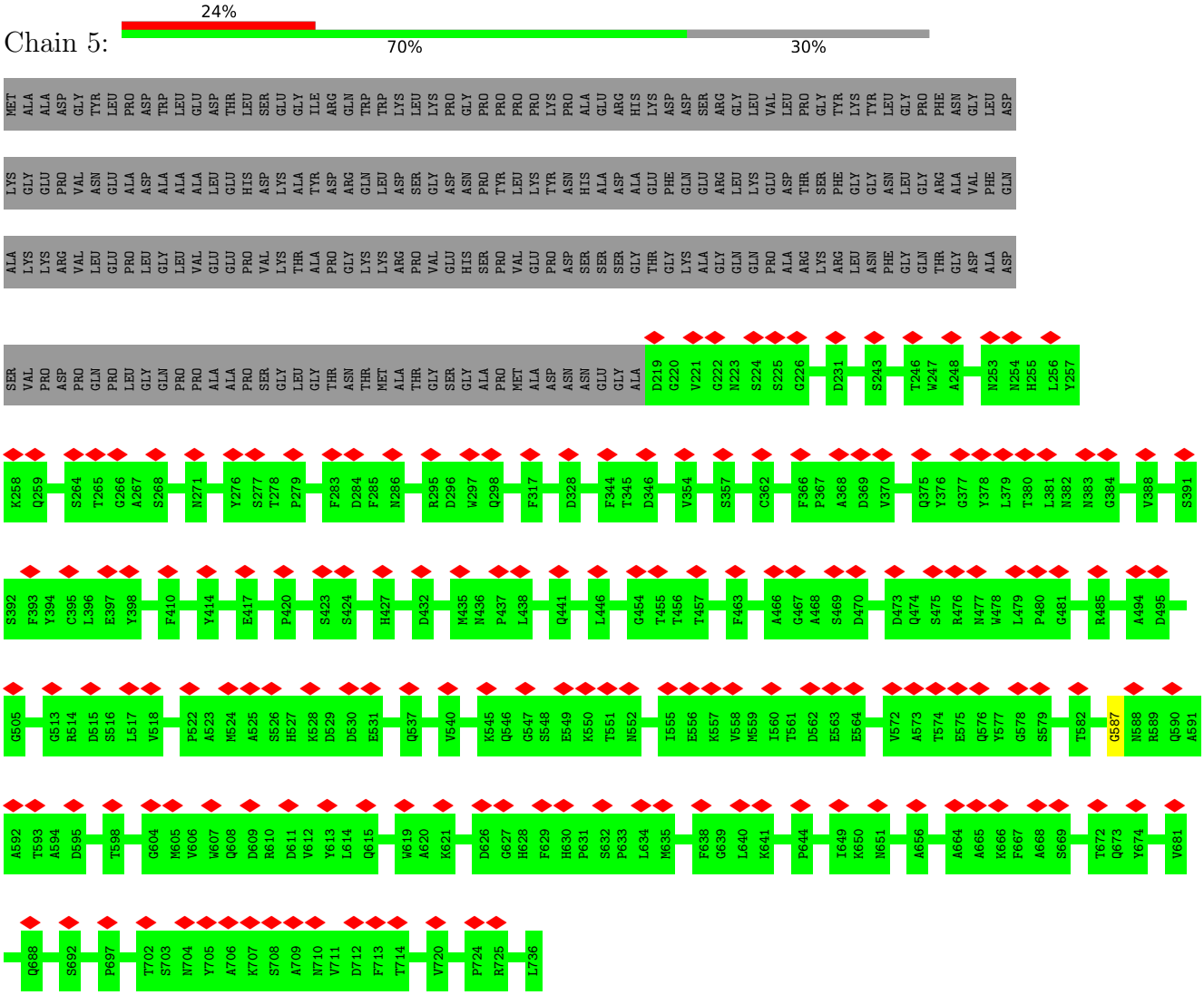
- Molecule 1: Capsid protein VP1

Chain 4:



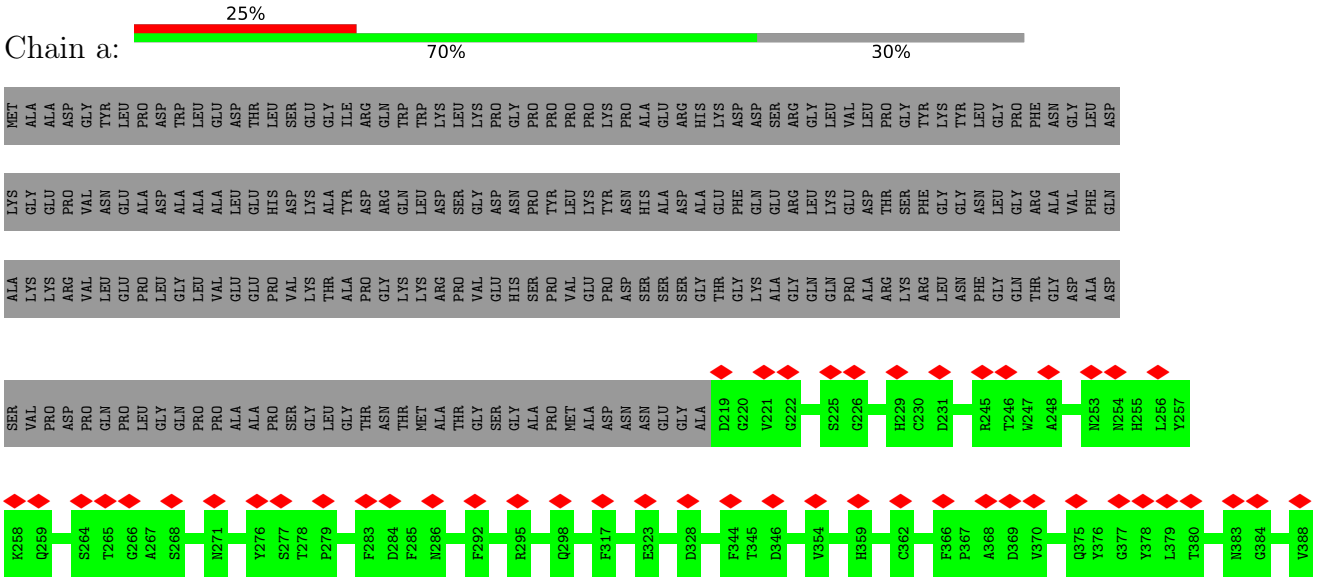
- Molecule 1: Capsid protein VP1

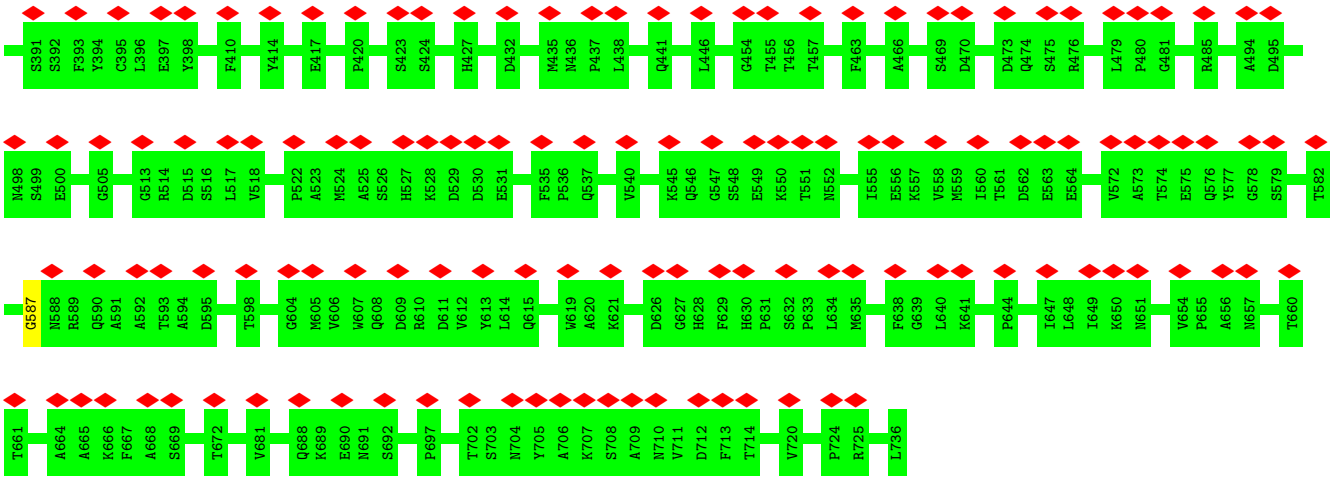
Chain 5:



• Molecule 1: Capsid protein VP1

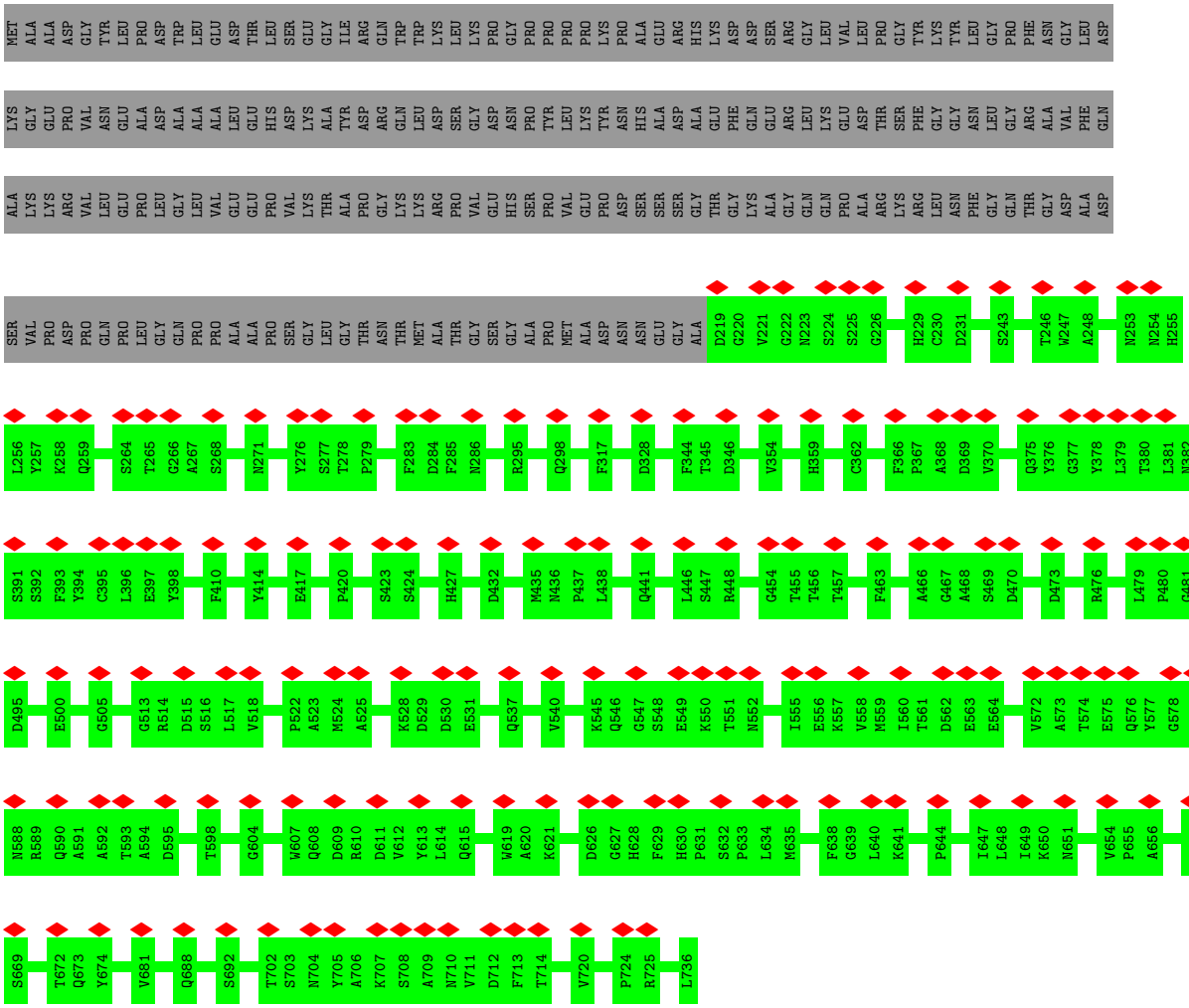
Chain a:





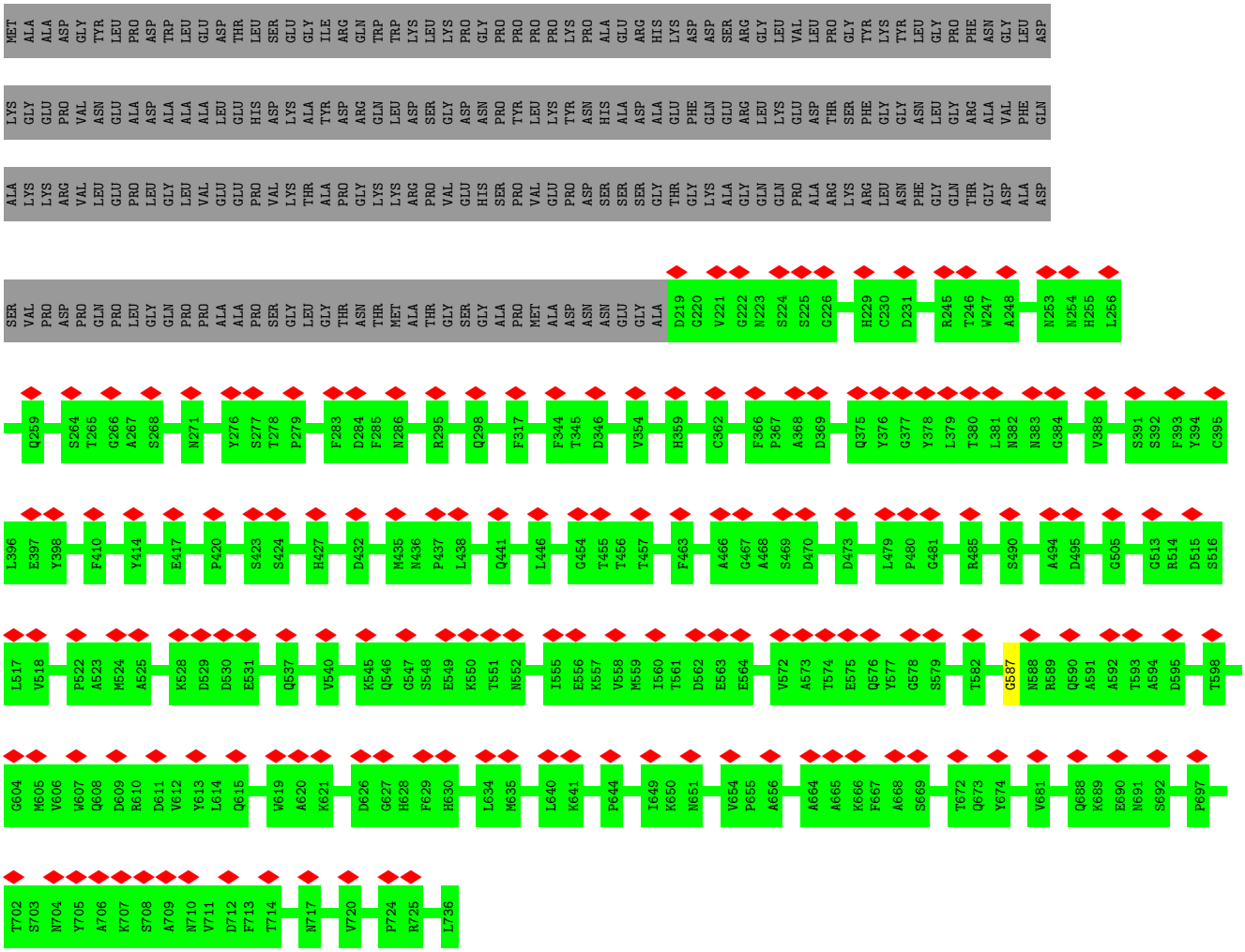
- Molecule 1: Capsid protein VP1

Chain b:



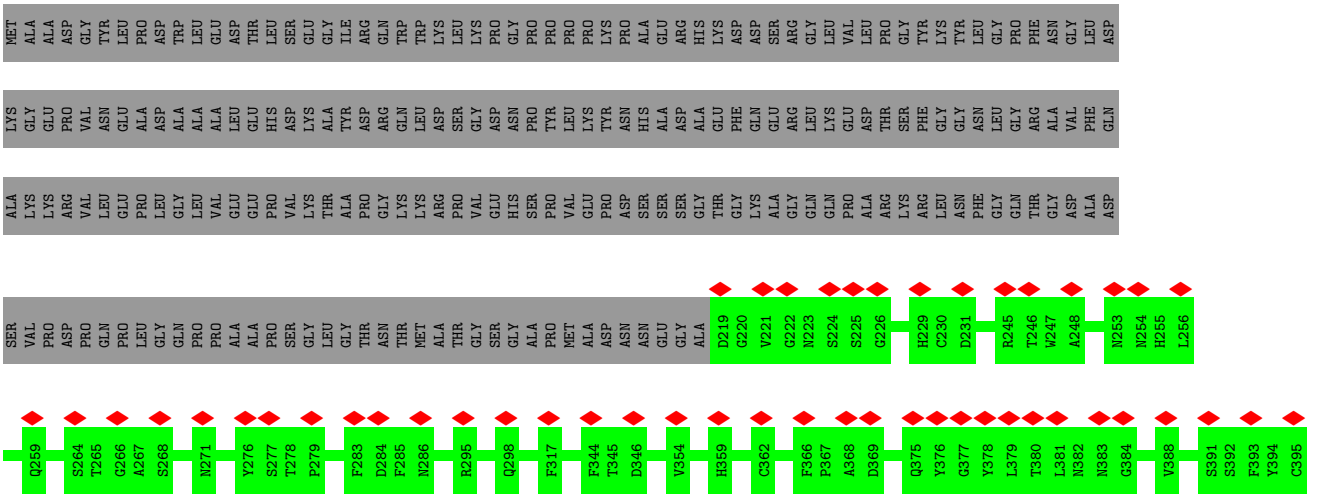
- Molecule 1: Capsid protein VP1

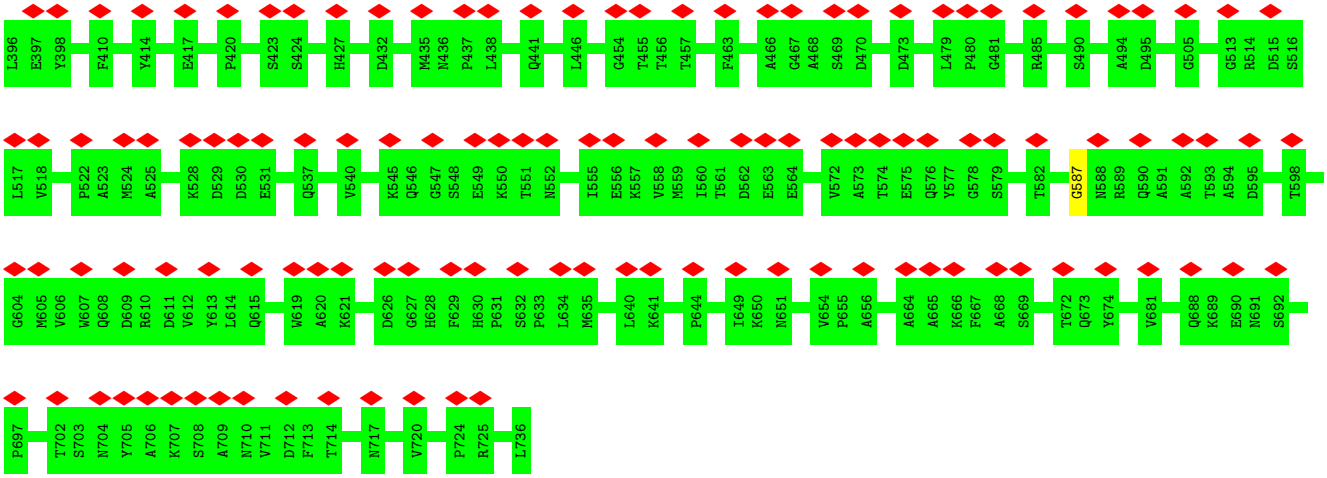
Chain c: 23% 70% 30%



- Molecule 1: Capsid protein VP1

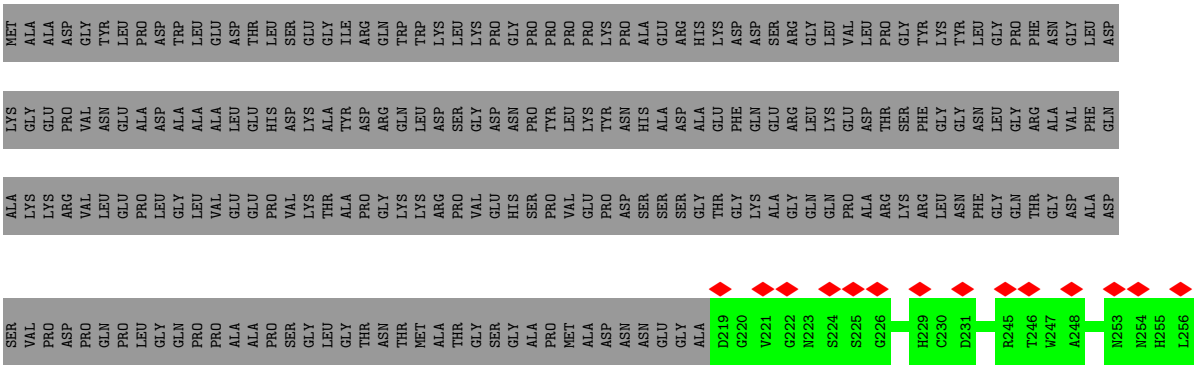
Chain d: 23% 70% 30%





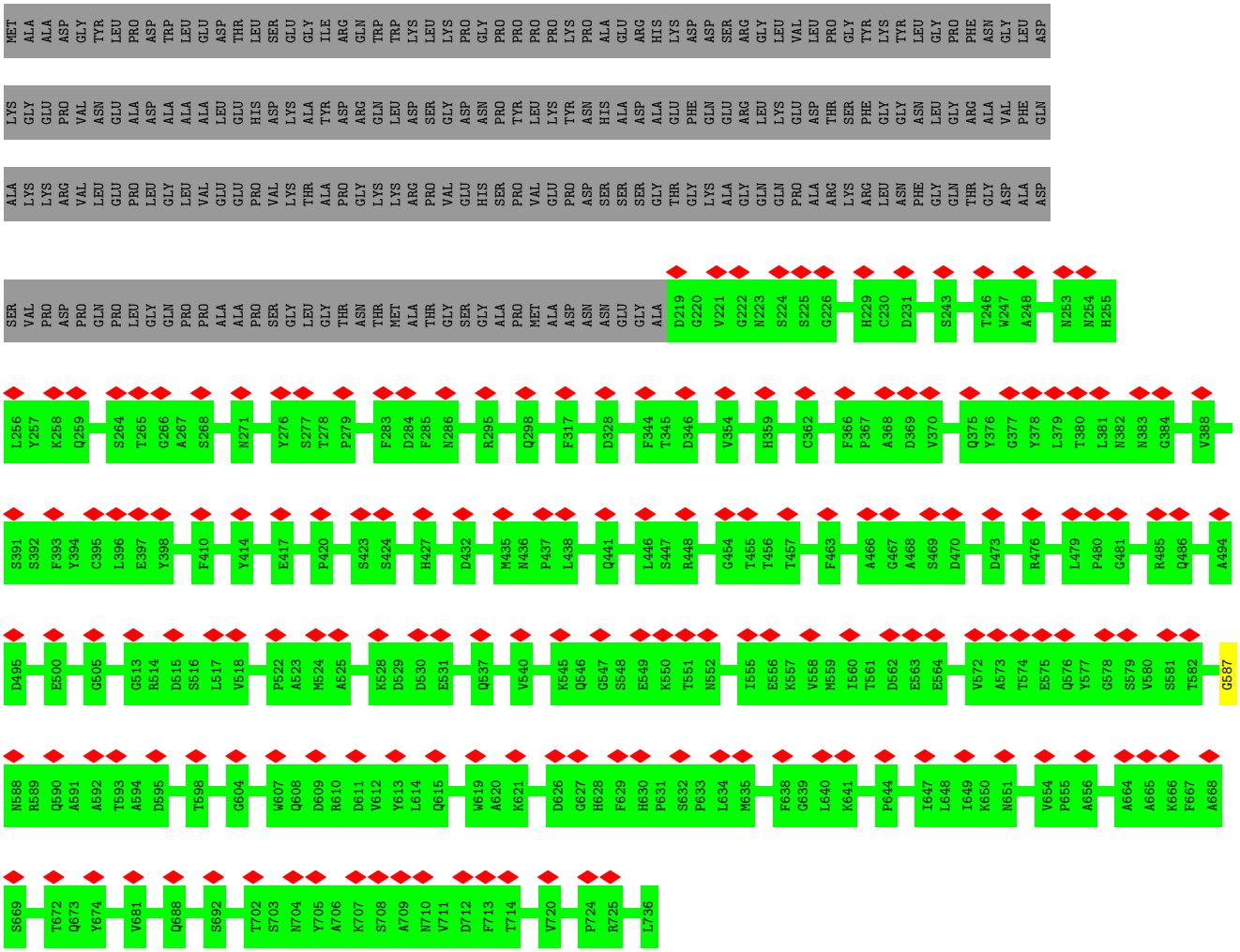
- Molecule 1: Capsid protein VP1

Chain e:



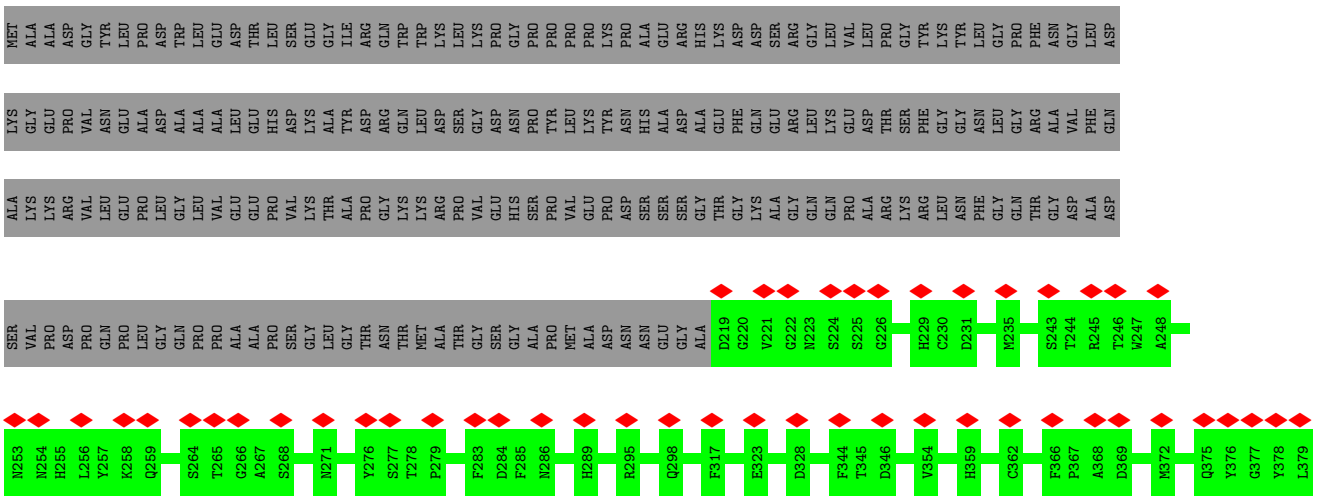
- Molecule 1: Capsid protein VP1

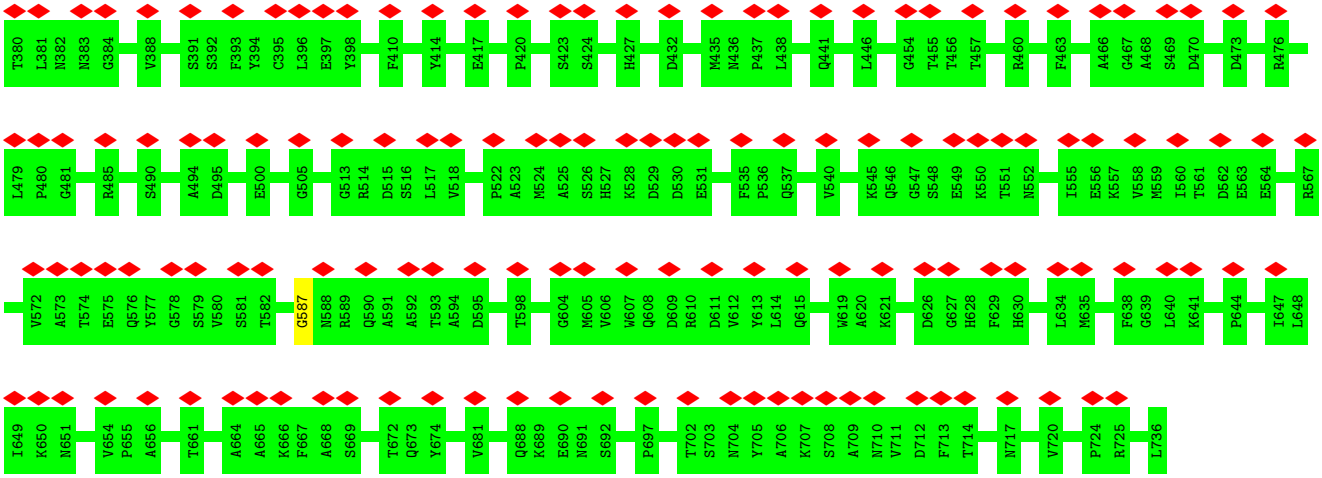
Chain f: 24% 70% 30%



- Molecule 1: Capsid protein VP1

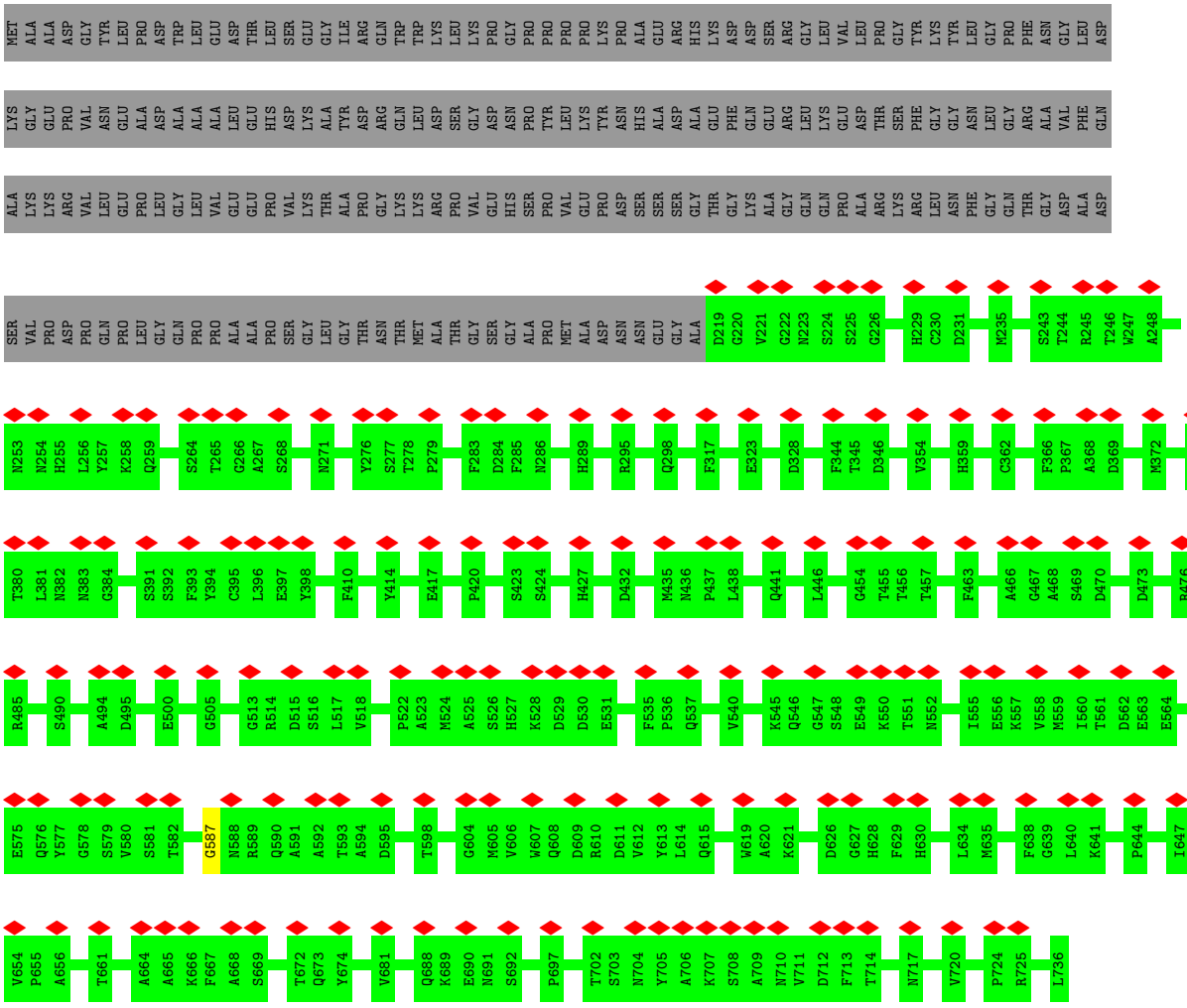
Chain g: 26% 70% 30%





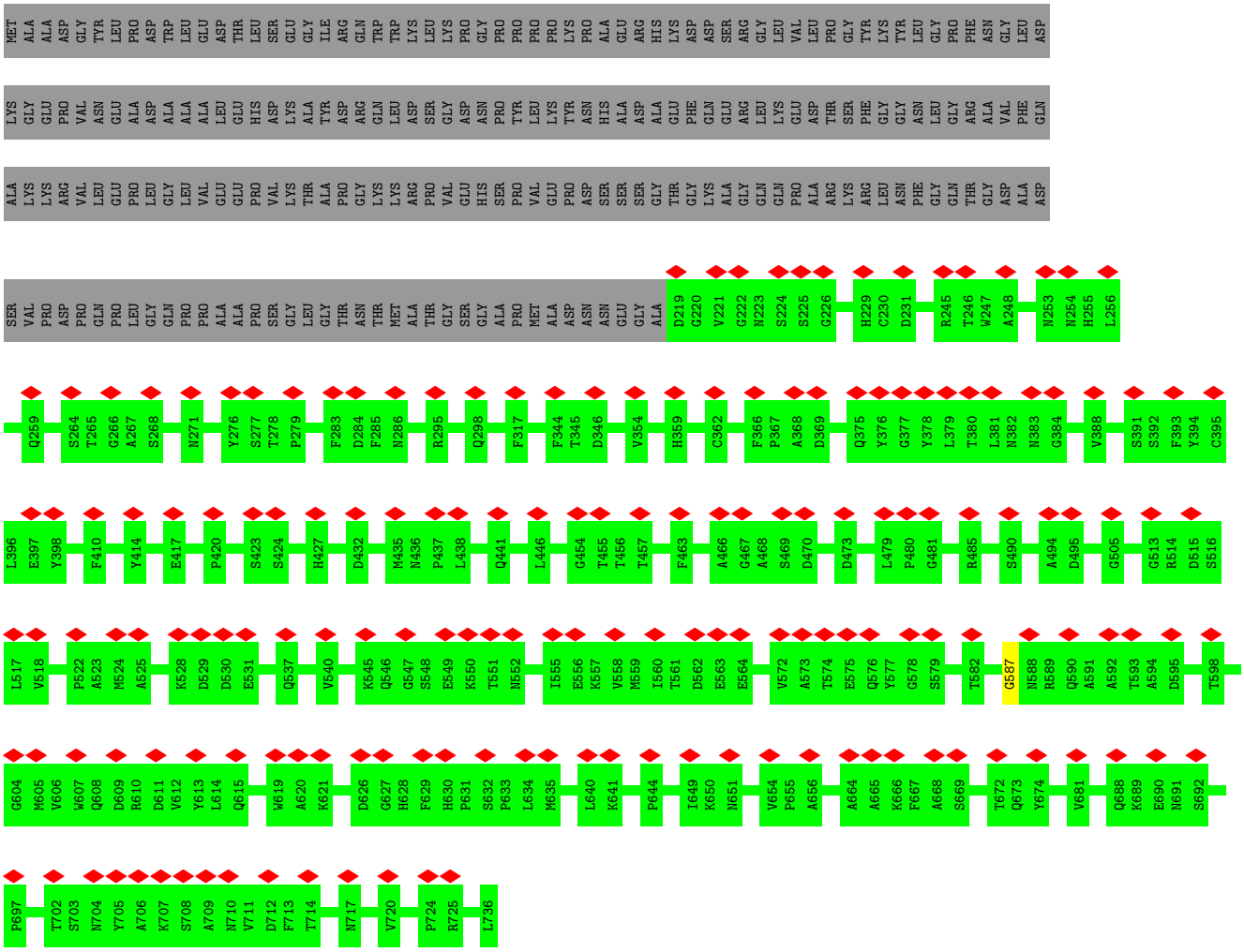
- Molecule 1: Capsid protein VP1

Chain h:



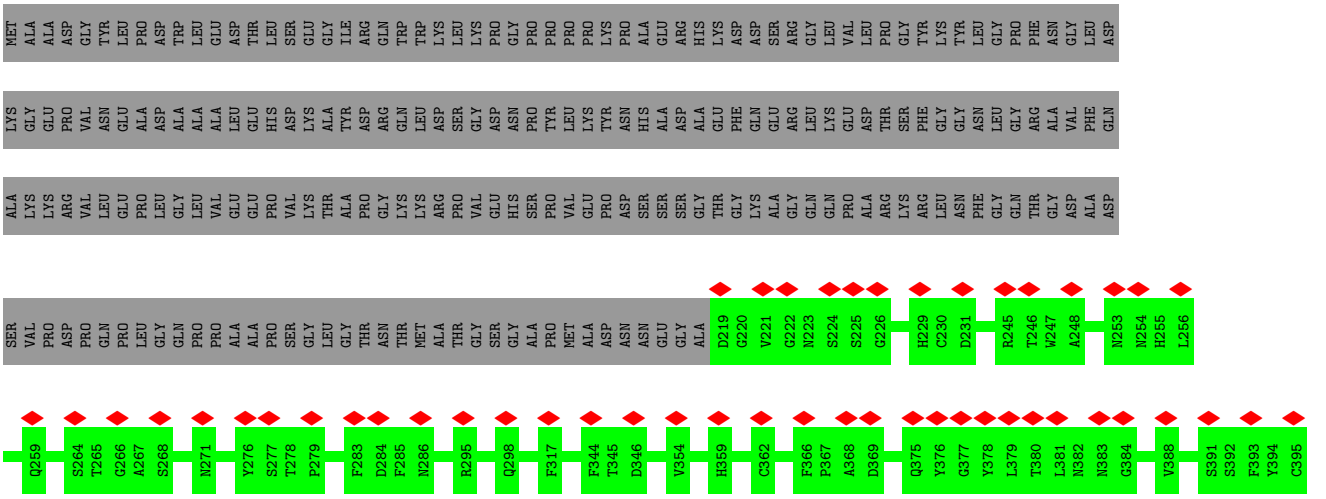
- Molecule 1: Capsid protein VP1

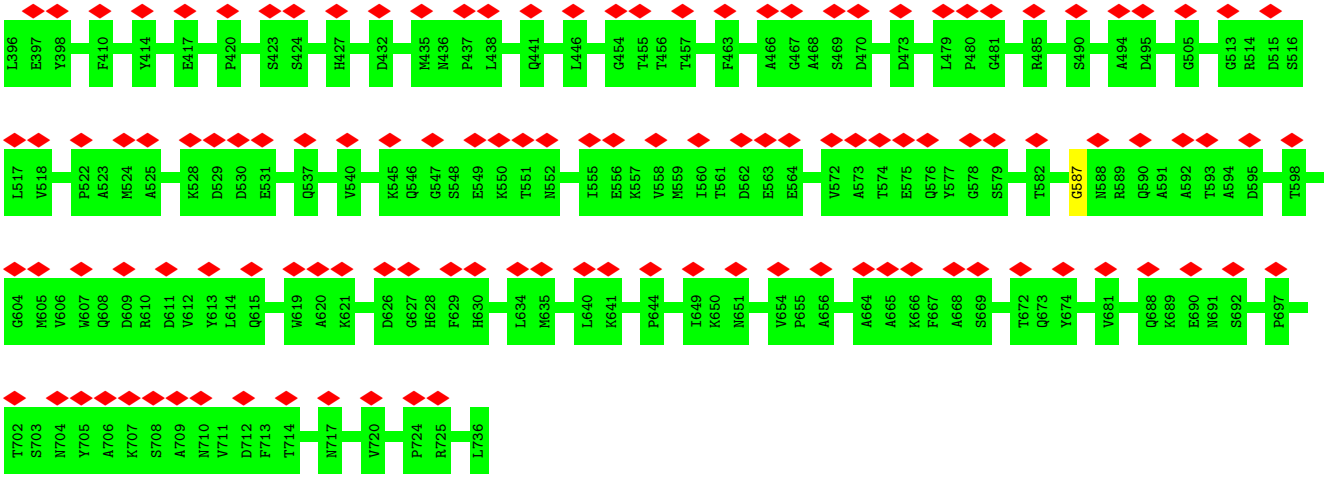
Chain i:



- Molecule 1: Capsid protein VP1

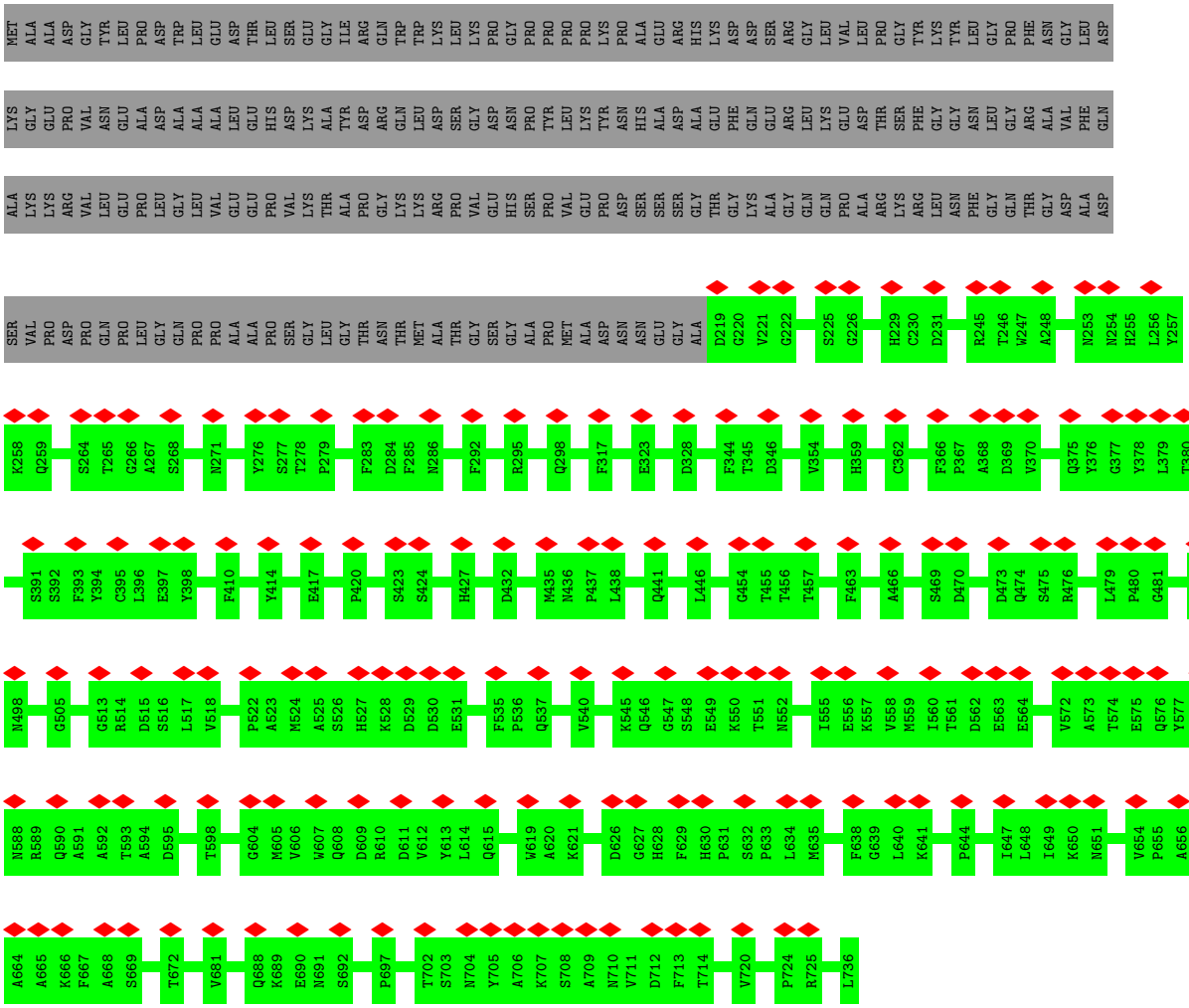
Chain j:





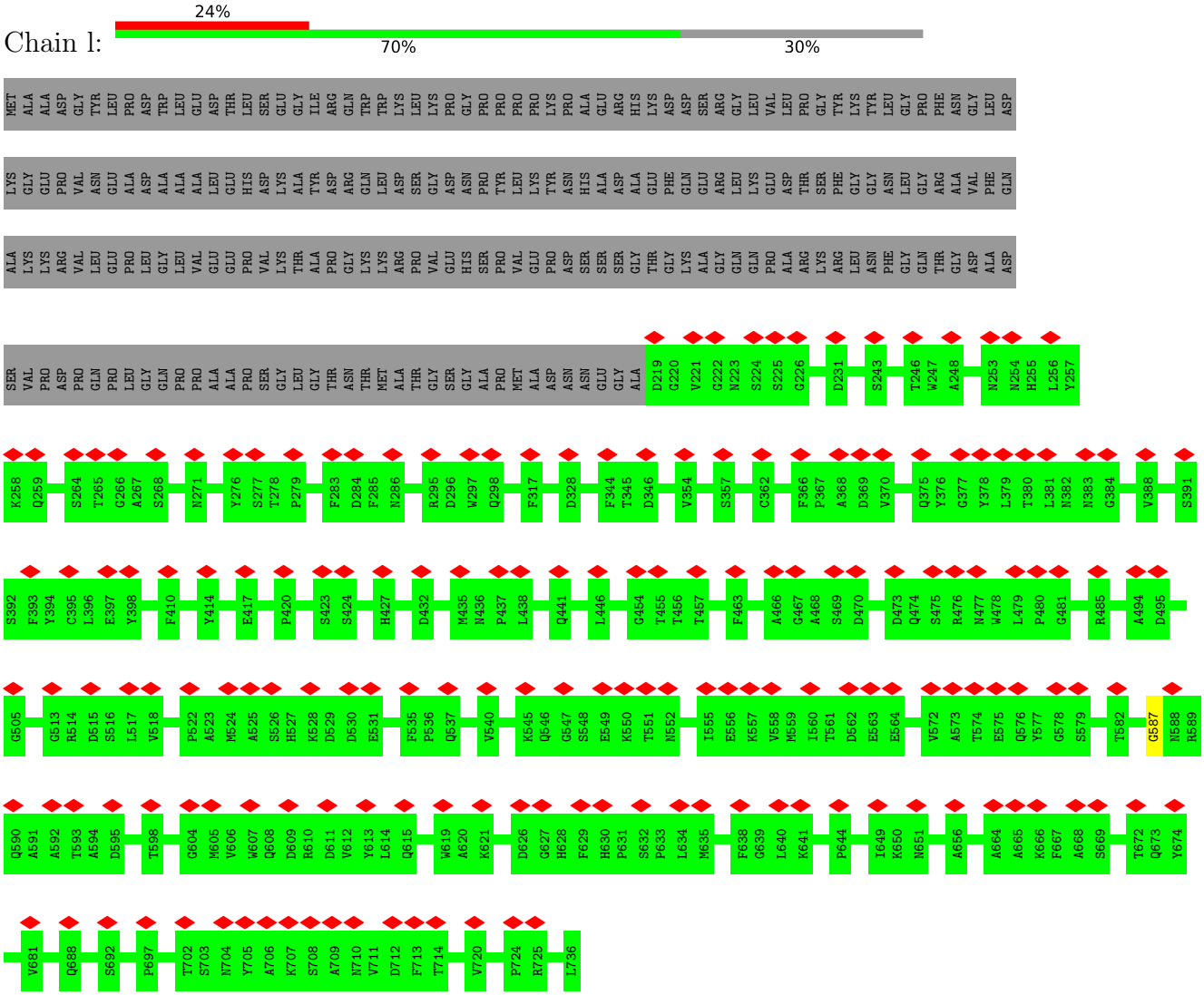
- Molecule 1: Capsid protein VP1

Chain k:



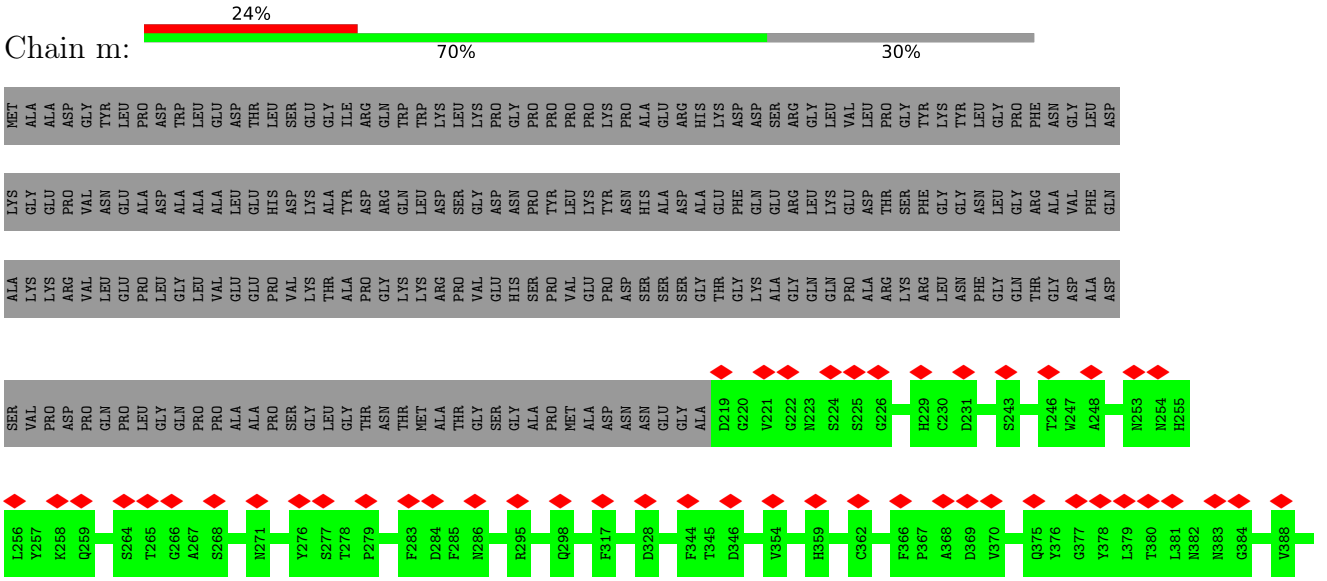
- Molecule 1: Capsid protein VP1

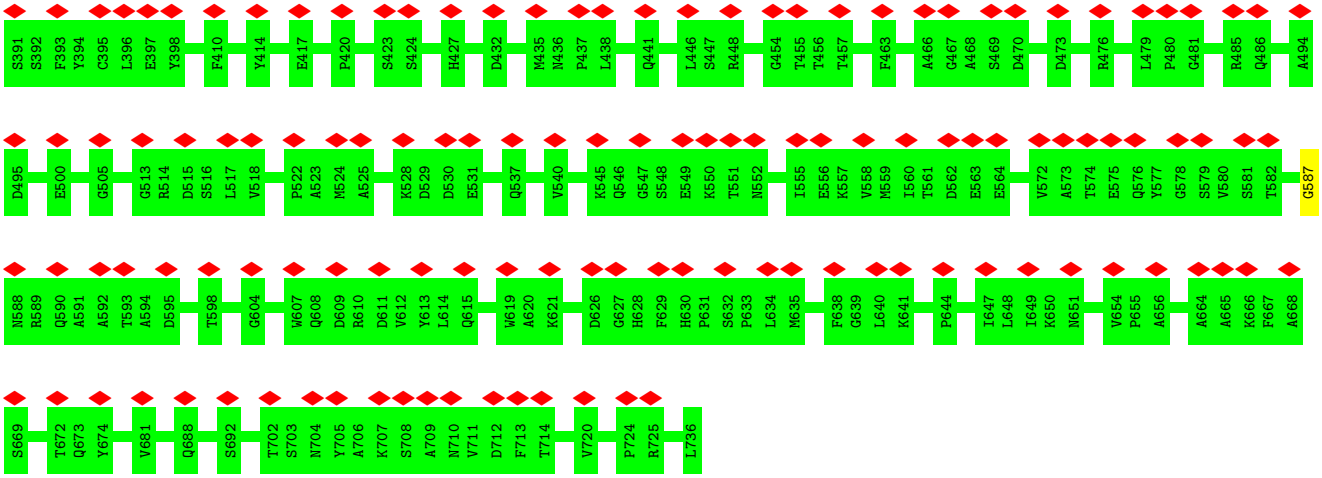
Chain l:



- Molecule 1: Capsid protein VP1

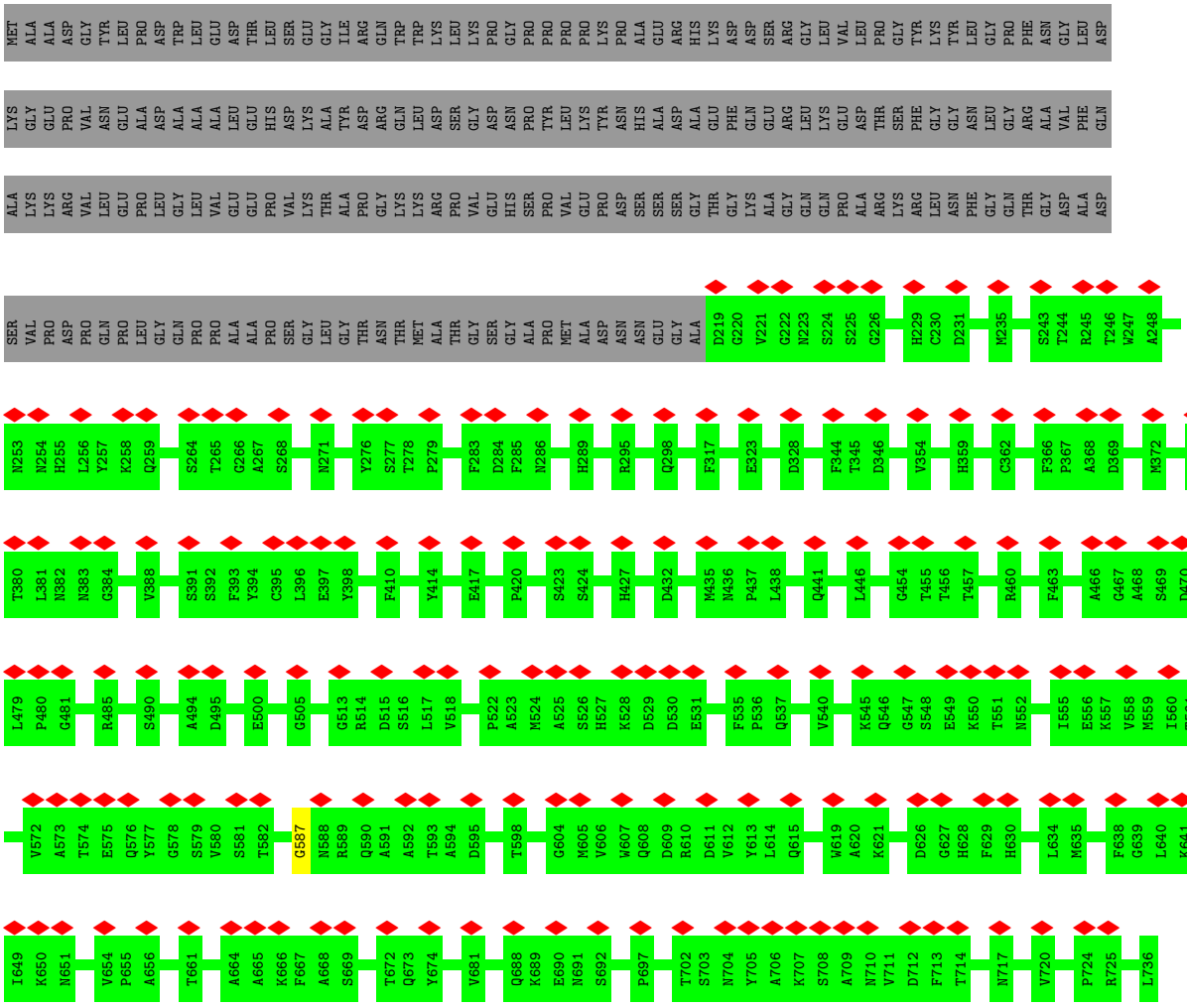
Chain m:





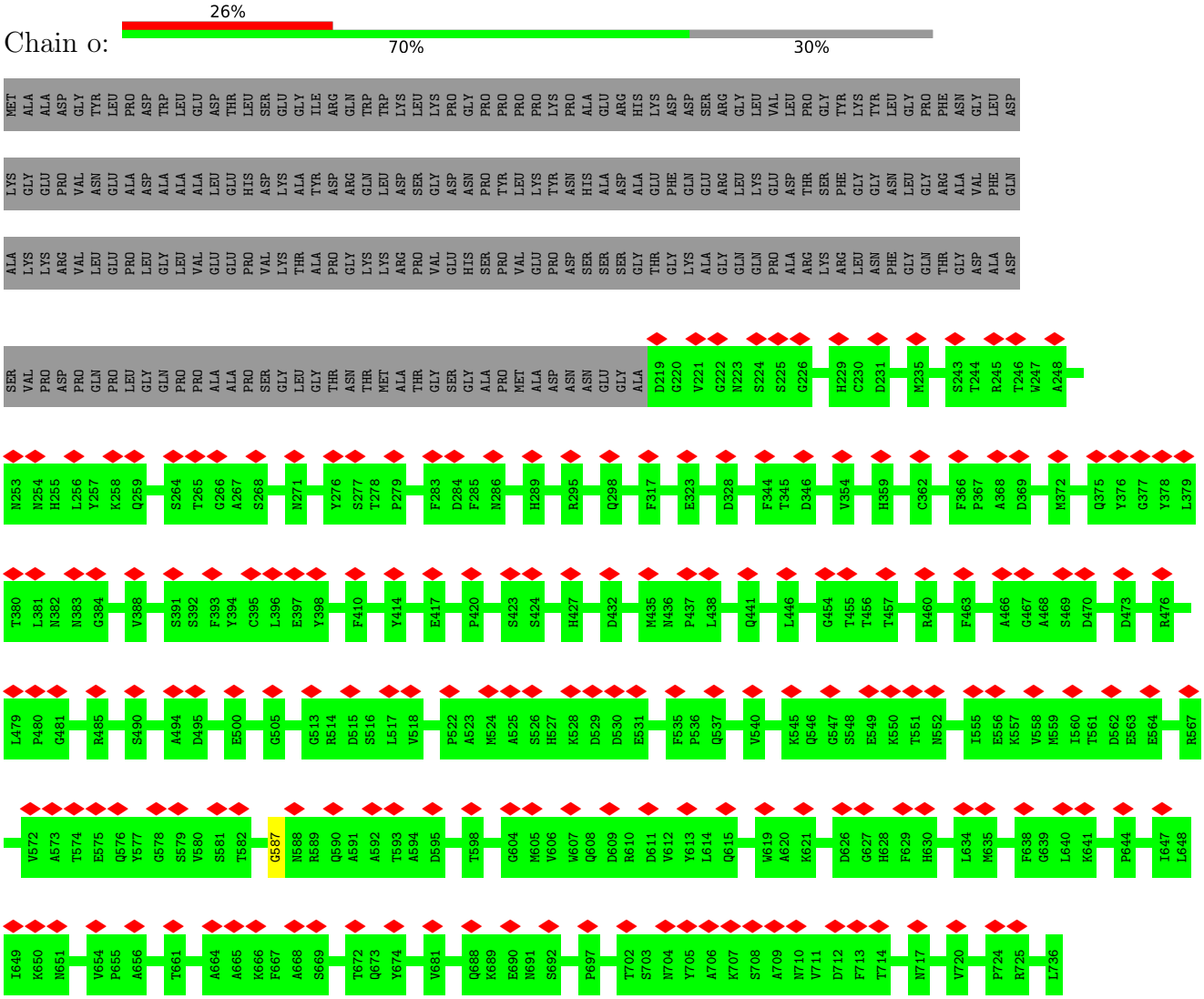
- Molecule 1: Capsid protein VP1

Chain n:



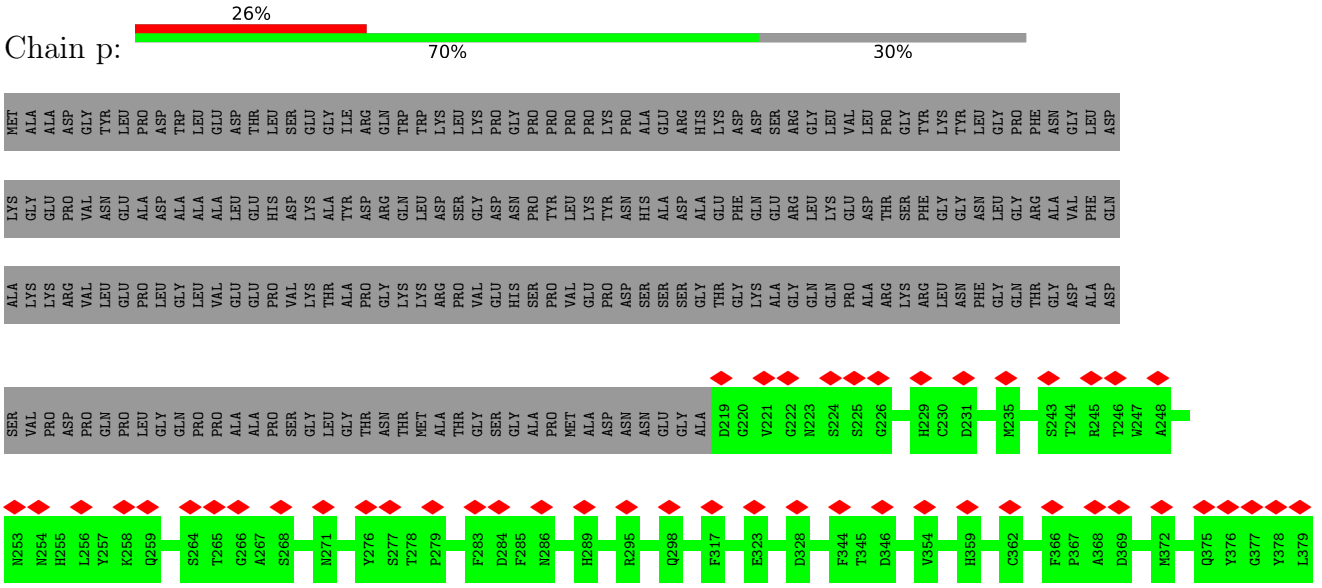
- Molecule 1: Capsid protein VP1

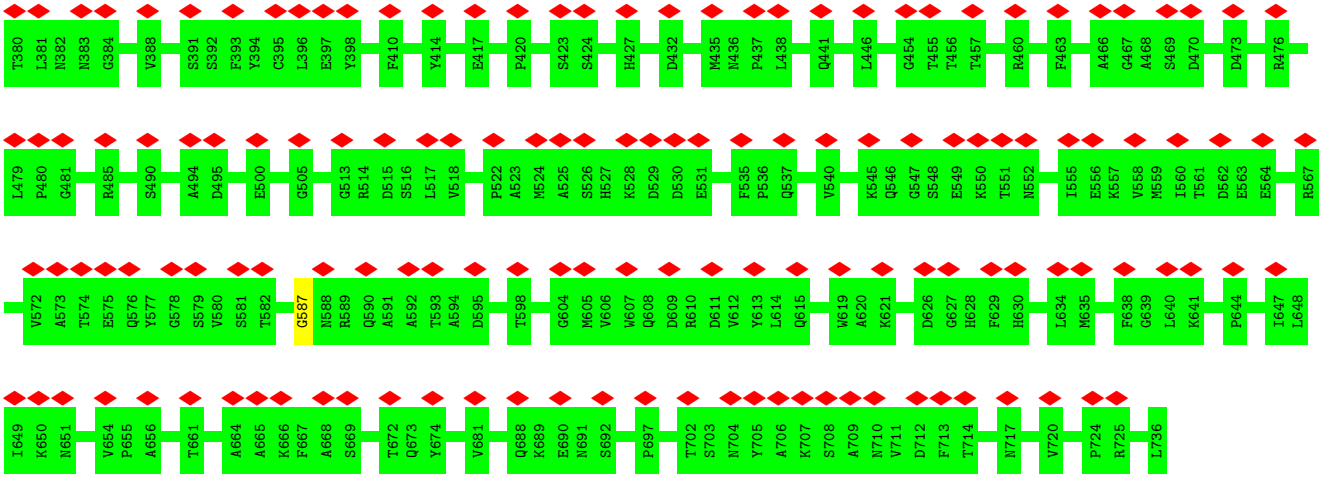
Chain o:



- Molecule 1: Capsid protein VP1

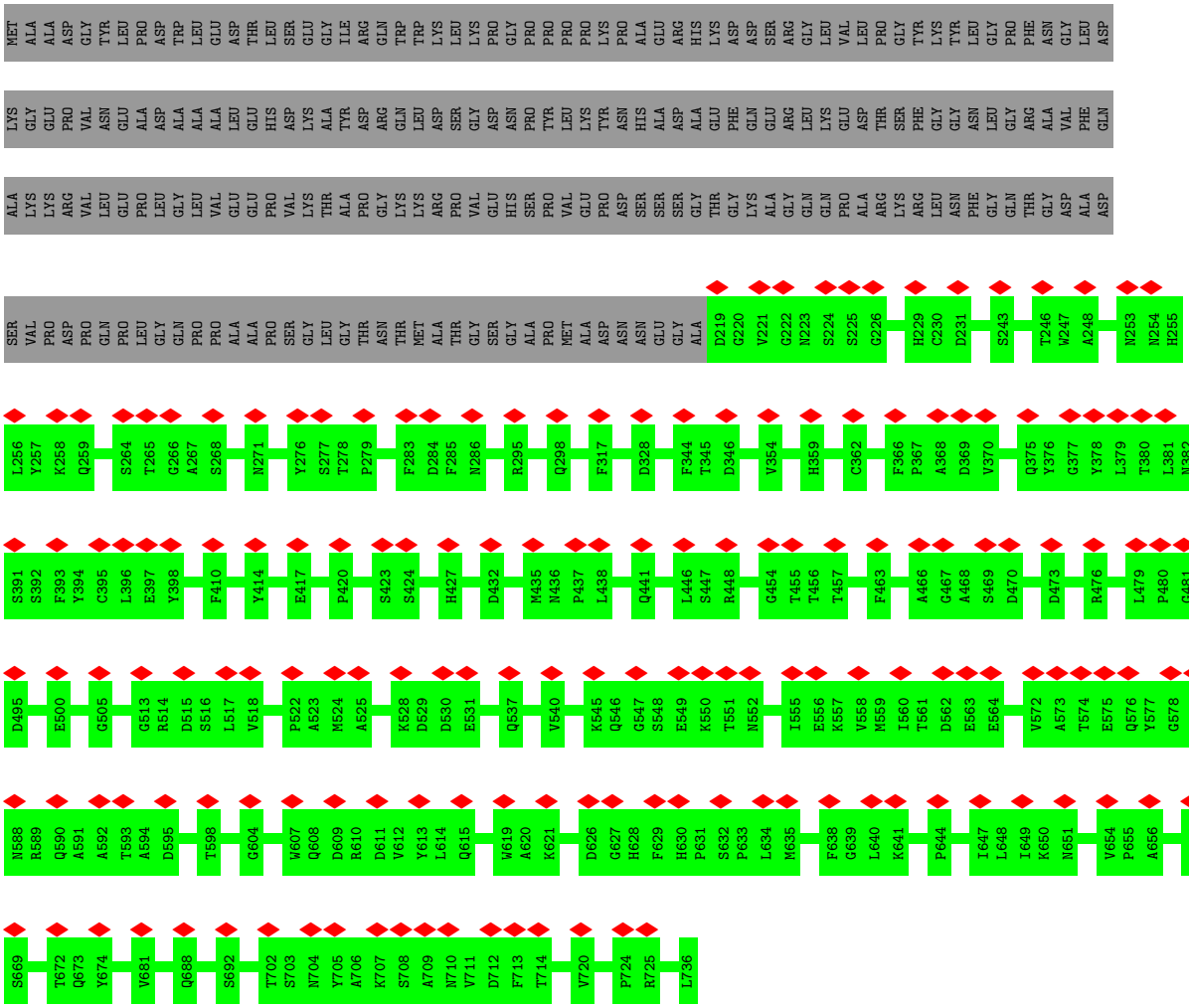
Chain p:





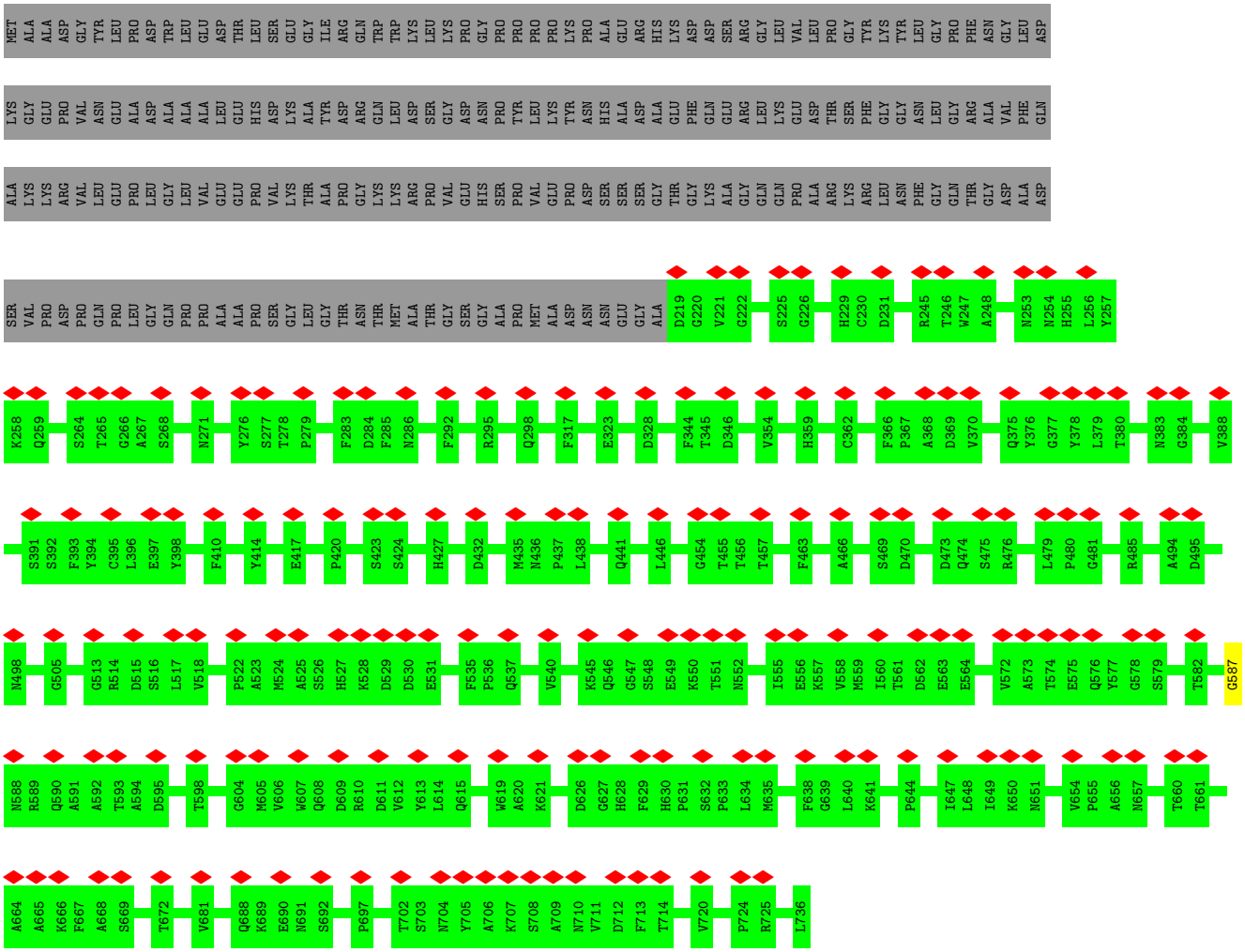
- Molecule 1: Capsid protein VP1

Chain q:



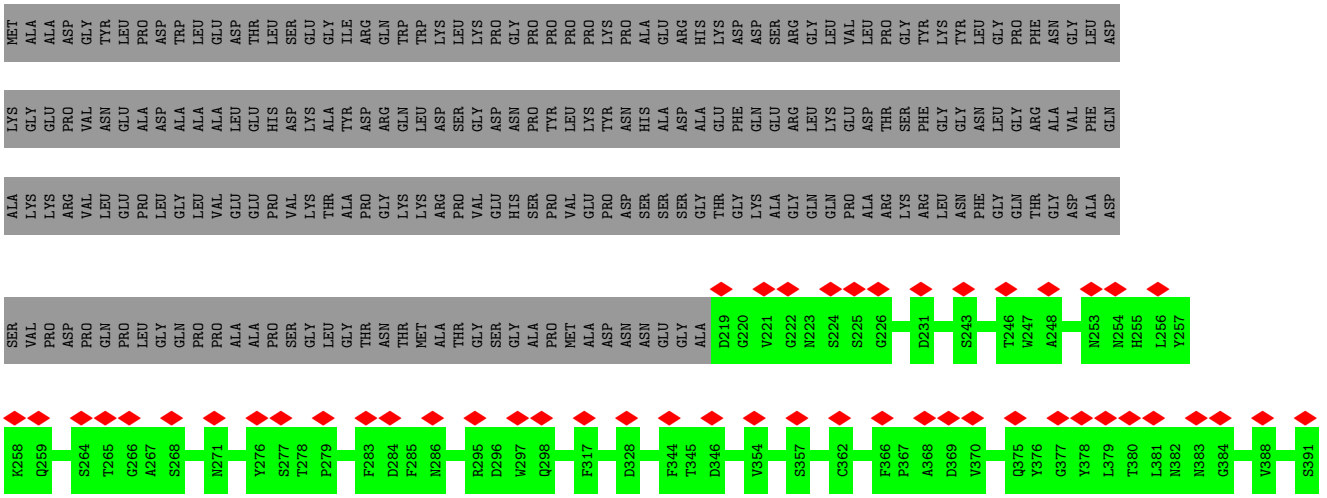
- Molecule 1: Capsid protein VP1

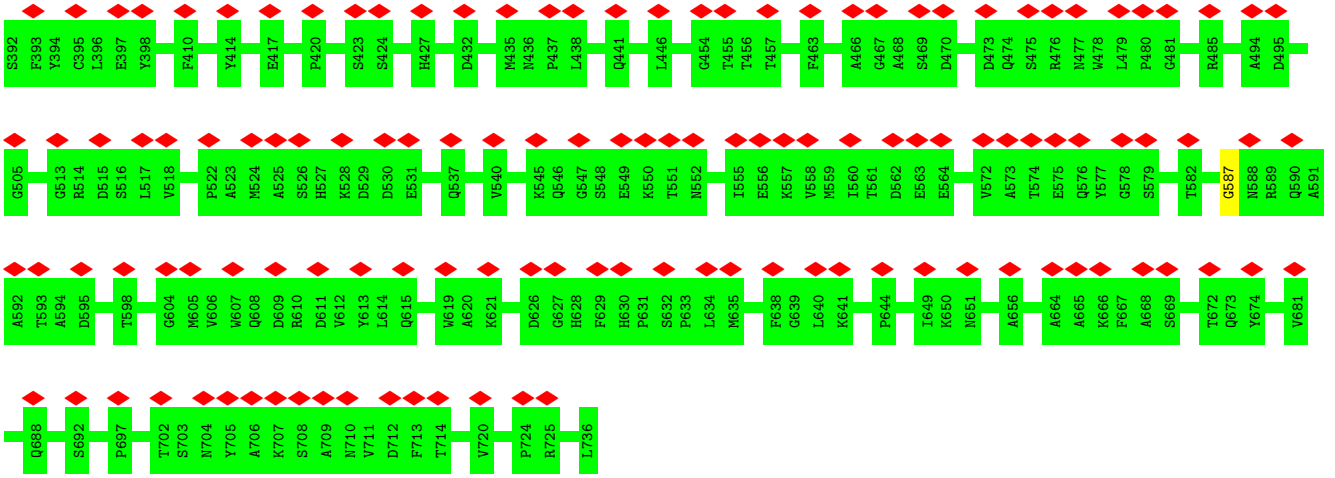
Chain r:



- Molecule 1: Capsid protein VP1

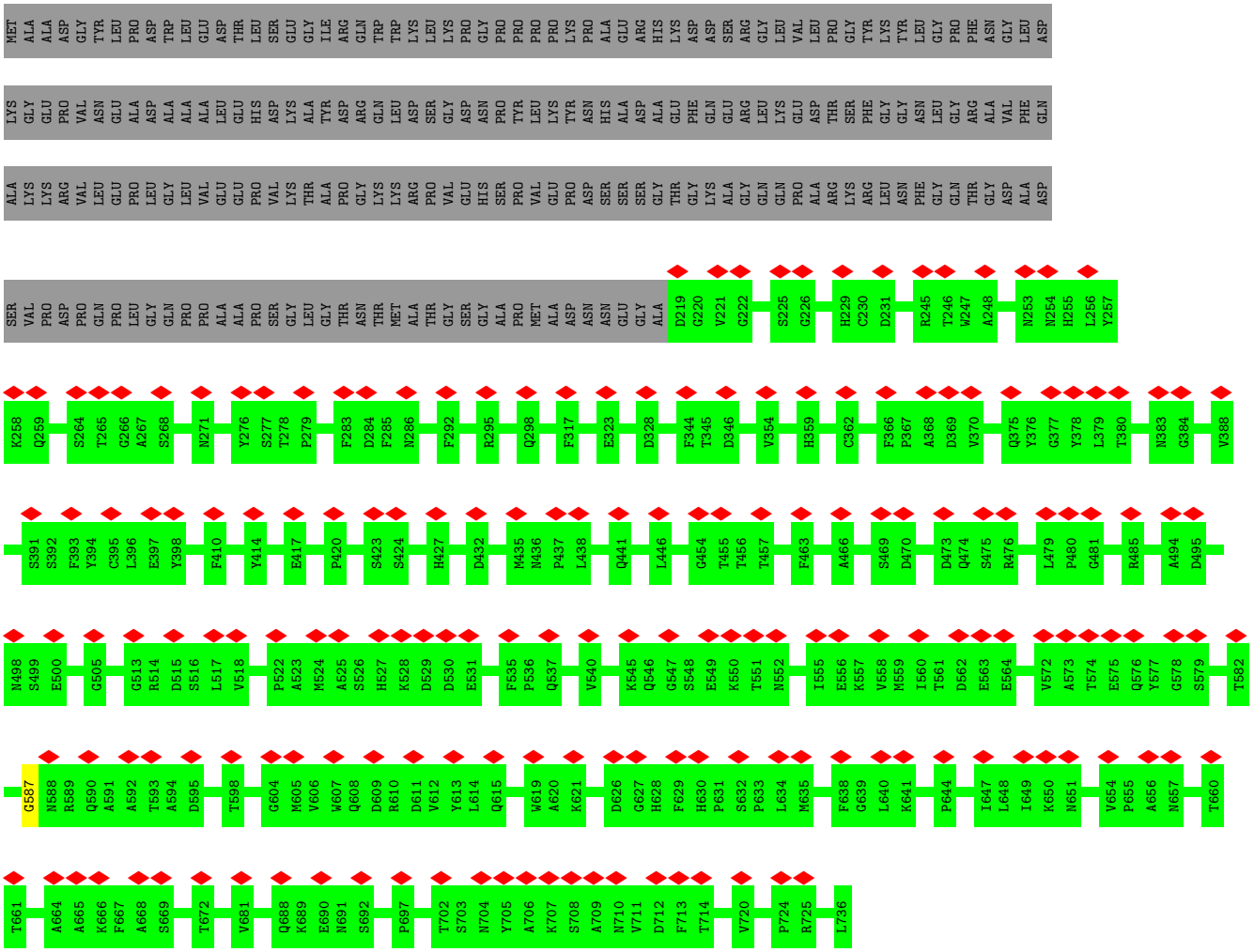
Chain s:





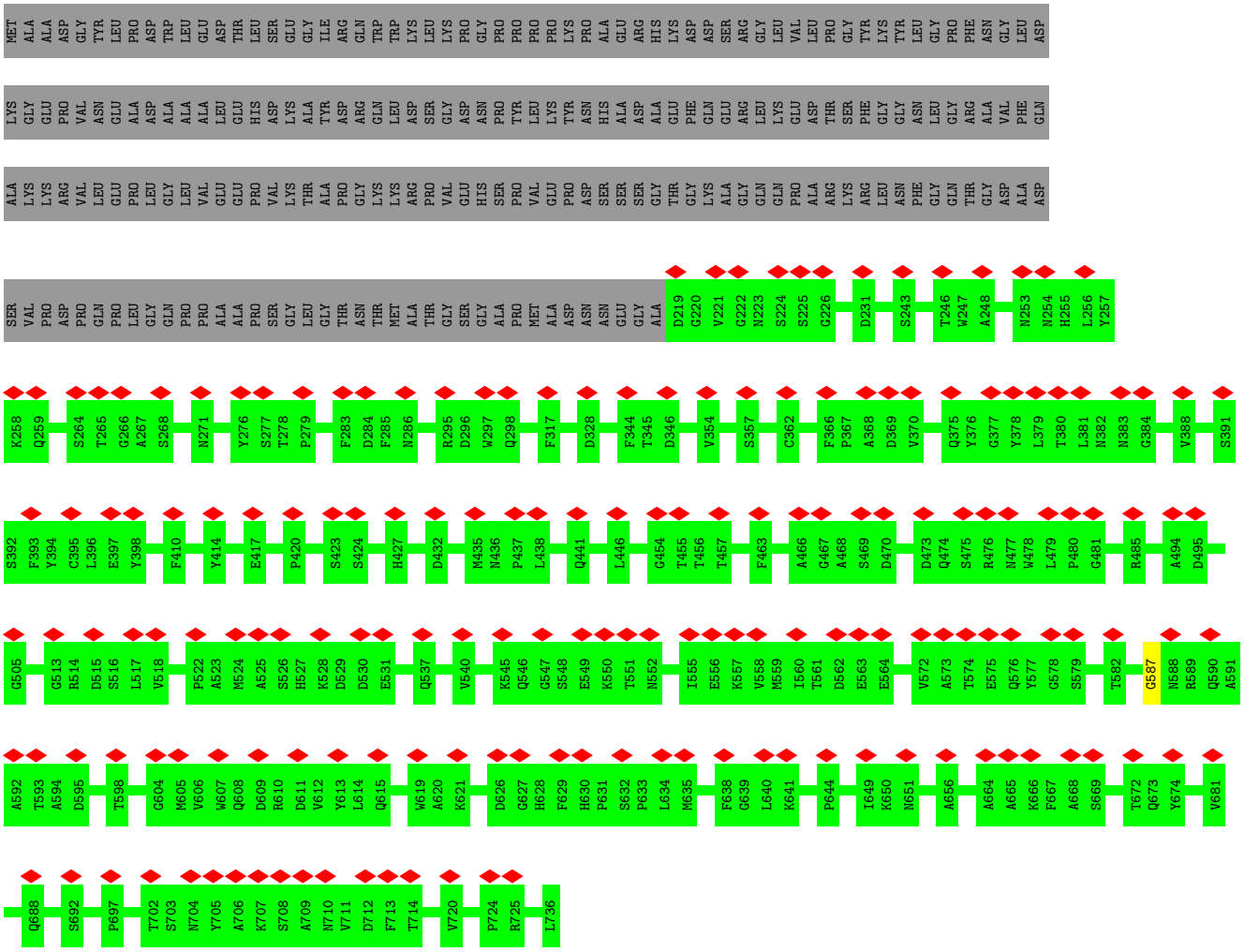
- Molecule 1: Capsid protein VP1

Chain t:



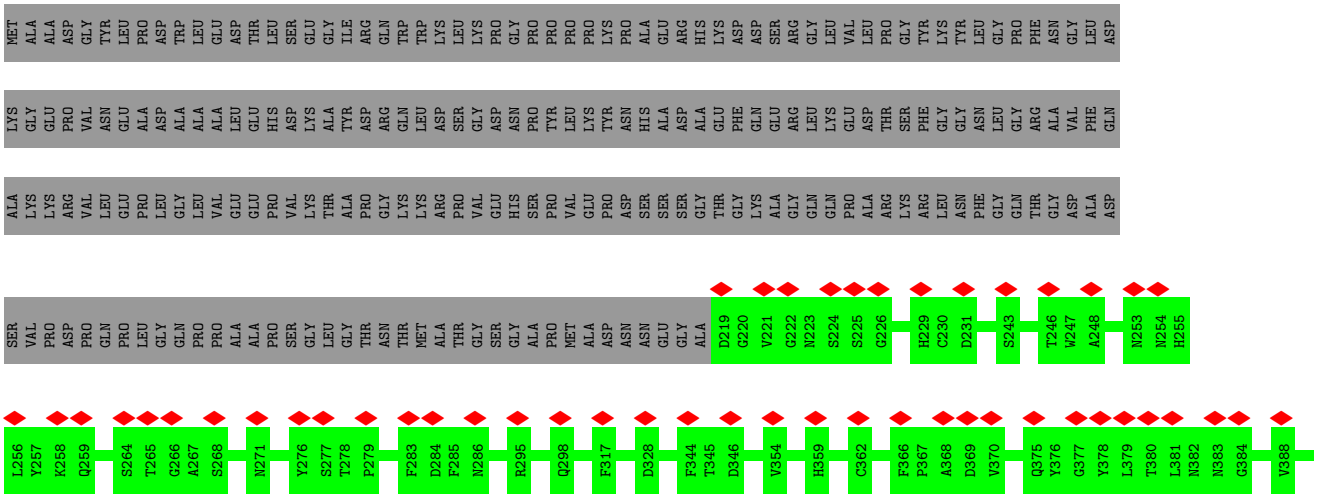
- Molecule 1: Capsid protein VP1

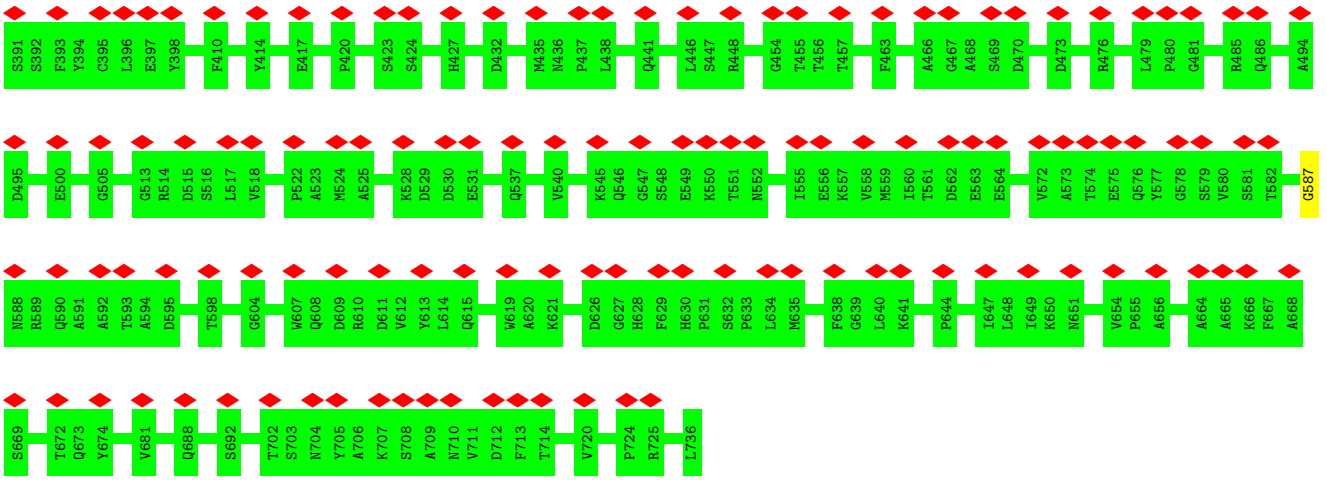
Chain u: 24% 70% 30%



- Molecule 1: Capsid protein VP1

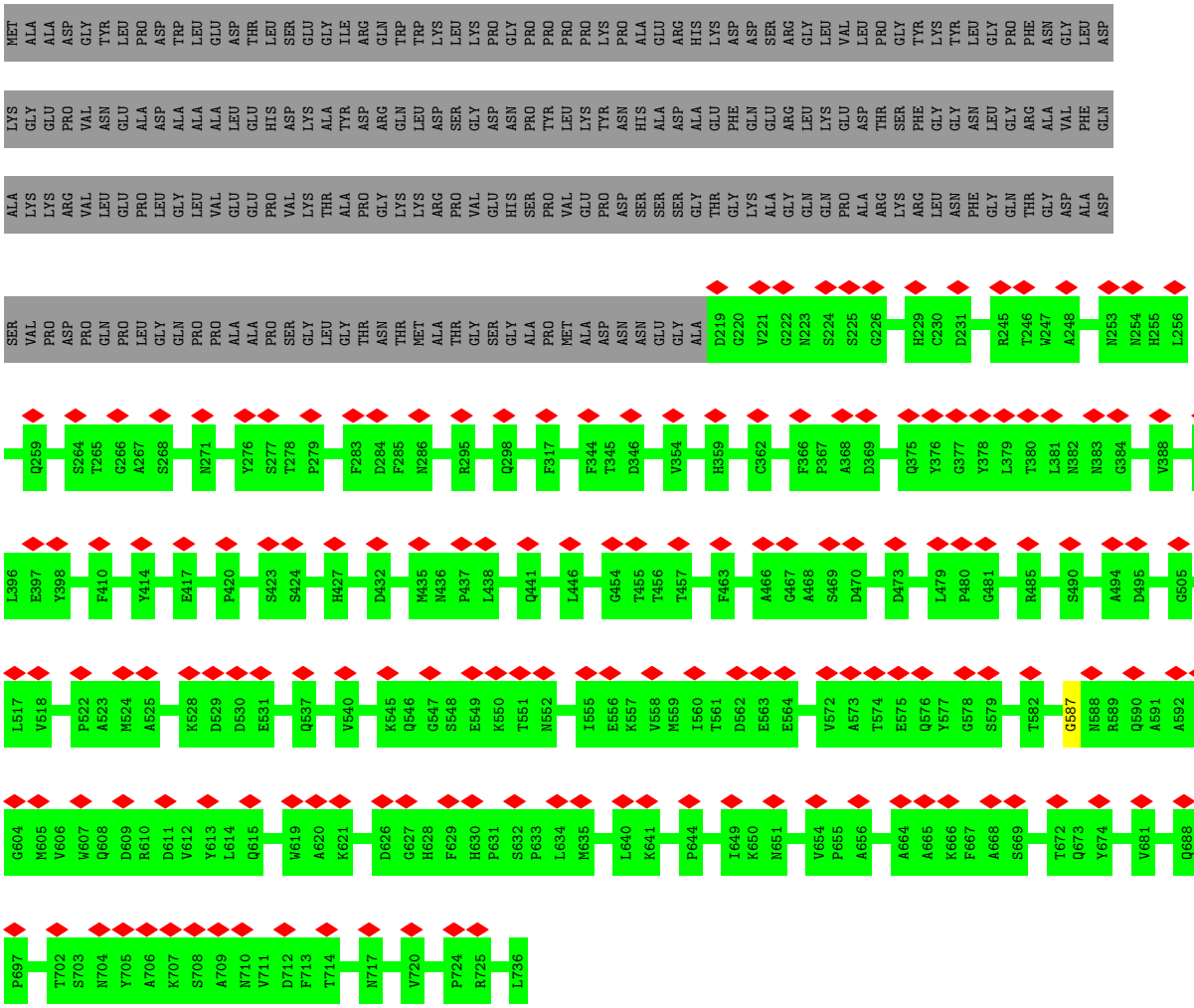
Chain v: 24% 70% 30%





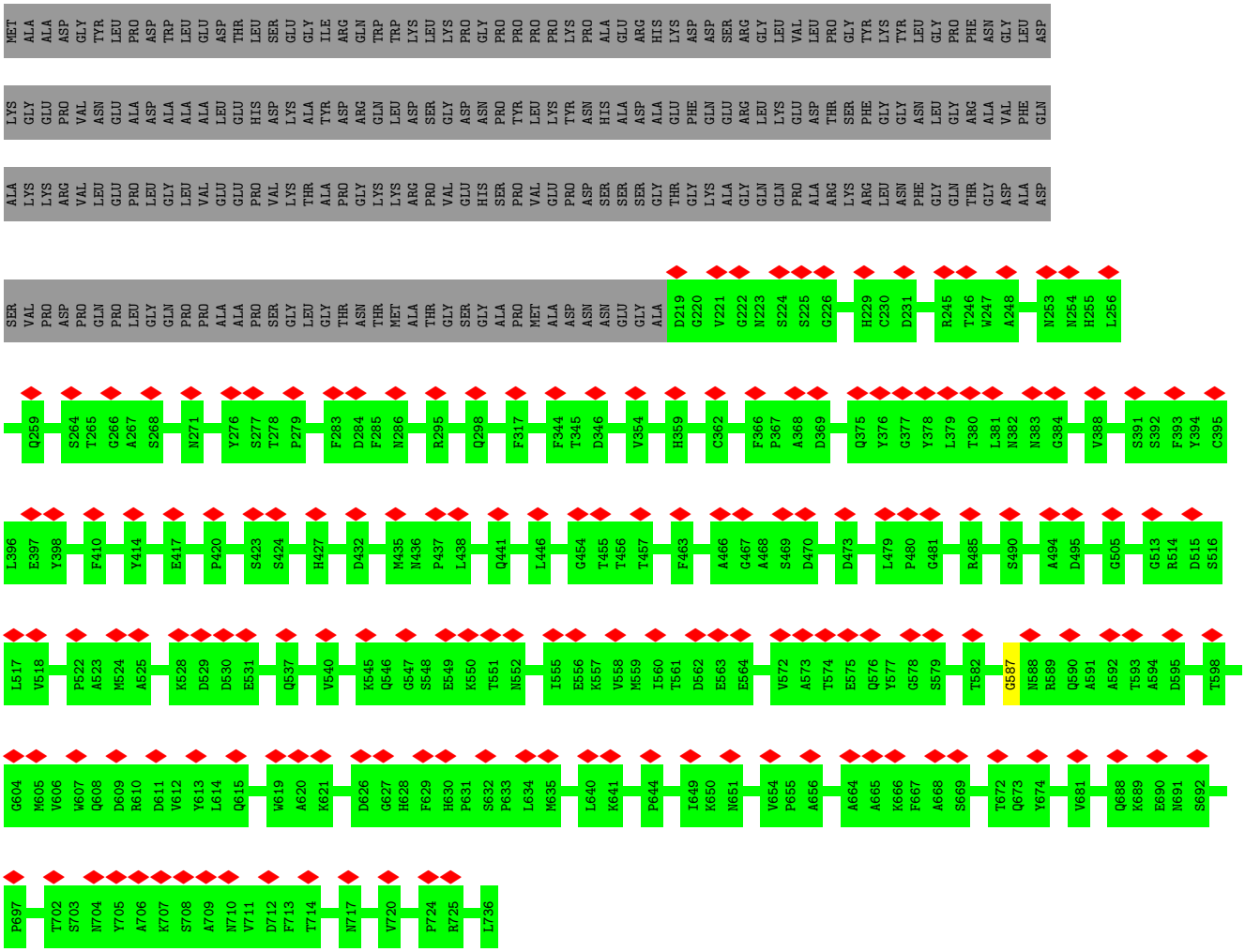
- Molecule 1: Capsid protein VP1

Chain w: 23% 70% 30%



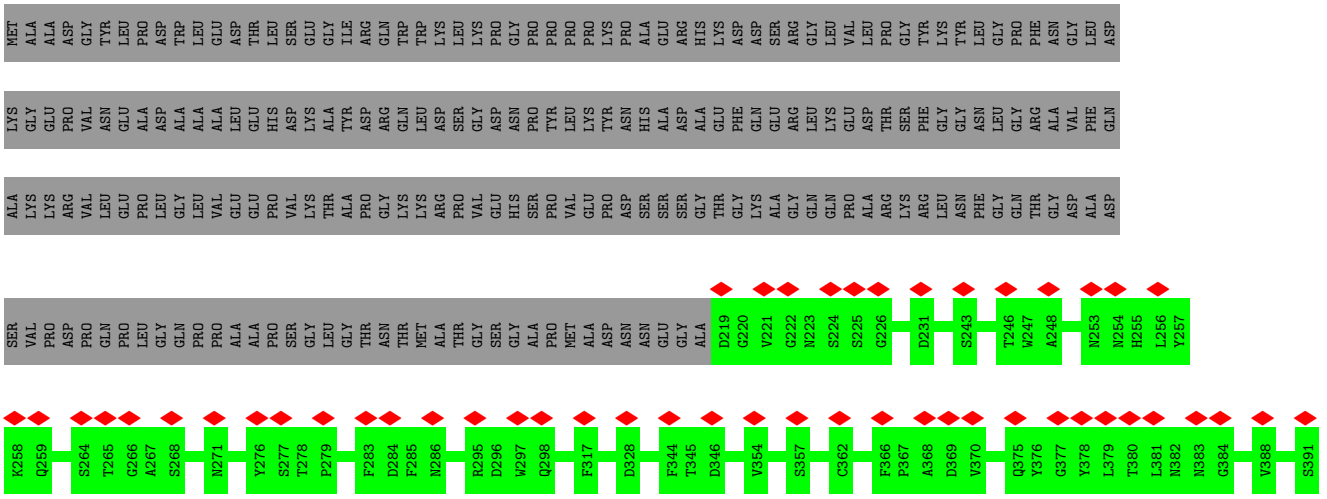
- Molecule 1: Capsid protein VP1

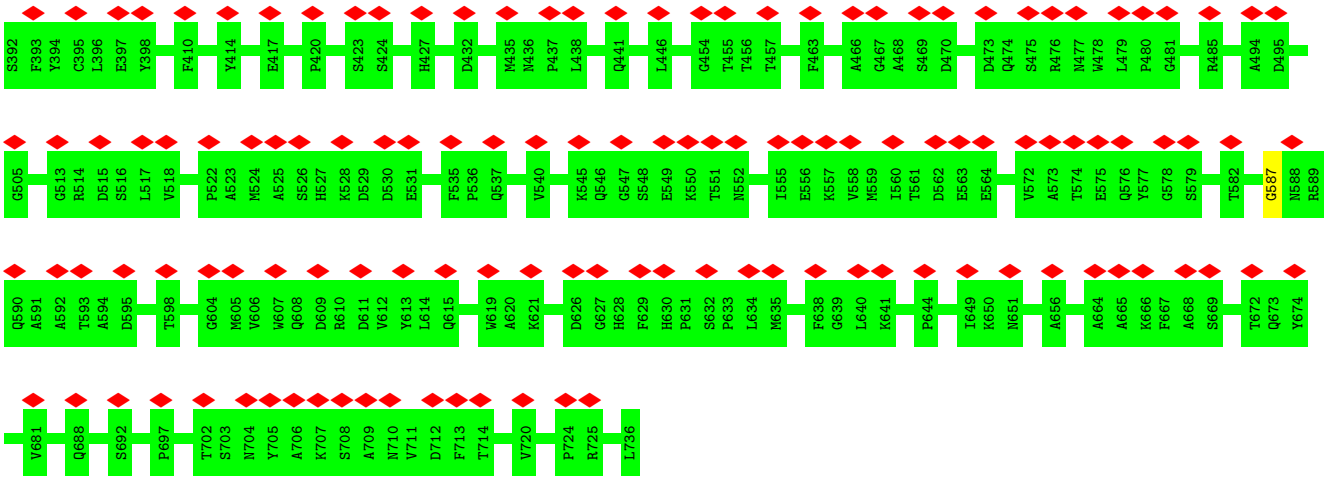
Chain x:



- Molecule 1: Capsid protein VP1

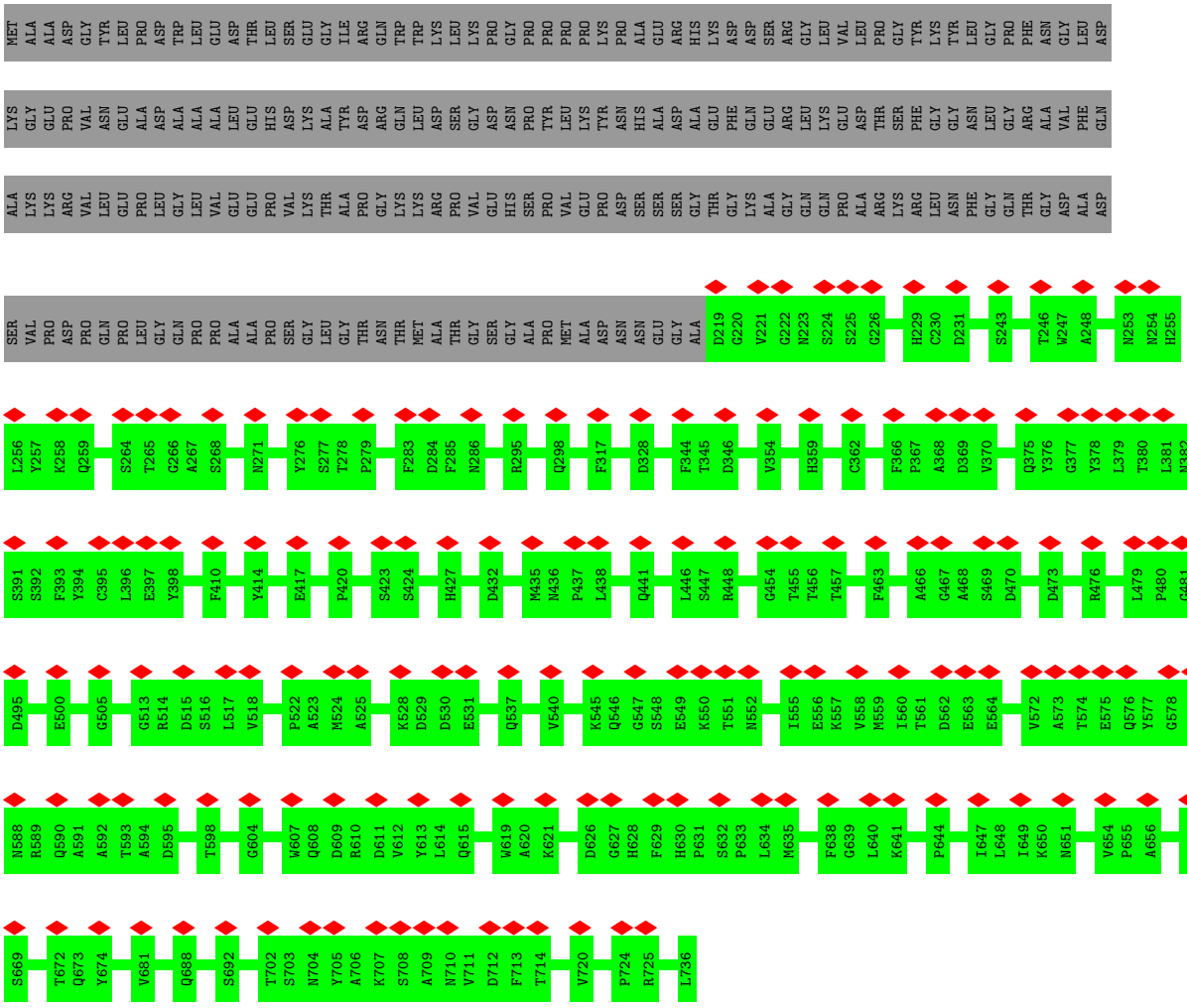
Chain y:





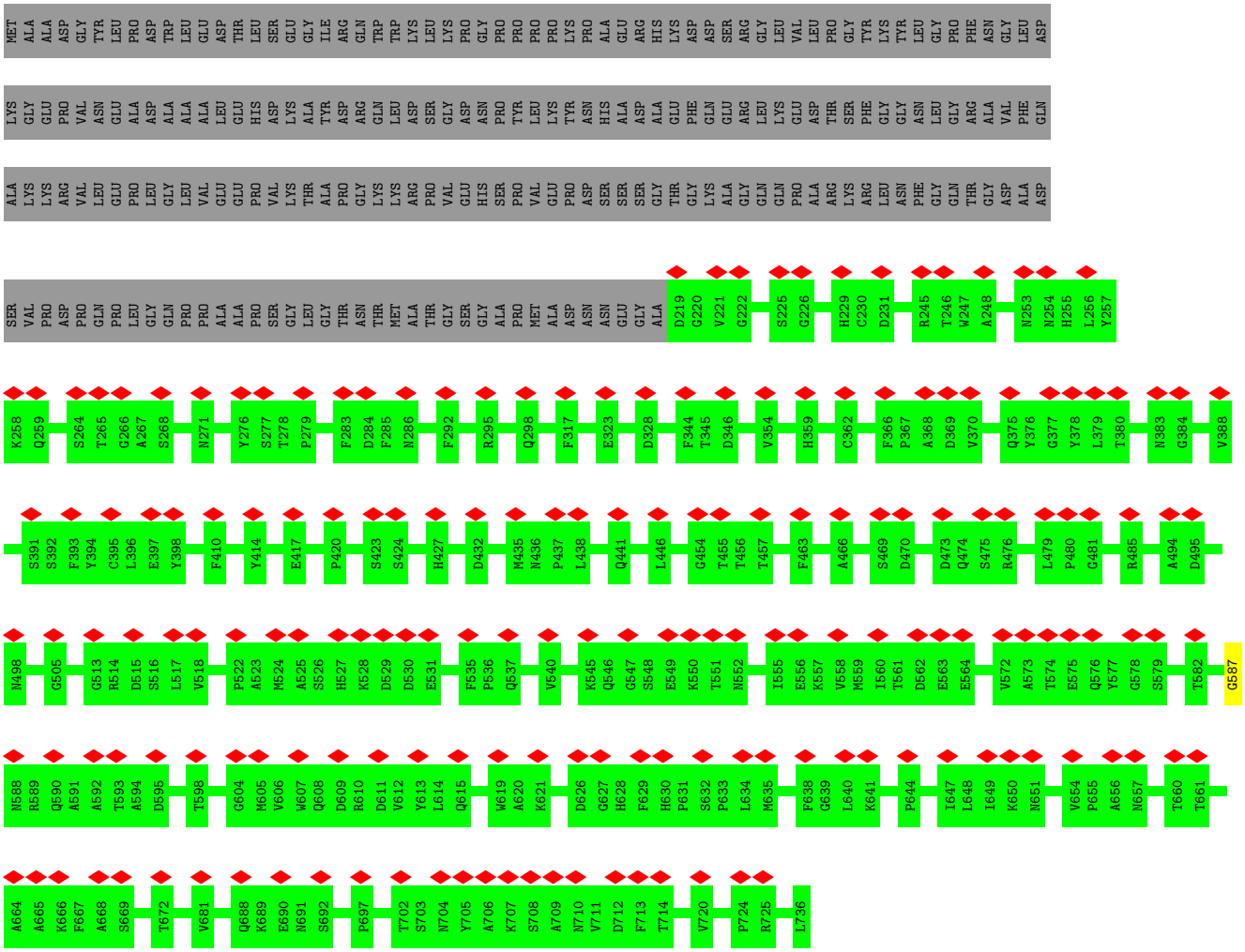
- Molecule 1: Capsid protein VP1

Chain z:



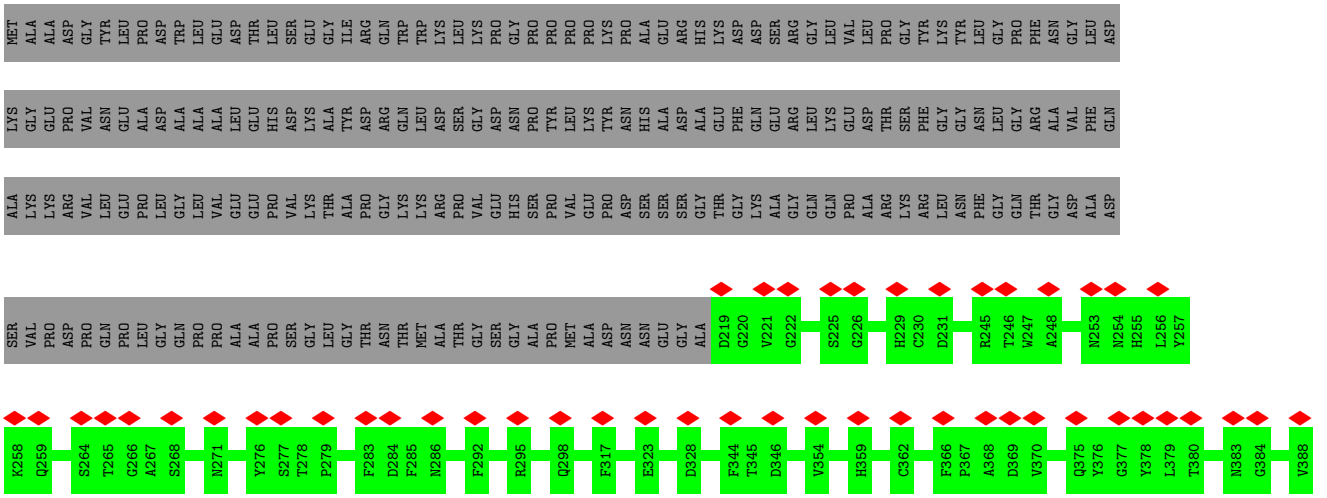
- Molecule 1: Capsid protein VP1

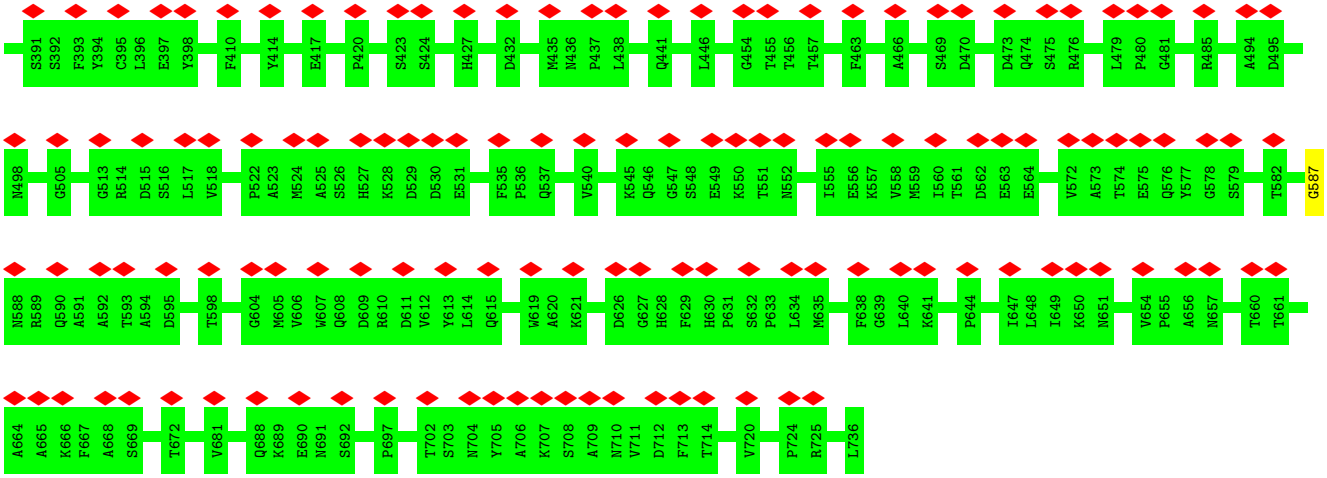
Chain 6:



- Molecule 1: Capsid protein VP1

Chain 7:

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E417
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D432
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L446
G454 T455 T456 T457
F463
A466
S469 D470
D473 Q474 S475 R476
L479 P480 G481
R485
A494 D495
N498
G505
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P522 A523 M524 A525 S526 H527 K528 D529 D530 E531
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V540
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T582
G587
N588 R589 Q590 A591 A592 T593 A594 D595
T598
G604 M605 V606 W607 Q608 D609 R610 D611 V612 Y613 L614 Q615
W619 A620 K621
D626 G627 H628 F629 H630 P631 S632 P633 L634 M635
F638 G639 L640 K641
P644
I647 L648 I649 K650 M651
V654 P655 A656 M657
T660 T661
A664 A665 K666 F667 A668 S669
T672
V681
Q688 K689 E690 N691 S692
P697
T702 S703 N704 Y705 A706 K707 S708 A709 N710 V711 D712 F713 T714
V720
P724 R725
L736

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24618	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 ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	16.777	Depositor
Minimum map value	-8.740	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	379.05, 379.05, 379.05	wwPDB
Map dimensions	399, 399, 399	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.53	0/4265	0.53	0/5814
1	1	0.53	0/4265	0.53	0/5814
1	2	0.53	0/4265	0.53	0/5814
1	3	0.53	0/4265	0.53	0/5814
1	4	0.53	0/4265	0.53	0/5814
1	5	0.53	0/4265	0.53	0/5814
1	6	0.53	0/4265	0.53	0/5814
1	7	0.53	0/4265	0.53	0/5814
1	A	0.53	0/4265	0.53	0/5814
1	B	0.53	0/4265	0.53	0/5814
1	C	0.53	0/4265	0.53	0/5814
1	D	0.53	0/4265	0.53	0/5814
1	E	0.53	0/4265	0.53	0/5814
1	F	0.53	0/4265	0.53	0/5814
1	G	0.53	0/4265	0.53	0/5814
1	H	0.53	0/4265	0.53	0/5814
1	I	0.53	0/4265	0.53	0/5814
1	J	0.53	0/4265	0.53	0/5814
1	K	0.53	0/4265	0.53	0/5814
1	L	0.53	0/4265	0.53	0/5814
1	M	0.53	0/4265	0.53	0/5814
1	N	0.53	0/4265	0.53	0/5814
1	O	0.53	0/4265	0.53	0/5814
1	P	0.53	0/4265	0.53	0/5814
1	Q	0.53	0/4265	0.53	0/5814
1	R	0.53	0/4265	0.53	0/5814
1	S	0.53	0/4265	0.53	0/5814
1	T	0.53	0/4265	0.53	0/5814
1	U	0.53	0/4265	0.53	0/5814
1	V	0.53	0/4265	0.53	0/5814
1	W	0.53	0/4265	0.53	0/5814
1	X	0.53	0/4265	0.53	0/5814
1	Y	0.53	0/4265	0.53	0/5814
1	Z	0.53	0/4265	0.53	0/5814

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.53	0/4265	0.53	0/5814
1	b	0.53	0/4265	0.53	0/5814
1	c	0.53	0/4265	0.53	0/5814
1	d	0.53	0/4265	0.53	0/5814
1	e	0.53	0/4265	0.53	0/5814
1	f	0.53	0/4265	0.53	0/5814
1	g	0.53	0/4265	0.53	0/5814
1	h	0.53	0/4265	0.53	0/5814
1	i	0.53	0/4265	0.53	0/5814
1	j	0.53	0/4265	0.53	0/5814
1	k	0.53	0/4265	0.53	0/5814
1	l	0.53	0/4265	0.53	0/5814
1	m	0.53	0/4265	0.53	0/5814
1	n	0.53	0/4265	0.53	0/5814
1	o	0.53	0/4265	0.53	0/5814
1	p	0.53	0/4265	0.53	0/5814
1	q	0.53	0/4265	0.53	0/5814
1	r	0.53	0/4265	0.53	0/5814
1	s	0.53	0/4265	0.53	0/5814
1	t	0.53	0/4265	0.53	0/5814
1	u	0.53	0/4265	0.53	0/5814
1	v	0.53	0/4265	0.53	0/5814
1	w	0.53	0/4265	0.53	0/5814
1	x	0.53	0/4265	0.53	0/5814
1	y	0.53	0/4265	0.53	0/5814
1	z	0.53	0/4265	0.53	0/5814
All	All	0.53	0/255900	0.53	0/348840

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	587	GLY	Peptide
1	1	587	GLY	Peptide
1	2	587	GLY	Peptide
1	3	587	GLY	Peptide
1	4	587	GLY	Peptide
1	5	587	GLY	Peptide
1	6	587	GLY	Peptide
1	7	587	GLY	Peptide
1	A	587	GLY	Peptide
1	B	587	GLY	Peptide
1	C	587	GLY	Peptide
1	D	587	GLY	Peptide
1	E	587	GLY	Peptide
1	F	587	GLY	Peptide
1	G	587	GLY	Peptide
1	H	587	GLY	Peptide
1	I	587	GLY	Peptide
1	J	587	GLY	Peptide
1	K	587	GLY	Peptide
1	L	587	GLY	Peptide
1	M	587	GLY	Peptide
1	N	587	GLY	Peptide
1	O	587	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	P	587	GLY	Peptide
1	Q	587	GLY	Peptide
1	R	587	GLY	Peptide
1	S	587	GLY	Peptide
1	T	587	GLY	Peptide
1	U	587	GLY	Peptide
1	V	587	GLY	Peptide
1	W	587	GLY	Peptide
1	X	587	GLY	Peptide
1	Y	587	GLY	Peptide
1	Z	587	GLY	Peptide
1	a	587	GLY	Peptide
1	b	587	GLY	Peptide
1	c	587	GLY	Peptide
1	d	587	GLY	Peptide
1	e	587	GLY	Peptide
1	f	587	GLY	Peptide
1	g	587	GLY	Peptide
1	h	587	GLY	Peptide
1	i	587	GLY	Peptide
1	j	587	GLY	Peptide
1	k	587	GLY	Peptide
1	l	587	GLY	Peptide
1	m	587	GLY	Peptide
1	n	587	GLY	Peptide
1	o	587	GLY	Peptide
1	p	587	GLY	Peptide
1	q	587	GLY	Peptide
1	r	587	GLY	Peptide
1	s	587	GLY	Peptide
1	t	587	GLY	Peptide
1	u	587	GLY	Peptide
1	v	587	GLY	Peptide
1	w	587	GLY	Peptide
1	x	587	GLY	Peptide
1	y	587	GLY	Peptide
1	z	587	GLY	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	1	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	2	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	3	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	4	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	5	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	6	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	7	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	A	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	B	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	C	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	D	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	E	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	F	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	G	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	H	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	I	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	J	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	K	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	L	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	M	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	N	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	O	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	P	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	Q	516/736 (70%)	507 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	S	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	T	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	U	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	V	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	W	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	X	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	Y	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	Z	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	a	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	b	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	c	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	d	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	e	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	f	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	g	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	h	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	i	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	j	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	k	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	l	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	m	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	n	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	o	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	p	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	q	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	r	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	s	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	t	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	u	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	v	516/736 (70%)	506 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	516/736 (70%)	507 (98%)	9 (2%)	0	100	100
1	x	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	y	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	z	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
All	All	30960/44160 (70%)	30384 (98%)	576 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	457/628 (73%)	457 (100%)	0	100	100
1	1	457/628 (73%)	457 (100%)	0	100	100
1	2	457/628 (73%)	457 (100%)	0	100	100
1	3	457/628 (73%)	457 (100%)	0	100	100
1	4	457/628 (73%)	457 (100%)	0	100	100
1	5	457/628 (73%)	457 (100%)	0	100	100
1	6	457/628 (73%)	457 (100%)	0	100	100
1	7	457/628 (73%)	457 (100%)	0	100	100
1	A	457/628 (73%)	457 (100%)	0	100	100
1	B	457/628 (73%)	457 (100%)	0	100	100
1	C	457/628 (73%)	457 (100%)	0	100	100
1	D	457/628 (73%)	457 (100%)	0	100	100
1	E	457/628 (73%)	457 (100%)	0	100	100
1	F	457/628 (73%)	457 (100%)	0	100	100
1	G	457/628 (73%)	457 (100%)	0	100	100
1	H	457/628 (73%)	457 (100%)	0	100	100
1	I	457/628 (73%)	457 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	457/628 (73%)	457 (100%)	0	100	100
1	K	457/628 (73%)	457 (100%)	0	100	100
1	L	457/628 (73%)	457 (100%)	0	100	100
1	M	457/628 (73%)	457 (100%)	0	100	100
1	N	457/628 (73%)	457 (100%)	0	100	100
1	O	457/628 (73%)	457 (100%)	0	100	100
1	P	457/628 (73%)	457 (100%)	0	100	100
1	Q	457/628 (73%)	457 (100%)	0	100	100
1	R	457/628 (73%)	457 (100%)	0	100	100
1	S	457/628 (73%)	457 (100%)	0	100	100
1	T	457/628 (73%)	457 (100%)	0	100	100
1	U	457/628 (73%)	457 (100%)	0	100	100
1	V	457/628 (73%)	457 (100%)	0	100	100
1	W	457/628 (73%)	457 (100%)	0	100	100
1	X	457/628 (73%)	457 (100%)	0	100	100
1	Y	457/628 (73%)	457 (100%)	0	100	100
1	Z	457/628 (73%)	457 (100%)	0	100	100
1	a	457/628 (73%)	457 (100%)	0	100	100
1	b	457/628 (73%)	457 (100%)	0	100	100
1	c	457/628 (73%)	457 (100%)	0	100	100
1	d	457/628 (73%)	457 (100%)	0	100	100
1	e	457/628 (73%)	457 (100%)	0	100	100
1	f	457/628 (73%)	457 (100%)	0	100	100
1	g	457/628 (73%)	457 (100%)	0	100	100
1	h	457/628 (73%)	457 (100%)	0	100	100
1	i	457/628 (73%)	457 (100%)	0	100	100
1	j	457/628 (73%)	457 (100%)	0	100	100
1	k	457/628 (73%)	457 (100%)	0	100	100
1	l	457/628 (73%)	457 (100%)	0	100	100
1	m	457/628 (73%)	457 (100%)	0	100	100
1	n	457/628 (73%)	457 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	457/628 (73%)	457 (100%)	0	100	100
1	p	457/628 (73%)	457 (100%)	0	100	100
1	q	457/628 (73%)	457 (100%)	0	100	100
1	r	457/628 (73%)	457 (100%)	0	100	100
1	s	457/628 (73%)	457 (100%)	0	100	100
1	t	457/628 (73%)	457 (100%)	0	100	100
1	u	457/628 (73%)	457 (100%)	0	100	100
1	v	457/628 (73%)	457 (100%)	0	100	100
1	w	457/628 (73%)	457 (100%)	0	100	100
1	x	457/628 (73%)	457 (100%)	0	100	100
1	y	457/628 (73%)	457 (100%)	0	100	100
1	z	457/628 (73%)	457 (100%)	0	100	100
All	All	27420/37680 (73%)	27420 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (855) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	298	GLN
1	A	335	ASN
1	A	342	GLN
1	A	383	ASN
1	A	408	ASN
1	A	458	GLN
1	A	462	GLN
1	A	519	ASN
1	A	552	ASN
1	A	599	GLN
1	A	608	GLN
1	A	628	HIS
1	A	646	GLN
1	B	289	HIS
1	B	298	GLN
1	B	335	ASN
1	B	342	GLN
1	B	383	ASN

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Mol	Chain	Res	Type
1	B	408	ASN
1	B	458	GLN
1	B	462	GLN
1	B	519	ASN
1	B	552	ASN
1	B	599	GLN
1	B	608	GLN
1	B	628	HIS
1	B	646	GLN
1	C	289	HIS
1	C	298	GLN
1	C	335	ASN
1	C	342	GLN
1	C	383	ASN
1	C	408	ASN
1	C	458	GLN
1	C	462	GLN
1	C	519	ASN
1	C	552	ASN
1	C	585	GLN
1	C	599	GLN
1	C	608	GLN
1	C	628	HIS
1	C	646	GLN
1	D	289	HIS
1	D	298	GLN
1	D	335	ASN
1	D	342	GLN
1	D	383	ASN
1	D	408	ASN
1	D	458	GLN
1	D	462	GLN
1	D	519	ASN
1	D	552	ASN
1	D	585	GLN
1	D	599	GLN
1	D	608	GLN
1	D	628	HIS
1	D	646	GLN
1	E	289	HIS
1	E	298	GLN
1	E	335	ASN

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Mol	Chain	Res	Type
1	E	342	GLN
1	E	383	ASN
1	E	408	ASN
1	E	458	GLN
1	E	462	GLN
1	E	519	ASN
1	E	552	ASN
1	E	585	GLN
1	E	599	GLN
1	E	608	GLN
1	E	628	HIS
1	E	646	GLN
1	F	289	HIS
1	F	298	GLN
1	F	335	ASN
1	F	342	GLN
1	F	383	ASN
1	F	408	ASN
1	F	458	GLN
1	F	462	GLN
1	F	519	ASN
1	F	552	ASN
1	F	599	GLN
1	F	608	GLN
1	F	628	HIS
1	F	646	GLN
1	G	289	HIS
1	G	298	GLN
1	G	335	ASN
1	G	342	GLN
1	G	383	ASN
1	G	408	ASN
1	G	458	GLN
1	G	462	GLN
1	G	519	ASN
1	G	552	ASN
1	G	599	GLN
1	G	608	GLN
1	G	628	HIS
1	G	646	GLN
1	H	289	HIS
1	H	298	GLN

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Mol	Chain	Res	Type
1	H	335	ASN
1	H	383	ASN
1	H	408	ASN
1	H	458	GLN
1	H	462	GLN
1	H	519	ASN
1	H	552	ASN
1	H	599	GLN
1	H	608	GLN
1	H	628	HIS
1	H	646	GLN
1	I	289	HIS
1	I	298	GLN
1	I	335	ASN
1	I	342	GLN
1	I	383	ASN
1	I	408	ASN
1	I	458	GLN
1	I	462	GLN
1	I	519	ASN
1	I	552	ASN
1	I	599	GLN
1	I	608	GLN
1	I	628	HIS
1	I	646	GLN
1	J	289	HIS
1	J	298	GLN
1	J	335	ASN
1	J	342	GLN
1	J	383	ASN
1	J	408	ASN
1	J	458	GLN
1	J	462	GLN
1	J	519	ASN
1	J	552	ASN
1	J	599	GLN
1	J	608	GLN
1	J	628	HIS
1	J	646	GLN
1	K	289	HIS
1	K	298	GLN
1	K	335	ASN

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Mol	Chain	Res	Type
1	K	342	GLN
1	K	383	ASN
1	K	408	ASN
1	K	458	GLN
1	K	462	GLN
1	K	519	ASN
1	K	552	ASN
1	K	599	GLN
1	K	608	GLN
1	K	628	HIS
1	K	646	GLN
1	L	289	HIS
1	L	298	GLN
1	L	335	ASN
1	L	342	GLN
1	L	383	ASN
1	L	408	ASN
1	L	458	GLN
1	L	462	GLN
1	L	519	ASN
1	L	552	ASN
1	L	599	GLN
1	L	608	GLN
1	L	628	HIS
1	L	646	GLN
1	M	289	HIS
1	M	298	GLN
1	M	335	ASN
1	M	342	GLN
1	M	383	ASN
1	M	408	ASN
1	M	458	GLN
1	M	462	GLN
1	M	519	ASN
1	M	552	ASN
1	M	599	GLN
1	M	608	GLN
1	M	628	HIS
1	M	646	GLN
1	N	289	HIS
1	N	298	GLN
1	N	335	ASN

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Mol	Chain	Res	Type
1	N	342	GLN
1	N	383	ASN
1	N	408	ASN
1	N	458	GLN
1	N	462	GLN
1	N	519	ASN
1	N	552	ASN
1	N	599	GLN
1	N	608	GLN
1	N	628	HIS
1	N	646	GLN
1	O	289	HIS
1	O	298	GLN
1	O	335	ASN
1	O	342	GLN
1	O	383	ASN
1	O	408	ASN
1	O	458	GLN
1	O	462	GLN
1	O	519	ASN
1	O	552	ASN
1	O	599	GLN
1	O	608	GLN
1	O	628	HIS
1	O	646	GLN
1	P	289	HIS
1	P	298	GLN
1	P	335	ASN
1	P	342	GLN
1	P	383	ASN
1	P	408	ASN
1	P	458	GLN
1	P	462	GLN
1	P	519	ASN
1	P	552	ASN
1	P	585	GLN
1	P	599	GLN
1	P	608	GLN
1	P	628	HIS
1	P	646	GLN
1	Q	289	HIS
1	Q	298	GLN

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Mol	Chain	Res	Type
1	Q	335	ASN
1	Q	342	GLN
1	Q	383	ASN
1	Q	408	ASN
1	Q	458	GLN
1	Q	462	GLN
1	Q	519	ASN
1	Q	552	ASN
1	Q	599	GLN
1	Q	608	GLN
1	Q	628	HIS
1	Q	646	GLN
1	R	289	HIS
1	R	298	GLN
1	R	335	ASN
1	R	342	GLN
1	R	383	ASN
1	R	408	ASN
1	R	458	GLN
1	R	462	GLN
1	R	519	ASN
1	R	552	ASN
1	R	599	GLN
1	R	608	GLN
1	R	628	HIS
1	R	646	GLN
1	S	289	HIS
1	S	298	GLN
1	S	335	ASN
1	S	342	GLN
1	S	383	ASN
1	S	408	ASN
1	S	458	GLN
1	S	462	GLN
1	S	519	ASN
1	S	552	ASN
1	S	585	GLN
1	S	599	GLN
1	S	608	GLN
1	S	628	HIS
1	S	646	GLN
1	T	289	HIS

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Mol	Chain	Res	Type
1	T	298	GLN
1	T	335	ASN
1	T	342	GLN
1	T	383	ASN
1	T	408	ASN
1	T	458	GLN
1	T	462	GLN
1	T	519	ASN
1	T	552	ASN
1	T	599	GLN
1	T	608	GLN
1	T	628	HIS
1	T	646	GLN
1	U	289	HIS
1	U	298	GLN
1	U	335	ASN
1	U	342	GLN
1	U	383	ASN
1	U	408	ASN
1	U	458	GLN
1	U	462	GLN
1	U	519	ASN
1	U	552	ASN
1	U	599	GLN
1	U	608	GLN
1	U	628	HIS
1	U	646	GLN
1	V	289	HIS
1	V	298	GLN
1	V	335	ASN
1	V	342	GLN
1	V	383	ASN
1	V	408	ASN
1	V	458	GLN
1	V	462	GLN
1	V	519	ASN
1	V	552	ASN
1	V	599	GLN
1	V	608	GLN
1	V	628	HIS
1	V	646	GLN
1	W	289	HIS

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Mol	Chain	Res	Type
1	W	298	GLN
1	W	335	ASN
1	W	342	GLN
1	W	383	ASN
1	W	408	ASN
1	W	458	GLN
1	W	462	GLN
1	W	519	ASN
1	W	552	ASN
1	W	599	GLN
1	W	608	GLN
1	W	628	HIS
1	W	646	GLN
1	X	289	HIS
1	X	298	GLN
1	X	335	ASN
1	X	342	GLN
1	X	383	ASN
1	X	408	ASN
1	X	458	GLN
1	X	462	GLN
1	X	519	ASN
1	X	552	ASN
1	X	599	GLN
1	X	608	GLN
1	X	628	HIS
1	X	646	GLN
1	Y	289	HIS
1	Y	298	GLN
1	Y	335	ASN
1	Y	342	GLN
1	Y	383	ASN
1	Y	408	ASN
1	Y	458	GLN
1	Y	462	GLN
1	Y	519	ASN
1	Y	552	ASN
1	Y	599	GLN
1	Y	608	GLN
1	Y	628	HIS
1	Y	646	GLN
1	Z	289	HIS

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Mol	Chain	Res	Type
1	Z	298	GLN
1	Z	335	ASN
1	Z	342	GLN
1	Z	383	ASN
1	Z	408	ASN
1	Z	458	GLN
1	Z	462	GLN
1	Z	519	ASN
1	Z	552	ASN
1	Z	599	GLN
1	Z	608	GLN
1	Z	628	HIS
1	Z	646	GLN
1	0	289	HIS
1	0	298	GLN
1	0	335	ASN
1	0	342	GLN
1	0	383	ASN
1	0	408	ASN
1	0	458	GLN
1	0	462	GLN
1	0	519	ASN
1	0	552	ASN
1	0	599	GLN
1	0	608	GLN
1	0	628	HIS
1	0	646	GLN
1	1	289	HIS
1	1	298	GLN
1	1	335	ASN
1	1	342	GLN
1	1	383	ASN
1	1	408	ASN
1	1	458	GLN
1	1	462	GLN
1	1	519	ASN
1	1	552	ASN
1	1	599	GLN
1	1	608	GLN
1	1	628	HIS
1	1	646	GLN
1	2	289	HIS

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Mol	Chain	Res	Type
1	2	298	GLN
1	2	335	ASN
1	2	342	GLN
1	2	383	ASN
1	2	408	ASN
1	2	458	GLN
1	2	462	GLN
1	2	519	ASN
1	2	552	ASN
1	2	585	GLN
1	2	599	GLN
1	2	608	GLN
1	2	628	HIS
1	2	646	GLN
1	3	289	HIS
1	3	298	GLN
1	3	335	ASN
1	3	342	GLN
1	3	383	ASN
1	3	408	ASN
1	3	458	GLN
1	3	462	GLN
1	3	519	ASN
1	3	552	ASN
1	3	599	GLN
1	3	608	GLN
1	3	628	HIS
1	3	646	GLN
1	4	289	HIS
1	4	298	GLN
1	4	335	ASN
1	4	342	GLN
1	4	383	ASN
1	4	408	ASN
1	4	458	GLN
1	4	462	GLN
1	4	519	ASN
1	4	552	ASN
1	4	599	GLN
1	4	608	GLN
1	4	628	HIS
1	4	646	GLN

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Mol	Chain	Res	Type
1	5	289	HIS
1	5	298	GLN
1	5	335	ASN
1	5	342	GLN
1	5	383	ASN
1	5	408	ASN
1	5	458	GLN
1	5	462	GLN
1	5	519	ASN
1	5	552	ASN
1	5	599	GLN
1	5	608	GLN
1	5	628	HIS
1	5	646	GLN
1	a	289	HIS
1	a	298	GLN
1	a	335	ASN
1	a	342	GLN
1	a	383	ASN
1	a	408	ASN
1	a	458	GLN
1	a	462	GLN
1	a	519	ASN
1	a	552	ASN
1	a	599	GLN
1	a	608	GLN
1	a	628	HIS
1	a	646	GLN
1	b	289	HIS
1	b	298	GLN
1	b	335	ASN
1	b	342	GLN
1	b	383	ASN
1	b	408	ASN
1	b	458	GLN
1	b	462	GLN
1	b	519	ASN
1	b	552	ASN
1	b	585	GLN
1	b	599	GLN
1	b	608	GLN
1	b	628	HIS

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Mol	Chain	Res	Type
1	b	646	GLN
1	c	289	HIS
1	c	298	GLN
1	c	335	ASN
1	c	342	GLN
1	c	383	ASN
1	c	408	ASN
1	c	458	GLN
1	c	462	GLN
1	c	519	ASN
1	c	552	ASN
1	c	599	GLN
1	c	608	GLN
1	c	628	HIS
1	c	646	GLN
1	d	289	HIS
1	d	298	GLN
1	d	335	ASN
1	d	342	GLN
1	d	383	ASN
1	d	408	ASN
1	d	458	GLN
1	d	462	GLN
1	d	519	ASN
1	d	552	ASN
1	d	599	GLN
1	d	608	GLN
1	d	628	HIS
1	d	646	GLN
1	e	289	HIS
1	e	298	GLN
1	e	335	ASN
1	e	342	GLN
1	e	383	ASN
1	e	408	ASN
1	e	458	GLN
1	e	462	GLN
1	e	519	ASN
1	e	552	ASN
1	e	585	GLN
1	e	599	GLN
1	e	608	GLN

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Mol	Chain	Res	Type
1	e	628	HIS
1	e	646	GLN
1	f	289	HIS
1	f	298	GLN
1	f	335	ASN
1	f	342	GLN
1	f	383	ASN
1	f	408	ASN
1	f	458	GLN
1	f	462	GLN
1	f	519	ASN
1	f	552	ASN
1	f	599	GLN
1	f	608	GLN
1	f	628	HIS
1	f	646	GLN
1	g	289	HIS
1	g	298	GLN
1	g	335	ASN
1	g	342	GLN
1	g	383	ASN
1	g	408	ASN
1	g	458	GLN
1	g	462	GLN
1	g	519	ASN
1	g	552	ASN
1	g	599	GLN
1	g	608	GLN
1	g	628	HIS
1	g	646	GLN
1	h	289	HIS
1	h	298	GLN
1	h	335	ASN
1	h	342	GLN
1	h	383	ASN
1	h	408	ASN
1	h	458	GLN
1	h	462	GLN
1	h	519	ASN
1	h	552	ASN
1	h	599	GLN
1	h	608	GLN

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Mol	Chain	Res	Type
1	h	628	HIS
1	h	646	GLN
1	i	289	HIS
1	i	298	GLN
1	i	335	ASN
1	i	342	GLN
1	i	383	ASN
1	i	408	ASN
1	i	458	GLN
1	i	462	GLN
1	i	519	ASN
1	i	552	ASN
1	i	585	GLN
1	i	599	GLN
1	i	608	GLN
1	i	628	HIS
1	i	646	GLN
1	j	289	HIS
1	j	298	GLN
1	j	335	ASN
1	j	342	GLN
1	j	383	ASN
1	j	408	ASN
1	j	458	GLN
1	j	462	GLN
1	j	519	ASN
1	j	552	ASN
1	j	599	GLN
1	j	608	GLN
1	j	628	HIS
1	j	646	GLN
1	k	289	HIS
1	k	298	GLN
1	k	335	ASN
1	k	342	GLN
1	k	383	ASN
1	k	408	ASN
1	k	458	GLN
1	k	462	GLN
1	k	519	ASN
1	k	552	ASN
1	k	585	GLN

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Mol	Chain	Res	Type
1	k	599	GLN
1	k	608	GLN
1	k	628	HIS
1	k	646	GLN
1	l	289	HIS
1	l	298	GLN
1	l	335	ASN
1	l	342	GLN
1	l	383	ASN
1	l	408	ASN
1	l	458	GLN
1	l	462	GLN
1	l	519	ASN
1	l	552	ASN
1	l	599	GLN
1	l	608	GLN
1	l	628	HIS
1	l	646	GLN
1	m	289	HIS
1	m	298	GLN
1	m	335	ASN
1	m	342	GLN
1	m	383	ASN
1	m	408	ASN
1	m	458	GLN
1	m	462	GLN
1	m	519	ASN
1	m	552	ASN
1	m	599	GLN
1	m	608	GLN
1	m	628	HIS
1	m	646	GLN
1	n	289	HIS
1	n	298	GLN
1	n	335	ASN
1	n	342	GLN
1	n	383	ASN
1	n	408	ASN
1	n	458	GLN
1	n	462	GLN
1	n	519	ASN
1	n	552	ASN

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Mol	Chain	Res	Type
1	n	599	GLN
1	n	608	GLN
1	n	628	HIS
1	n	646	GLN
1	o	289	HIS
1	o	298	GLN
1	o	335	ASN
1	o	342	GLN
1	o	383	ASN
1	o	408	ASN
1	o	458	GLN
1	o	462	GLN
1	o	519	ASN
1	o	552	ASN
1	o	599	GLN
1	o	608	GLN
1	o	628	HIS
1	o	646	GLN
1	p	289	HIS
1	p	298	GLN
1	p	335	ASN
1	p	342	GLN
1	p	383	ASN
1	p	408	ASN
1	p	458	GLN
1	p	462	GLN
1	p	519	ASN
1	p	552	ASN
1	p	599	GLN
1	p	608	GLN
1	p	628	HIS
1	p	646	GLN
1	q	289	HIS
1	q	298	GLN
1	q	335	ASN
1	q	342	GLN
1	q	383	ASN
1	q	408	ASN
1	q	458	GLN
1	q	462	GLN
1	q	519	ASN
1	q	552	ASN

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Mol	Chain	Res	Type
1	q	599	GLN
1	q	608	GLN
1	q	628	HIS
1	q	646	GLN
1	r	289	HIS
1	r	298	GLN
1	r	335	ASN
1	r	342	GLN
1	r	383	ASN
1	r	408	ASN
1	r	458	GLN
1	r	462	GLN
1	r	519	ASN
1	r	552	ASN
1	r	585	GLN
1	r	599	GLN
1	r	608	GLN
1	r	628	HIS
1	r	646	GLN
1	s	289	HIS
1	s	298	GLN
1	s	335	ASN
1	s	342	GLN
1	s	383	ASN
1	s	408	ASN
1	s	458	GLN
1	s	462	GLN
1	s	519	ASN
1	s	552	ASN
1	s	599	GLN
1	s	608	GLN
1	s	628	HIS
1	s	646	GLN
1	t	289	HIS
1	t	298	GLN
1	t	335	ASN
1	t	342	GLN
1	t	383	ASN
1	t	408	ASN
1	t	458	GLN
1	t	462	GLN
1	t	519	ASN

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Mol	Chain	Res	Type
1	t	552	ASN
1	t	585	GLN
1	t	599	GLN
1	t	608	GLN
1	t	628	HIS
1	t	646	GLN
1	u	289	HIS
1	u	298	GLN
1	u	335	ASN
1	u	342	GLN
1	u	383	ASN
1	u	408	ASN
1	u	458	GLN
1	u	462	GLN
1	u	519	ASN
1	u	552	ASN
1	u	585	GLN
1	u	599	GLN
1	u	608	GLN
1	u	628	HIS
1	u	646	GLN
1	v	289	HIS
1	v	298	GLN
1	v	335	ASN
1	v	342	GLN
1	v	383	ASN
1	v	408	ASN
1	v	458	GLN
1	v	519	ASN
1	v	552	ASN
1	v	585	GLN
1	v	599	GLN
1	v	608	GLN
1	v	628	HIS
1	v	646	GLN
1	w	289	HIS
1	w	298	GLN
1	w	335	ASN
1	w	342	GLN
1	w	383	ASN
1	w	408	ASN
1	w	458	GLN

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Mol	Chain	Res	Type
1	w	462	GLN
1	w	519	ASN
1	w	552	ASN
1	w	599	GLN
1	w	608	GLN
1	w	628	HIS
1	w	646	GLN
1	x	289	HIS
1	x	298	GLN
1	x	335	ASN
1	x	342	GLN
1	x	383	ASN
1	x	408	ASN
1	x	458	GLN
1	x	462	GLN
1	x	519	ASN
1	x	552	ASN
1	x	585	GLN
1	x	599	GLN
1	x	608	GLN
1	x	628	HIS
1	x	646	GLN
1	y	289	HIS
1	y	298	GLN
1	y	335	ASN
1	y	342	GLN
1	y	383	ASN
1	y	408	ASN
1	y	458	GLN
1	y	462	GLN
1	y	519	ASN
1	y	552	ASN
1	y	599	GLN
1	y	608	GLN
1	y	628	HIS
1	y	646	GLN
1	z	289	HIS
1	z	298	GLN
1	z	335	ASN
1	z	342	GLN
1	z	383	ASN
1	z	408	ASN

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Mol	Chain	Res	Type
1	z	458	GLN
1	z	462	GLN
1	z	519	ASN
1	z	552	ASN
1	z	585	GLN
1	z	599	GLN
1	z	608	GLN
1	z	628	HIS
1	z	646	GLN
1	6	289	HIS
1	6	298	GLN
1	6	335	ASN
1	6	342	GLN
1	6	383	ASN
1	6	408	ASN
1	6	458	GLN
1	6	462	GLN
1	6	519	ASN
1	6	552	ASN
1	6	599	GLN
1	6	608	GLN
1	6	628	HIS
1	6	646	GLN
1	7	289	HIS
1	7	298	GLN
1	7	335	ASN
1	7	342	GLN
1	7	383	ASN
1	7	408	ASN
1	7	458	GLN
1	7	462	GLN
1	7	519	ASN
1	7	552	ASN
1	7	585	GLN
1	7	599	GLN
1	7	608	GLN
1	7	628	HIS
1	7	646	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

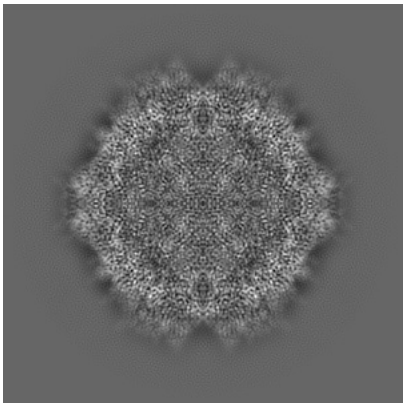
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7452. These allow visual inspection of the internal detail of the map and identification of artifacts.

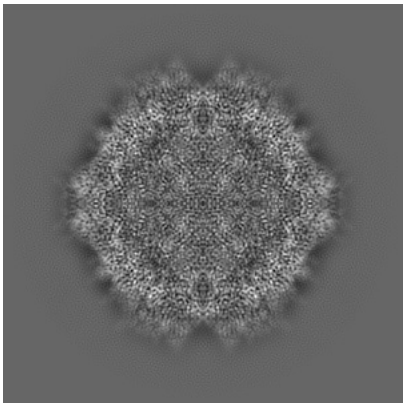
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

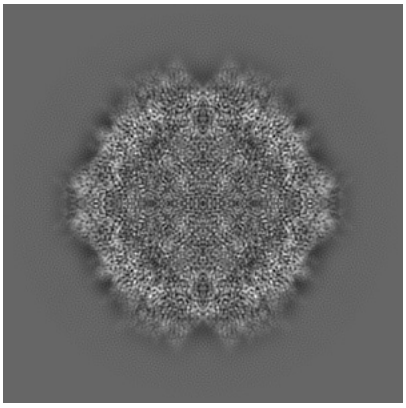
6.1.1 Primary map



X



Y

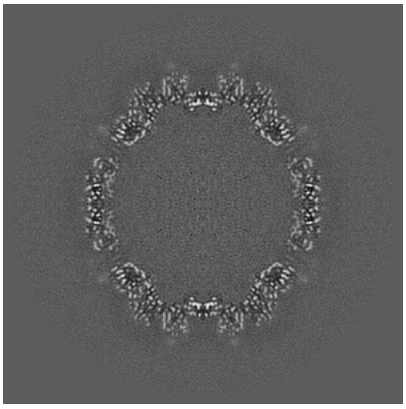


Z

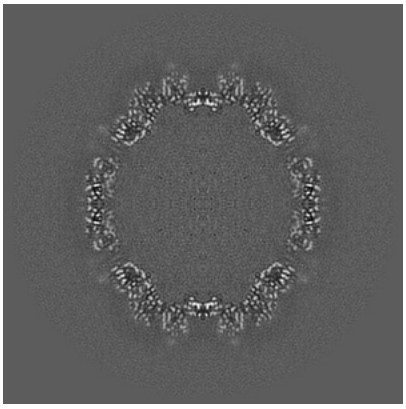
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

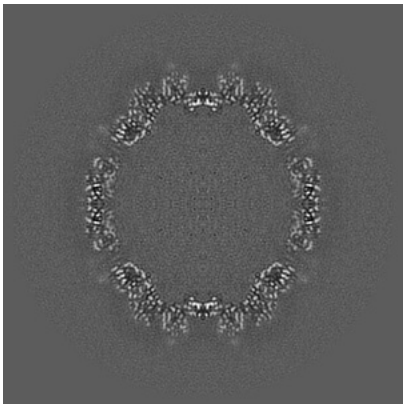
6.2.1 Primary map



X Index: 199



Y Index: 199

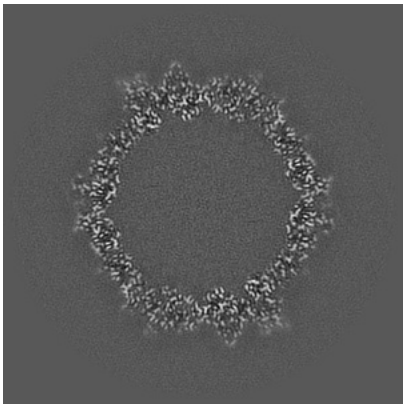


Z Index: 199

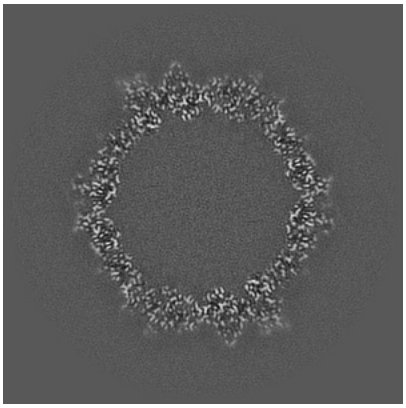
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

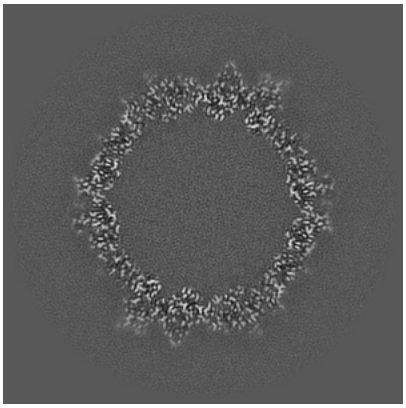
6.3.1 Primary map



X Index: 214



Y Index: 214

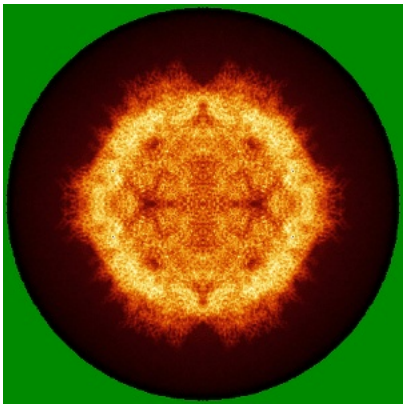


Z Index: 184

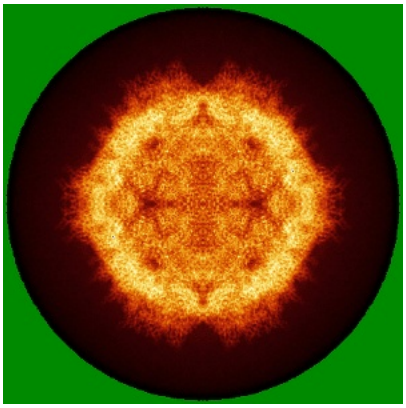
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

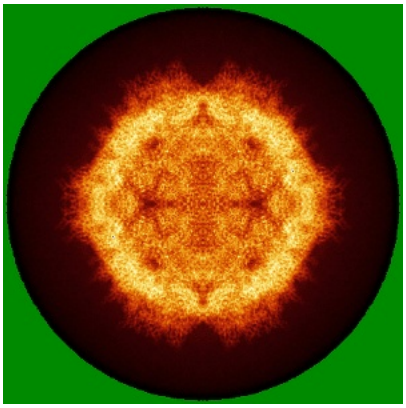
6.4.1 Primary map



X



Y

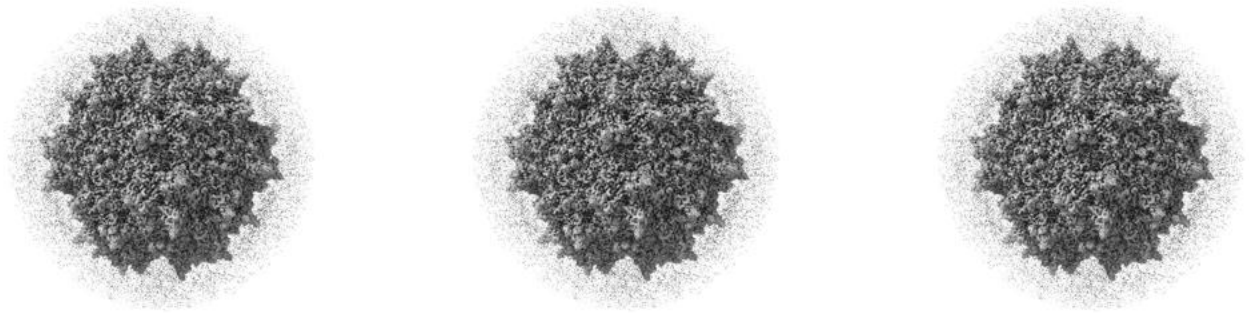


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

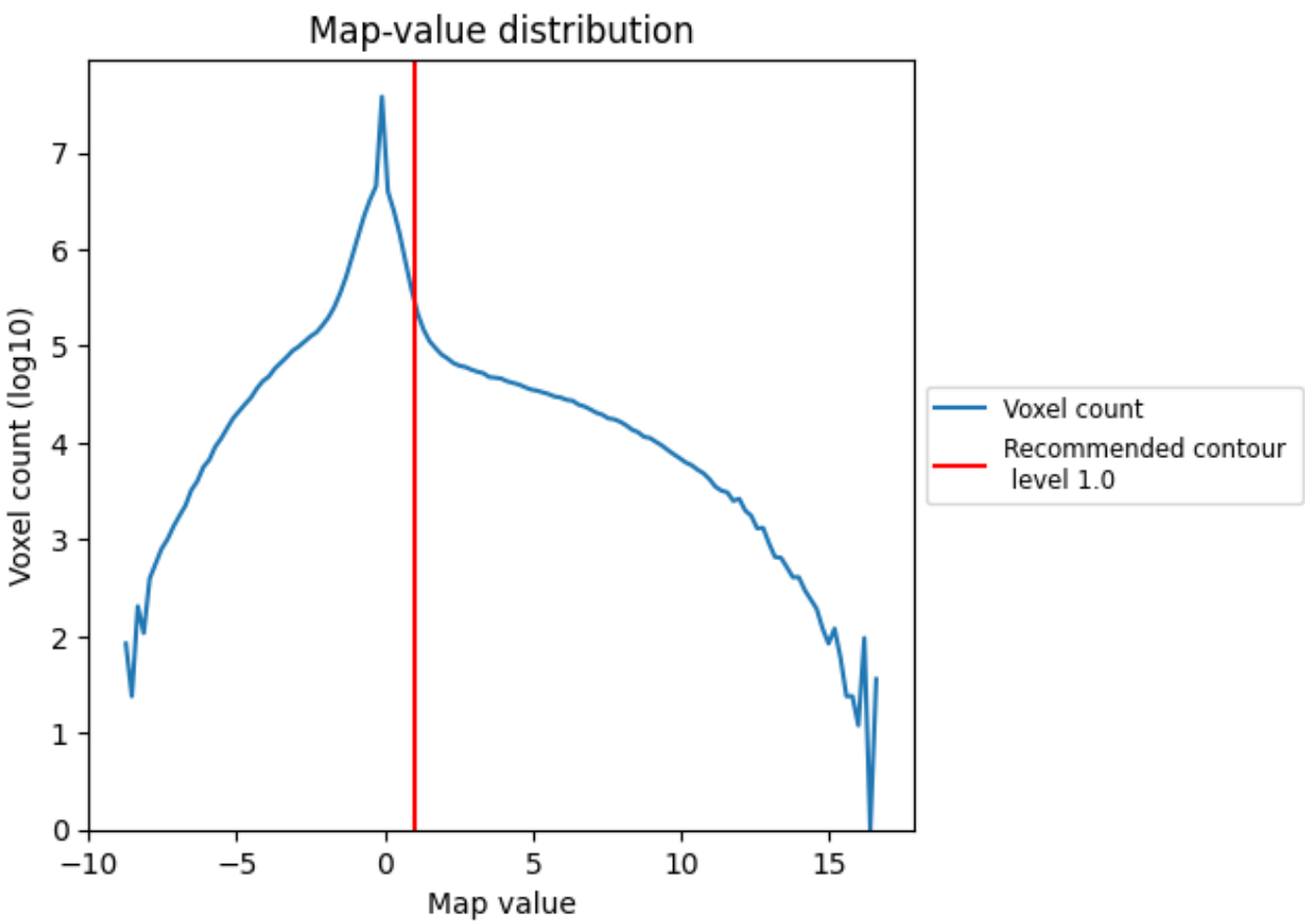
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

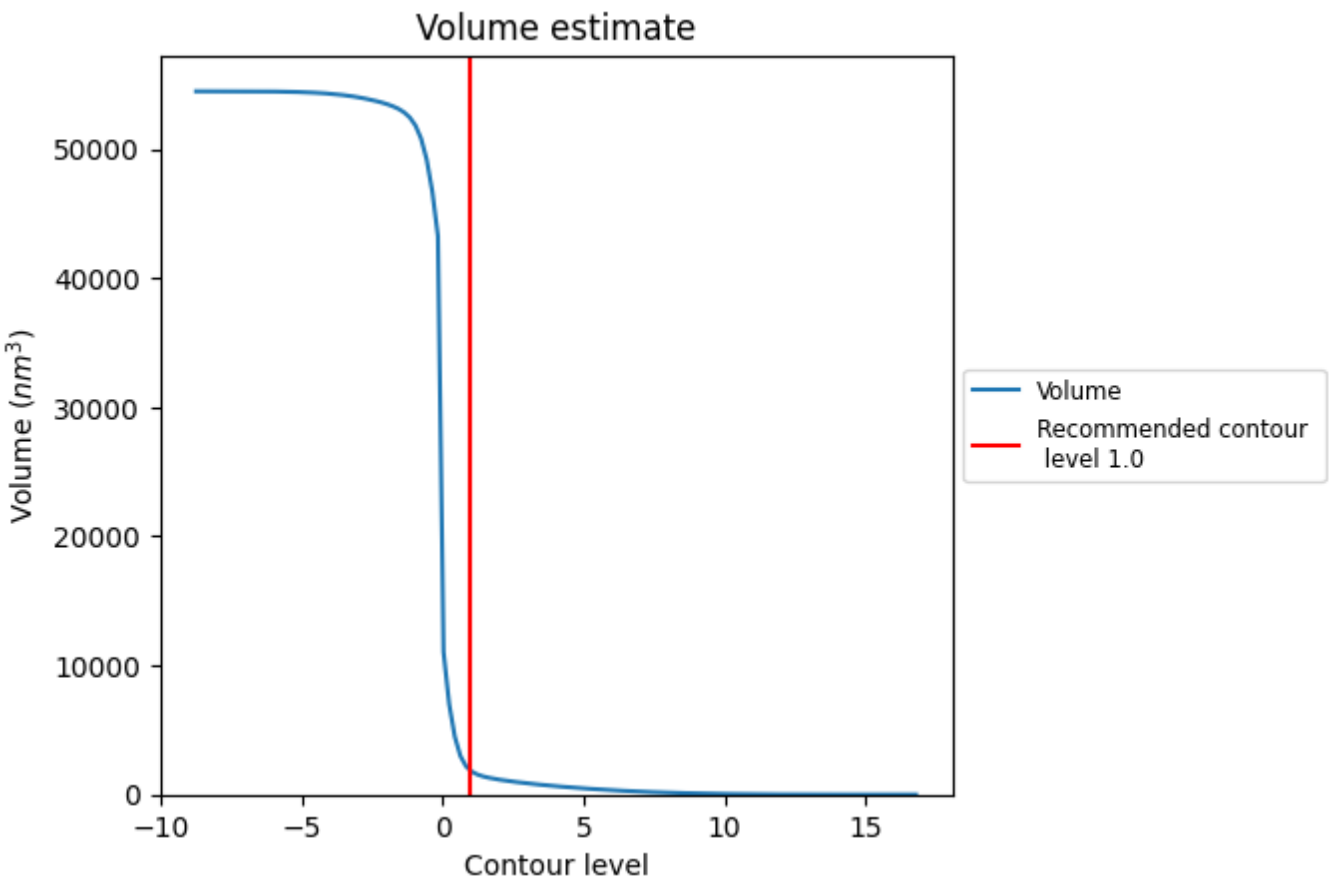
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

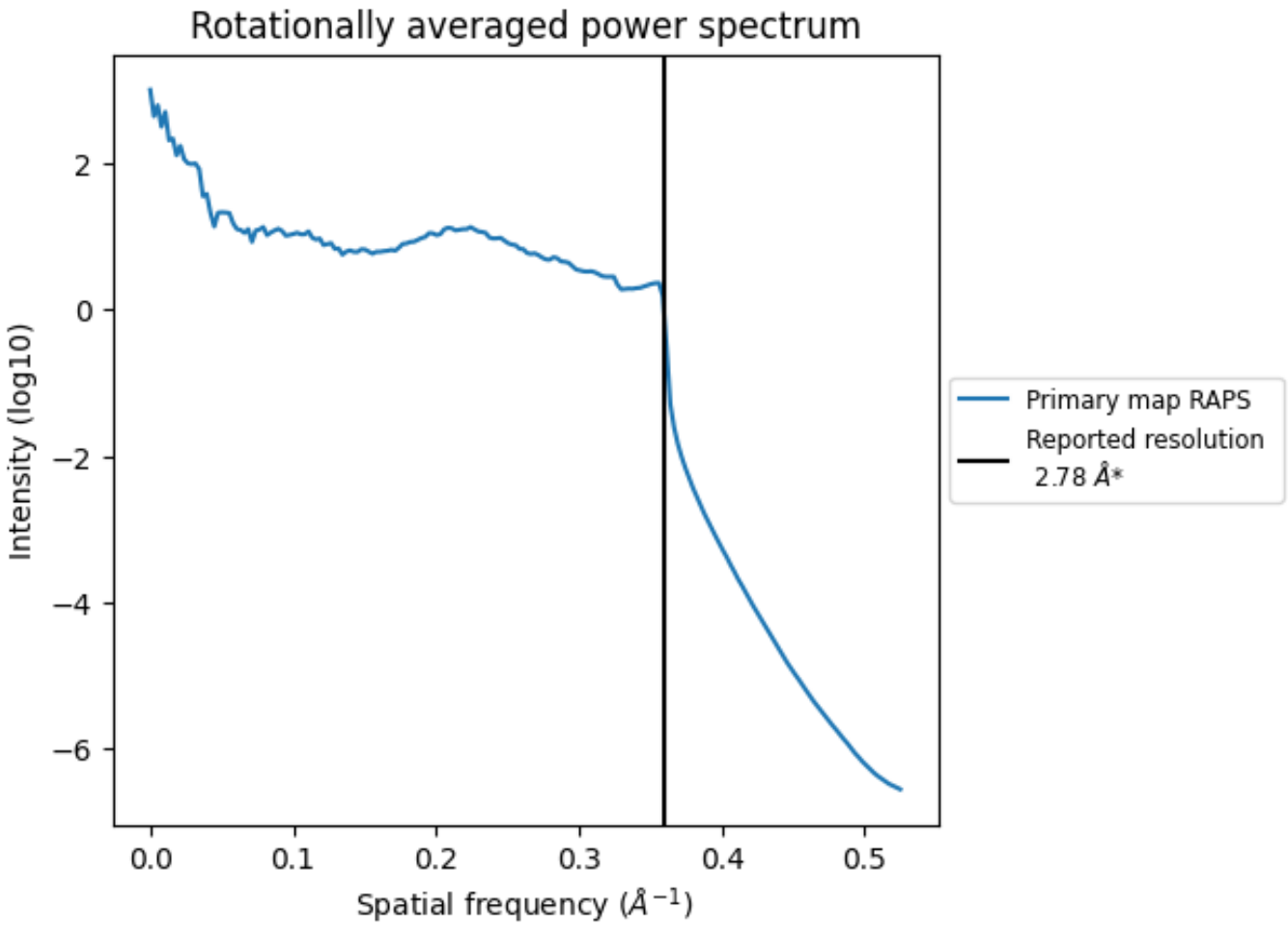
7.2 Volume estimate (i)



The volume at the recommended contour level is 1837 nm^3; this corresponds to an approximate mass of 1660 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

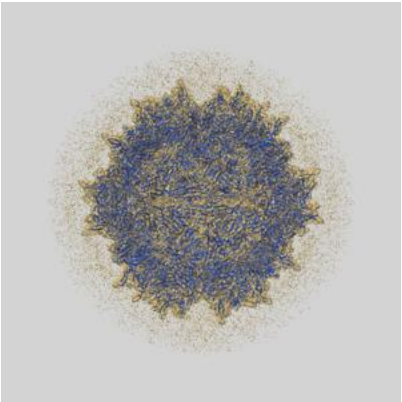
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

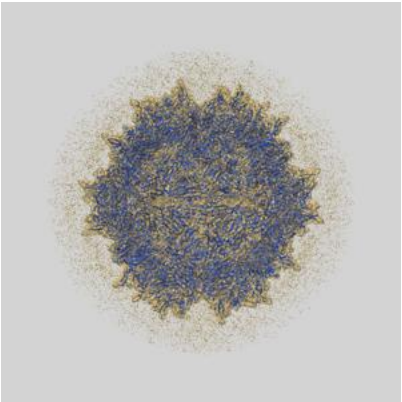
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7452 and PDB model 6CBE. Per-residue inclusion information can be found in section 3 on page 17.

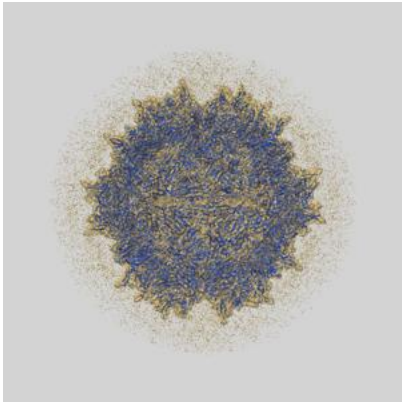
9.1 Map-model overlay (i)



X



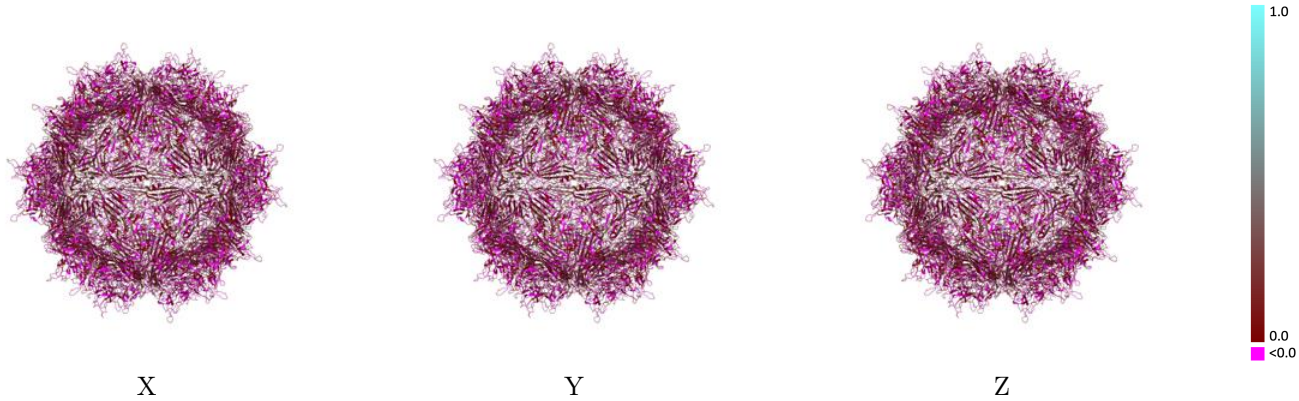
Y



Z

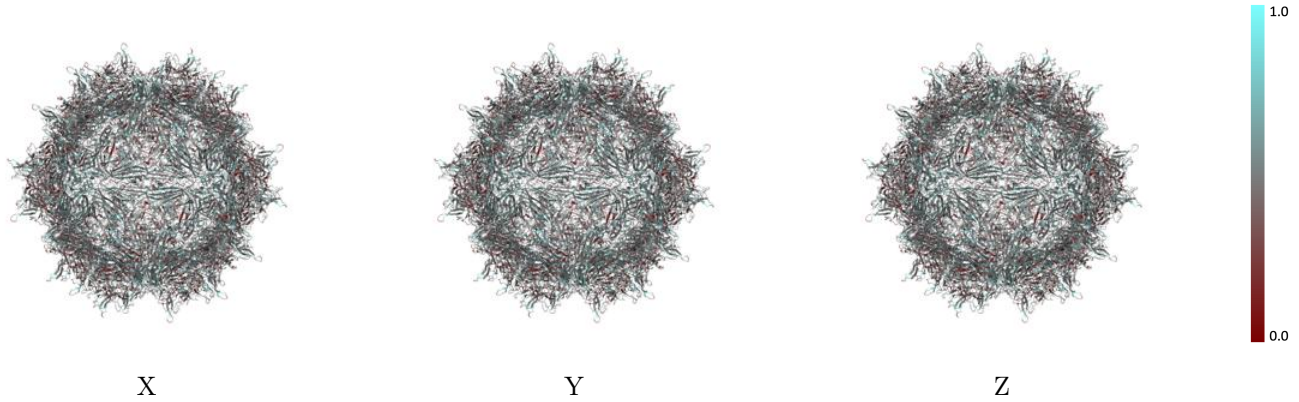
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



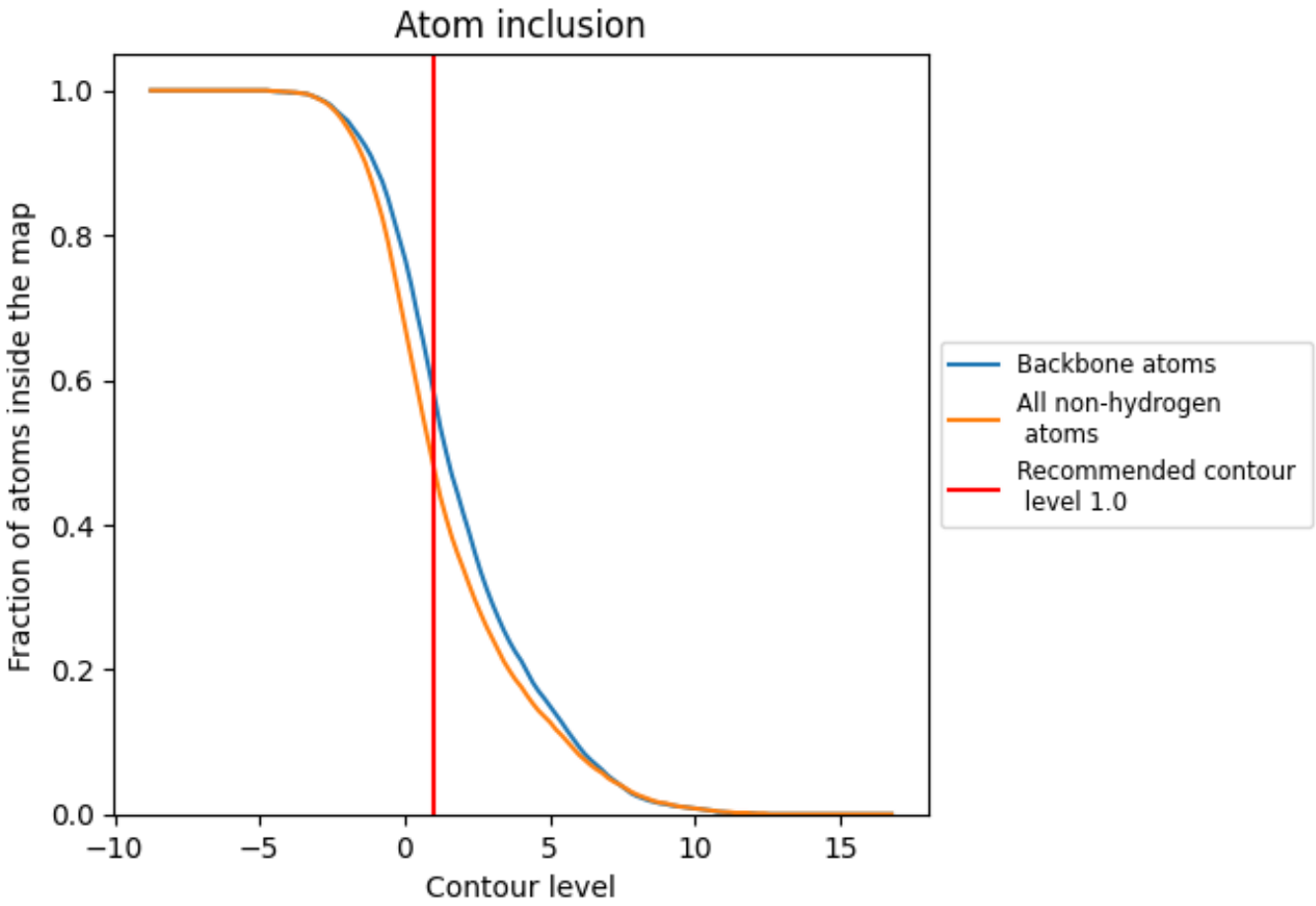
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4800	0.0960
0	0.4810	0.0980
1	0.4810	0.0960
2	0.4840	0.1060
3	0.4820	0.1020
4	0.4770	0.0940
5	0.4830	0.0820
6	0.4780	0.0990
7	0.4780	0.0970
A	0.4810	0.0930
B	0.4770	0.0910
C	0.4830	0.0880
D	0.4780	0.0870
E	0.4830	0.0890
F	0.4840	0.0970
G	0.4780	0.1000
H	0.4780	0.1000
I	0.4820	0.0970
J	0.4770	0.0990
K	0.4820	0.0990
L	0.4760	0.0930
M	0.4780	0.0940
N	0.4820	0.0970
O	0.4760	0.1040
P	0.4810	0.0920
Q	0.4830	0.0980
R	0.4810	0.1000
S	0.4780	0.1010
T	0.4780	0.1000
U	0.4820	0.1020
V	0.4770	0.1000
W	0.4820	0.1000
X	0.4760	0.0920
Y	0.4810	0.0950
Z	0.4840	0.0980

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Chain	Atom inclusion	Q-score
a	0.4780	0.0790
b	0.4810	0.0850
c	0.4840	0.0940
d	0.4840	0.0950
e	0.4830	0.0890
f	0.4810	0.1000
g	0.4770	0.1080
h	0.4760	0.1070
i	0.4830	0.1020
j	0.4840	0.1050
k	0.4780	0.1040
l	0.4820	0.1050
m	0.4810	0.1070
n	0.4760	0.0960
o	0.4760	0.0870
p	0.4770	0.0900
q	0.4810	0.0910
r	0.4780	0.0980
s	0.4820	0.0950
t	0.4780	0.0780
u	0.4820	0.0780
v	0.4810	0.0830
w	0.4830	0.0950
x	0.4830	0.0900
y	0.4820	0.0960
z	0.4810	0.0980