



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:33 PM UTC

PDB ID : 6CBE / pdb_00006cbe
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 wwPDB EM Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

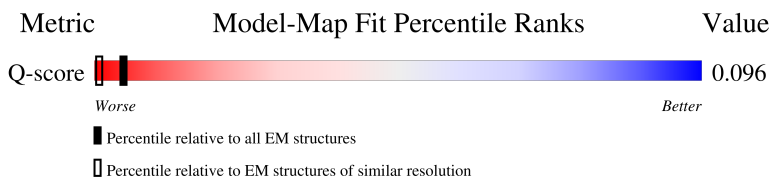
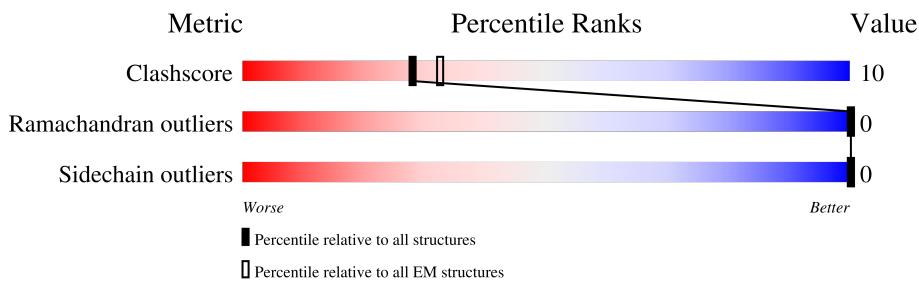
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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 $\leq 5\%$. 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	<p>24% (Poor fit), 55% (0 outliers), 15% (1 outlier), 30% (Not modelled)</p>
1	1	736	<p>24% (Poor fit), 55% (0 outliers), 15% (1 outlier), 30% (Not modelled)</p>
1	2	736	<p>23% (Poor fit), 55% (0 outliers), 15% (1 outlier), 30% (Not modelled)</p>
1	3	736	<p>24% (Poor fit), 54% (0 outliers), 16% (1 outlier), 30% (Not modelled)</p>

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Mol	Chain	Length	Quality of chain
1	4	736	26% 55% 16% 30%
1	5	736	24% 55% 16% 30%
1	6	736	25% 55% 15% 30%
1	7	736	25% 55% 15% 30%
1	A	736	24% 56% 15% 30%
1	B	736	26% 55% 15% 30%
1	C	736	24% 55% 15% 30%
1	D	736	25% 55% 15% 30%
1	E	736	23% 55% 15% 30%
1	F	736	23% 55% 16% 30%
1	G	736	25% 55% 15% 30%
1	H	736	25% 55% 16% 30%
1	I	736	24% 55% 15% 30%
1	J	736	26% 55% 15% 30%
1	K	736	24% 55% 15% 30%
1	L	736	26% 55% 16% 30%
1	M	736	25% 55% 15% 30%
1	N	736	24% 55% 15% 30%
1	O	736	26% 55% 15% 30%
1	P	736	24% 55% 16% 30%
1	Q	736	23% 55% 15% 30%
1	R	736	24% 55% 15% 30%
1	S	736	25% 55% 15% 30%
1	T	736	25% 55% 15% 30%
1	U	736	24% 55% 15% 30%

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Mol	Chain	Length	Quality of chain
1	V	736	26% 55% 16% 30%
1	W	736	24% 55% 15% 30%
1	X	736	26% 55% 15% 30%
1	Y	736	24% 56% 15% 30%
1	Z	736	23% 55% 16% 30%
1	a	736	25% 55% 15% 30%
1	b	736	24% 55% 15% 30%
1	c	736	23% 55% 16% 30%
1	d	736	23% 54% 16% 30%
1	e	736	23% 55% 15% 30%
1	f	736	24% 55% 15% 30%
1	g	736	26% 55% 15% 30%
1	h	736	25% 55% 15% 30%
1	i	736	23% 55% 16% 30%
1	j	736	23% 55% 16% 30%
1	k	736	25% 55% 15% 30%
1	l	736	24% 55% 15% 30%
1	m	736	24% 55% 16% 30%
1	n	736	26% 54% 16% 30%
1	o	736	26% 55% 15% 30%
1	p	736	26% 55% 15% 30%
1	q	736	24% 55% 16% 30%
1	r	736	25% 55% 15% 30%
1	s	736	24% 55% 15% 30%
1	t	736	25% 55% 15% 30%

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Mol	Chain	Length	Quality of chain
1	u	736	
1	v	736	
1	w	736	
1	x	736	
1	y	736	
1	z	736	

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

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

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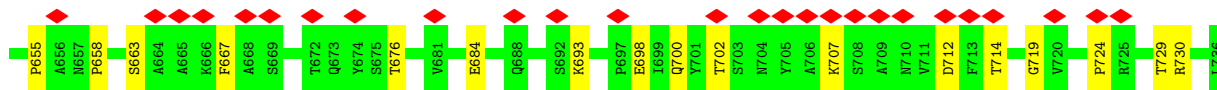
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Chain	Residue	Modelled	Actual	Comment	Reference
r	265	THR	-	insertion	UNP P03135
r	706	ALA	ASN	conflict	UNP P03135
r	709	ALA	VAL	conflict	UNP P03135
r	717	ASN	THR	conflict	UNP P03135
s	263	ALA	GLN	conflict	UNP P03135
s	265	THR	-	insertion	UNP P03135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

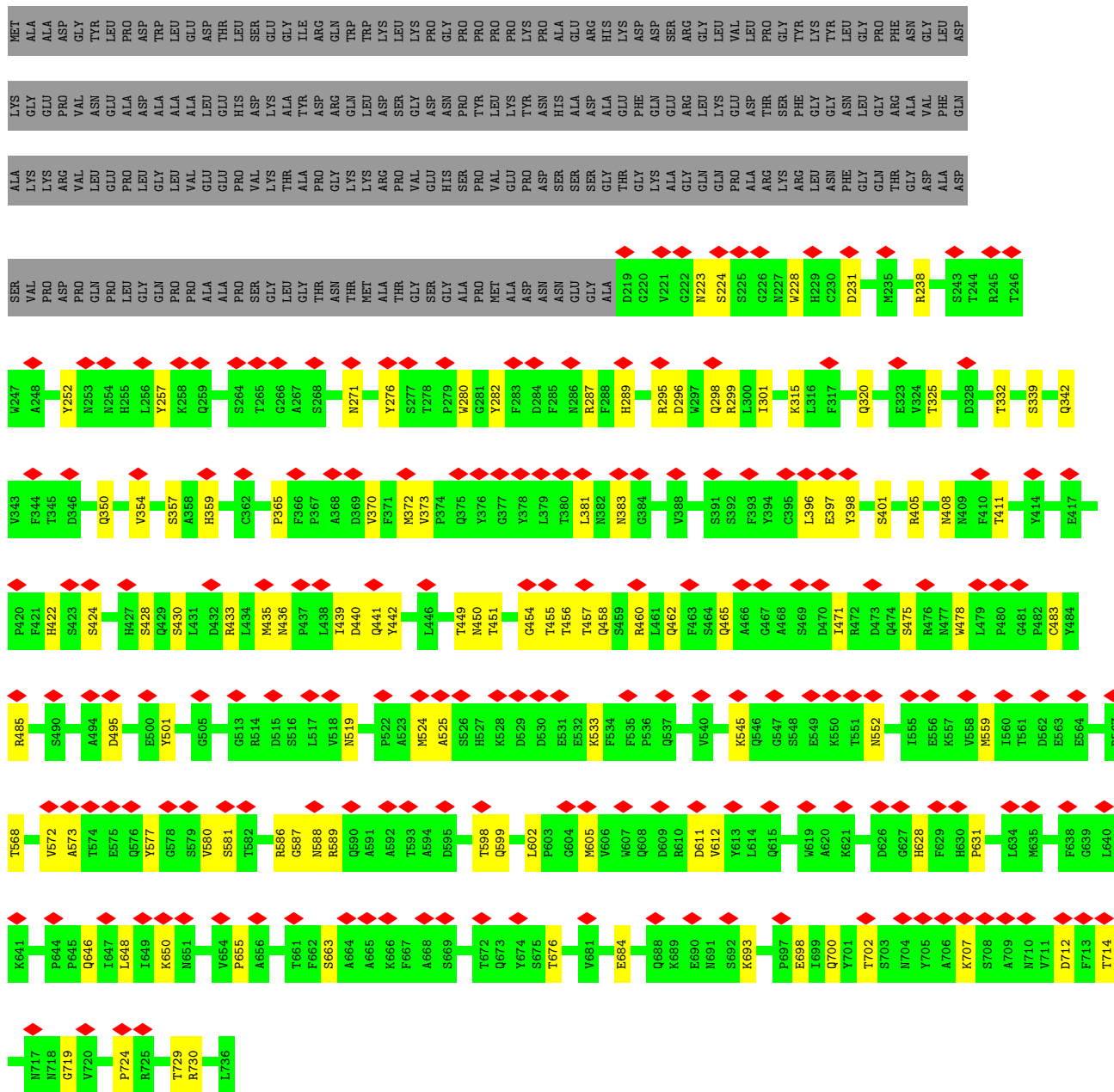
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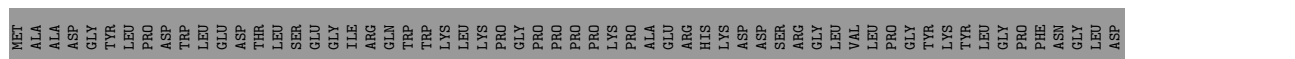
Chain	Residue	Modelled	Actual	Comment	Reference
z	709	ALA	VAL	conflict	UNP P03135
z	717	ASN	THR	conflict	UNP P03135
6	263	ALA	GLN	conflict	UNP P03135
6	265	THR	-	insertion	UNP P03135
6	706	ALA	ASN	conflict	UNP P03135
6	709	ALA	VAL	conflict	UNP P03135
6	717	ASN	THR	conflict	UNP P03135
7	263	ALA	GLN	conflict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

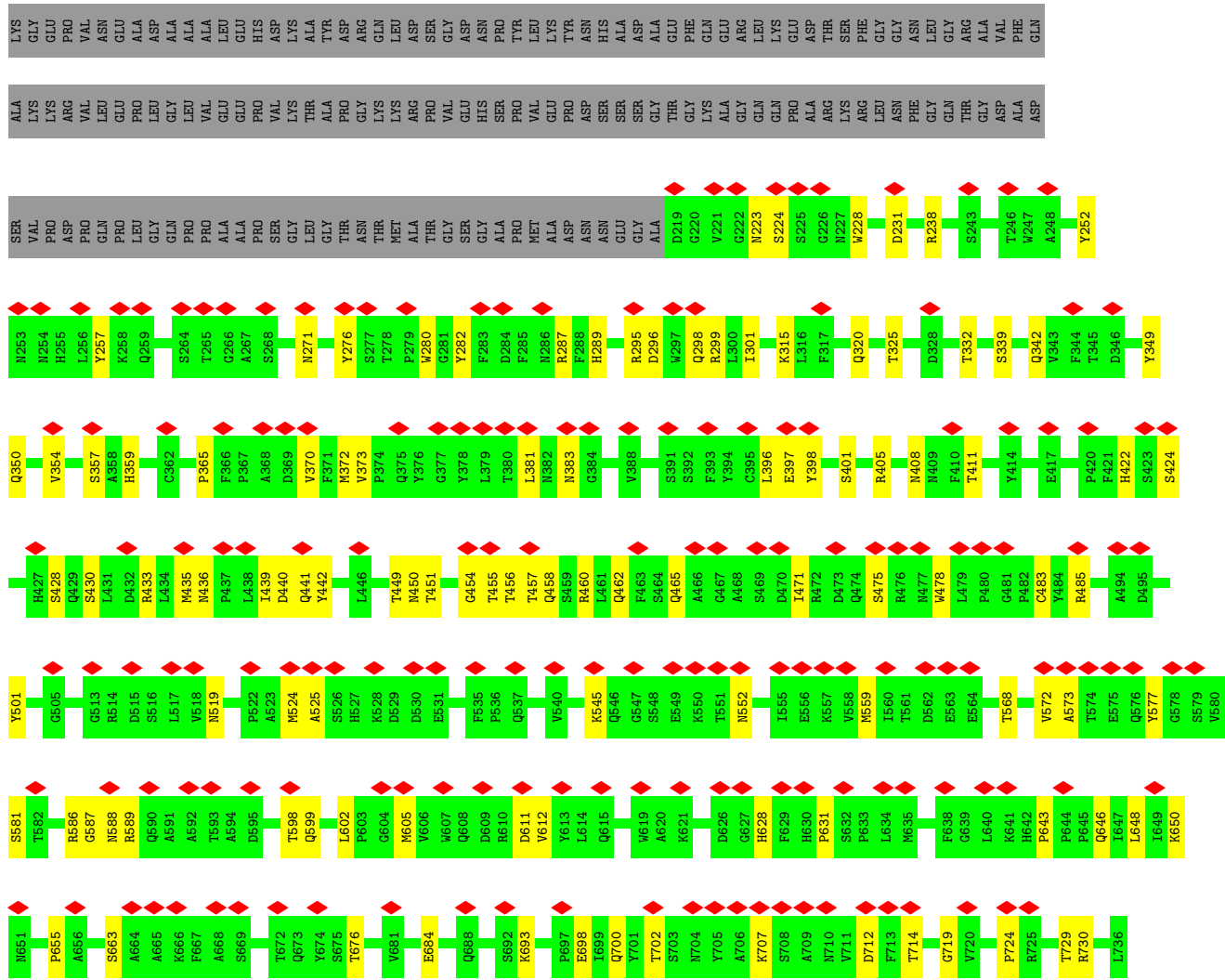


• Molecule 1: Capsid protein VP1

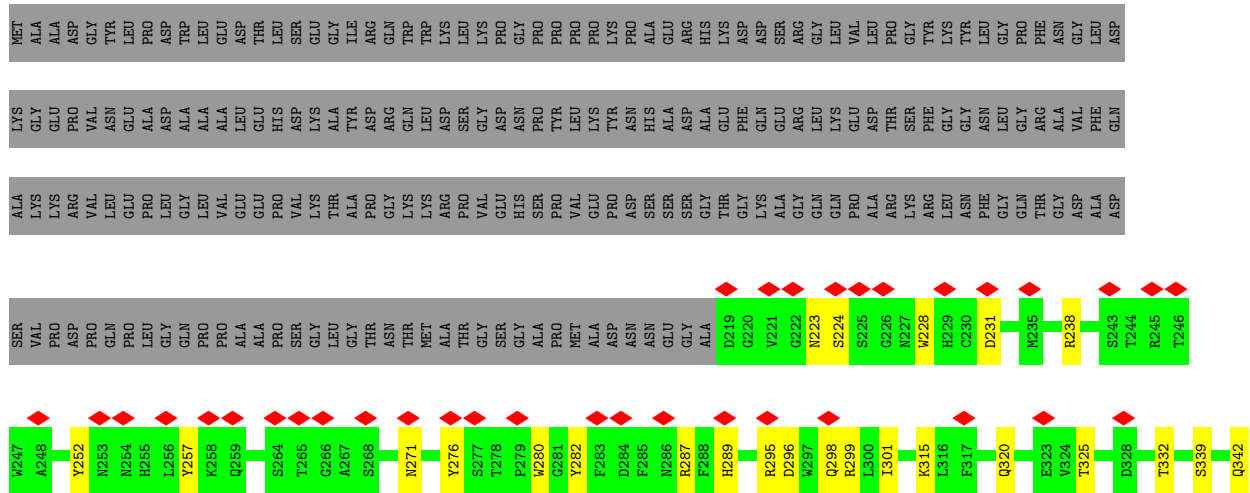


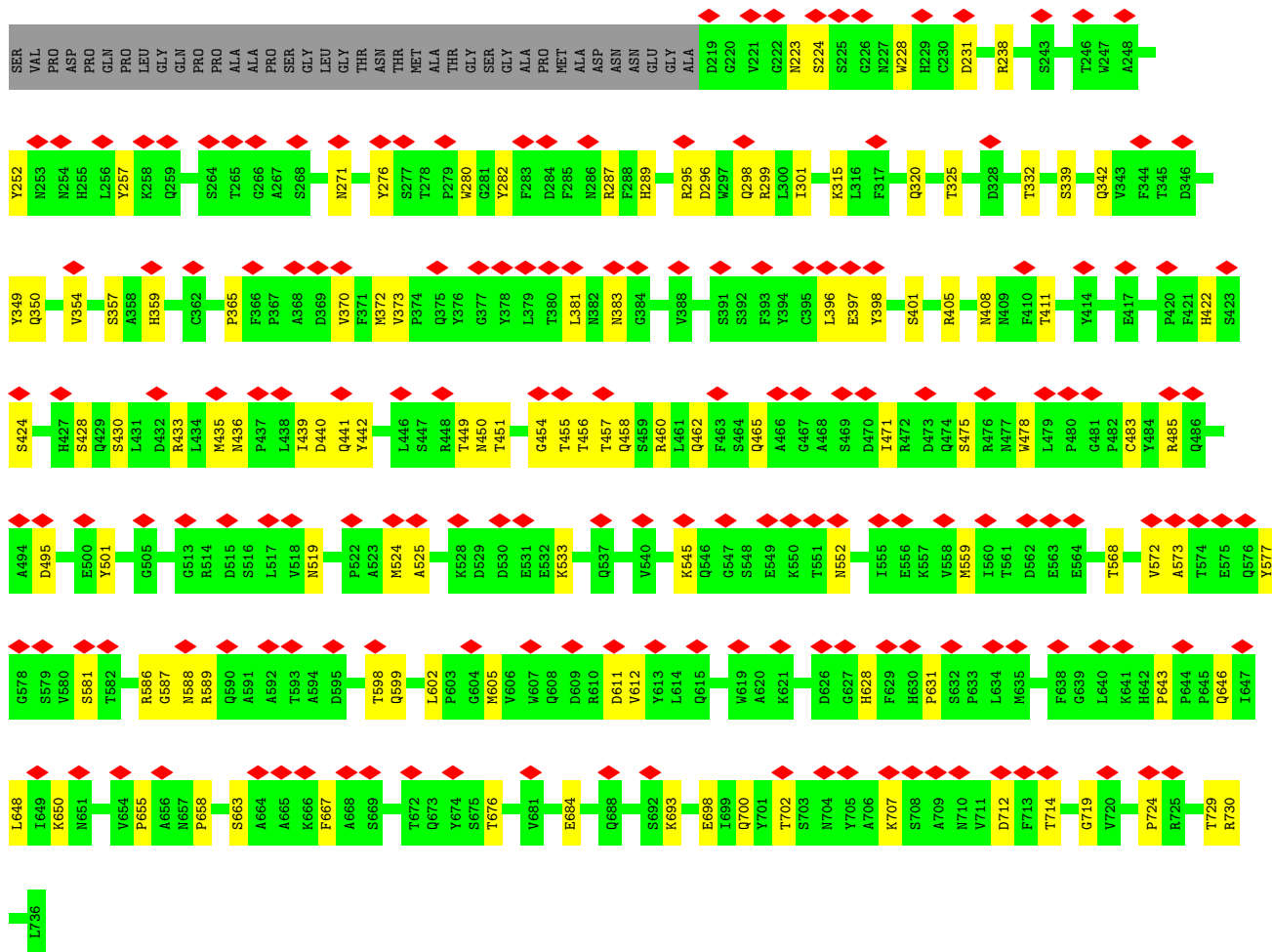
• Molecule 1: Capsid protein VP1



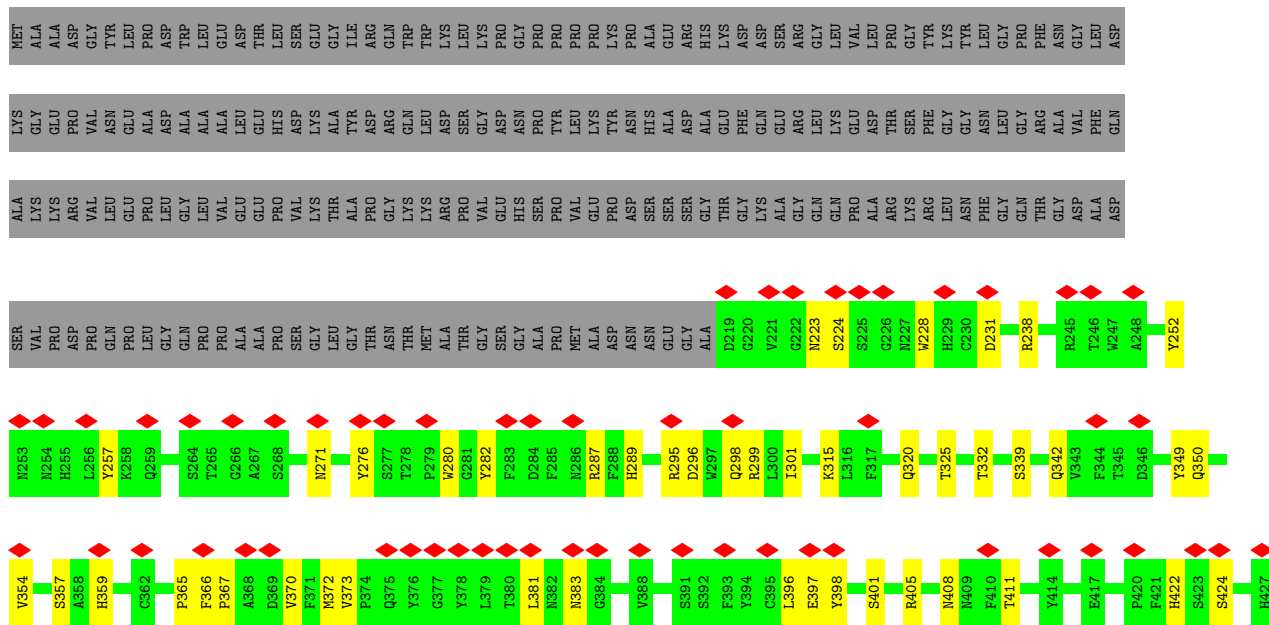


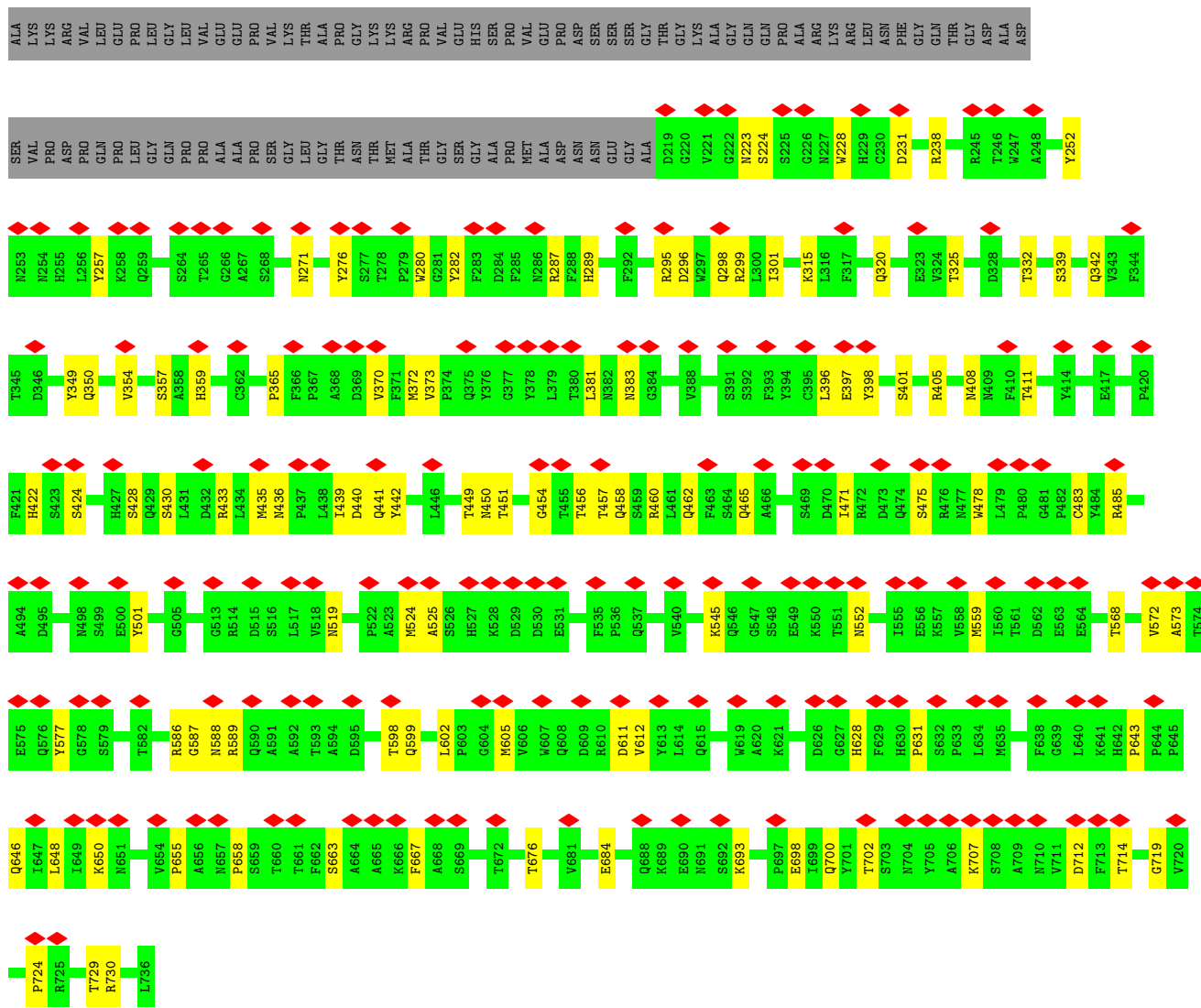
● Molecule 1: Capsid protein VP1



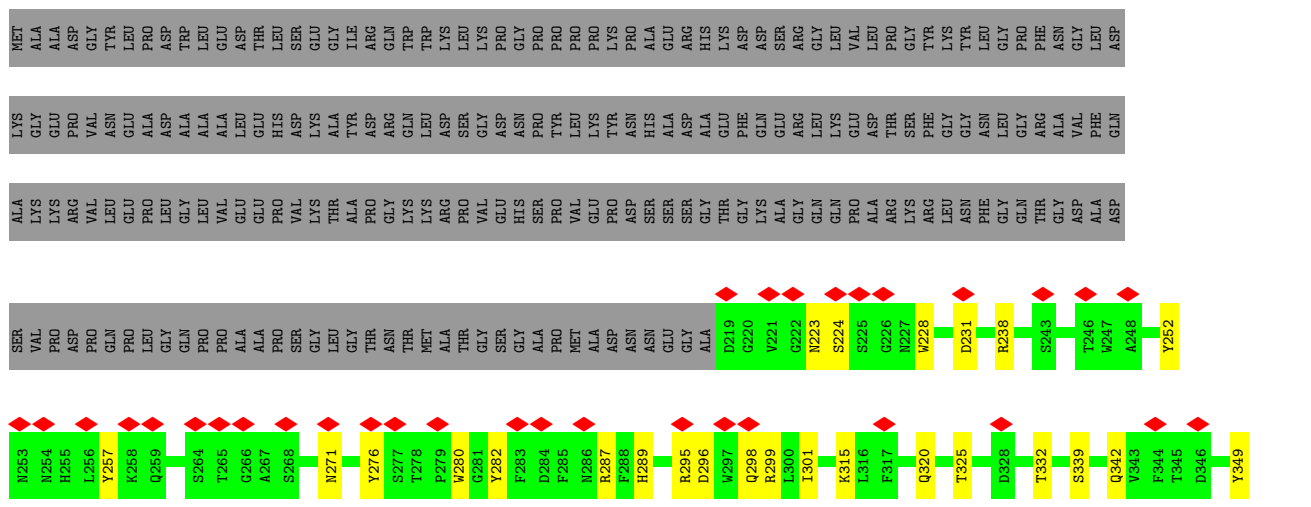


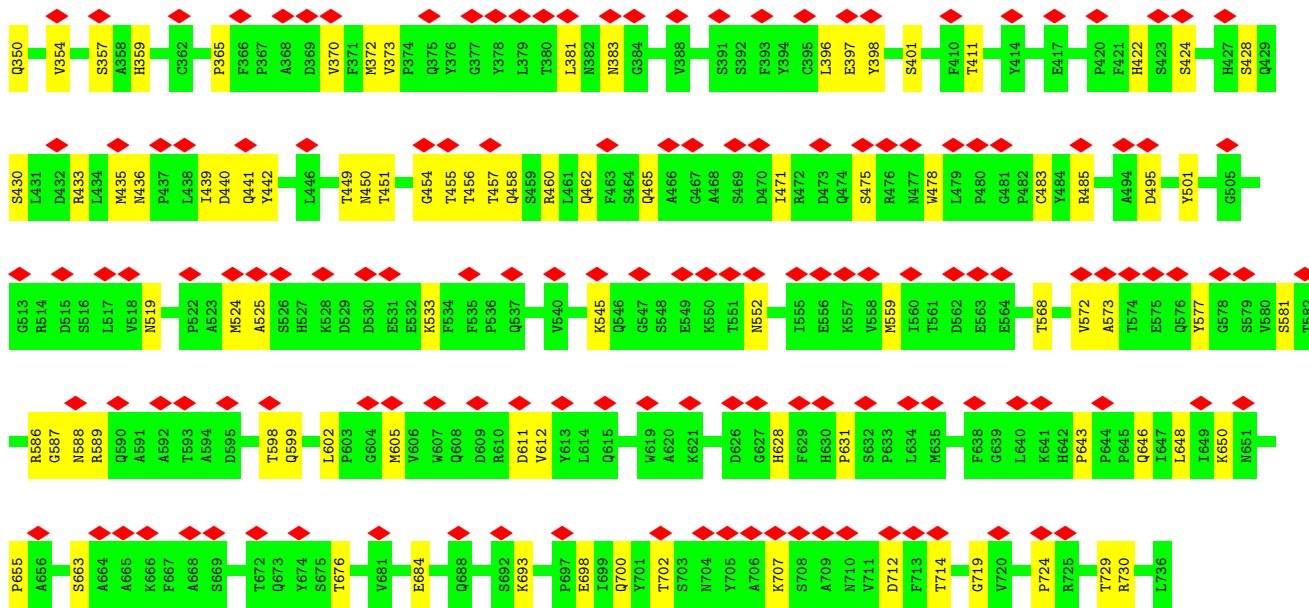
- Molecule 1: Capsid protein VP1



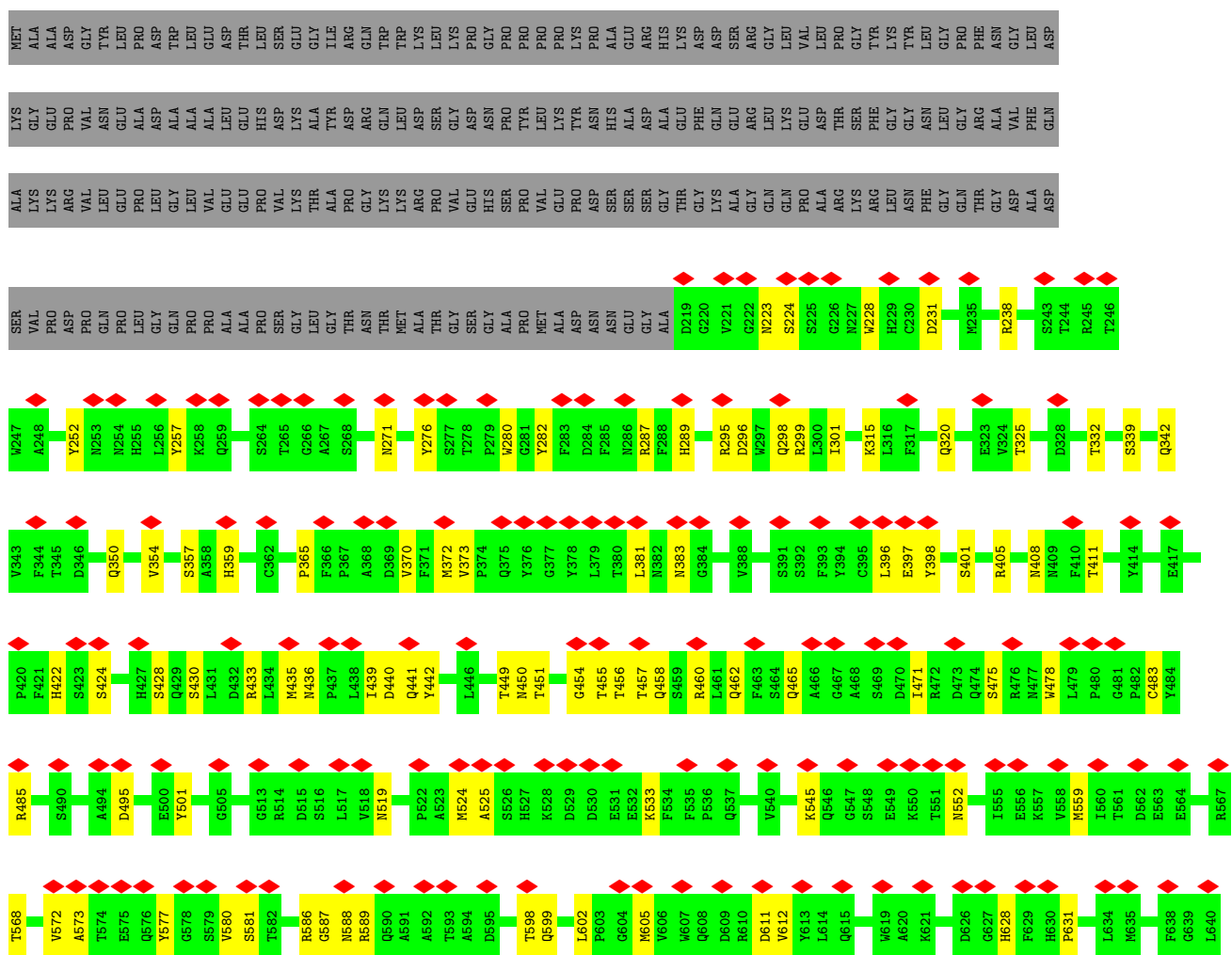


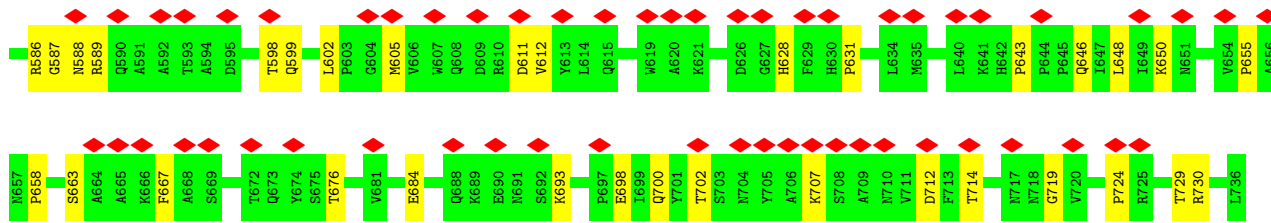
• Molecule 1: Capsid protein VP1



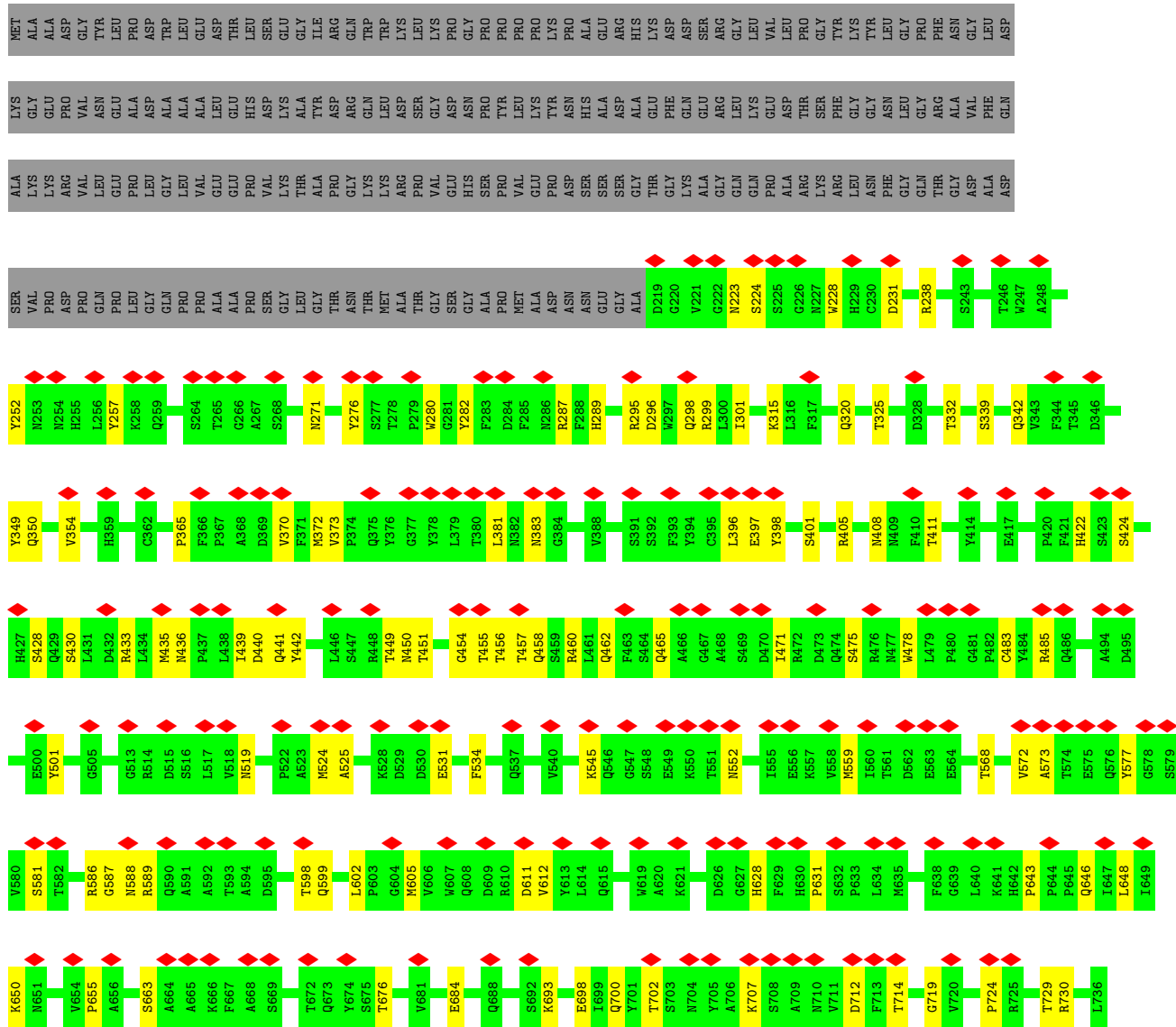


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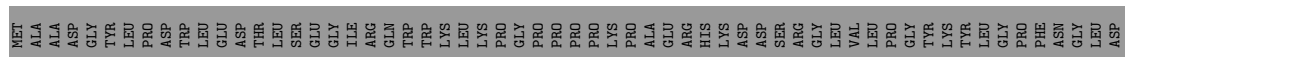


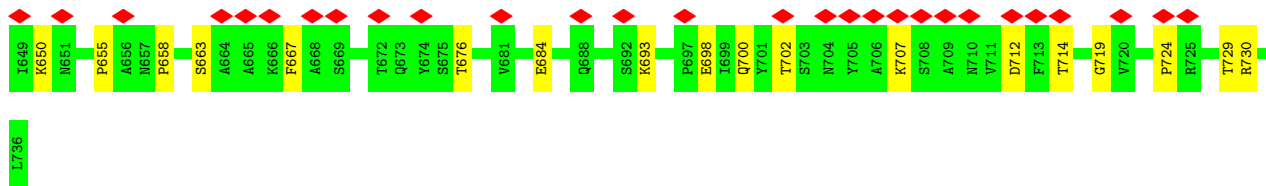


• Molecule 1: Capsid protein VP1

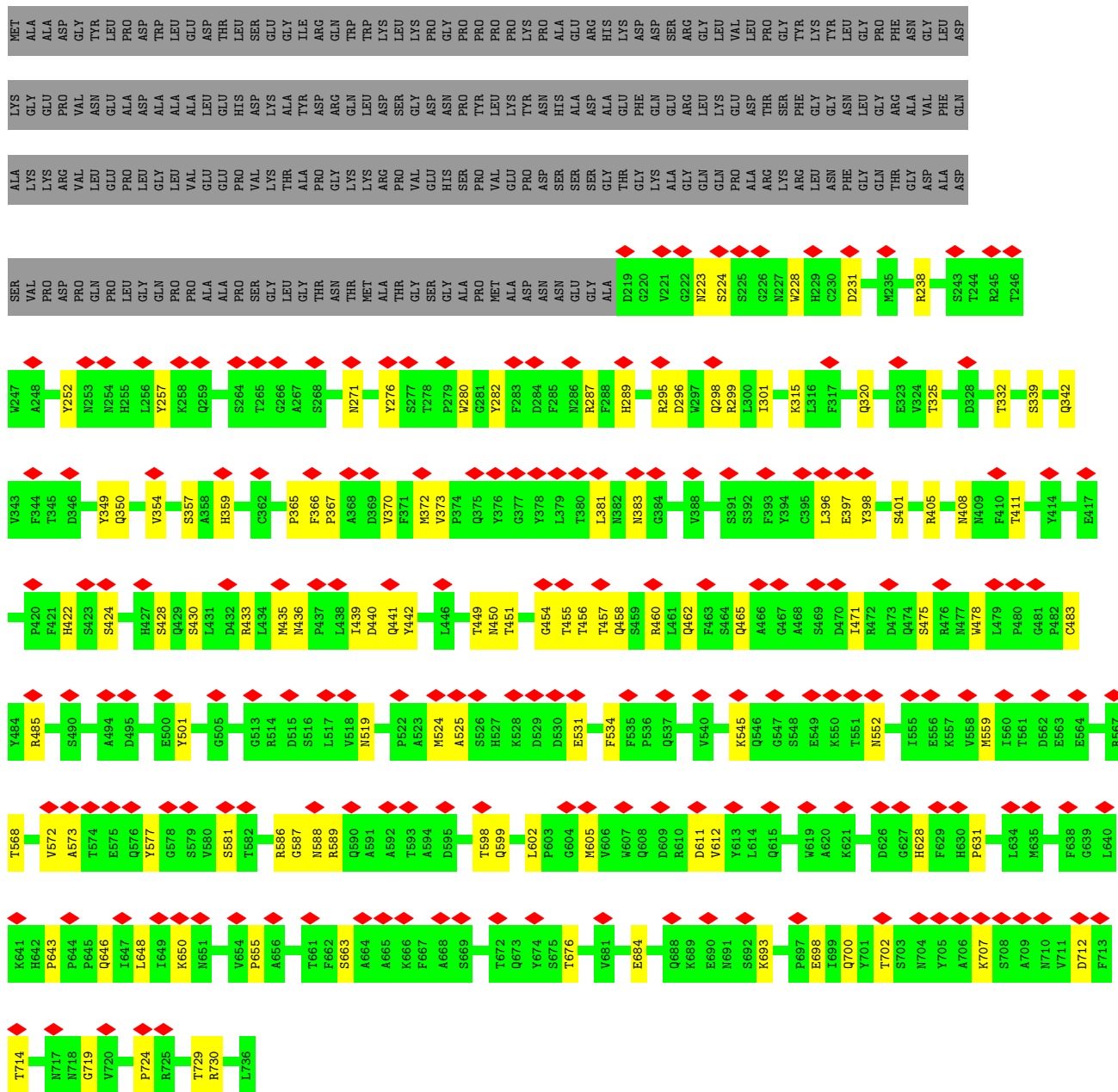


• Molecule 1: Capsid protein VP1



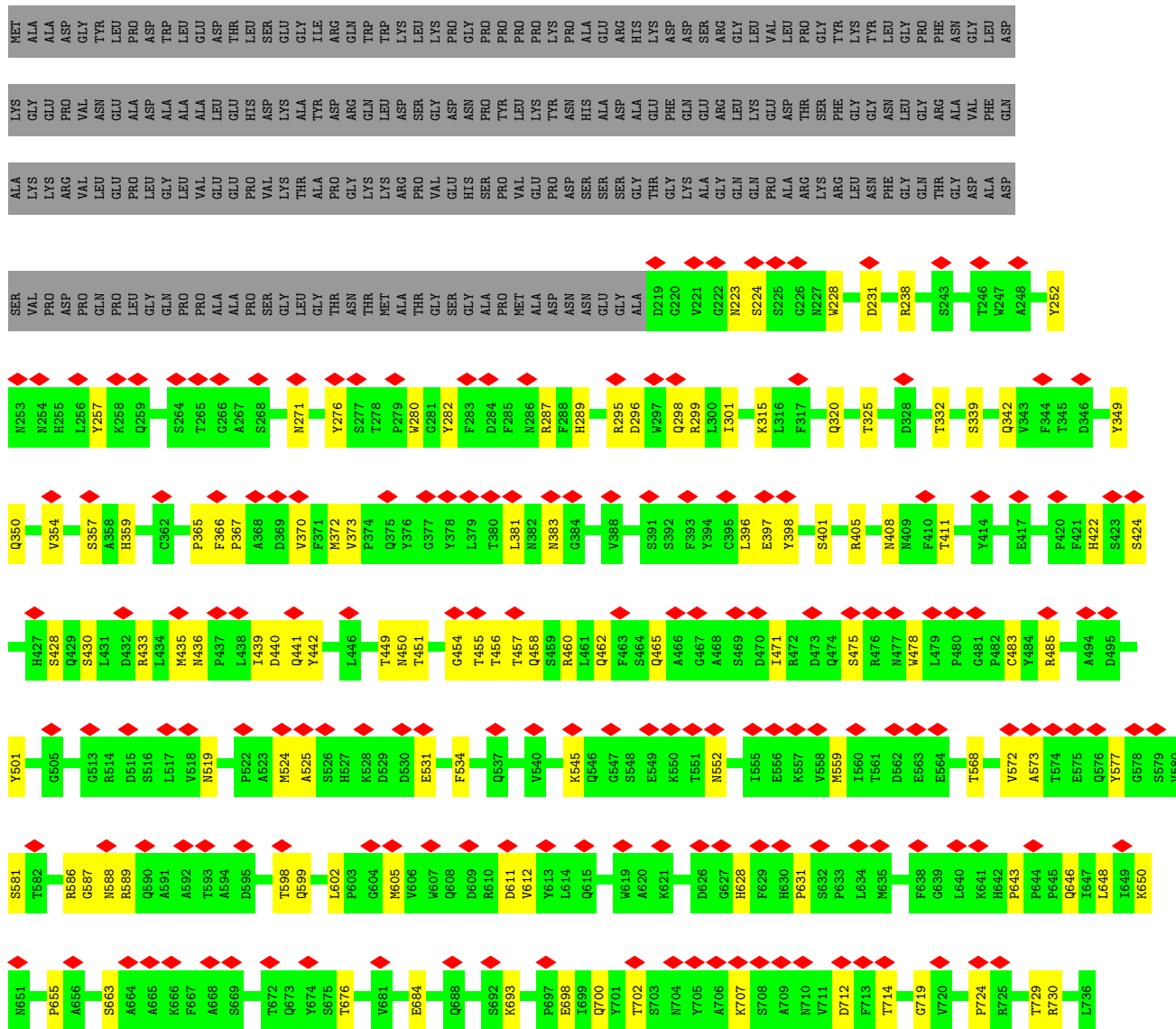


• Molecule 1: Capsid protein VP1

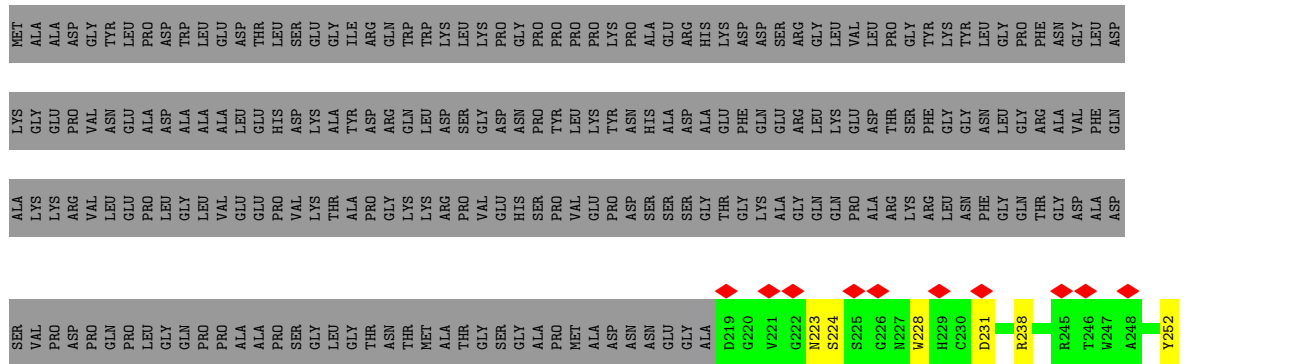


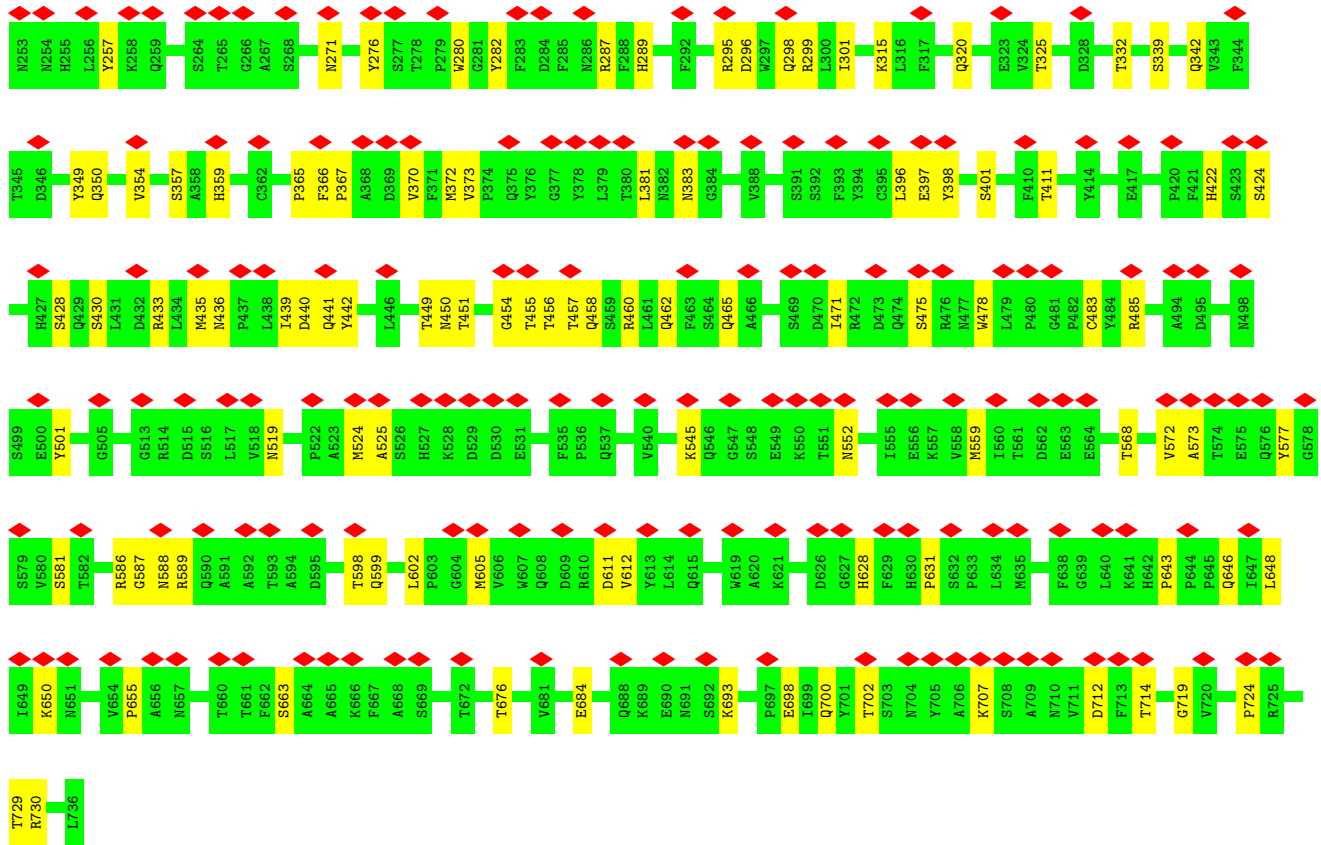
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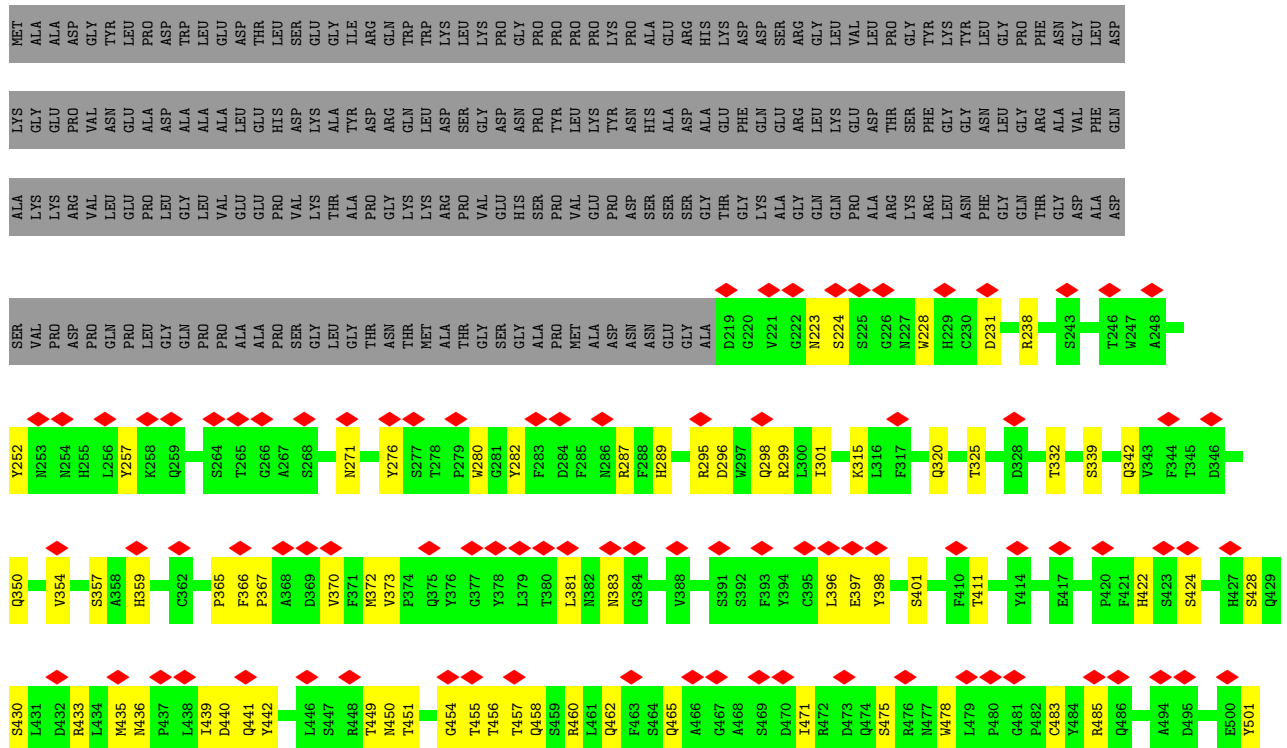


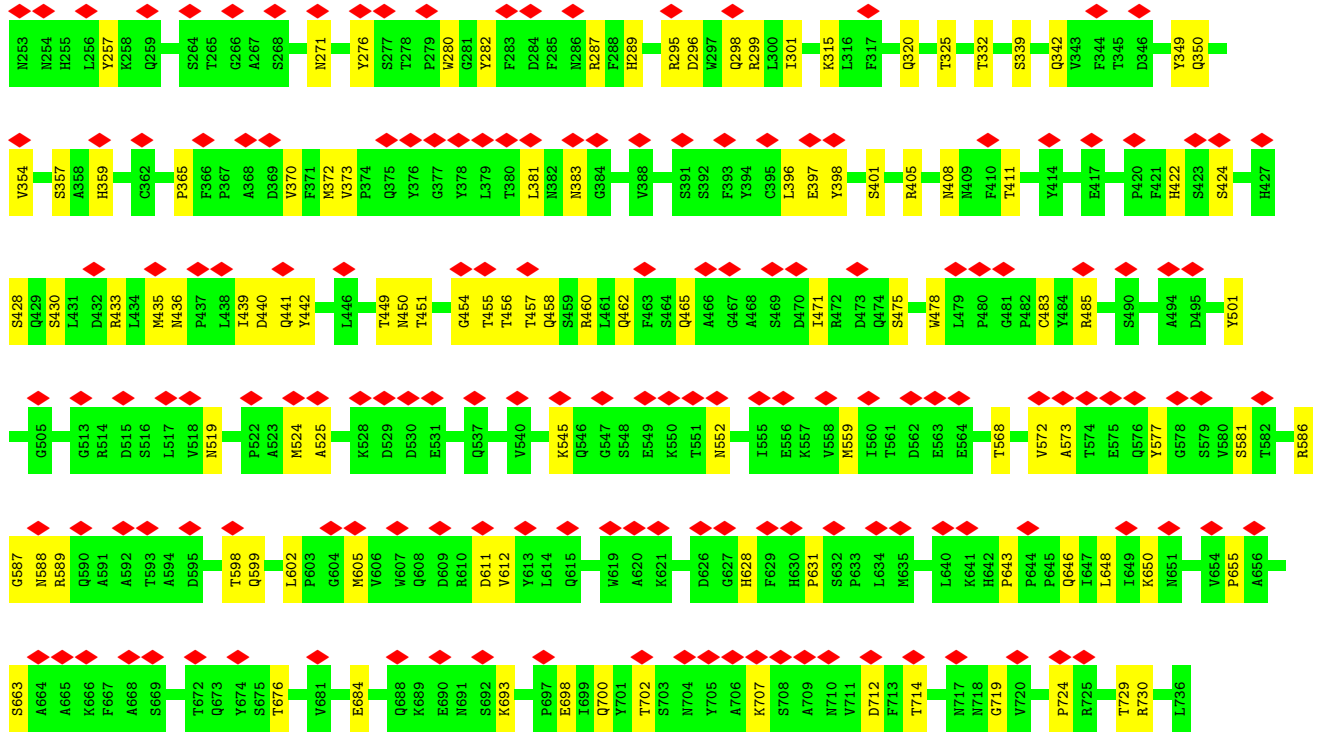
● Molecule 1: Capsid protein VP1



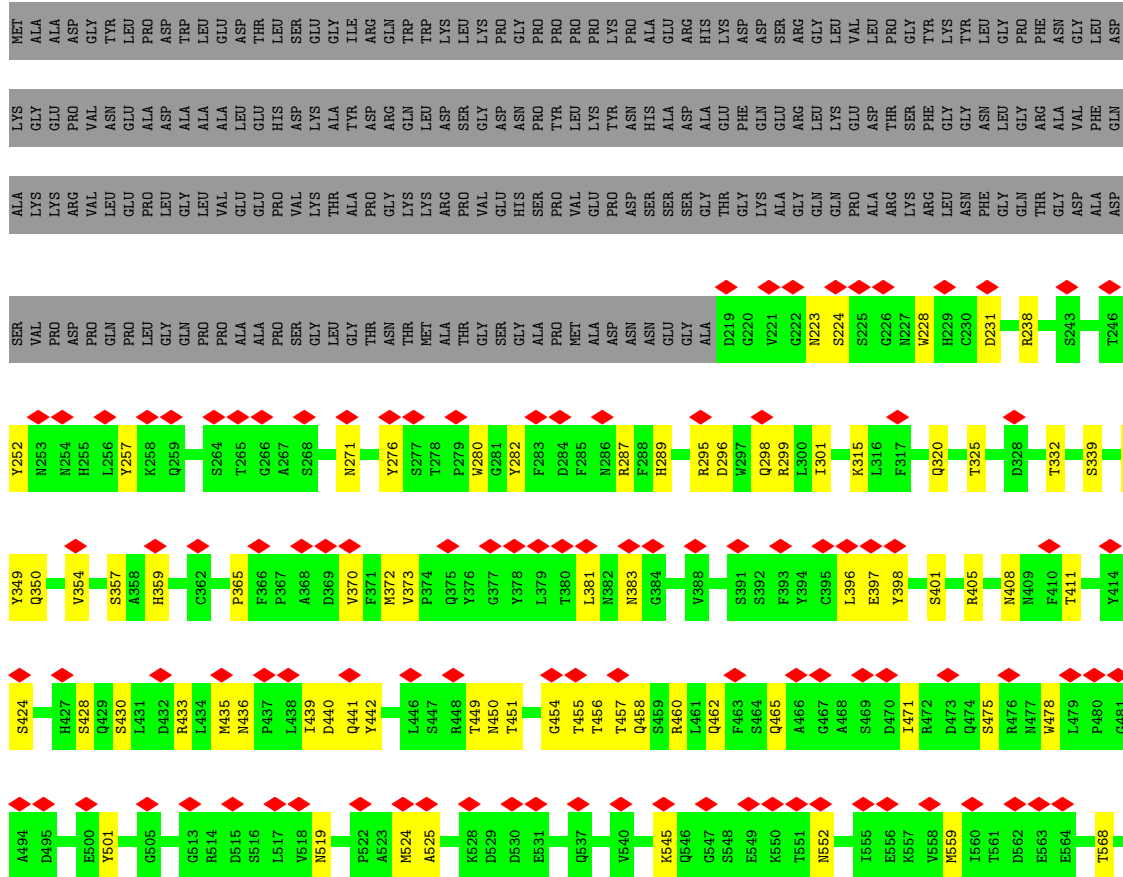


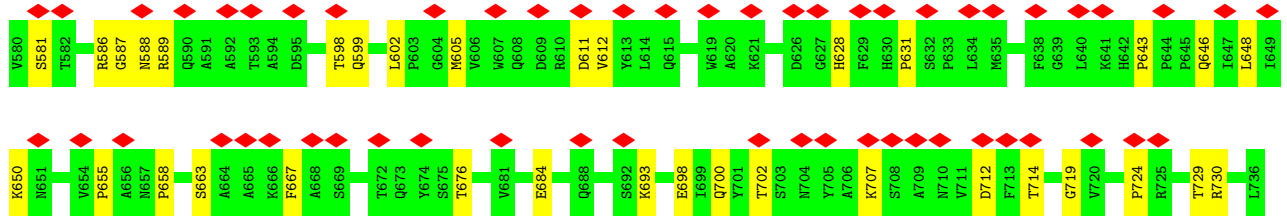
• Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1

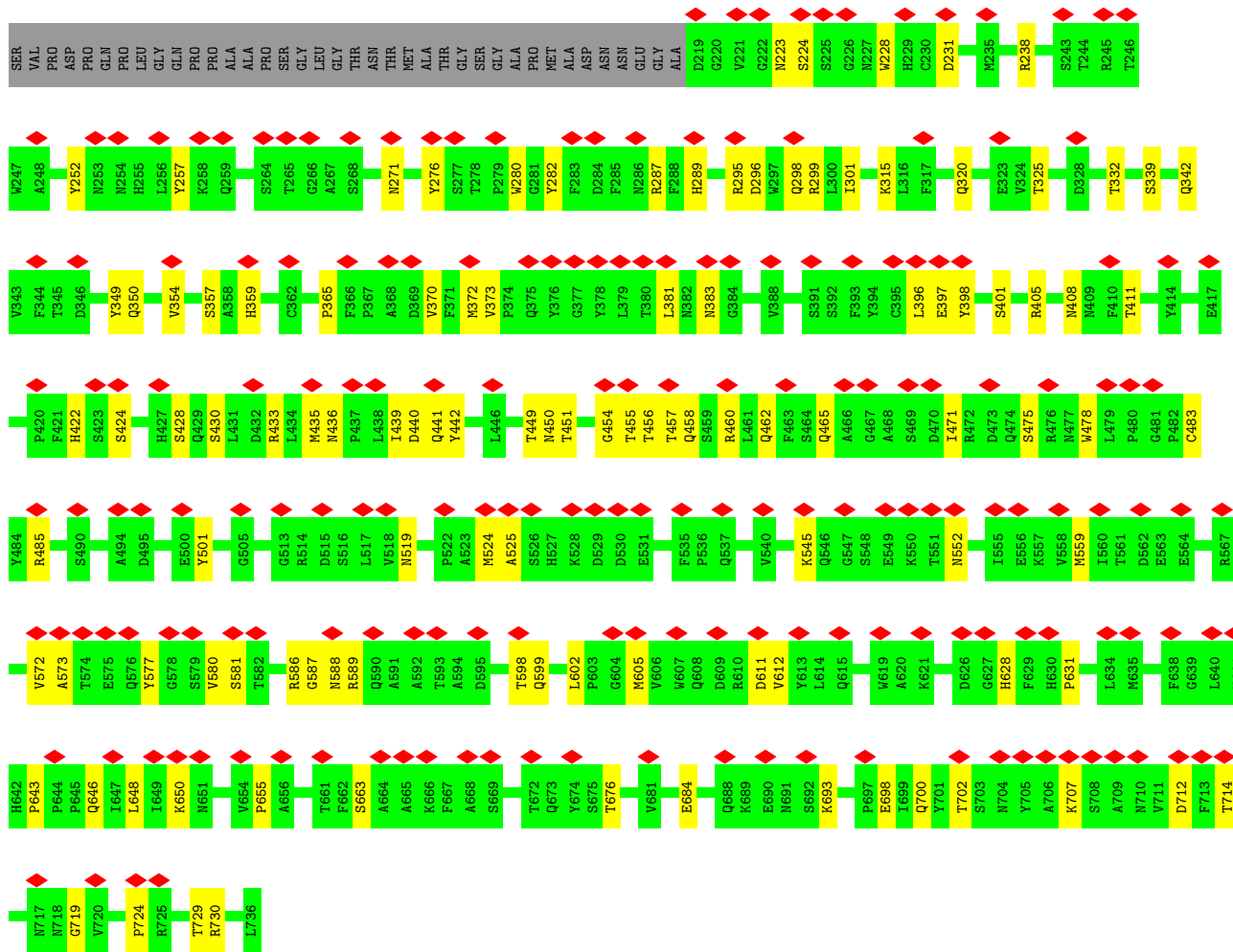




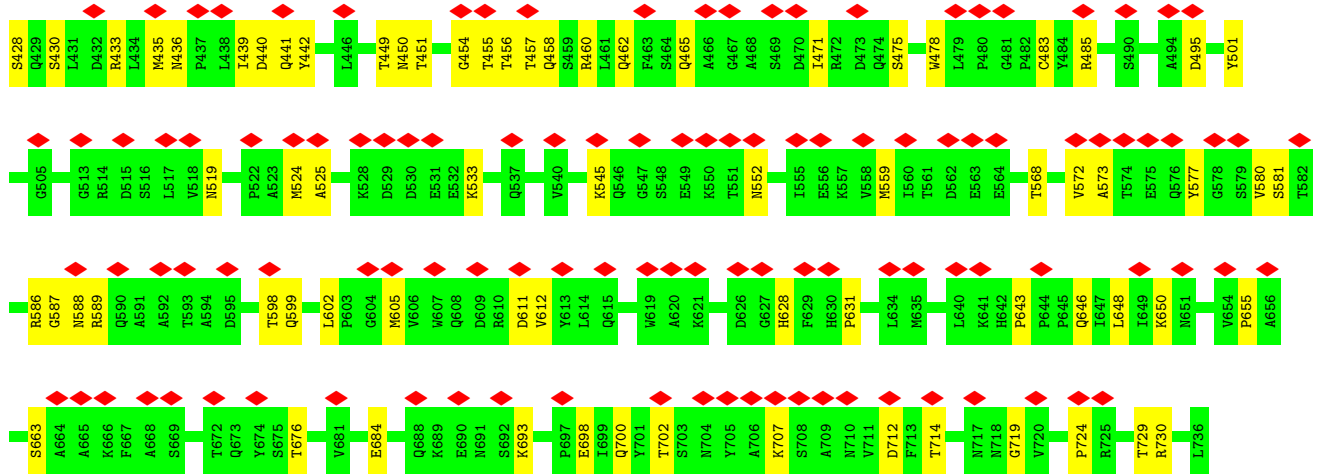
• Molecule 1: Capsid protein VP1



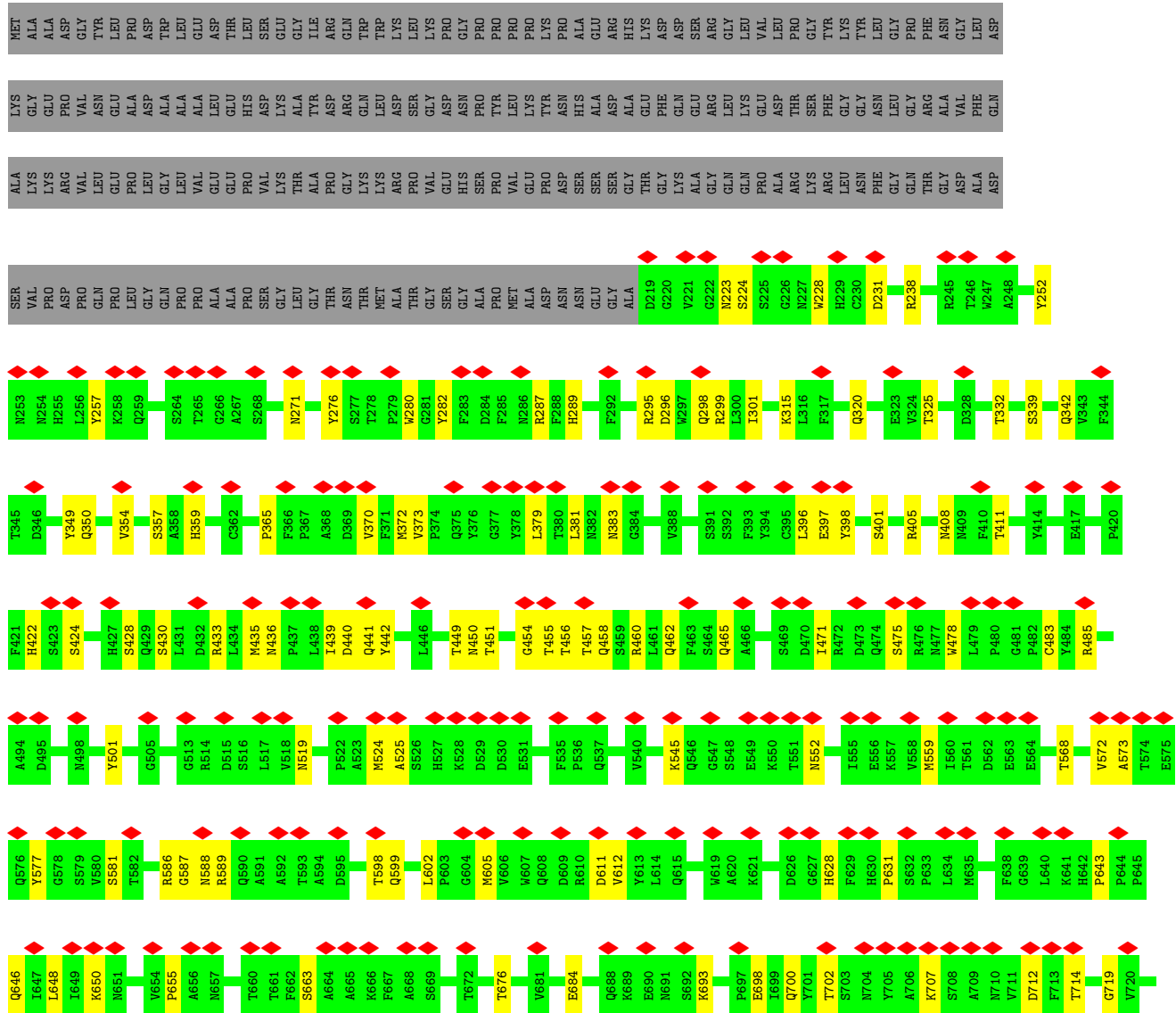
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LYS	GLY	PRO	VAL	ASN	GLY	ALA	ASP	LEU	ALA	ALA	LEU	LEU	LEU	GLY	A664	A665	K666	F667	A668	S669	T672	Q673	Y674	S675	T676	V681	E684	Q688	S692	K693	E698	I699	Q700	Y701	T702	S703	N704	Y705	A706	K707	S708	A709	N710	V711	F713	T714	G719	V720	P724	R725	T729	R730	L736								
ALA	LYS	ARG	VAL	LEU	PRO	GLY	PRO	GLY	PRO	VAL	LYS	THR	ALA	GLY	A664	A665	K666	F667	A668	S669	T672	Q673	Y674	S675	T676	V681	E684	Q688	S692	K693	E698	I699	Q700	Y701	T702	S703	N704	Y705	A706	K707	S708	A709	N710	V711	F713	T714	G719	V720	P724	R725	T729	R730	L736								

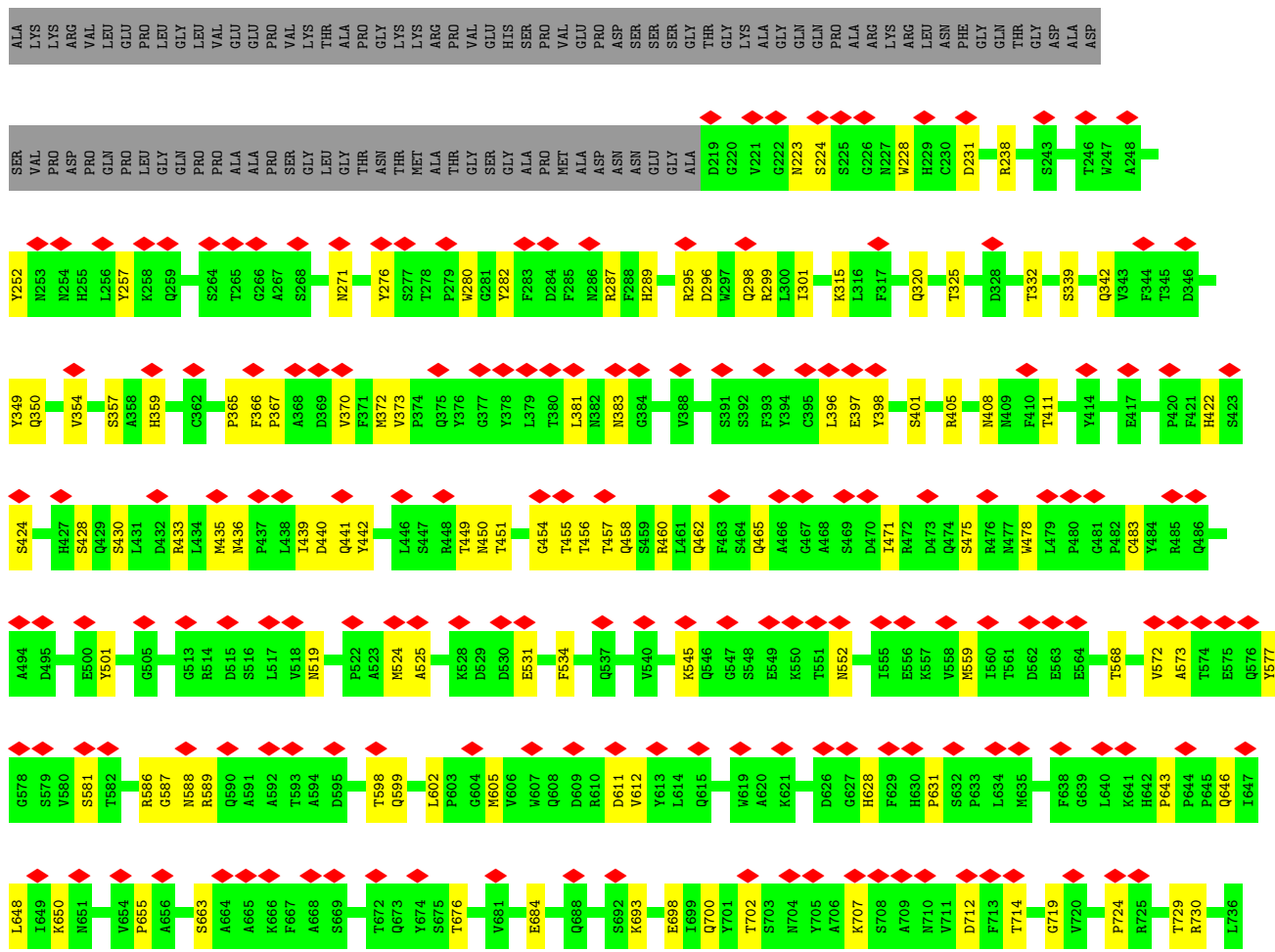


• Molecule 1: Capsid protein VP1

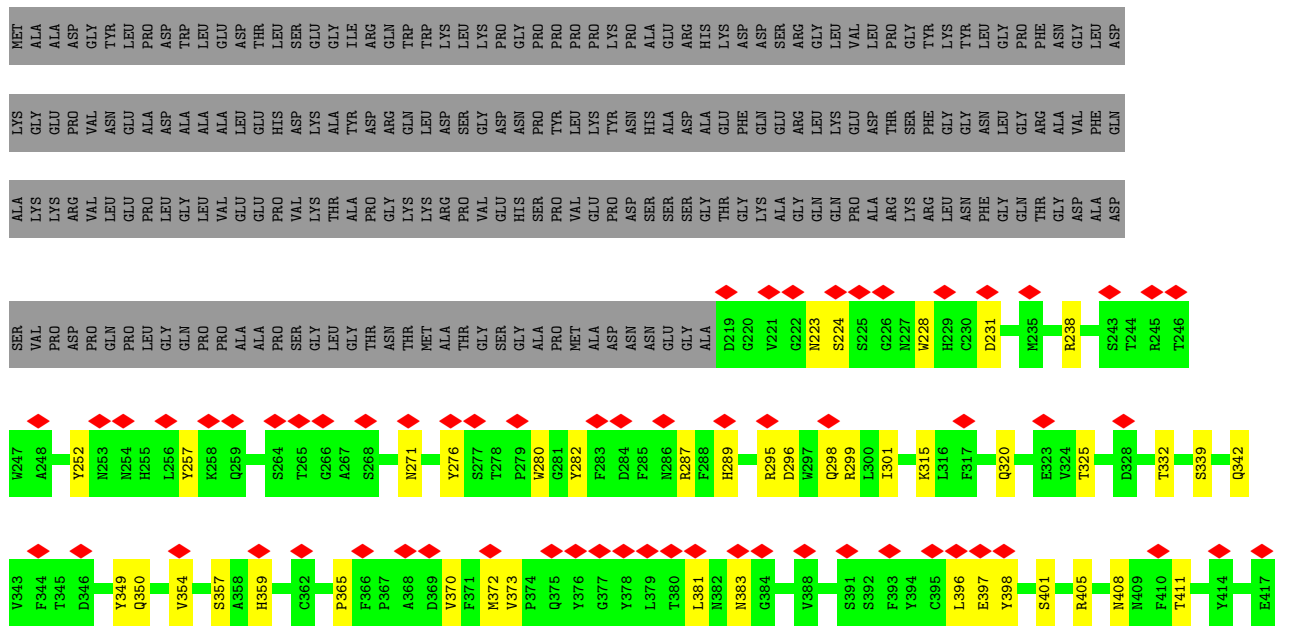


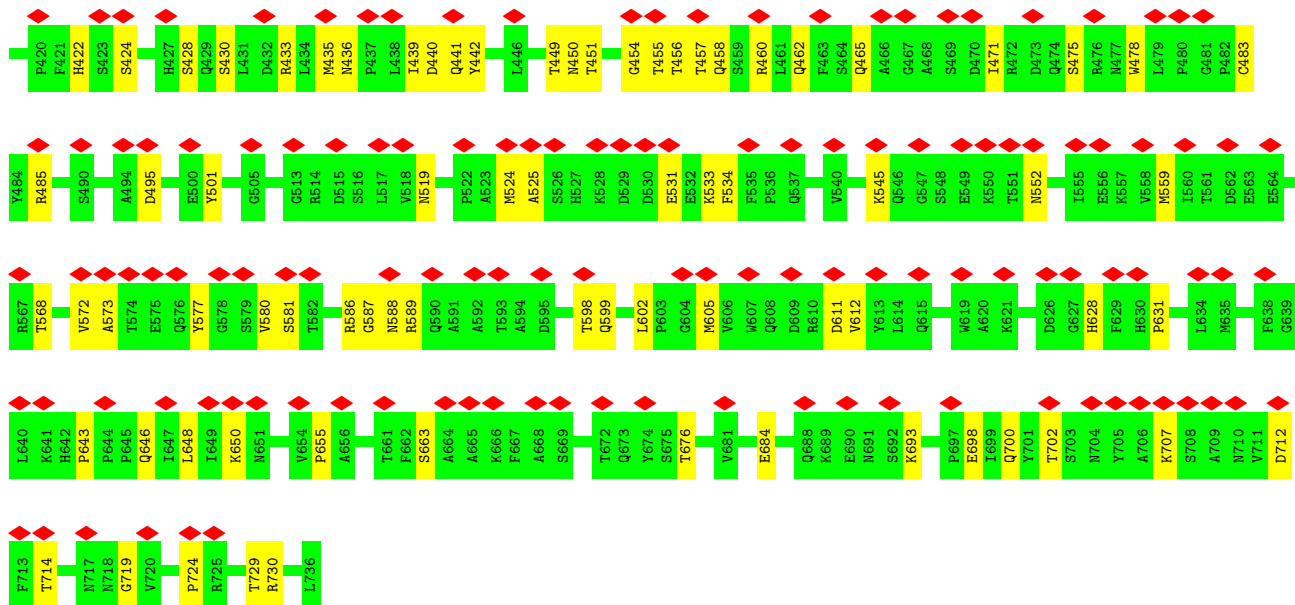
● Molecule 1: Capsid protein VP1



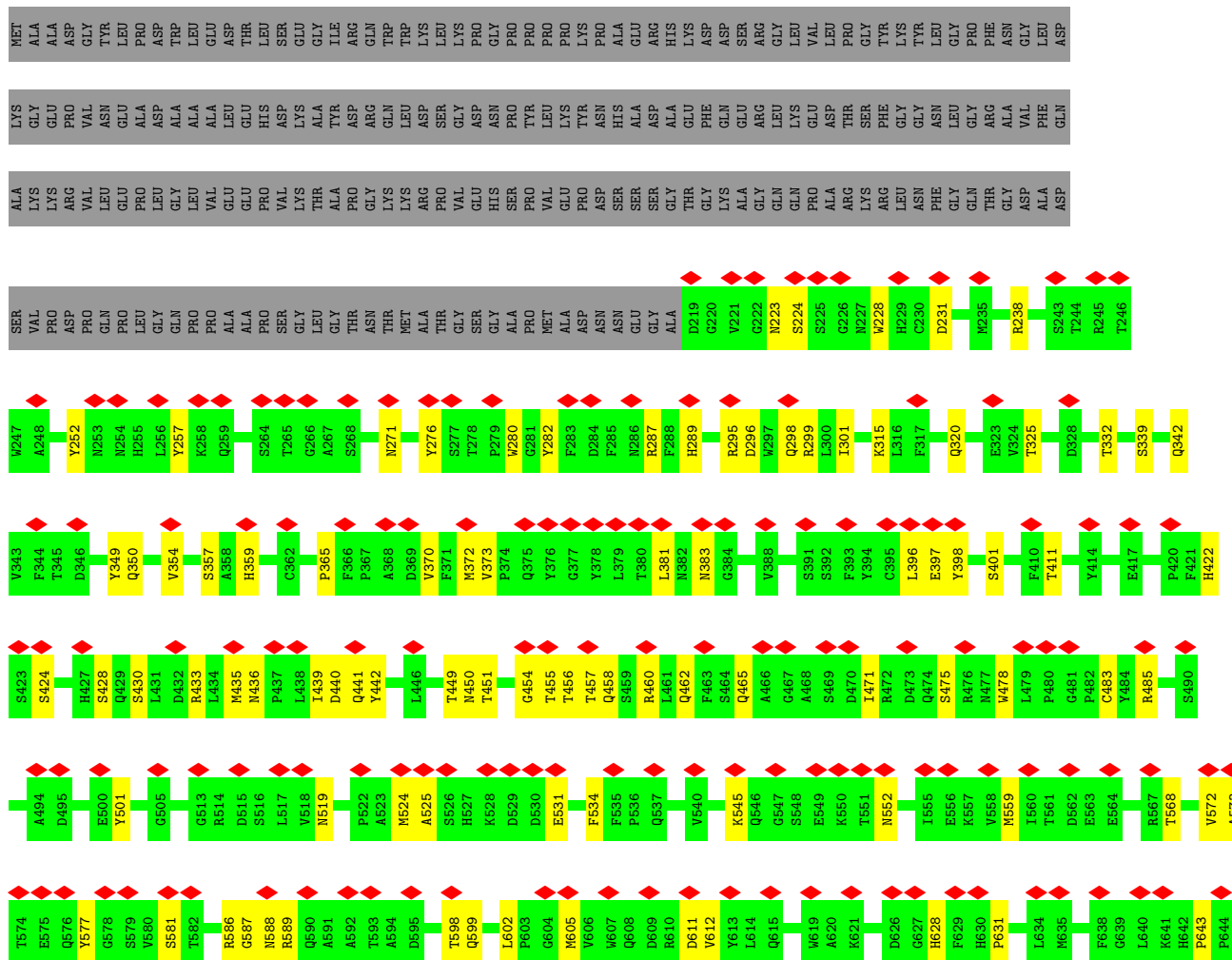


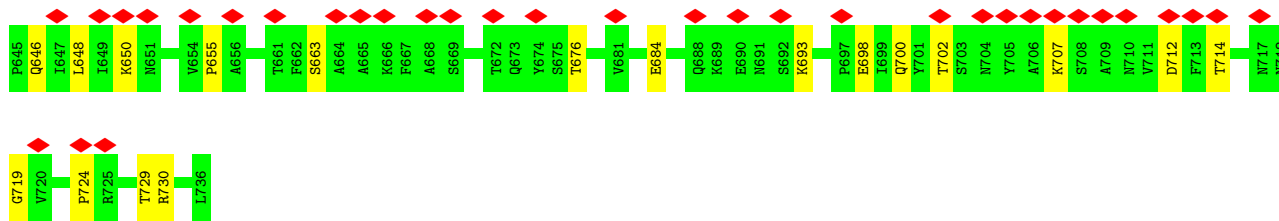
● Molecule 1: Capsid protein VP1





● Molecule 1: Capsid protein VP1

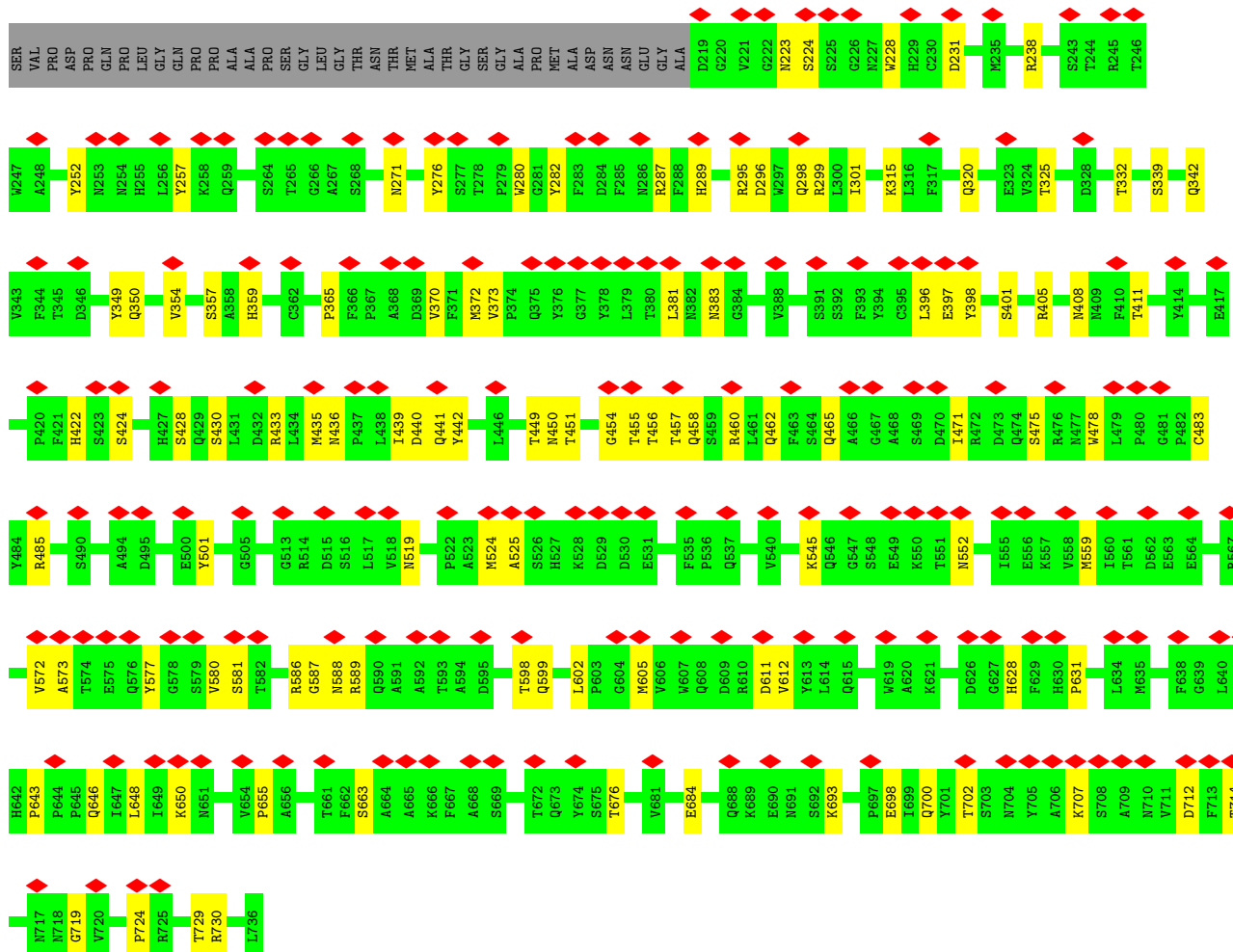




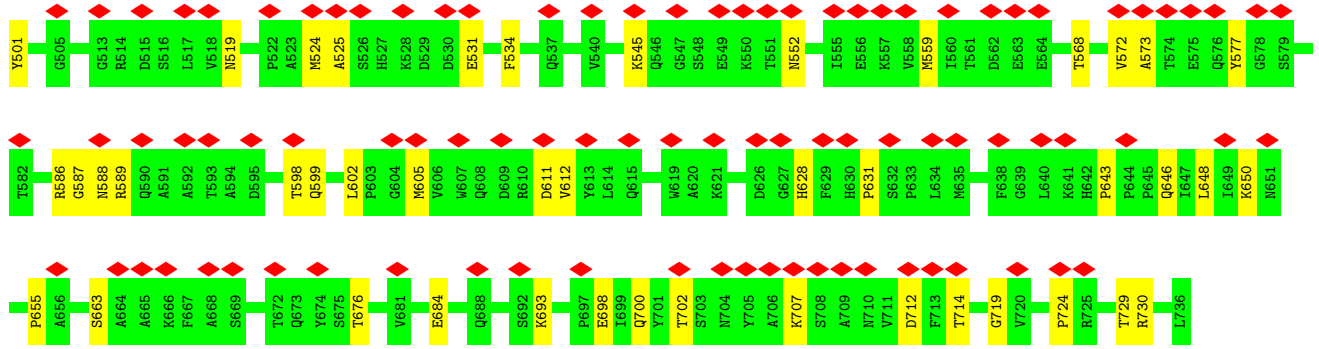
• Molecule 1: Capsid protein VP1



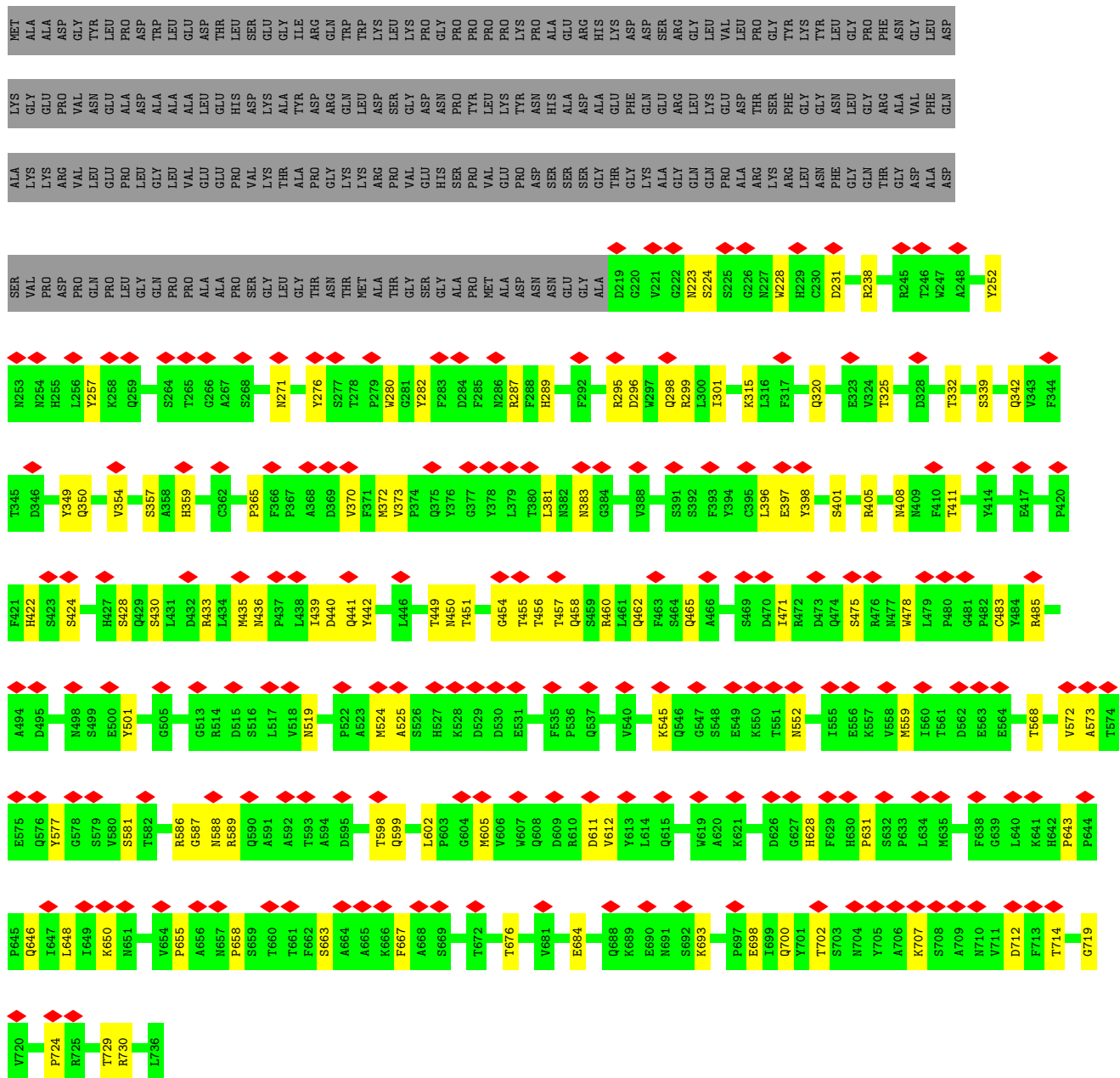
MET	ALA	ALA	ASP	GLY	TYR	PRO	ASP	TRP	LEU	ASP	T661	F662	S663	A664	A665	K666	F667	A668	S669	T672	Q673	Y674	S675	T676	V681	E684	Q688	K689	E690	M691	S692	K693	P697	E698	I699	Q700	Y701	T702	S703	N704	Y705	A706	K707	S708	A709	N710	V711	D712	F713	T714	N717	N718				
LYS	GLY	PRO	ARG	VAL	LEU	GLU	PRO	ALA	ASP	ALA	LEU	GLY	VAL	THR	ALA	TYR	ASP	ARG	GLN	TRP	LYS	LEU	TRP	LYS	LEU	LEU	LYS	PRO	GLY	ASN	ALA	GLU	ARG	GLY	LEU	VAL	LEU	ASP	THR	PRO	TYR	ASN	LEU	GLY	PRO	ARG	PHE	ASN	GLY	VAL	PHE	GLN	ASP			
ALA	LYS	LYS	ARG	VAL	LEU	GLU	PRO	LEU	GLY	VAL	PRO	VAL	VAL	THR	LYS	ALA	PRO	GLY	LYS	LYS	ARG	PRO	VAL	GLU	PRO	PRO	TYR	PRO	ALA	GLU	SER	ASP	GLY	THR	GLY	LEU	ALA	PRO	GLY	LEU	ALA	ALA	GLY	GLN	GLN	PRO	ALA	ALA	GLY	GLY	THR	GLY	ASP	ALA	ALA	ASP

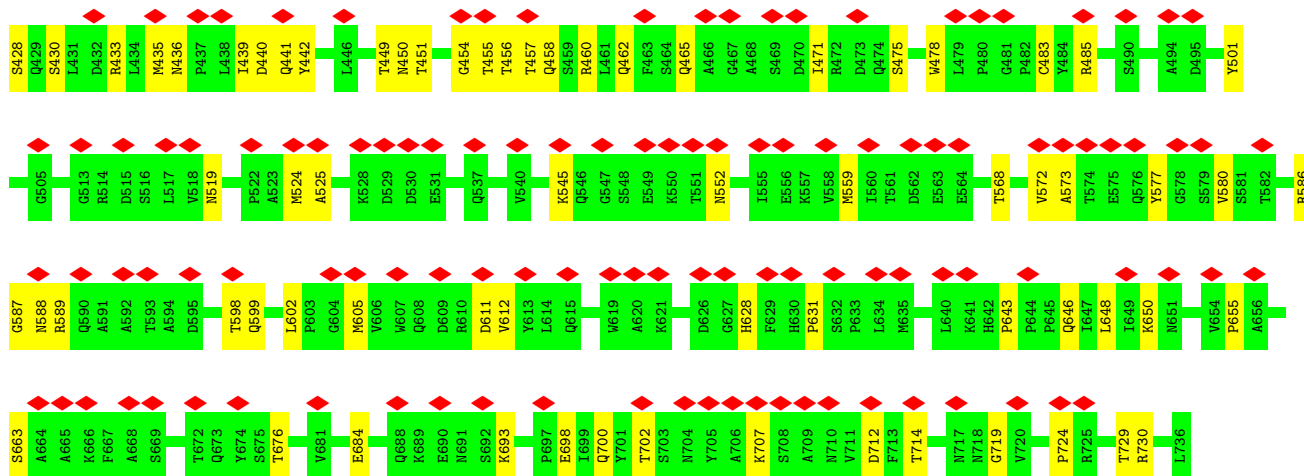


• Molecule 1: Capsid protein VP1

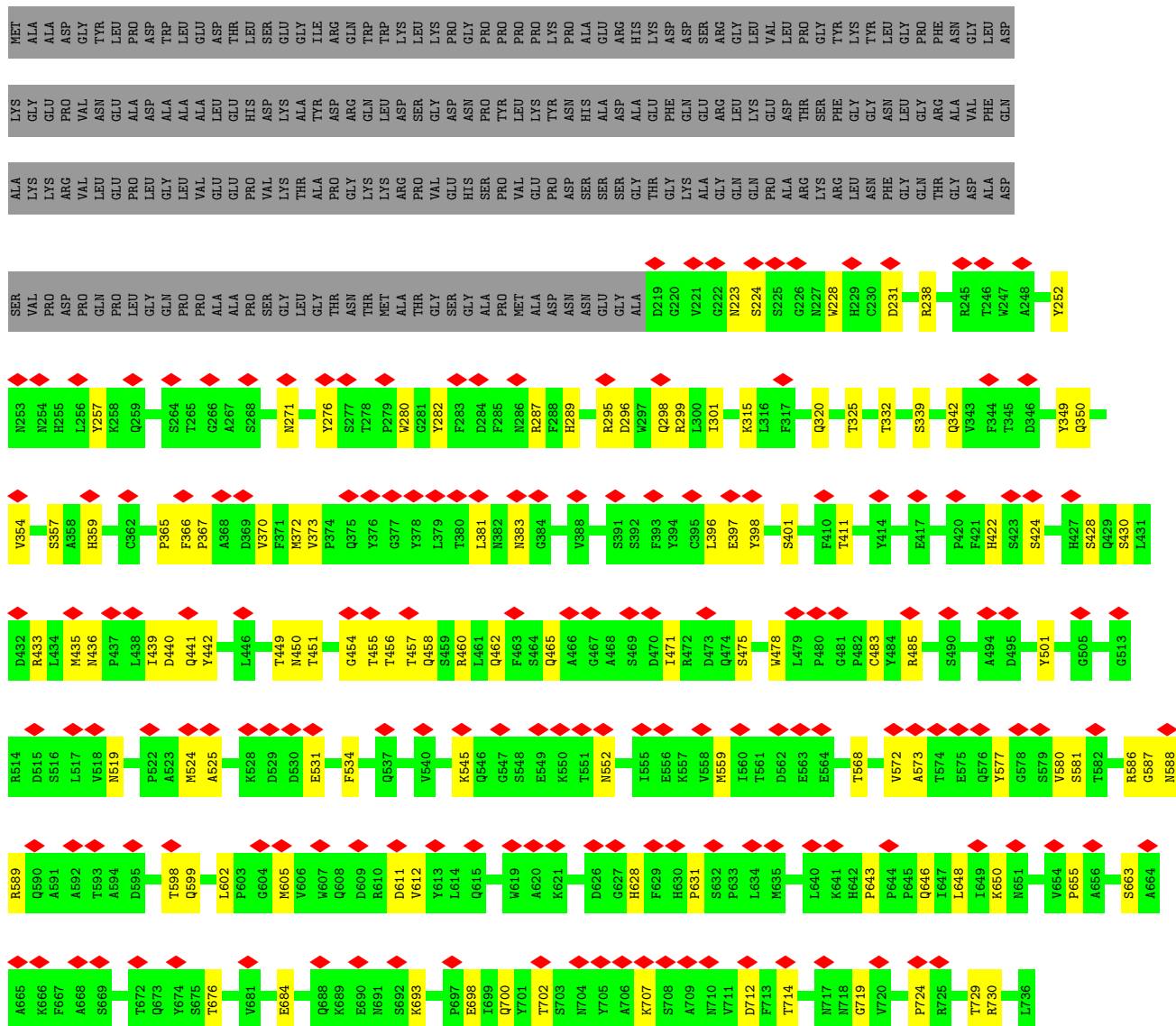


• Molecule 1: Capsid protein VP1

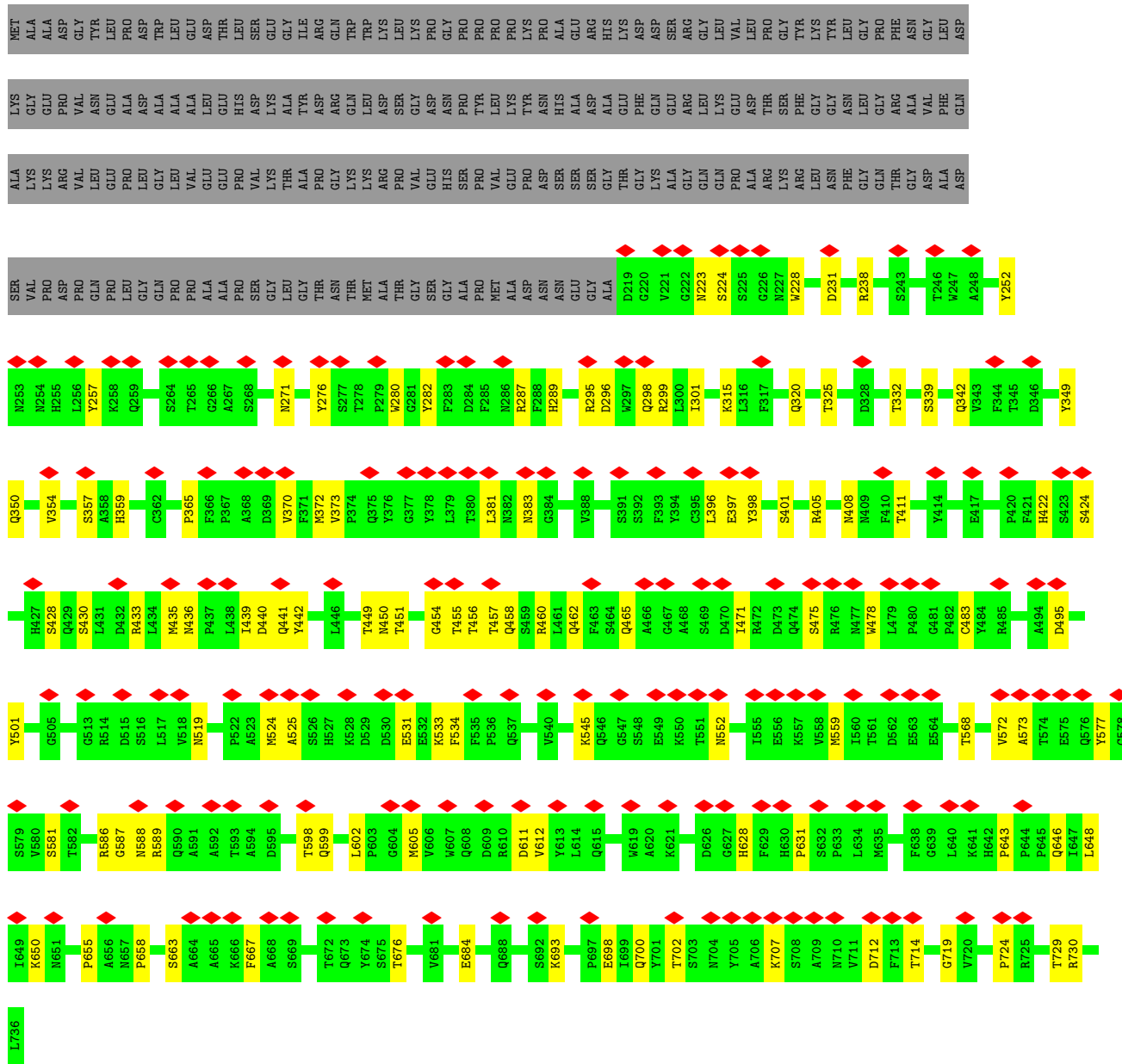




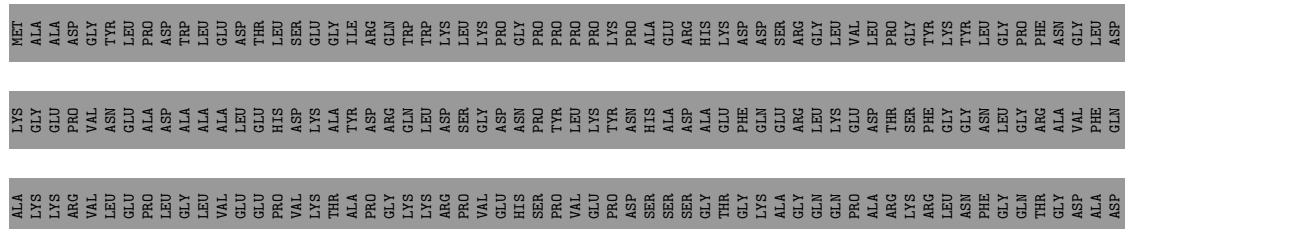
• Molecule 1: Capsid protein VP1

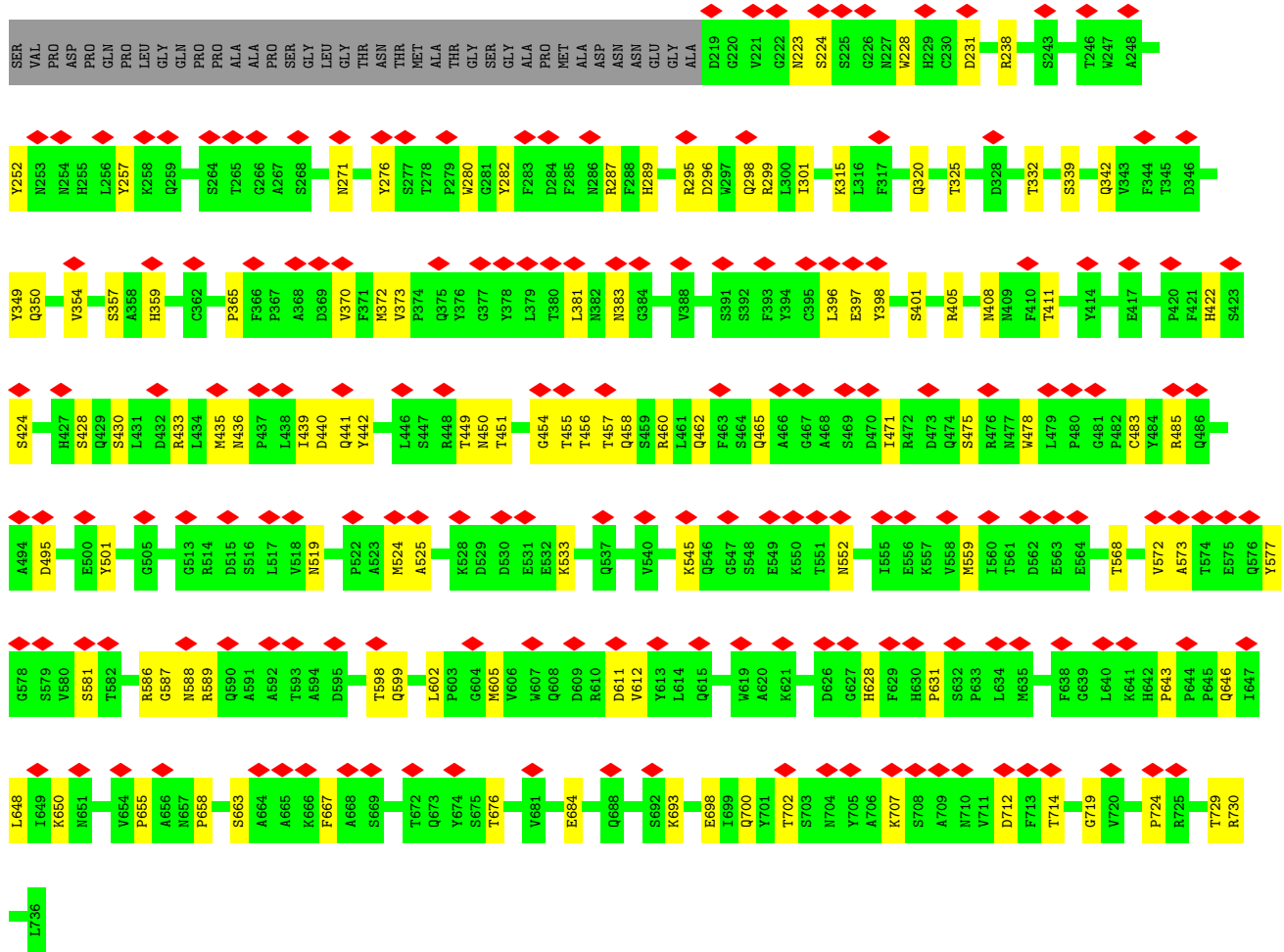


Molecule 1: Capsid protein VP1

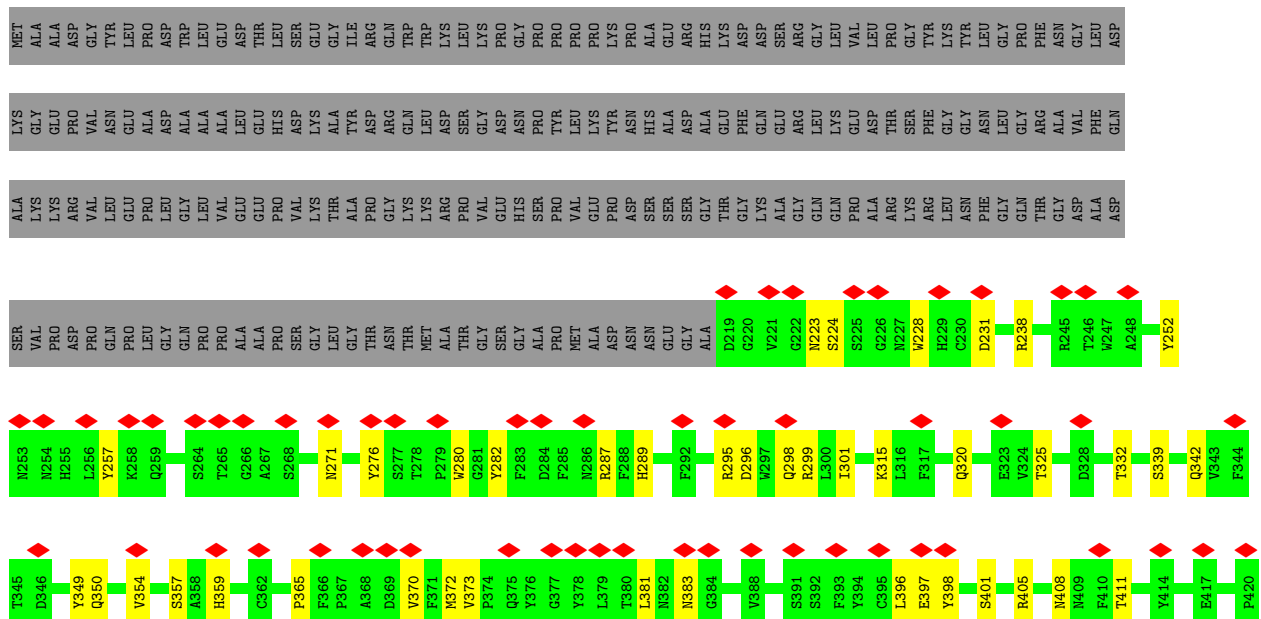


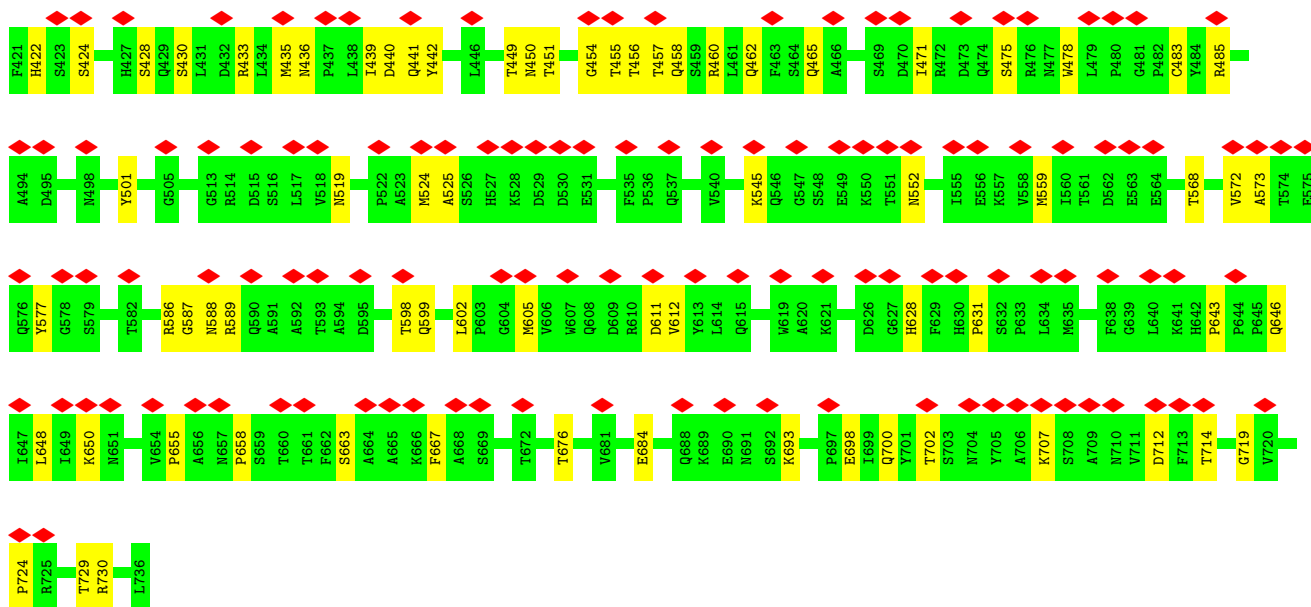
Molecule 1: Capsid protein VP1



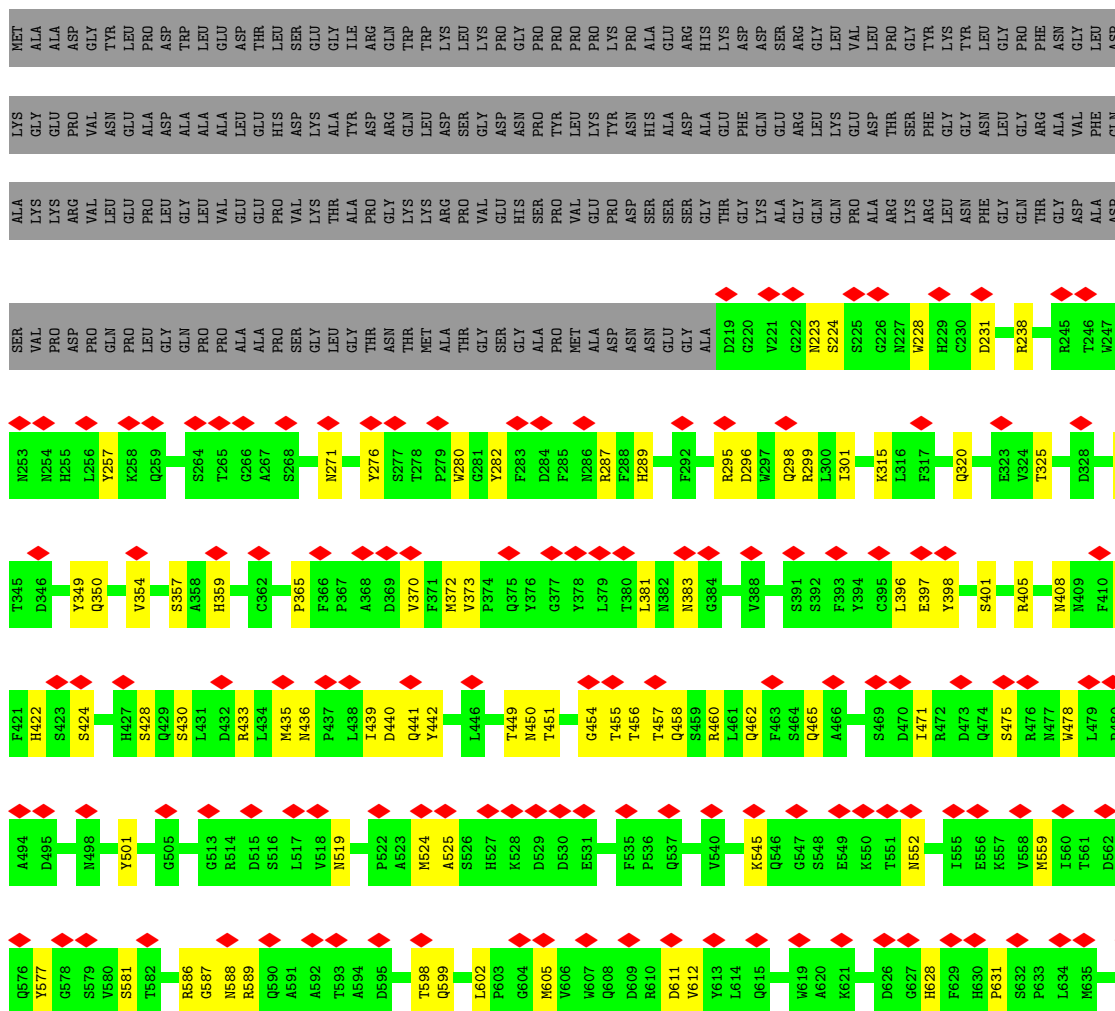


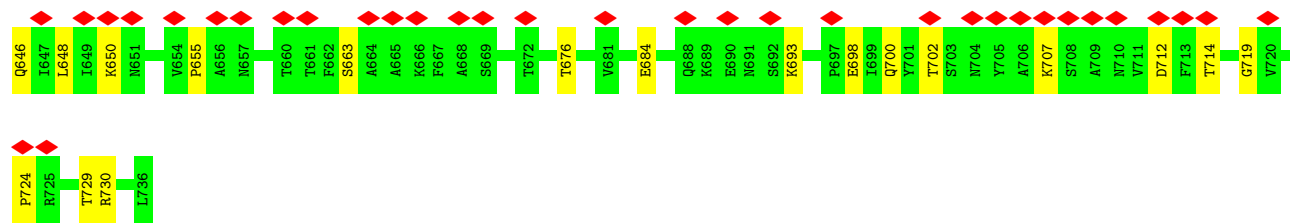
● Molecule 1: Capsid protein VP1





• Molecule 1: Capsid protein VP1





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	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	0.44	0/4265	0.50	0/5814
1	1	0.44	0/4265	0.50	0/5814
1	2	0.44	0/4265	0.50	0/5814
1	3	0.44	0/4265	0.50	0/5814
1	4	0.44	0/4265	0.50	0/5814
1	5	0.44	0/4265	0.50	0/5814
1	6	0.44	0/4265	0.50	0/5814
1	7	0.44	0/4265	0.50	0/5814
1	A	0.44	0/4265	0.50	0/5814
1	B	0.44	0/4265	0.50	0/5814
1	C	0.44	0/4265	0.50	0/5814
1	D	0.44	0/4265	0.50	0/5814
1	E	0.44	0/4265	0.50	0/5814
1	F	0.44	0/4265	0.50	0/5814
1	G	0.44	0/4265	0.50	0/5814
1	H	0.44	0/4265	0.50	0/5814
1	I	0.44	0/4265	0.50	0/5814
1	J	0.44	0/4265	0.50	0/5814
1	K	0.44	0/4265	0.50	0/5814
1	L	0.44	0/4265	0.50	0/5814
1	M	0.44	0/4265	0.50	0/5814
1	N	0.44	0/4265	0.50	0/5814
1	O	0.44	0/4265	0.50	0/5814
1	P	0.44	0/4265	0.50	0/5814
1	Q	0.44	0/4265	0.50	0/5814
1	R	0.44	0/4265	0.50	0/5814
1	S	0.44	0/4265	0.50	0/5814
1	T	0.44	0/4265	0.50	0/5814
1	U	0.44	0/4265	0.50	0/5814
1	V	0.44	0/4265	0.50	0/5814
1	W	0.44	0/4265	0.50	0/5814
1	X	0.44	0/4265	0.50	0/5814
1	Y	0.44	0/4265	0.50	0/5814
1	Z	0.44	0/4265	0.50	0/5814

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.44	0/4265	0.50	0/5814
1	b	0.44	0/4265	0.50	0/5814
1	c	0.44	0/4265	0.50	0/5814
1	d	0.44	0/4265	0.50	0/5814
1	e	0.44	0/4265	0.50	0/5814
1	f	0.44	0/4265	0.50	0/5814
1	g	0.44	0/4265	0.50	0/5814
1	h	0.44	0/4265	0.50	0/5814
1	i	0.44	0/4265	0.50	0/5814
1	j	0.44	0/4265	0.50	0/5814
1	k	0.44	0/4265	0.50	0/5814
1	l	0.44	0/4265	0.50	0/5814
1	m	0.44	0/4265	0.50	0/5814
1	n	0.44	0/4265	0.50	0/5814
1	o	0.44	0/4265	0.50	0/5814
1	p	0.44	0/4265	0.50	0/5814
1	q	0.44	0/4265	0.50	0/5814
1	r	0.44	0/4265	0.50	0/5814
1	s	0.44	0/4265	0.50	0/5814
1	t	0.44	0/4265	0.50	0/5814
1	u	0.44	0/4265	0.50	0/5814
1	v	0.44	0/4265	0.50	0/5814
1	w	0.44	0/4265	0.50	0/5814
1	x	0.44	0/4265	0.50	0/5814
1	y	0.44	0/4265	0.50	0/5814
1	z	0.44	0/4265	0.50	0/5814
All	All	0.44	0/255900	0.50	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.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4142	0	3894	101	0
1	1	4142	0	3894	102	0
1	2	4142	0	3894	102	0
1	3	4142	0	3894	102	0
1	4	4142	0	3894	104	0
1	5	4142	0	3894	103	0
1	6	4142	0	3894	101	0
1	7	4142	0	3894	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4142	0	3894	100	0
1	B	4142	0	3894	103	0
1	C	4142	0	3894	102	0
1	D	4142	0	3894	102	0
1	E	4142	0	3894	103	0
1	F	4142	0	3894	103	0
1	G	4142	0	3894	100	0
1	H	4142	0	3894	102	0
1	I	4142	0	3894	100	0
1	J	4142	0	3894	103	0
1	K	4142	0	3894	101	0
1	L	4142	0	3894	104	0
1	M	4142	0	3894	102	0
1	N	4142	0	3894	102	0
1	O	4142	0	3894	101	0
1	P	4142	0	3894	103	0
1	Q	4142	0	3894	102	0
1	R	4142	0	3894	101	0
1	S	4142	0	3894	101	0
1	T	4142	0	3894	100	0
1	U	4142	0	3894	102	0
1	V	4142	0	3894	104	0
1	W	4142	0	3894	100	0
1	X	4142	0	3894	103	0
1	Y	4142	0	3894	99	0
1	Z	4142	0	3894	103	0
1	a	4142	0	3894	101	0
1	b	4142	0	3894	102	0
1	c	4142	0	3894	103	0
1	d	4142	0	3894	105	0
1	e	4142	0	3894	102	0
1	f	4142	0	3894	103	0
1	g	4142	0	3894	102	0
1	h	4142	0	3894	103	0
1	i	4142	0	3894	103	0
1	j	4142	0	3894	104	0
1	k	4142	0	3894	102	0
1	l	4142	0	3894	101	0
1	m	4142	0	3894	103	0
1	n	4142	0	3894	105	0
1	o	4142	0	3894	102	0
1	p	4142	0	3894	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	q	4142	0	3894	102	0
1	r	4142	0	3894	101	0
1	s	4142	0	3894	100	0
1	t	4142	0	3894	102	0
1	u	4142	0	3894	103	0
1	v	4142	0	3894	103	0
1	w	4142	0	3894	103	0
1	x	4142	0	3894	104	0
1	y	4142	0	3894	102	0
1	z	4142	0	3894	104	0
All	All	248520	0	233640	4623	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 10.

The worst 5 of 4623 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:R:430:SER:HA	1:R:568:THR:HG23	1.58	0.86
1:O:430:SER:HA	1:O:568:THR:HG23	1.58	0.86
1:D:430:SER:HA	1:D:568:THR:HG23	1.58	0.86
1:t:430:SER:HA	1:t:568:THR:HG23	1.58	0.86
1:I:430:SER:HA	1:I:568:THR:HG23	1.58	0.86

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	0	516/736 (70%)	506 (98%)	10 (2%)	0	100	100
1	1	516/736 (70%)	506 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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. 5 of 1028 such sidechains are listed below:

Mol	Chain	Res	Type
1	w	462	GLN
1	x	628	HIS
1	w	458	GLN
1	W	465	GLN
1	V	718	ASN

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 oligosaccharides 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

There are no chain breaks in this entry.

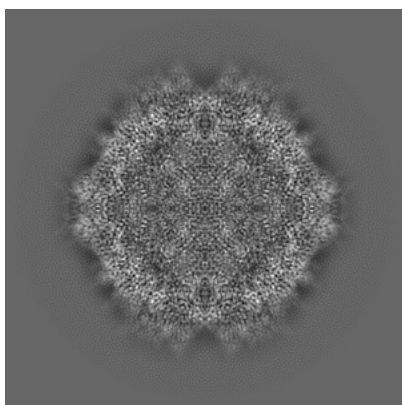
6 Map visualisation [i](#)

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.

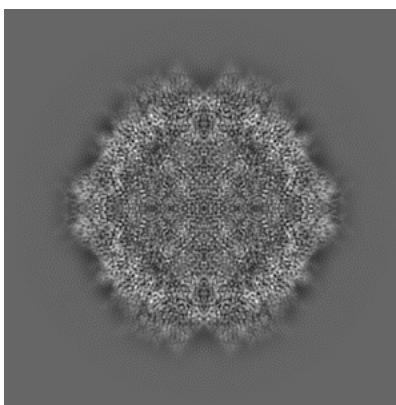
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

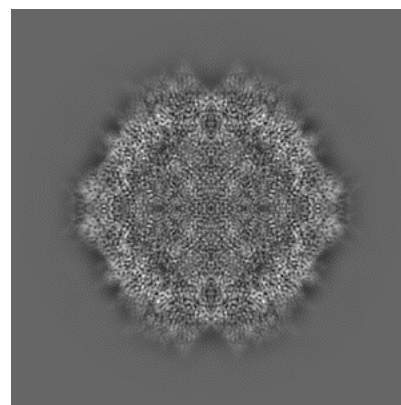
6.1.1 Primary map



X



Y

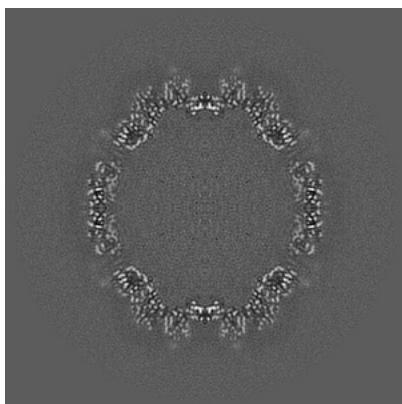


Z

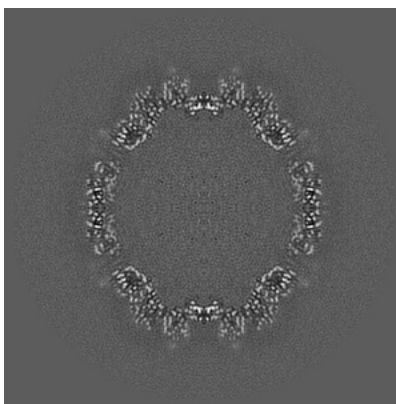
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

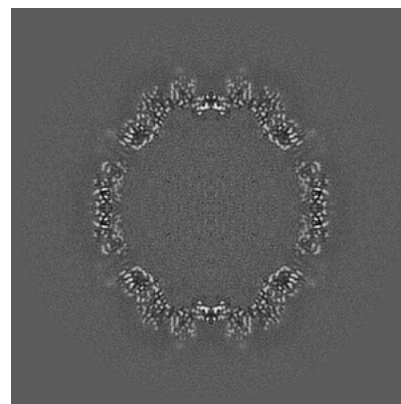
6.2.1 Primary map



X Index: 199



Y Index: 199

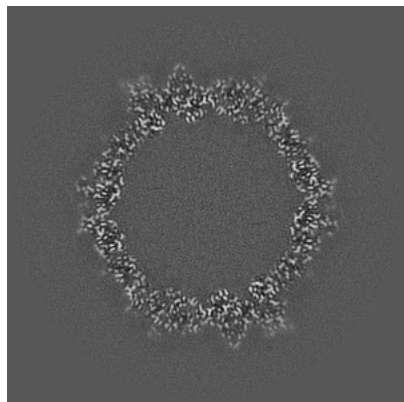


Z Index: 199

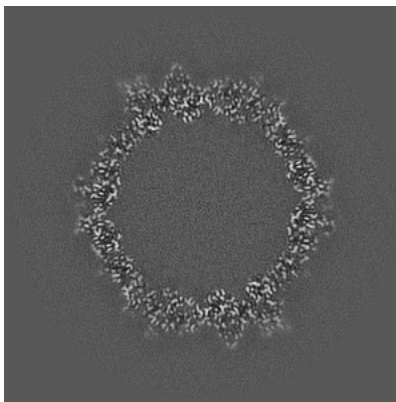
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

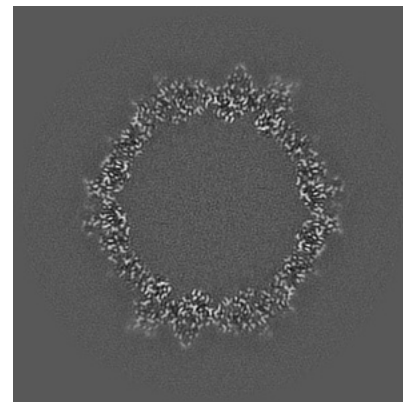
6.3.1 Primary map



X Index: 214



Y Index: 214

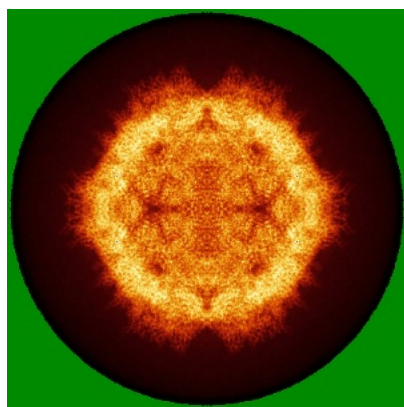


Z Index: 184

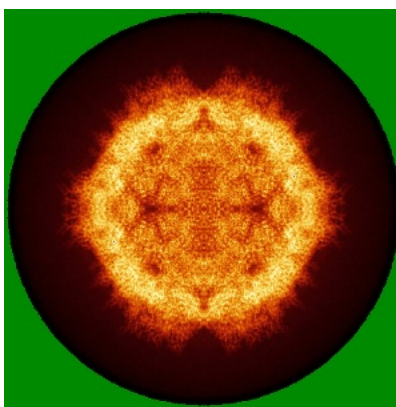
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

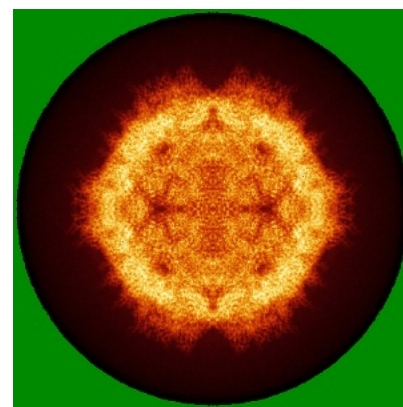
6.4.1 Primary map



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

This section was not generated.

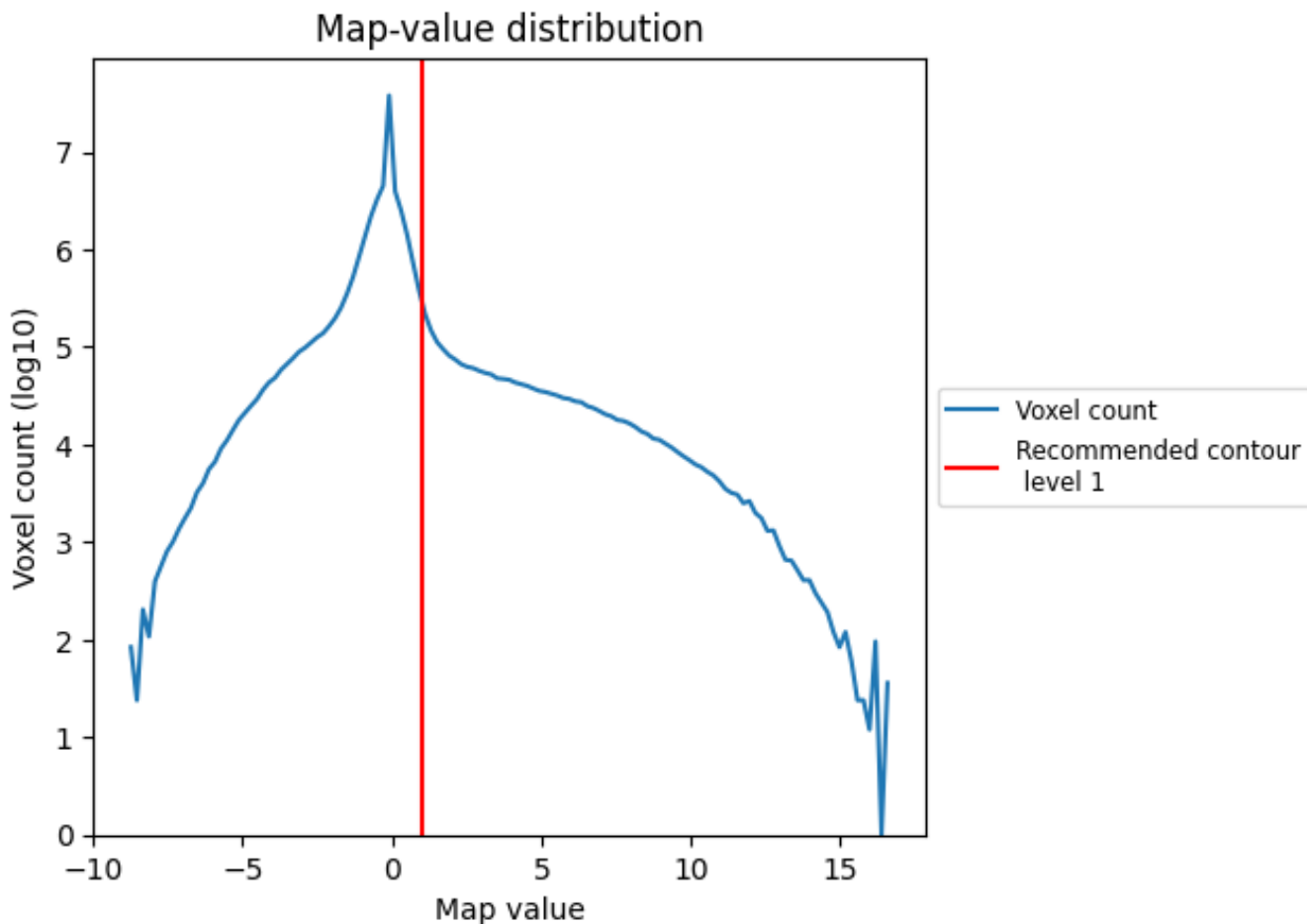
6.6 Mask visualisation

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

7 Map analysis [i](#)

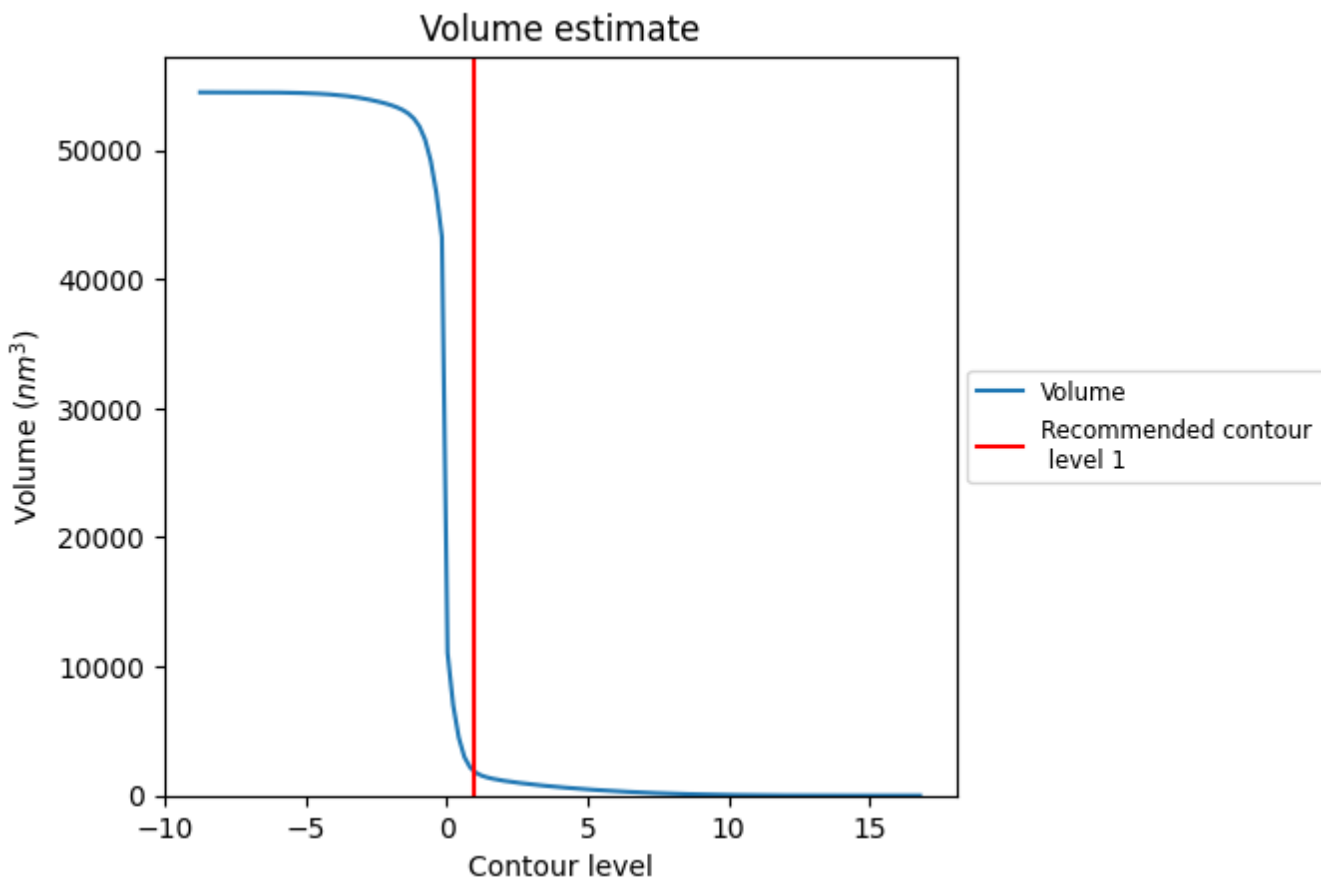
This section contains the results of statistical analysis of the map.

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.

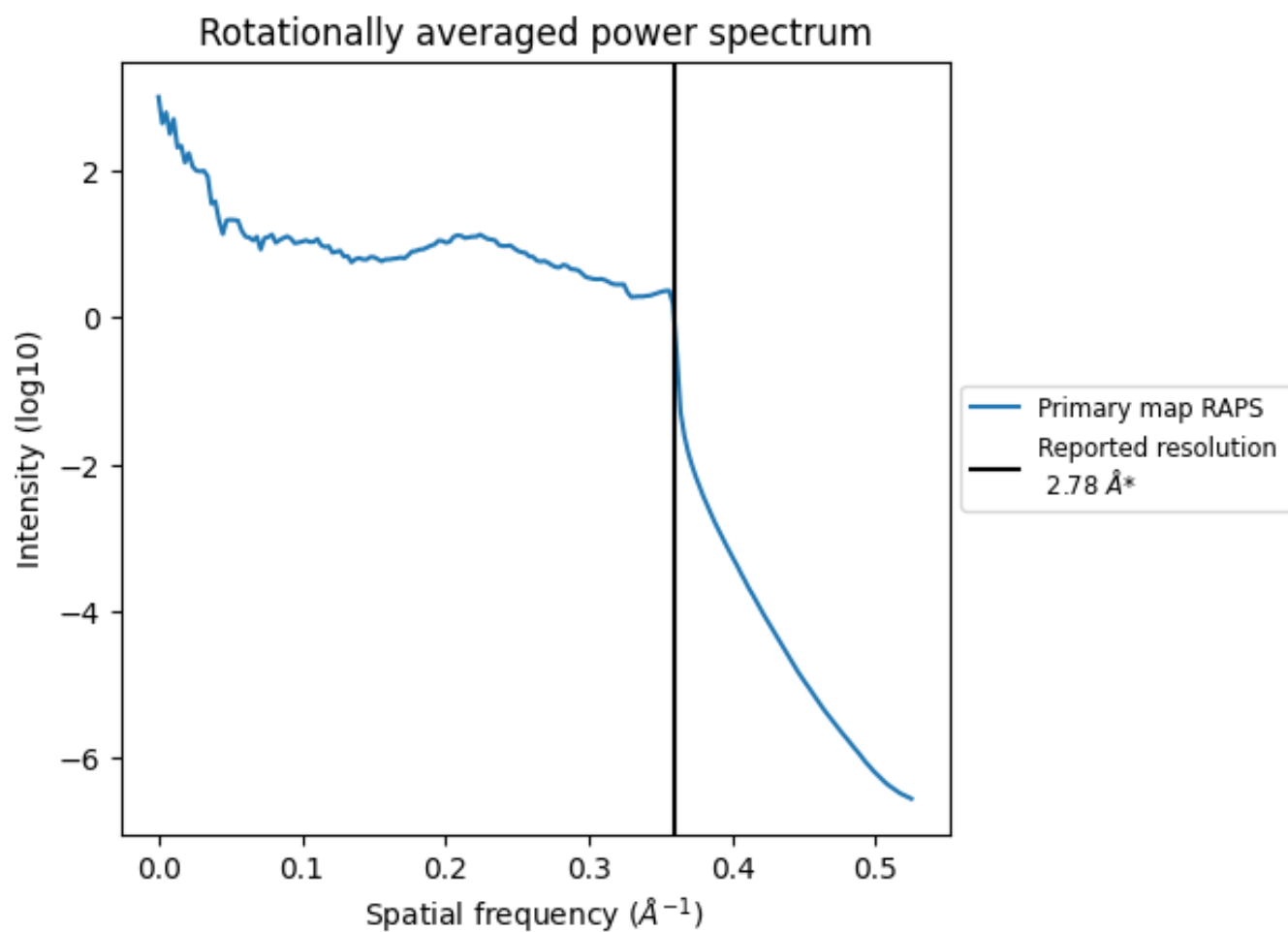
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1837 nm³; 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\AA^{-1}

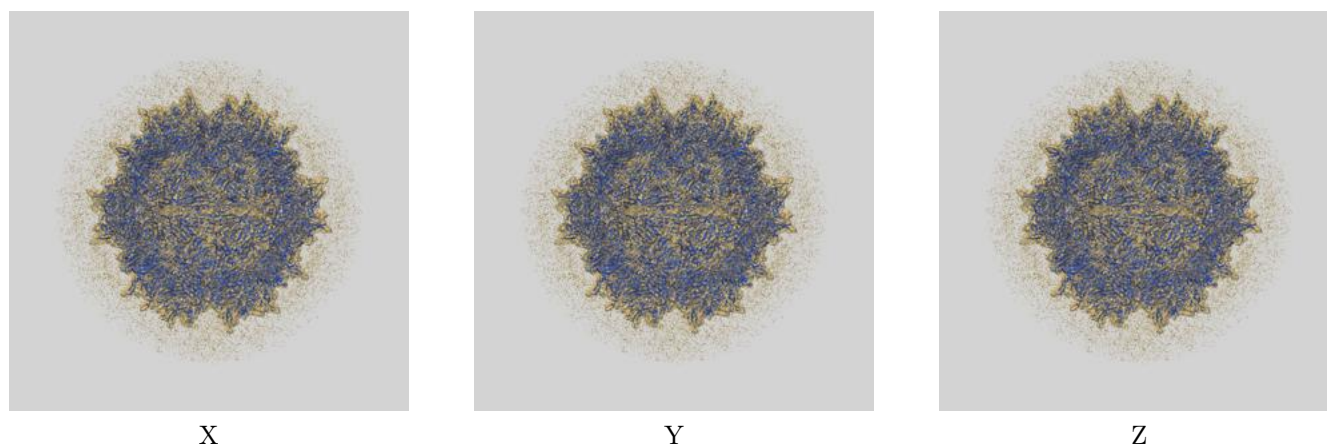
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

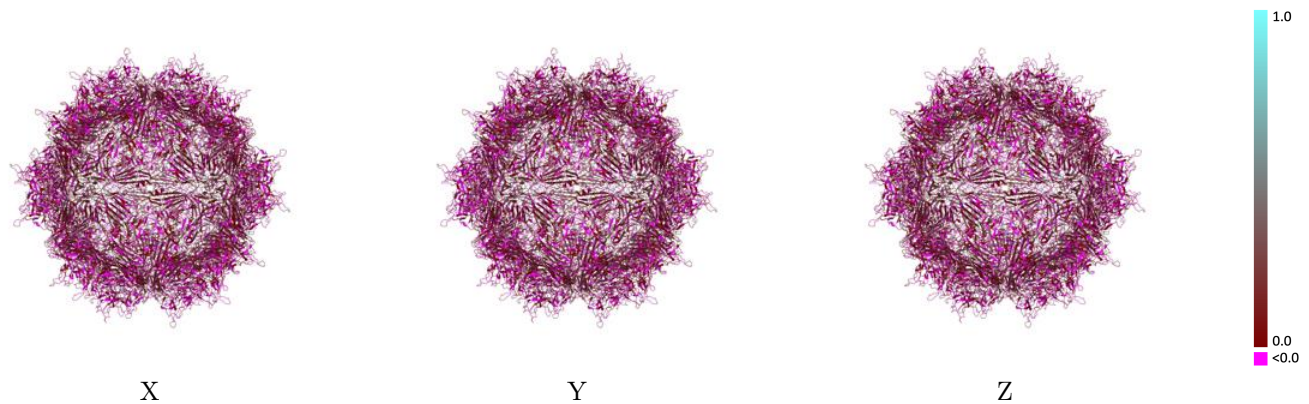
This section contains information regarding the fit between EMDB map EMD-7452 and PDB model 6CBE. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



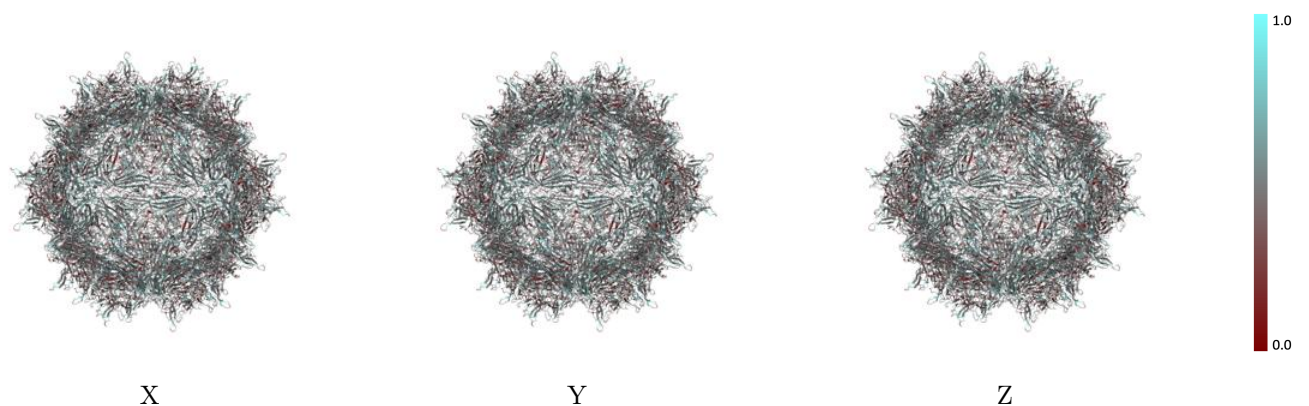
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



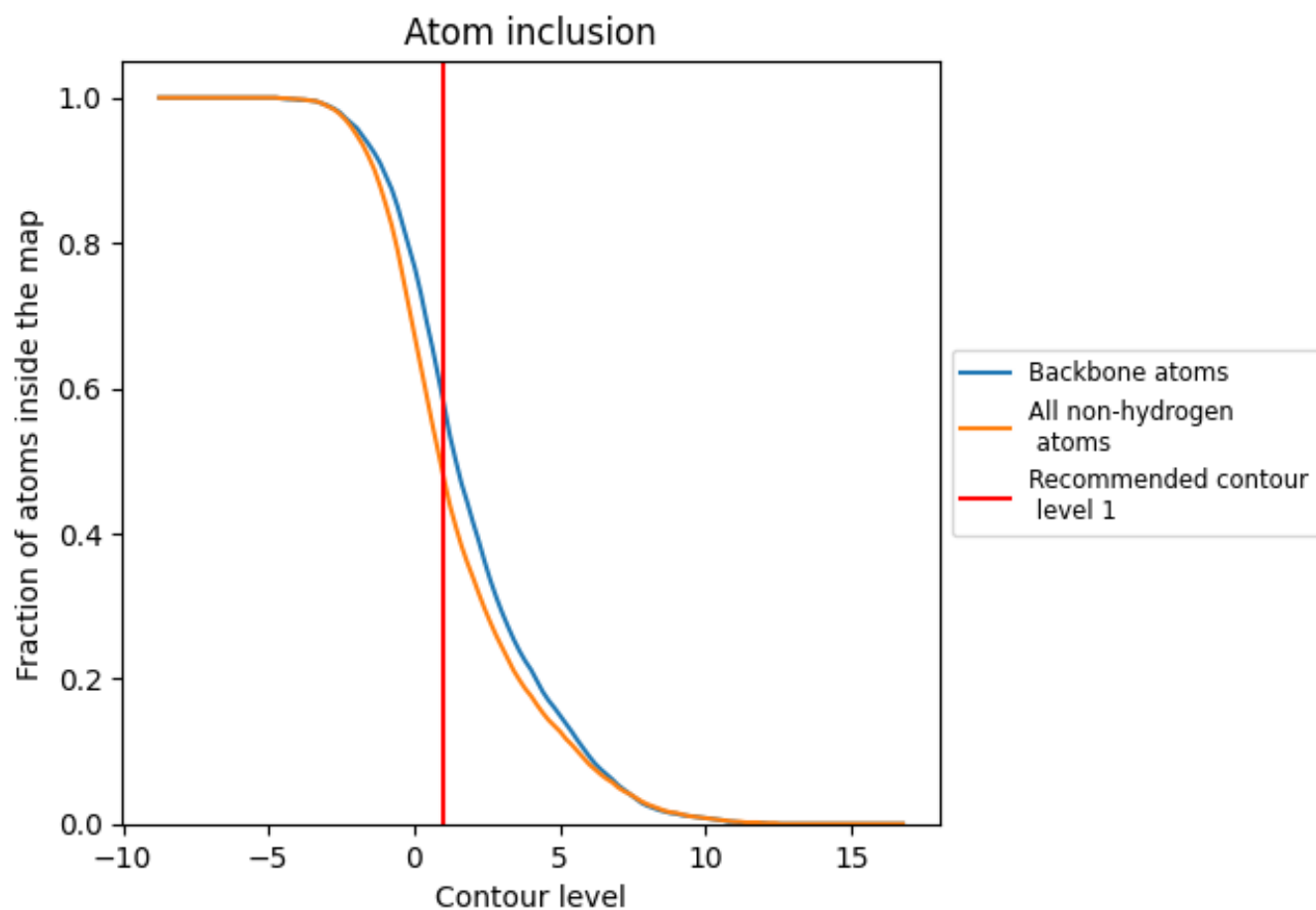
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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).

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) 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