



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 05:07 AM UTC

PDB ID : 5IPI / pdb_00005ipi
EMDB ID : EMD-8099
Title : Structure of Adeno-associated virus type 2 VLP
Authors : Drouin, L.M.; Lins, B.; Janssen, M.E.; Bennet, A.; Chipman, P.; McKenna, R.; Chen, W.; Muzyczka, N.; Cardone, G.; Baker, T.S.; Agbandje-McKenna, M.
Deposited on : 2016-03-09
Resolution : 3.80 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:

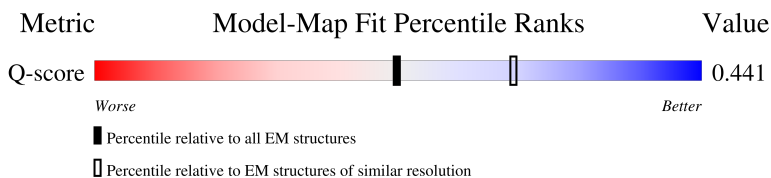
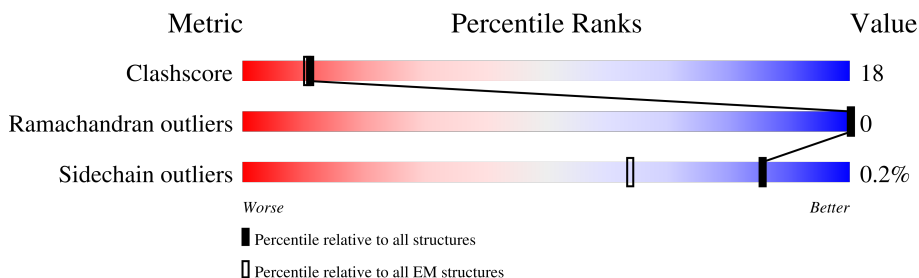
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.80 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	10198 (3.30 - 4.30)

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	1	735	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">44%</div> <div style="text-align: right;">25%</div> <div style="text-align: right;">30%</div> </div>
1	2	735	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">45%</div> <div style="text-align: right;">24%</div> <div style="text-align: right;">30%</div> </div>
1	3	735	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">16%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">44%</div> <div style="text-align: right;">25%</div> <div style="text-align: right;">30%</div> </div>
1	4	735	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">44%</div> <div style="text-align: right;">25%</div> <div style="text-align: right;">30%</div> </div>

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Mol	Chain	Length	Quality of chain			
1	5	735	17%	44%	25%	30%
1	6	735	17%	44%	25%	30%
1	7	735	16%	44%	26%	30%
1	8	735	16%	44%	25%	30%
1	A	735	17%	44%	26%	30%
1	B	735	17%	43%	26%	30%
1	C	735	16%	44%	25%	30%
1	D	735	17%	44%	25%	30%
1	E	735	16%	44%	26%	30%
1	F	735	17%	44%	25%	30%
1	G	735	17%	44%	26%	30%
1	H	735	17%	43%	26%	30%
1	I	735	17%	44%	25%	30%
1	J	735	17%	44%	25%	30%
1	K	735	17%	44%	26%	30%
1	L	735	17%	44%	25%	30%
1	M	735	16%	44%	25%	30%
1	N	735	17%	44%	26%	30%
1	O	735	17%	44%	25%	30%
1	P	735	17%	45%	25%	30%
1	Q	735	16%	44%	25%	30%
1	R	735	16%	44%	26%	30%
1	S	735	17%	44%	25%	30%
1	T	735	17%	44%	25%	30%
1	U	735	17%	44%	25%	30%

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Mol	Chain	Length	Quality of chain			
1	V	735	17%	43%	26%	30%
1	W	735	17%	44%	25%	30%
1	X	735	17%	45%	24%	30%
1	Y	735	16%	43%	26%	30%
1	Z	735	17%	44%	25%	30%
1	a	735	16%	44%	26%	30%
1	b	735	17%	43%	26%	30%
1	c	735	17%	44%	25%	30%
1	d	735	17%	45%	24%	30%
1	e	735	17%	45%	24%	30%
1	f	735	16%	44%	25%	30%
1	g	735	17%	44%	25%	30%
1	h	735	16%	44%	26%	30%
1	i	735	17%	44%	26%	30%
1	j	735	16%	44%	25%	30%
1	k	735	17%	44%	25%	30%
1	l	735	17%	44%	25%	30%
1	m	735	17%	44%	25%	30%
1	n	735	17%	44%	25%	30%
1	o	735	17%	43%	26%	30%
1	p	735	17%	44%	26%	30%
1	q	735	17%	45%	24%	30%
1	r	735	17%	43%	26%	30%
1	s	735	17%	43%	26%	30%
1	t	735	17%	44%	26%	30%

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Mol	Chain	Length	Quality of chain
1	u	735	<p>17% 43% 26% 30%</p>
1	v	735	<p>16% 44% 25% 30%</p>
1	w	735	<p>17% 45% 24% 30%</p>
1	x	735	<p>17% 45% 24% 30%</p>
1	y	735	<p>17% 43% 26% 30%</p>
1	z	735	<p>17% 45% 25% 30%</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 246360 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	511	4106	2588	716	789	13	0	0
1	B	511	4106	2588	716	789	13	0	0
1	C	511	4106	2588	716	789	13	0	0
1	D	511	4106	2588	716	789	13	0	0
1	E	511	4106	2588	716	789	13	0	0
1	F	511	4106	2588	716	789	13	0	0
1	G	511	4106	2588	716	789	13	0	0
1	H	511	4106	2588	716	789	13	0	0
1	I	511	4106	2588	716	789	13	0	0
1	J	511	4106	2588	716	789	13	0	0
1	K	511	4106	2588	716	789	13	0	0
1	L	511	4106	2588	716	789	13	0	0
1	M	511	4106	2588	716	789	13	0	0
1	N	511	4106	2588	716	789	13	0	0
1	O	511	4106	2588	716	789	13	0	0
1	P	511	4106	2588	716	789	13	0	0
1	Q	511	4106	2588	716	789	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	S	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	T	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	U	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	V	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	W	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	X	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	Y	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	Z	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	a	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	b	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	c	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	d	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	e	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	f	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	g	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	h	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	i	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	j	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	k	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		
1	l	511	Total	C	N	O	S	0	0
			4106	2588	716	789	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	n	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	o	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	p	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	q	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	r	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	s	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	t	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	u	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	v	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	w	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	x	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	y	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	z	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	1	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	2	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	3	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	4	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	5	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	6	511	Total 4106	C 2588	N 716	O 789	S 13	0	0
1	7	511	Total 4106	C 2588	N 716	O 789	S 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	511	4106	2588	716	789	13	0	0

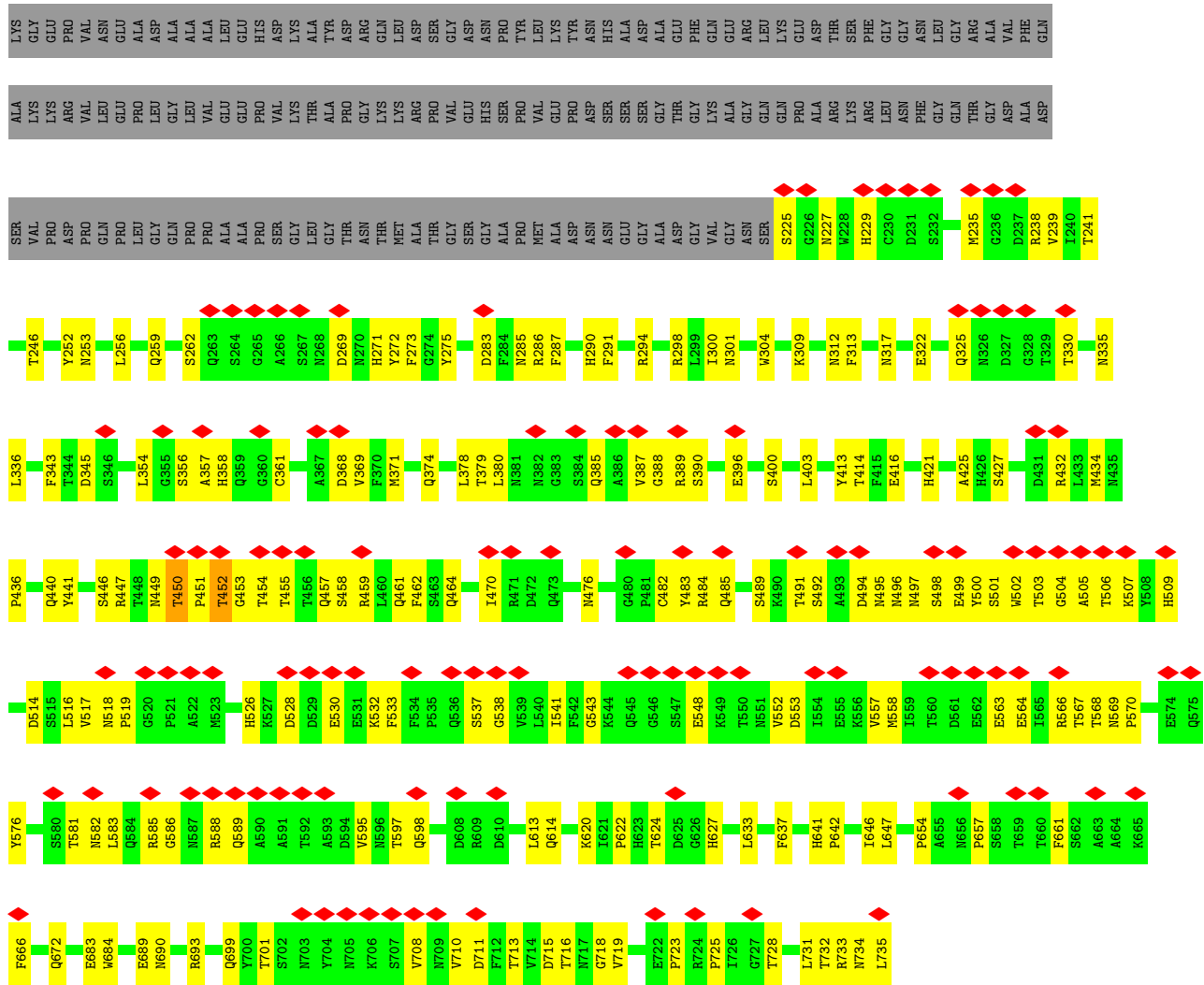
There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	THR	SER	conflict	UNP P03135
B	452	THR	SER	conflict	UNP P03135
C	452	THR	SER	conflict	UNP P03135
D	452	THR	SER	conflict	UNP P03135
E	452	THR	SER	conflict	UNP P03135
F	452	THR	SER	conflict	UNP P03135
G	452	THR	SER	conflict	UNP P03135
H	452	THR	SER	conflict	UNP P03135
I	452	THR	SER	conflict	UNP P03135
J	452	THR	SER	conflict	UNP P03135
K	452	THR	SER	conflict	UNP P03135
L	452	THR	SER	conflict	UNP P03135
M	452	THR	SER	conflict	UNP P03135
N	452	THR	SER	conflict	UNP P03135
O	452	THR	SER	conflict	UNP P03135
P	452	THR	SER	conflict	UNP P03135
Q	452	THR	SER	conflict	UNP P03135
R	452	THR	SER	conflict	UNP P03135
S	452	THR	SER	conflict	UNP P03135
T	452	THR	SER	conflict	UNP P03135
U	452	THR	SER	conflict	UNP P03135
V	452	THR	SER	conflict	UNP P03135
W	452	THR	SER	conflict	UNP P03135
X	452	THR	SER	conflict	UNP P03135
Y	452	THR	SER	conflict	UNP P03135
Z	452	THR	SER	conflict	UNP P03135
a	452	THR	SER	conflict	UNP P03135
b	452	THR	SER	conflict	UNP P03135
c	452	THR	SER	conflict	UNP P03135
d	452	THR	SER	conflict	UNP P03135
e	452	THR	SER	conflict	UNP P03135
f	452	THR	SER	conflict	UNP P03135
g	452	THR	SER	conflict	UNP P03135
h	452	THR	SER	conflict	UNP P03135
i	452	THR	SER	conflict	UNP P03135
j	452	THR	SER	conflict	UNP P03135

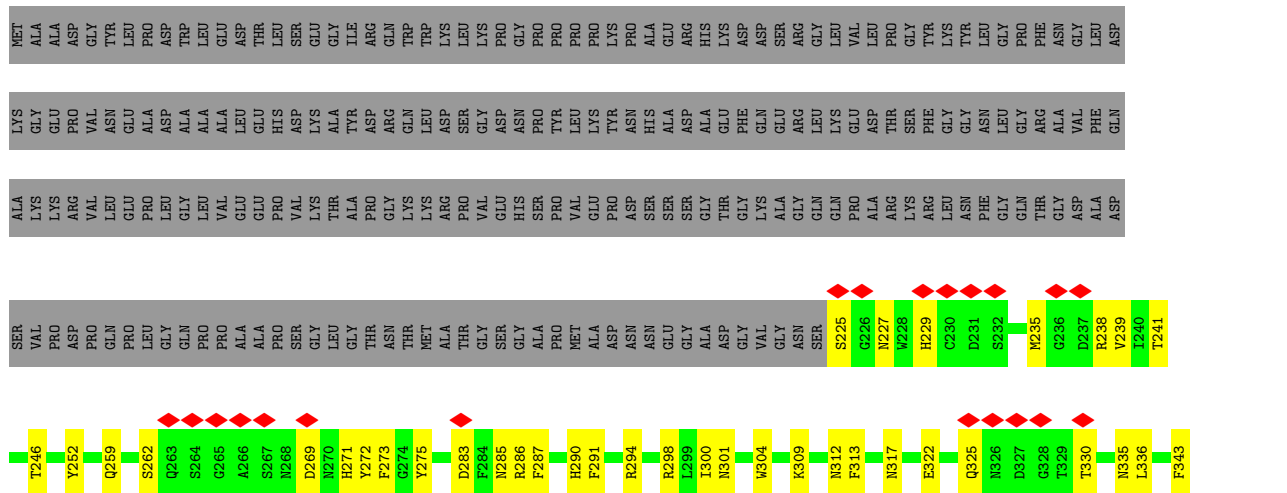
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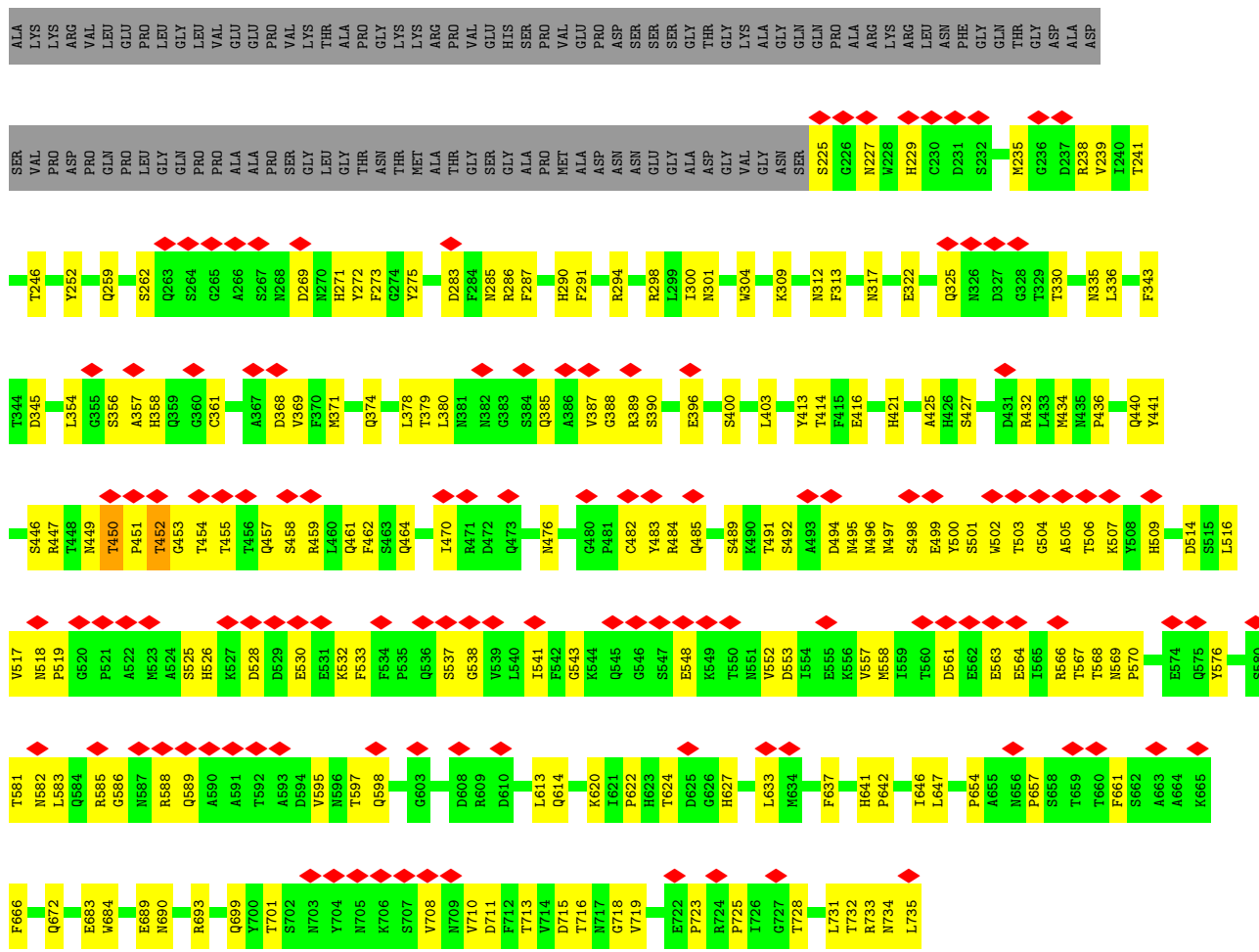
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Chain	Residue	Modelled	Actual	Comment	Reference
k	452	THR	SER	conflict	UNP P03135
l	452	THR	SER	conflict	UNP P03135
m	452	THR	SER	conflict	UNP P03135
n	452	THR	SER	conflict	UNP P03135
o	452	THR	SER	conflict	UNP P03135
p	452	THR	SER	conflict	UNP P03135
q	452	THR	SER	conflict	UNP P03135
r	452	THR	SER	conflict	UNP P03135
s	452	THR	SER	conflict	UNP P03135
t	452	THR	SER	conflict	UNP P03135
u	452	THR	SER	conflict	UNP P03135
v	452	THR	SER	conflict	UNP P03135
w	452	THR	SER	conflict	UNP P03135
x	452	THR	SER	conflict	UNP P03135
y	452	THR	SER	conflict	UNP P03135
z	452	THR	SER	conflict	UNP P03135
1	452	THR	SER	conflict	UNP P03135
2	452	THR	SER	conflict	UNP P03135
3	452	THR	SER	conflict	UNP P03135
4	452	THR	SER	conflict	UNP P03135
5	452	THR	SER	conflict	UNP P03135
6	452	THR	SER	conflict	UNP P03135
7	452	THR	SER	conflict	UNP P03135
8	452	THR	SER	conflict	UNP P03135

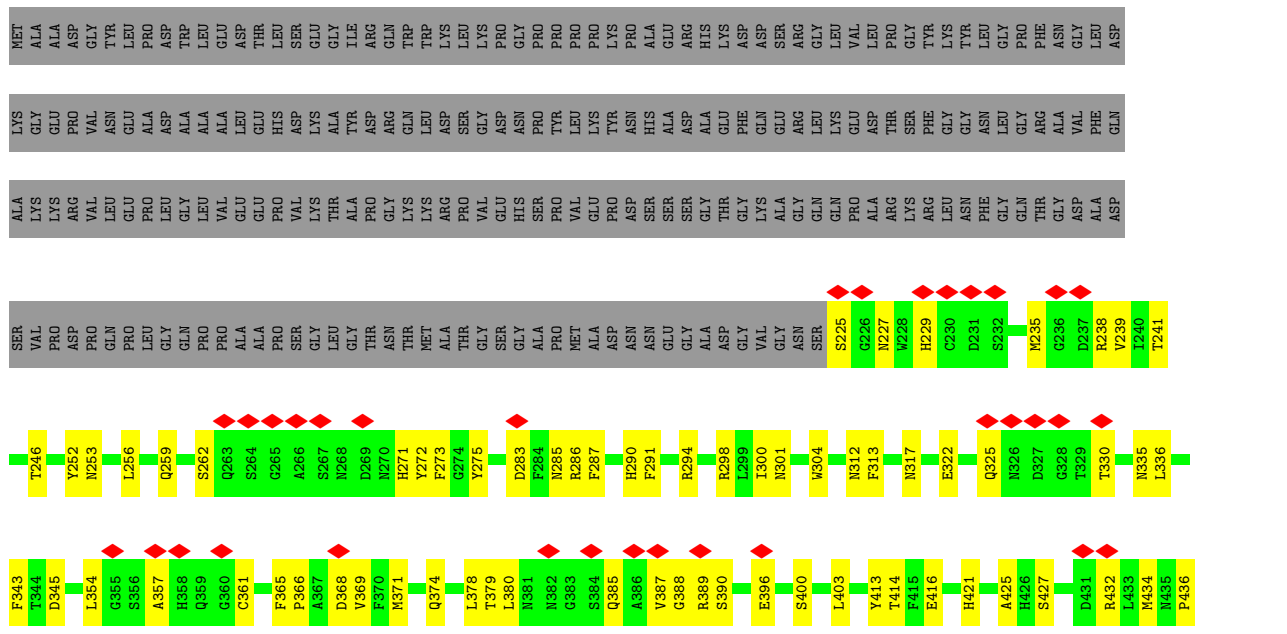


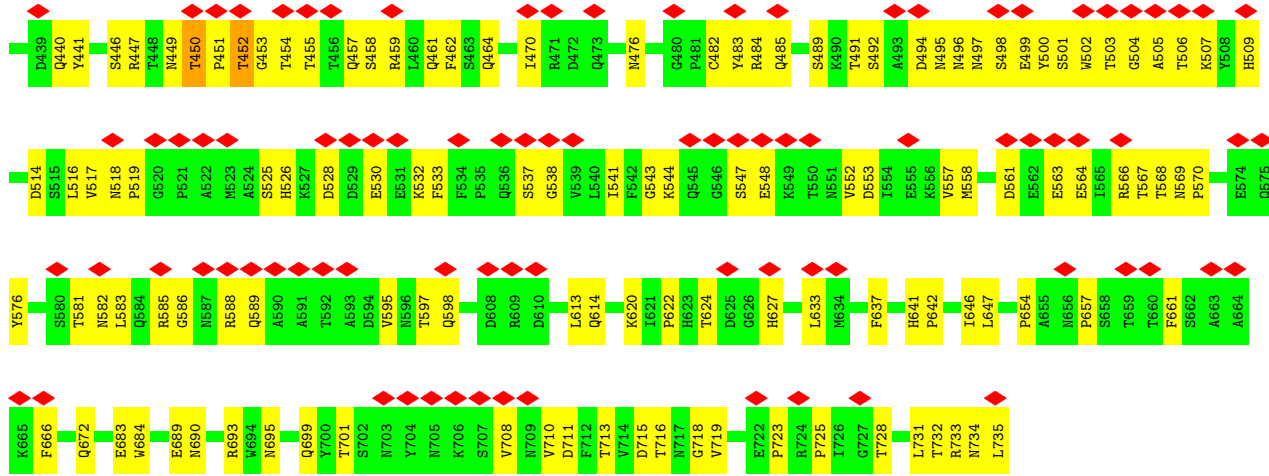
● Molecule 1: Capsid protein VP1



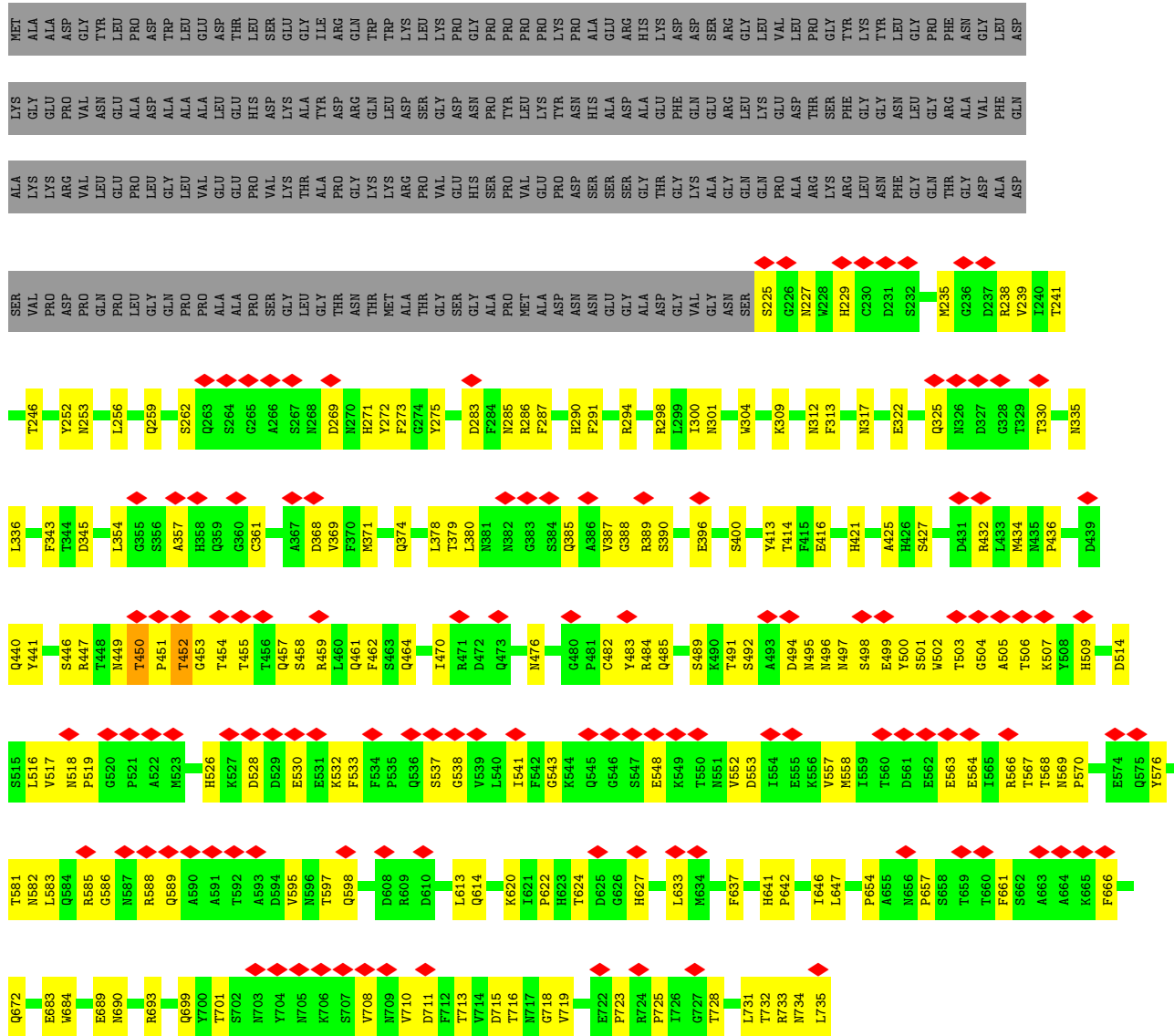


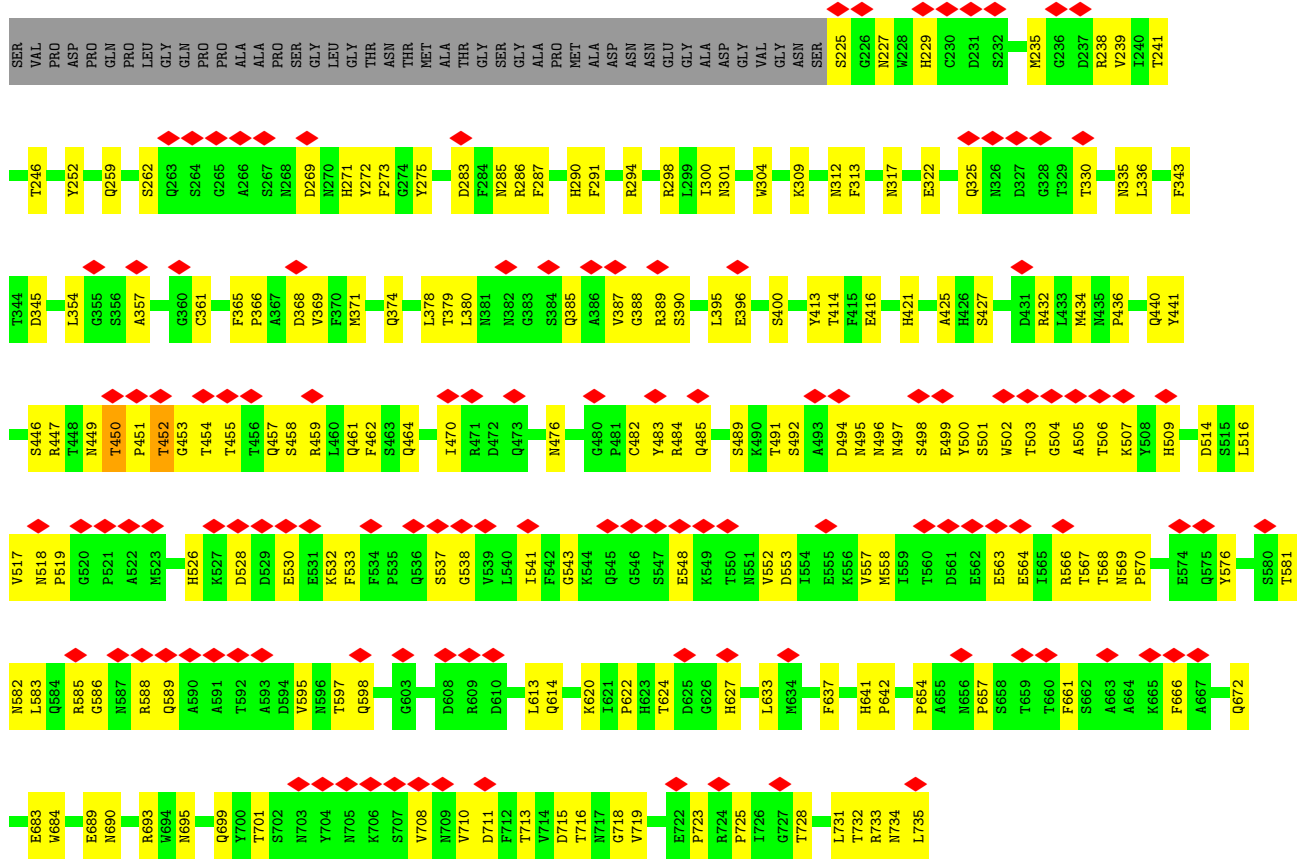
● Molecule 1: Capsid protein VP1



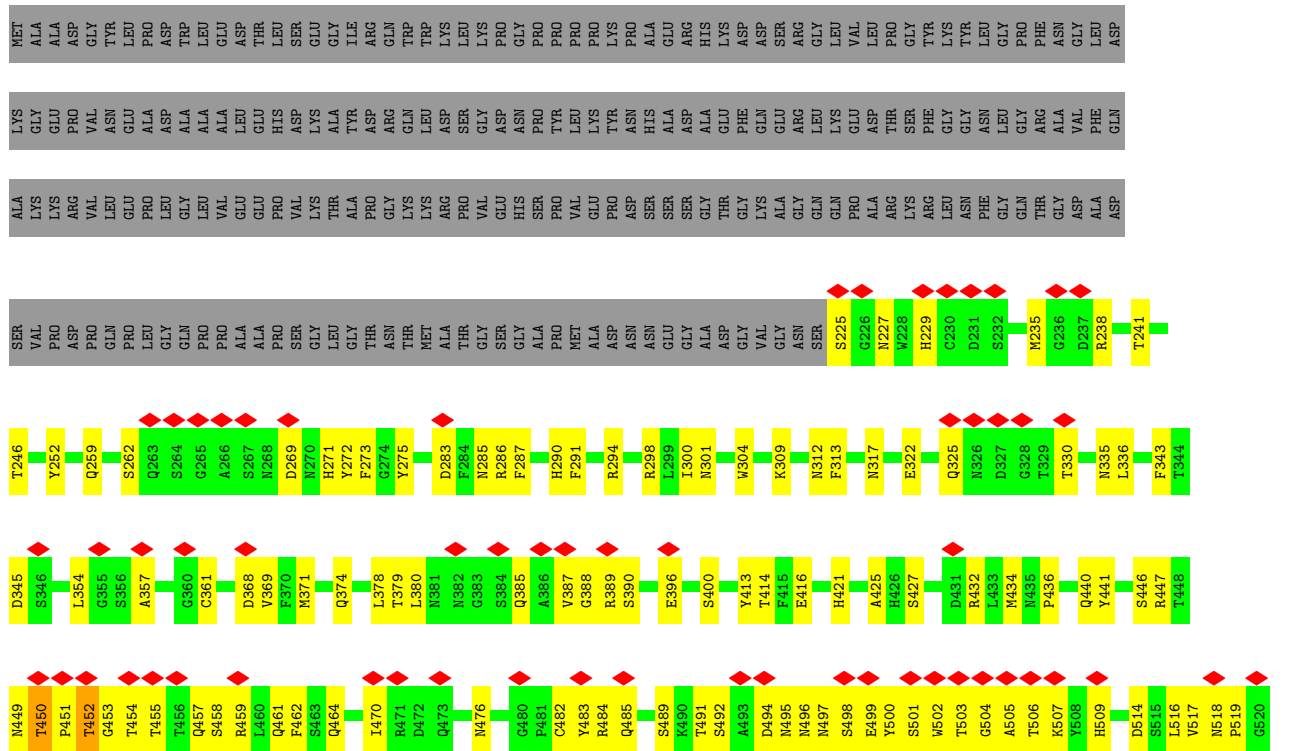
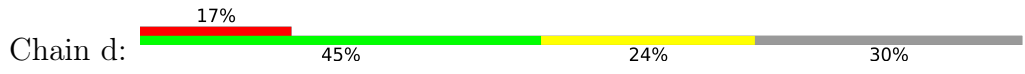


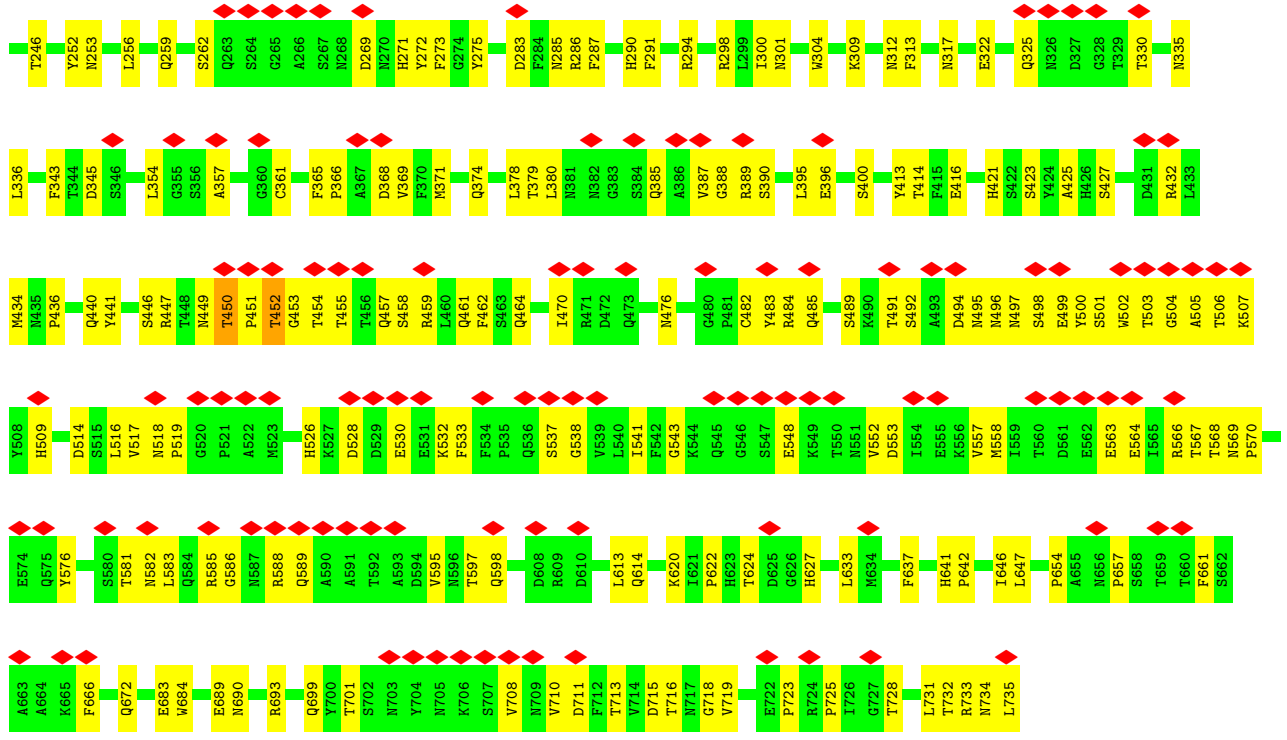
● Molecule 1: Capsid protein VP1



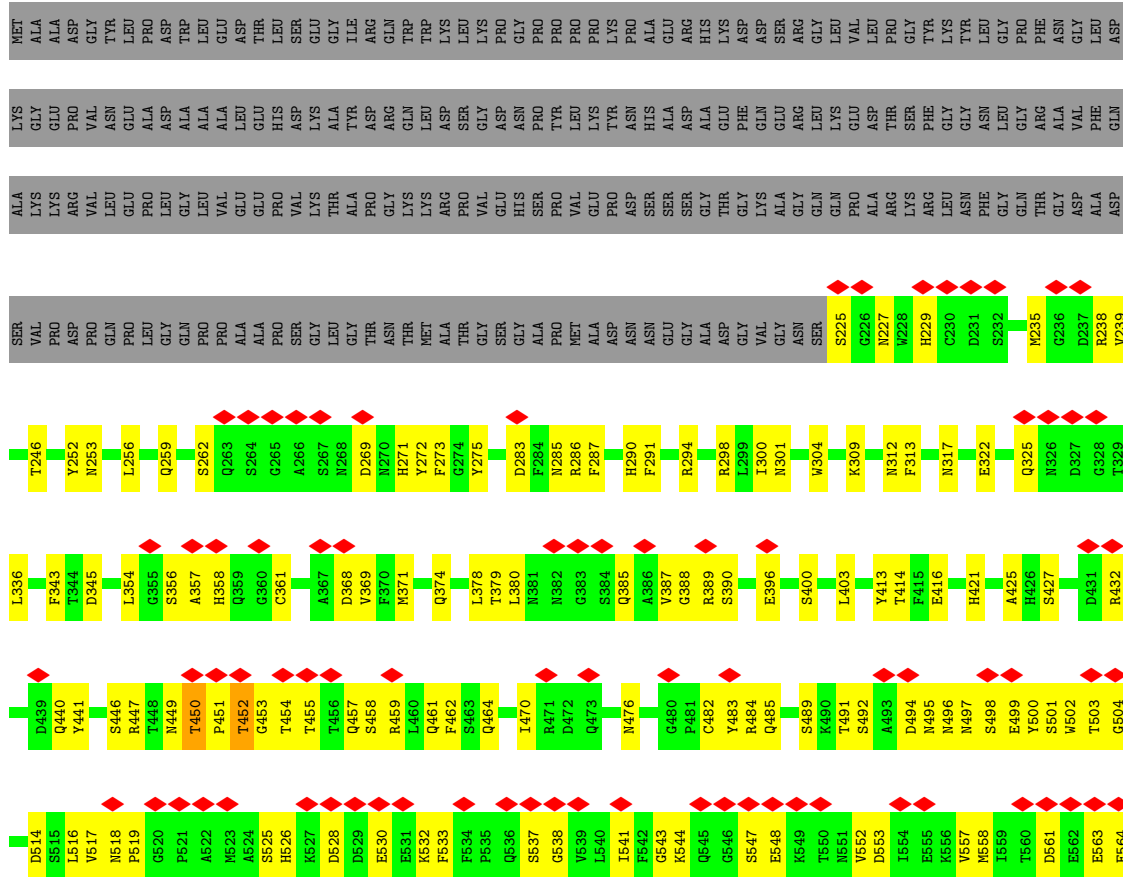


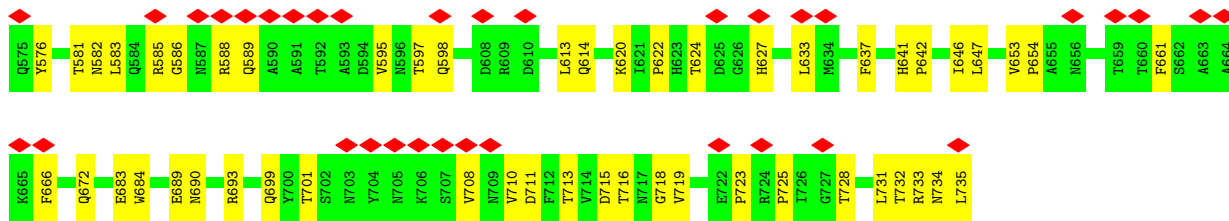
• Molecule 1: Capsid protein VP1



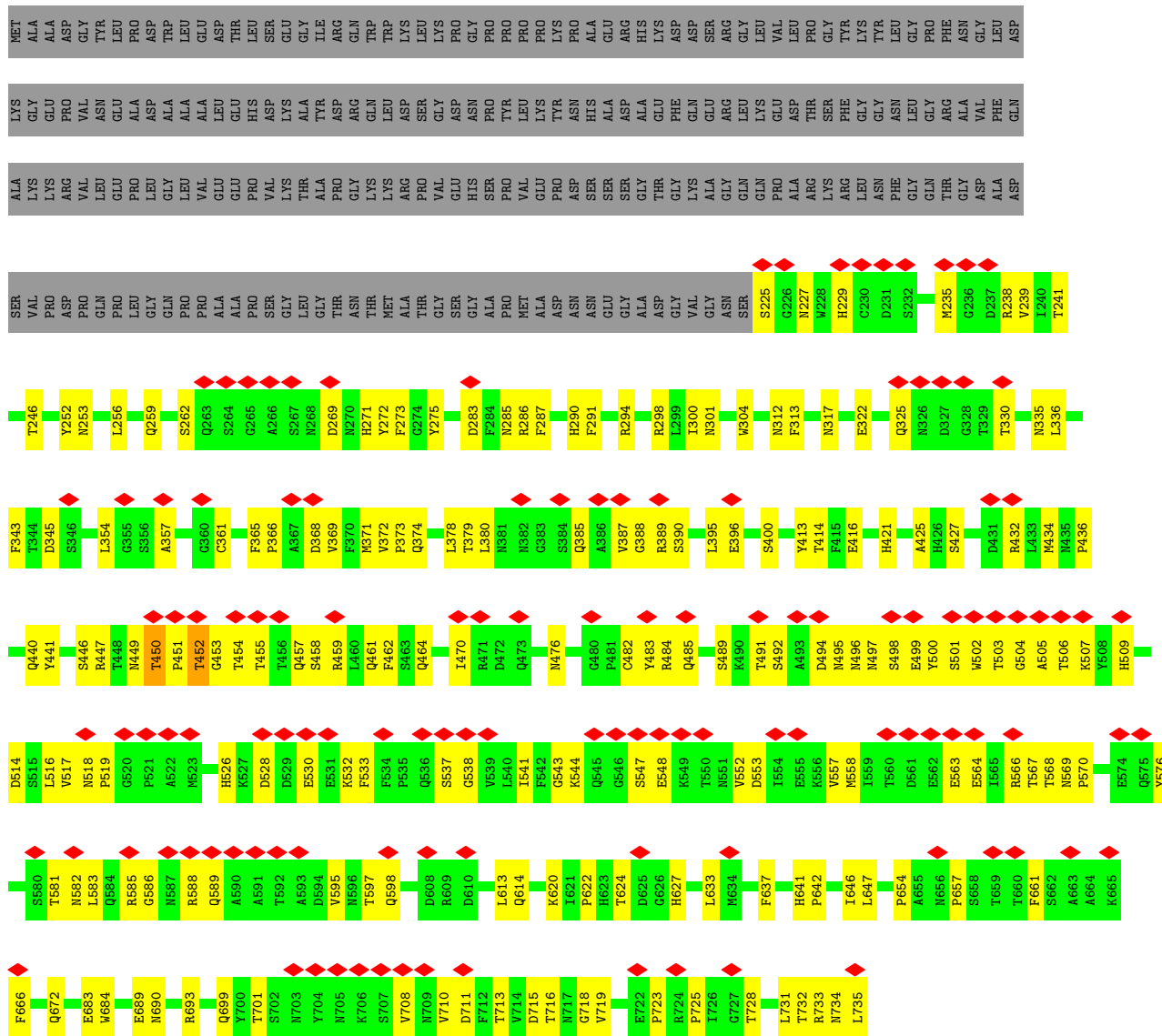


• Molecule 1: Capsid protein VP1

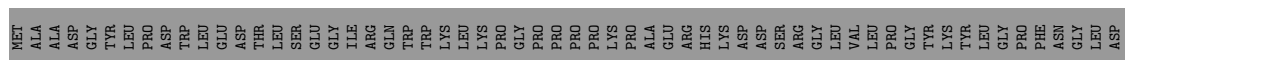
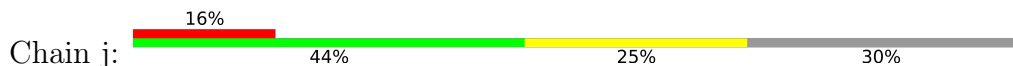


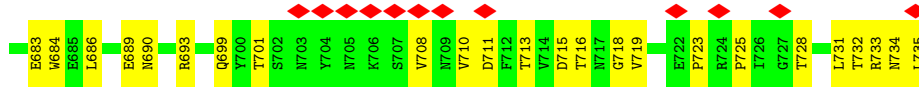


• Molecule 1: Capsid protein VP1

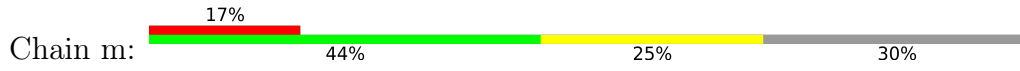


• Molecule 1: Capsid protein VP1

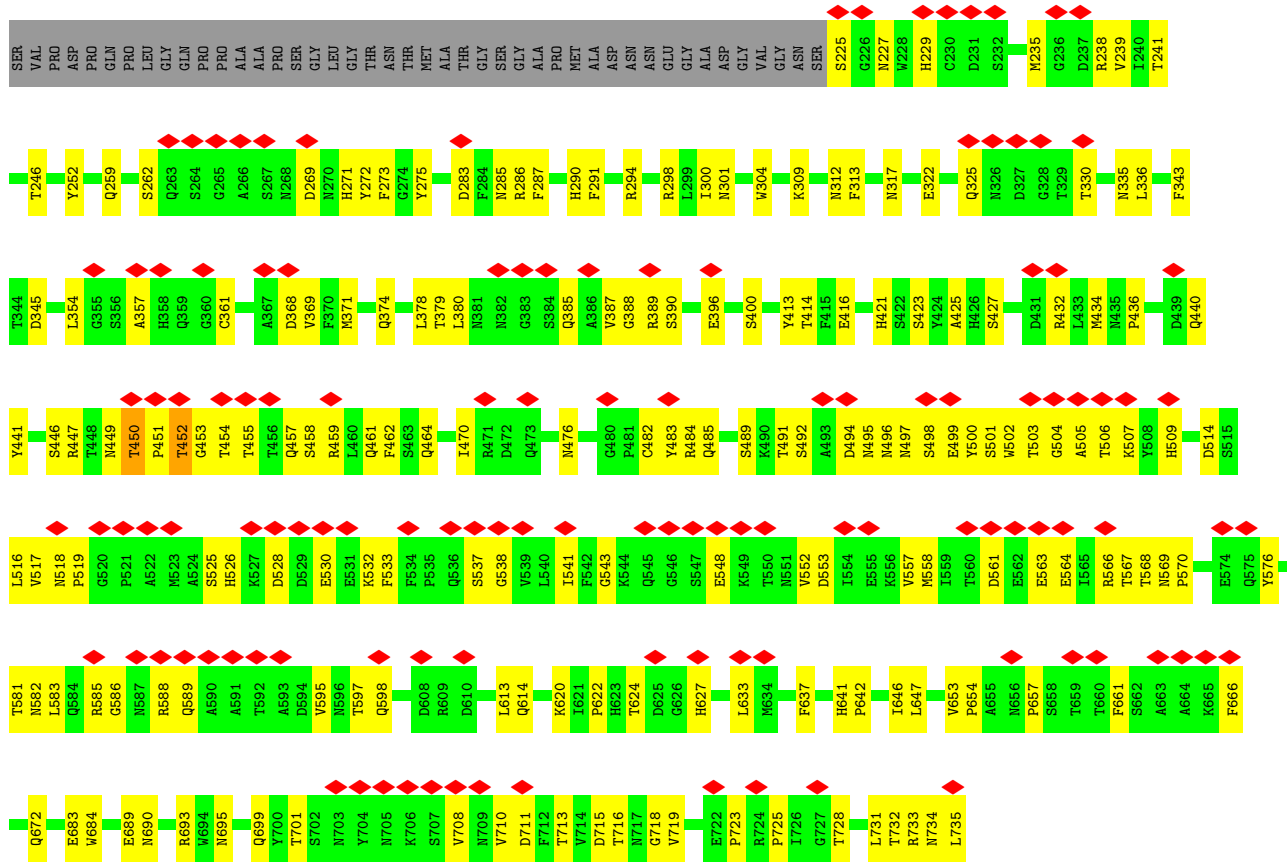




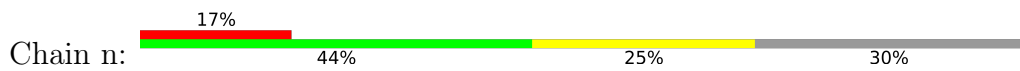
• Molecule 1: Capsid protein VP1



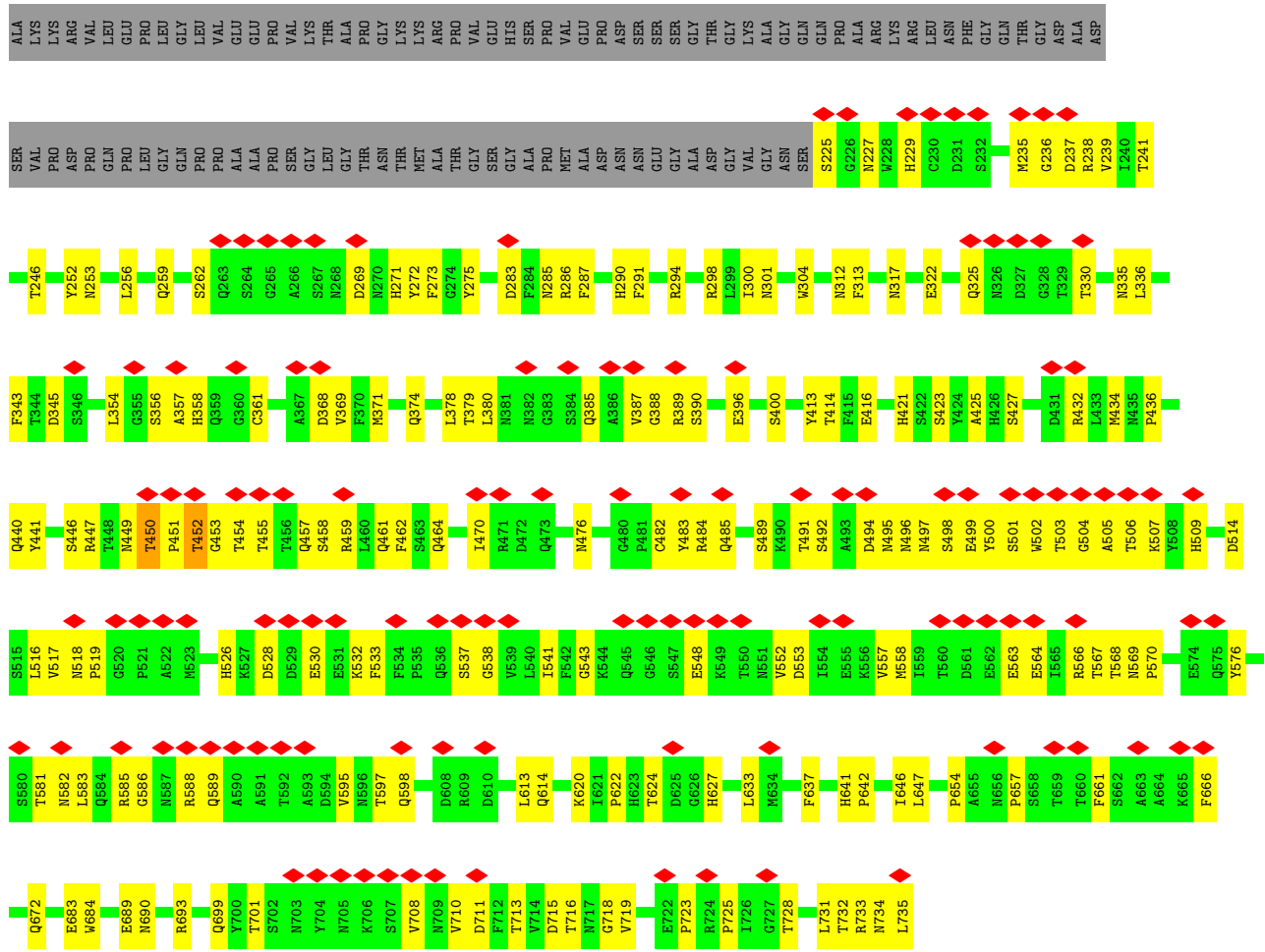
MET	ALA	ALA	ASP	GLY	TYR	LEU	PRO	ASP	TRP	LEU	GLU	ASP	THR	LEU	SER	GLY	GLY	ILE	ARG	GLN	TRP	LYS	LEU	TRP	LYS	PRO	LEU	LYS	VAL	D711	F712	T713	V714	D715	N716	G717	V718	V719	E722	P723	R724	P725	I726	G727	T728	L731	T732	R733	N734	L735						
LYS	GLY	GLU	PRO	VAL	ASN	GLU	ALA	ASP	ASP	ALA	ALA	LEU	GLU	HIS	SER	LYS	LYS	ALA	TYR	ARG	ASP	ARG	GLN	LEU	TRP	LYS	PRO	LEU	LYS	TYR	ASN	ALA	ALA	GLU	ASP	ALA	ALA	GLY	THR	PHE	GLY	ASP	GLY	VAL	LEU	ASP	THR	PRO	GLY	TYR	LEU	ASN	PHE	VAL	GLY	GLN
ALA	LYS	LYS	ARG	VAL	VAL	LEU	PRO	LEU	LEU	GLY	VAL	GLU	PRO	PRO	VAL	VAL	LYS	LYS	ALA	PRO	GLY	GLY	ARG	ASP	ARG	PRO	VAL	VAL	GLU	PRO	ASP	ASN	SER	SER	ALA	SER	GLY	THR	ALA	THR	GLY	GLN	PRO	ALA	ALA	VAL	GLY	THR	THR	GLY	ASP	ALA	ASP			



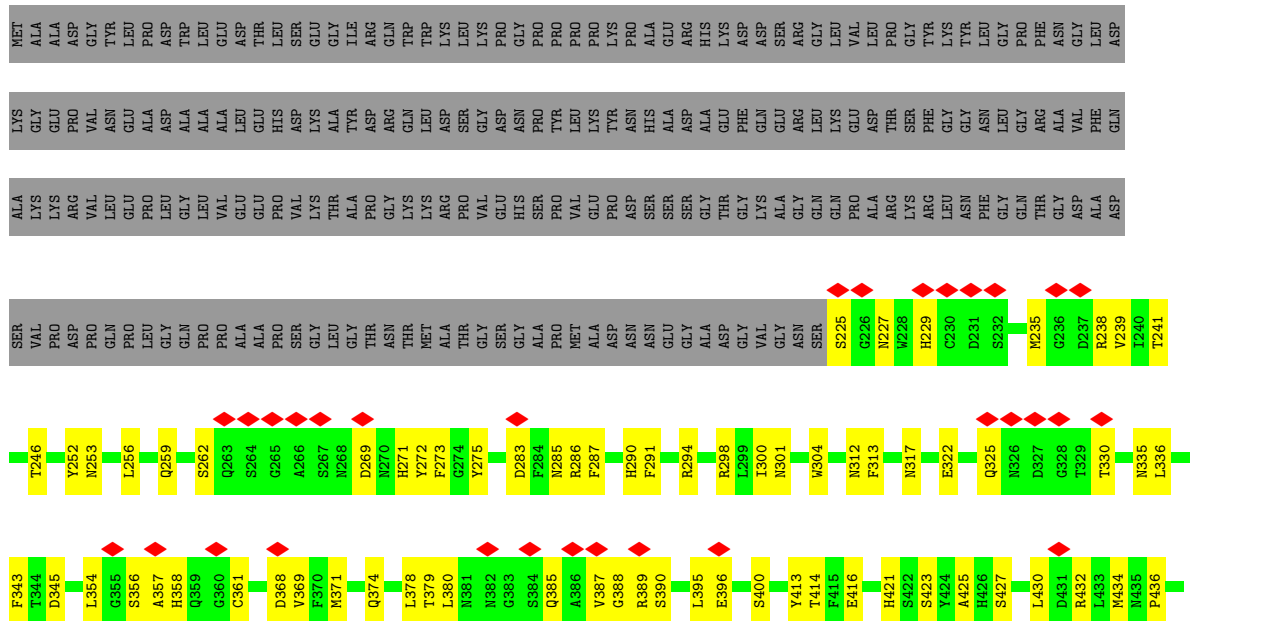
• Molecule 1: Capsid protein VP1

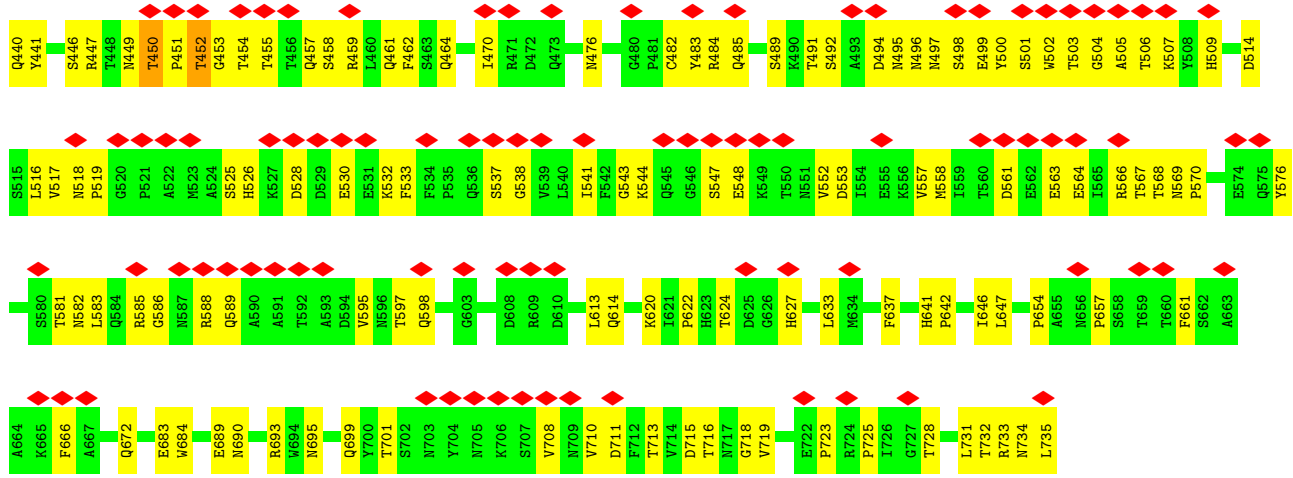


MET	ALA	ALA	ASP	GLY	TYR	LEU	PRO	ASP	TRP	LEU	GLU	ASP	THR	LEU	SER	GLY	GLY	ILE	ARG	GLN	TRP	LYS	LEU	TRP	LYS	PRO	LEU	LYS	VAL	D711	F712	T713	V714	D715	N716	G717	V718	V719	E722	P723	R724	P725	I726	G727	L731	T732	R733	N734	L735							
LYS	GLY	GLU	PRO	VAL	ASN	GLU	ALA	ASP	ASP	ALA	ALA	LEU	GLU	HIS	SER	LYS	LYS	ALA	TYR	ARG	ASP	ARG	GLN	LEU	TRP	LYS	PRO	LEU	LYS	TYR	ASN	ALA	ALA	GLU	ASP	ALA	ALA	GLY	THR	PHE	GLY	ASP	GLY	VAL	LEU	ASP	THR	PRO	GLY	TYR	LEU	ASN	PHE	VAL	GLY	GLN
MET	ALA	ALA	ASP	GLY	TYR	LEU	PRO	ASP	TRP	LEU	GLU	ASP	THR	LEU	SER	GLY	GLY	ILE	ARG	GLN	TRP	LYS	LEU	TRP	LYS	PRO	LEU	LYS	VAL	D711	F712	T713	V714	D715	N716	G717	V718	V719	E722	P723	R724	P725	I726	G727	L731	T732	R733	N734	L735							

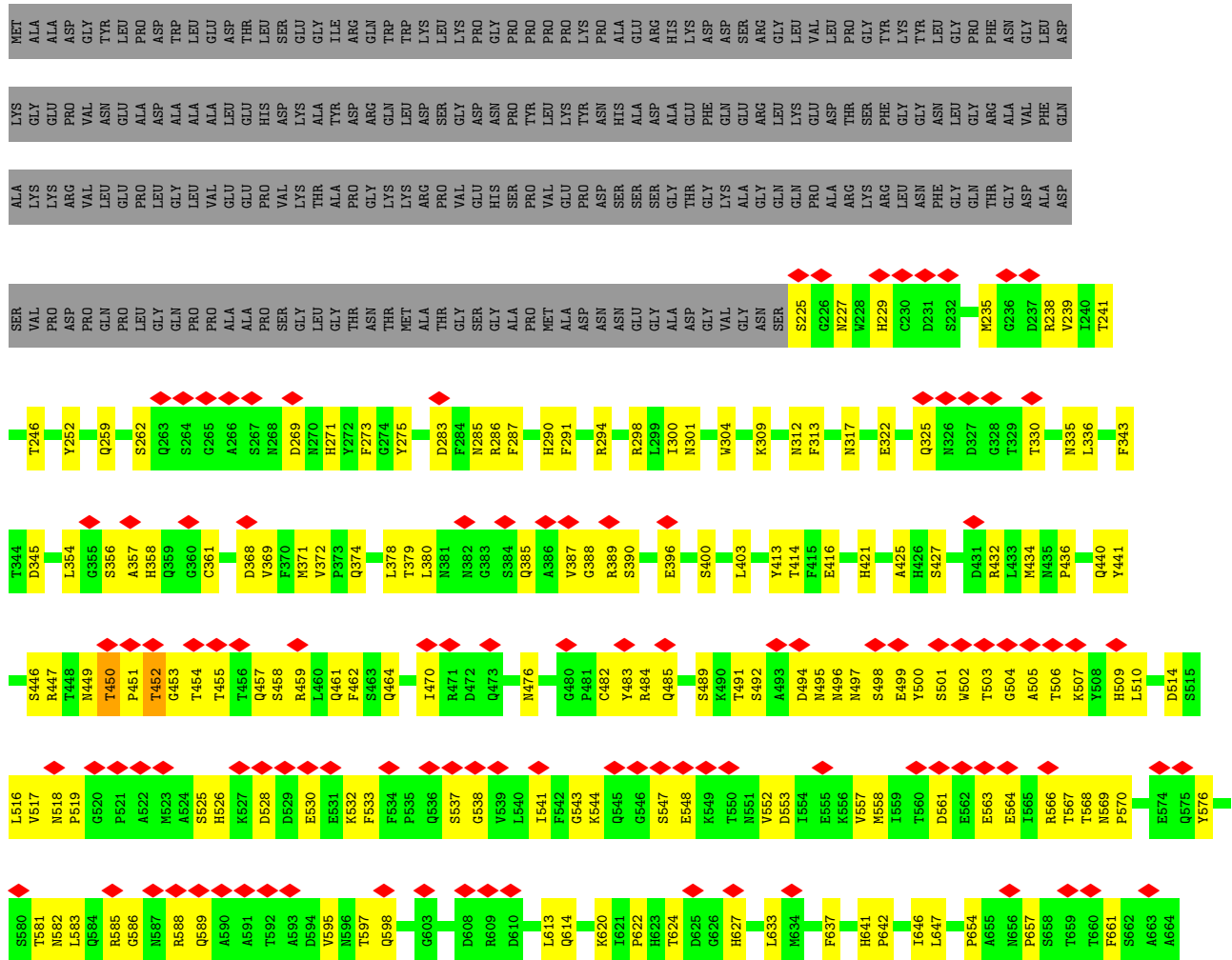


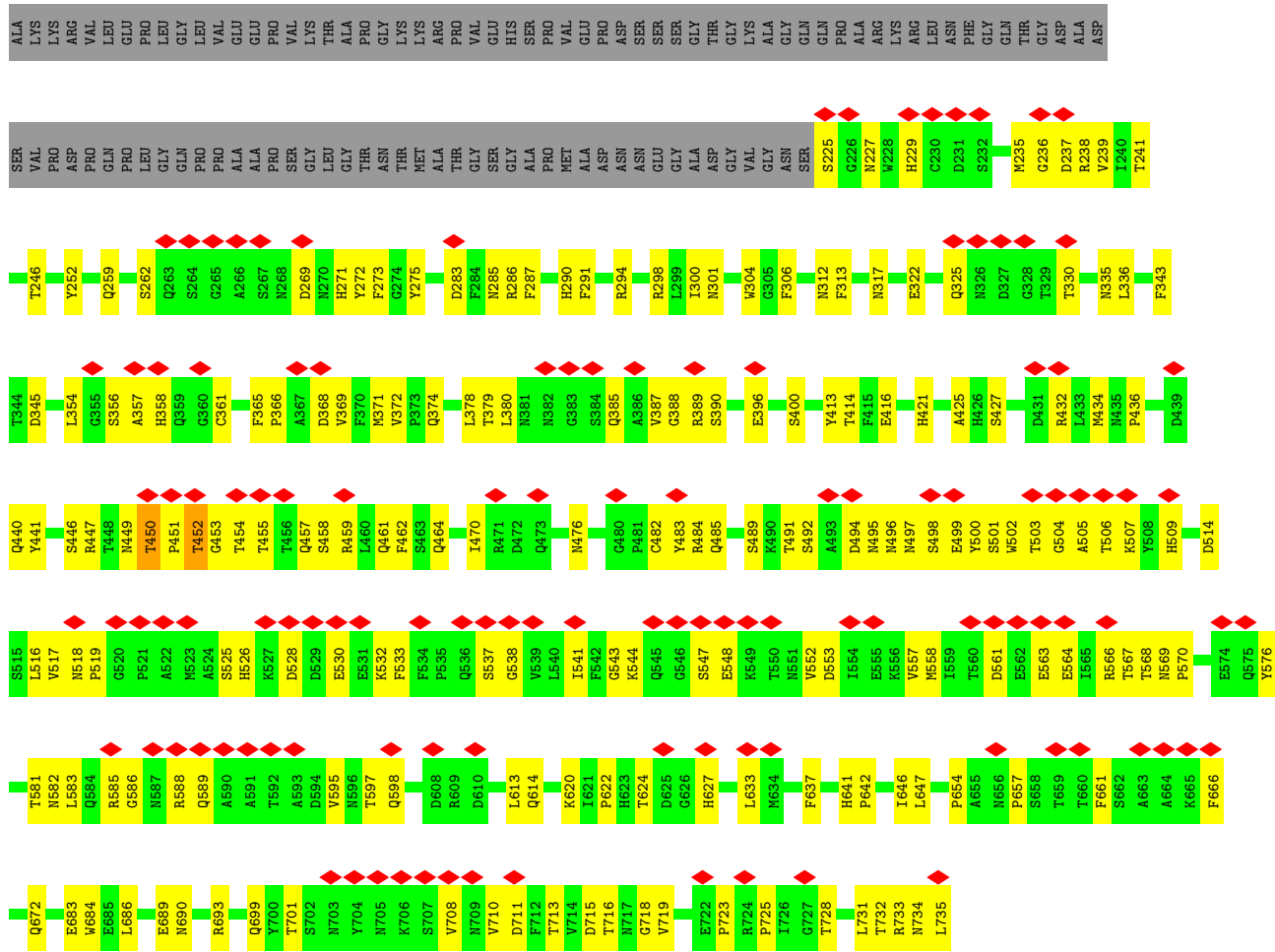
• Molecule 1: Capsid protein VP1



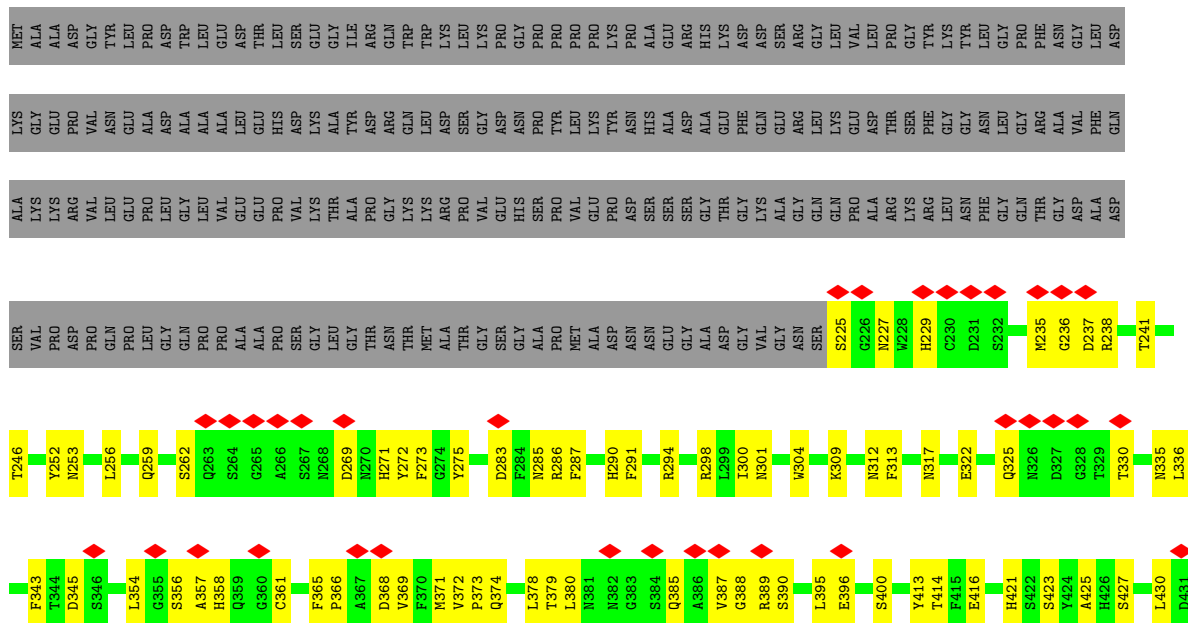


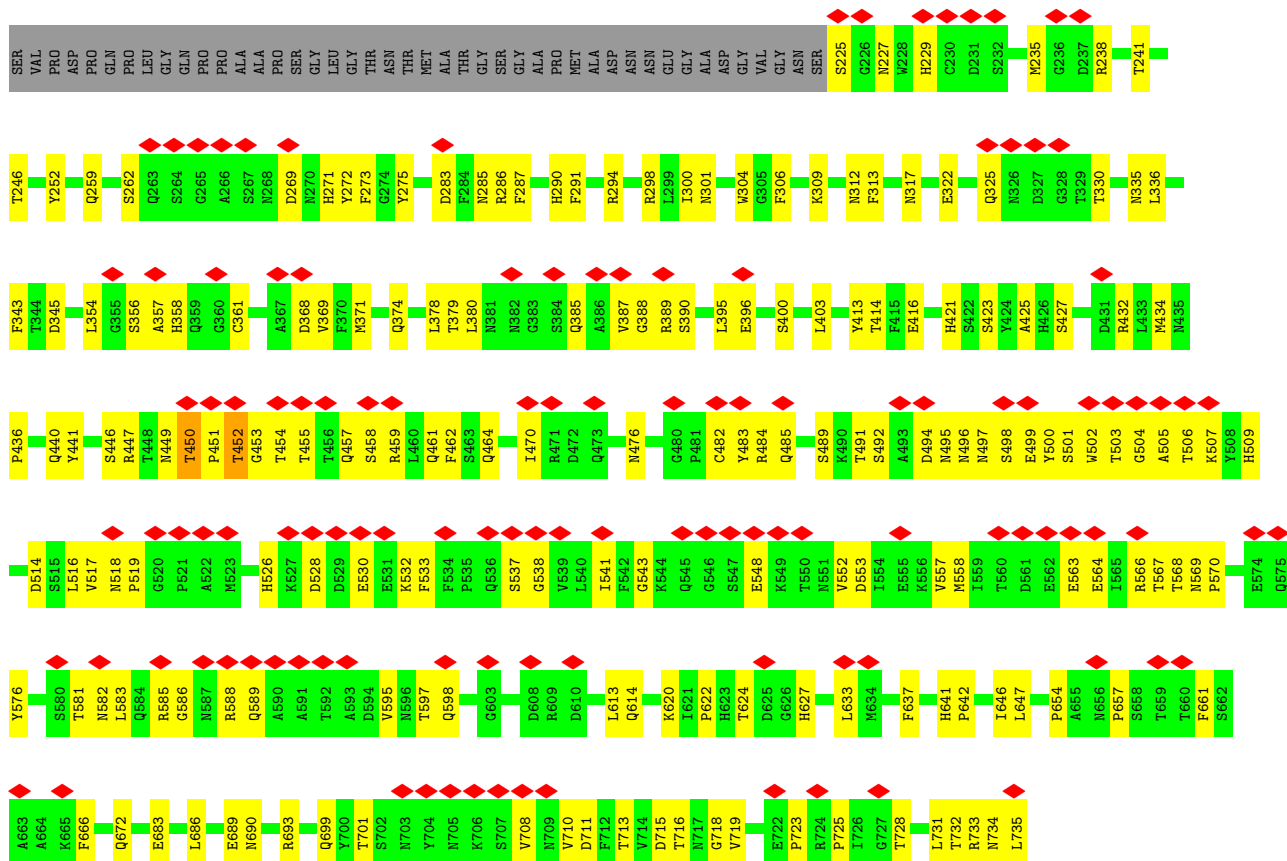
• Molecule 1: Capsid protein VP1



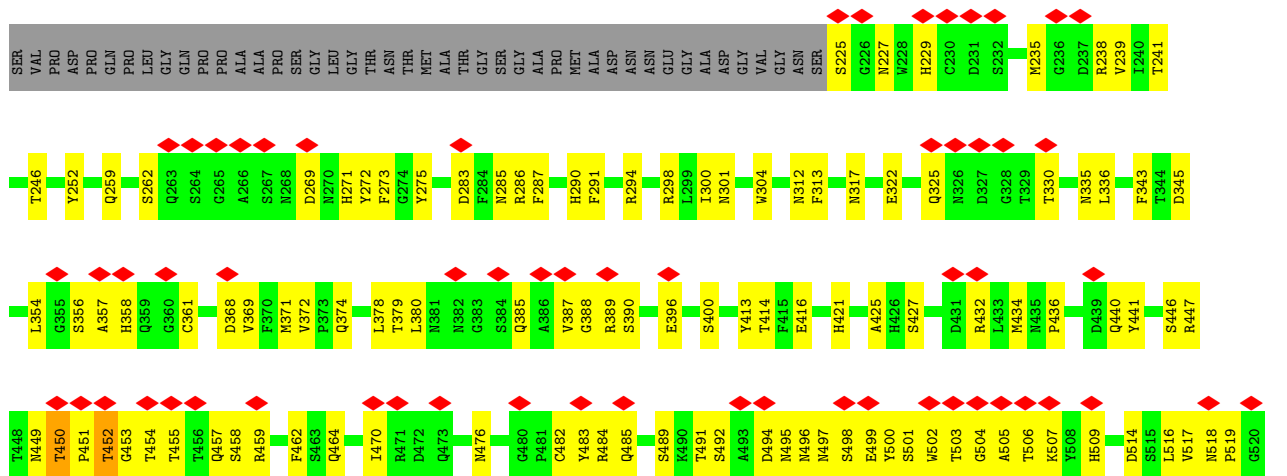
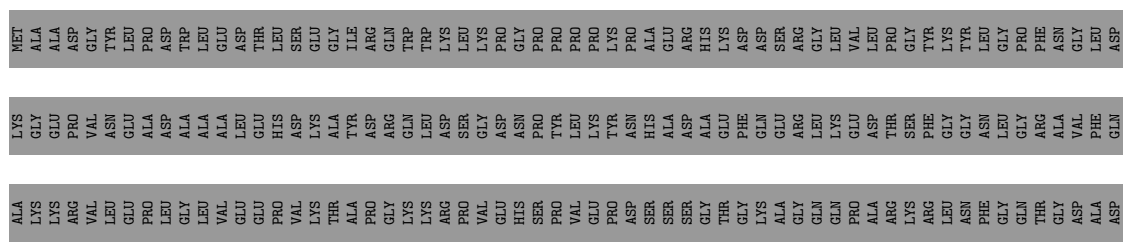
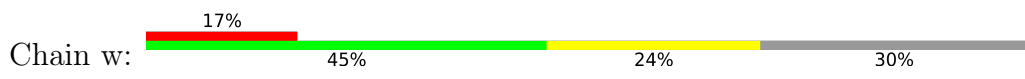


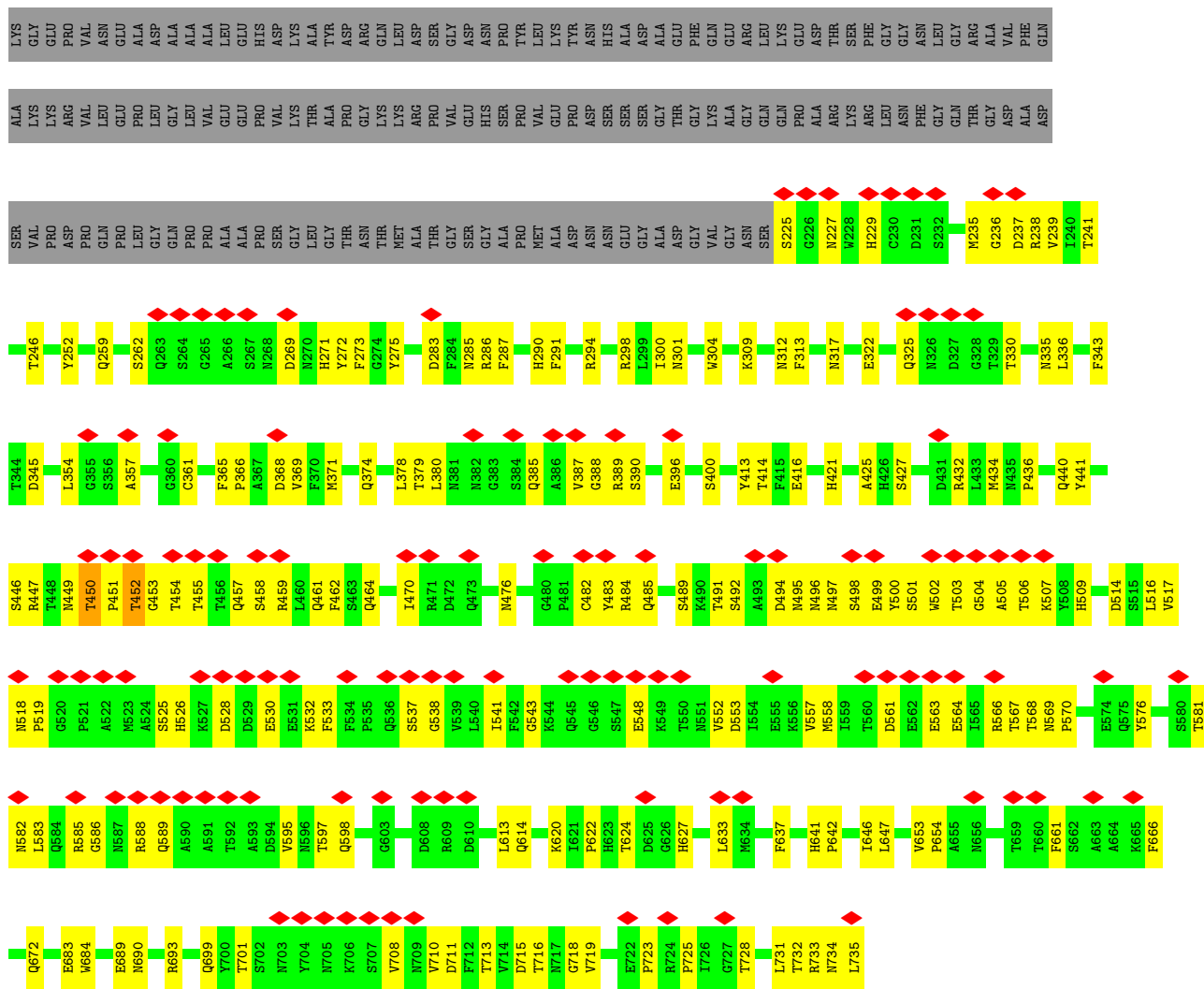
● Molecule 1: Capsid protein VP1



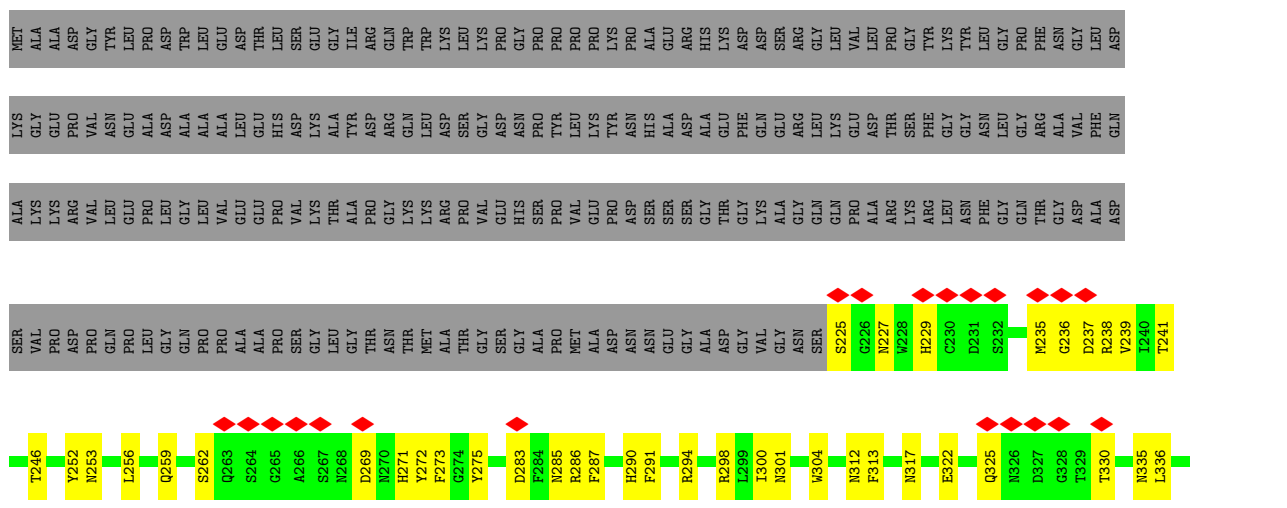


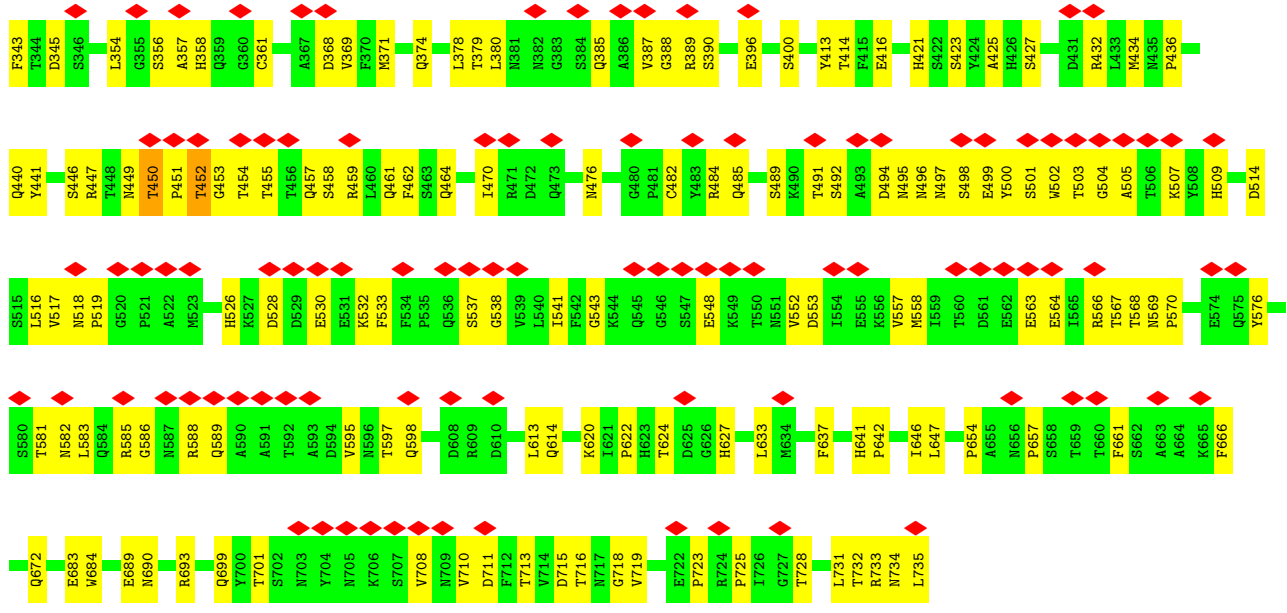
• Molecule 1: Capsid protein VP1



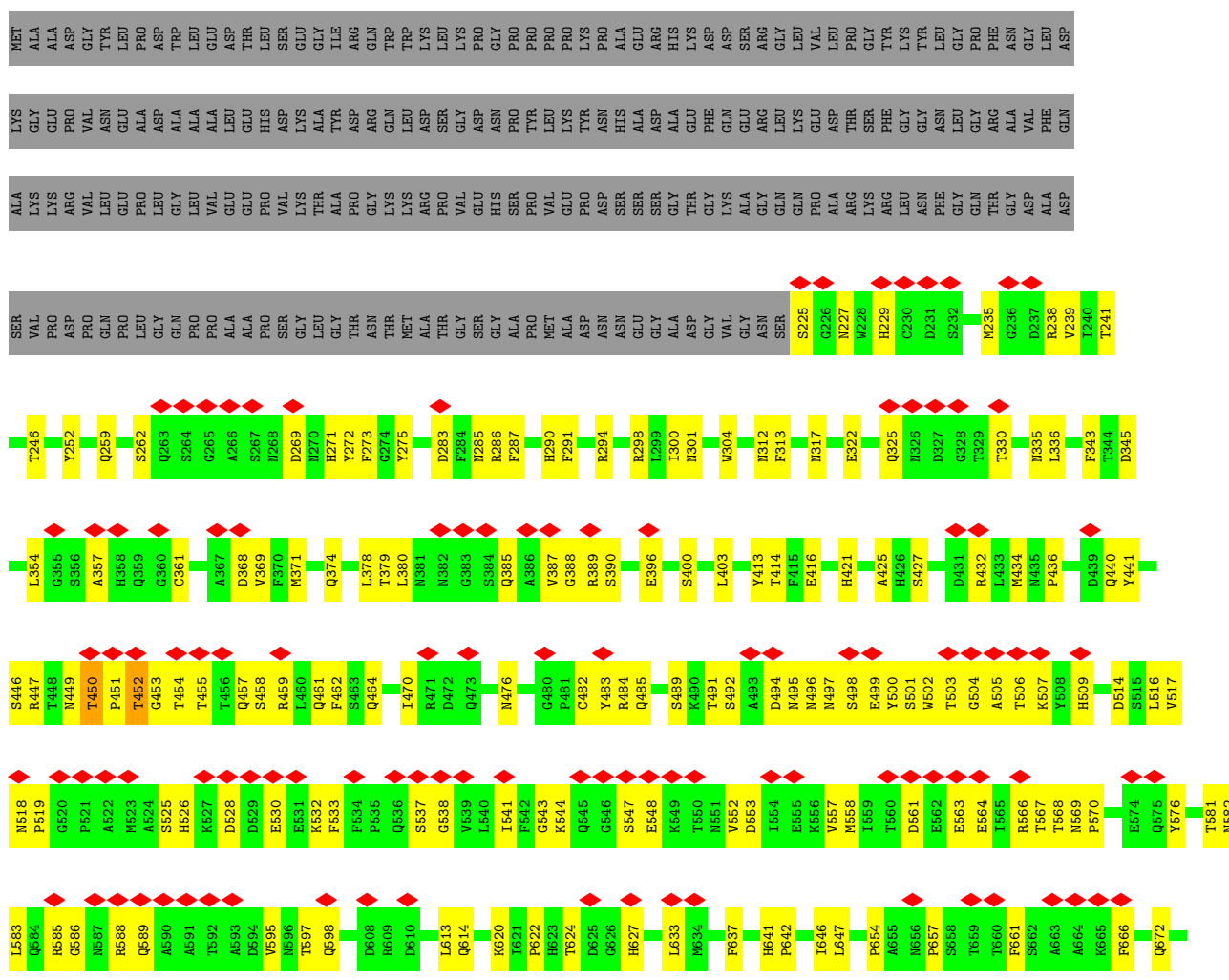


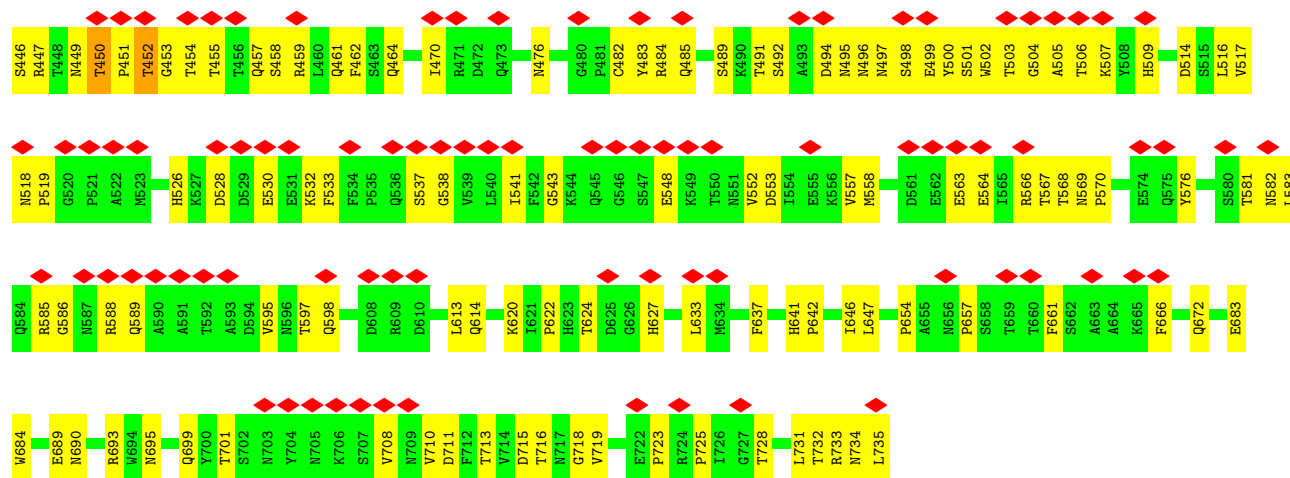
• Molecule 1: Capsid protein VP1





• 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	23039	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	56924	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	14.791	Depositor
Minimum map value	-15.532	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.9	Depositor
Map size (\AA)	361.9, 361.9, 361.9	wwPDB
Map dimensions	329, 329, 329	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	1	0.47	0/4229	0.66	3/5767 (0.1%)
1	2	0.47	0/4229	0.66	3/5767 (0.1%)
1	3	0.47	0/4229	0.66	3/5767 (0.1%)
1	4	0.47	0/4229	0.66	3/5767 (0.1%)
1	5	0.47	0/4229	0.66	3/5767 (0.1%)
1	6	0.47	0/4229	0.66	3/5767 (0.1%)
1	7	0.47	0/4229	0.66	3/5767 (0.1%)
1	8	0.47	0/4229	0.66	3/5767 (0.1%)
1	A	0.46	0/4229	0.66	3/5767 (0.1%)
1	B	0.47	0/4229	0.66	3/5767 (0.1%)
1	C	0.47	0/4229	0.66	3/5767 (0.1%)
1	D	0.47	0/4229	0.66	3/5767 (0.1%)
1	E	0.47	0/4229	0.66	3/5767 (0.1%)
1	F	0.47	0/4229	0.66	3/5767 (0.1%)
1	G	0.47	0/4229	0.66	3/5767 (0.1%)
1	H	0.47	0/4229	0.66	3/5767 (0.1%)
1	I	0.47	0/4229	0.66	3/5767 (0.1%)
1	J	0.47	0/4229	0.66	3/5767 (0.1%)
1	K	0.47	0/4229	0.66	3/5767 (0.1%)
1	L	0.46	0/4229	0.66	3/5767 (0.1%)
1	M	0.47	0/4229	0.66	3/5767 (0.1%)
1	N	0.47	0/4229	0.66	3/5767 (0.1%)
1	O	0.47	0/4229	0.66	3/5767 (0.1%)
1	P	0.46	0/4229	0.66	3/5767 (0.1%)
1	Q	0.47	0/4229	0.66	3/5767 (0.1%)
1	R	0.47	0/4229	0.66	3/5767 (0.1%)
1	S	0.47	0/4229	0.66	3/5767 (0.1%)
1	T	0.46	0/4229	0.66	3/5767 (0.1%)
1	U	0.47	0/4229	0.66	3/5767 (0.1%)
1	V	0.47	0/4229	0.66	3/5767 (0.1%)
1	W	0.47	0/4229	0.66	3/5767 (0.1%)
1	X	0.47	0/4229	0.66	3/5767 (0.1%)
1	Y	0.47	0/4229	0.66	3/5767 (0.1%)
1	Z	0.47	0/4229	0.66	3/5767 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.47	0/4229	0.66	3/5767 (0.1%)
1	b	0.47	0/4229	0.66	3/5767 (0.1%)
1	c	0.47	0/4229	0.66	3/5767 (0.1%)
1	d	0.47	0/4229	0.66	3/5767 (0.1%)
1	e	0.47	0/4229	0.66	3/5767 (0.1%)
1	f	0.47	0/4229	0.66	3/5767 (0.1%)
1	g	0.47	0/4229	0.66	3/5767 (0.1%)
1	h	0.47	0/4229	0.66	3/5767 (0.1%)
1	i	0.46	0/4229	0.66	3/5767 (0.1%)
1	j	0.47	0/4229	0.66	3/5767 (0.1%)
1	k	0.47	0/4229	0.66	3/5767 (0.1%)
1	l	0.47	0/4229	0.66	3/5767 (0.1%)
1	m	0.47	0/4229	0.66	3/5767 (0.1%)
1	n	0.47	0/4229	0.66	3/5767 (0.1%)
1	o	0.47	0/4229	0.66	3/5767 (0.1%)
1	p	0.46	0/4229	0.66	3/5767 (0.1%)
1	q	0.47	0/4229	0.66	3/5767 (0.1%)
1	r	0.46	0/4229	0.66	3/5767 (0.1%)
1	s	0.47	0/4229	0.66	3/5767 (0.1%)
1	t	0.47	0/4229	0.66	3/5767 (0.1%)
1	u	0.47	0/4229	0.66	3/5767 (0.1%)
1	v	0.47	0/4229	0.66	3/5767 (0.1%)
1	w	0.47	0/4229	0.66	3/5767 (0.1%)
1	x	0.47	0/4229	0.65	3/5767 (0.1%)
1	y	0.47	0/4229	0.66	3/5767 (0.1%)
1	z	0.47	0/4229	0.66	3/5767 (0.1%)
All	All	0.47	0/253740	0.66	180/346020 (0.1%)

There are no bond length outliers.

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	450	THR	CA-C-N	8.35	147.03	127.00
1	c	450	THR	C-N-CA	8.35	147.03	127.00
1	V	450	THR	CA-C-N	8.35	147.03	127.00
1	V	450	THR	C-N-CA	8.35	147.03	127.00
1	2	450	THR	CA-C-N	8.34	147.01	127.00

There are no chirality outliers.

There are no planarity outliers.

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	1	4106	0	3868	167	0
1	2	4106	0	3868	165	0
1	3	4106	0	3868	167	0
1	4	4106	0	3868	168	0
1	5	4106	0	3868	168	0
1	6	4106	0	3868	173	0
1	7	4106	0	3868	168	0
1	8	4106	0	3868	172	0
1	A	4106	0	3868	173	0
1	B	4106	0	3868	174	0
1	C	4106	0	3868	168	0
1	D	4106	0	3868	171	0
1	E	4106	0	3868	170	0
1	F	4106	0	3868	173	0
1	G	4106	0	3868	173	0
1	H	4106	0	3868	175	0
1	I	4106	0	3868	171	0
1	J	4106	0	3868	172	0
1	K	4106	0	3868	174	0
1	L	4106	0	3868	166	0
1	M	4106	0	3868	172	0
1	N	4106	0	3868	173	0
1	O	4106	0	3868	168	0
1	P	4106	0	3868	168	0
1	Q	4106	0	3868	167	0
1	R	4106	0	3868	174	0
1	S	4106	0	3868	172	0
1	T	4106	0	3868	170	0
1	U	4106	0	3868	172	0
1	V	4106	0	3868	175	0
1	W	4106	0	3868	168	0
1	X	4106	0	3868	166	0
1	Y	4106	0	3868	172	0
1	Z	4106	0	3868	169	0
1	a	4106	0	3868	172	0
1	b	4106	0	3868	174	0
1	c	4106	0	3868	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	4106	0	3868	164	0
1	e	4106	0	3868	167	0
1	f	4106	0	3868	172	0
1	g	4106	0	3868	172	0
1	h	4106	0	3868	173	0
1	i	4106	0	3868	172	0
1	j	4106	0	3868	173	0
1	k	4106	0	3868	169	0
1	l	4106	0	3868	166	0
1	m	4106	0	3868	171	0
1	n	4106	0	3868	171	0
1	o	4106	0	3868	174	0
1	p	4106	0	3868	172	0
1	q	4106	0	3868	168	0
1	r	4106	0	3868	172	0
1	s	4106	0	3868	175	0
1	t	4106	0	3868	174	0
1	u	4106	0	3868	173	0
1	v	4106	0	3868	167	0
1	w	4106	0	3868	165	0
1	x	4106	0	3868	166	0
1	y	4106	0	3868	175	0
1	z	4106	0	3868	163	0
All	All	246360	0	232080	8720	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 18.

The worst 5 of 8720 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:e:371:MET:HE1	1:h:661:PHE:HA	1.55	0.89
1:N:371:MET:HE1	1:m:661:PHE:HA	1.55	0.89
1:M:371:MET:HE1	1:N:661:PHE:HA	1.55	0.88
1:Q:371:MET:HE1	1:S:661:PHE:HA	1.55	0.88
1:k:661:PHE:HA	1:w:371:MET:HE1	1.56	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	2	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	3	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	4	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	5	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	6	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	7	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	8	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	A	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	B	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	C	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	D	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	E	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	F	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	G	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	H	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	I	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	J	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	K	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	L	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	M	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	N	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	O	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	P	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	Q	509/735 (69%)	469 (92%)	40 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	S	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	T	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	U	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	V	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	W	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	X	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	Y	509/735 (69%)	468 (92%)	41 (8%)	0	100	100
1	Z	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	a	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	b	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	c	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	d	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	e	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	f	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	g	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	h	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	i	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	j	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	k	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	l	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	m	509/735 (69%)	468 (92%)	41 (8%)	0	100	100
1	n	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	o	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	p	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	q	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	r	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	s	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	t	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	u	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	v	509/735 (69%)	469 (92%)	40 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	x	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	y	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
1	z	509/735 (69%)	469 (92%)	40 (8%)	0	100	100
All	All	30540/44100 (69%)	28138 (92%)	2402 (8%)	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	1	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	2	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	3	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	4	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	5	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	6	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	7	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	8	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	A	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	B	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	C	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	D	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	E	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	F	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	G	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	H	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	I	455/630 (72%)	454 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	K	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	L	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	M	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	N	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	O	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	P	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	Q	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	R	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	S	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	T	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	U	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	V	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	W	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	X	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	Y	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	Z	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	a	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	b	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	c	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	d	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	e	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	f	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	g	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	h	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	i	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	j	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	k	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	l	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	m	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	n	455/630 (72%)	454 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	p	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	q	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	r	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	s	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	t	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	u	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	v	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	w	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	x	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	y	455/630 (72%)	454 (100%)	1 (0%)	87	87
1	z	455/630 (72%)	454 (100%)	1 (0%)	87	87
All	All	27300/37800 (72%)	27240 (100%)	60 (0%)	85	87

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

Mol	Chain	Res	Type
1	c	452	THR
1	4	452	THR
1	j	452	THR
1	3	452	THR
1	8	452	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 610 such sidechains are listed below:

Mol	Chain	Res	Type
1	t	457	GLN
1	5	485	GLN
1	u	598	GLN
1	t	449	ASN
1	y	650	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 [i](#)

There are no chain breaks in this entry.

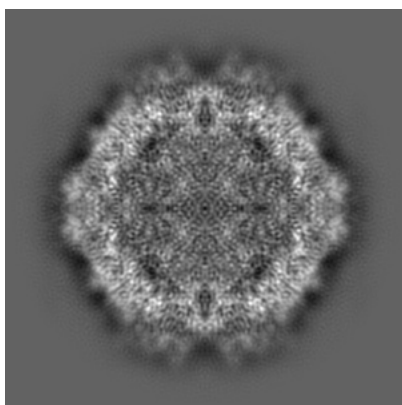
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8099. These allow visual inspection of the internal detail of the map and identification of artifacts.

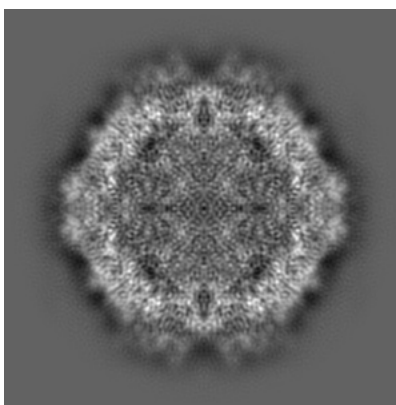
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

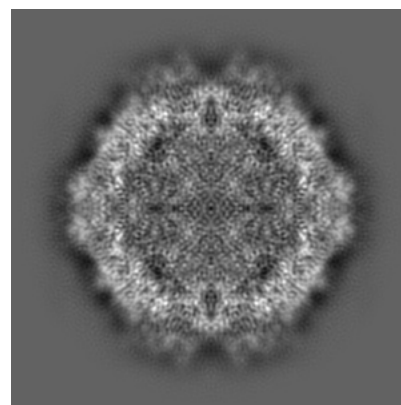
6.1.1 Primary map



X



Y

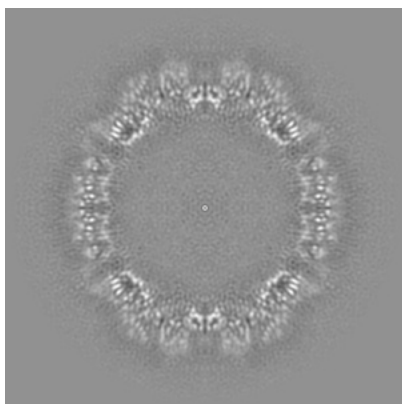


Z

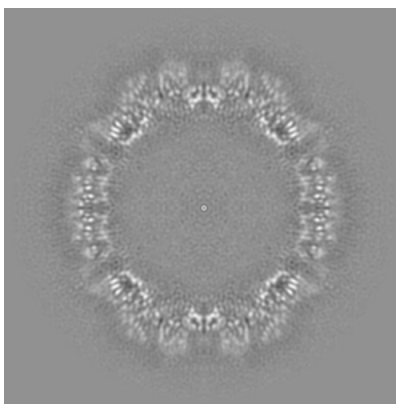
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

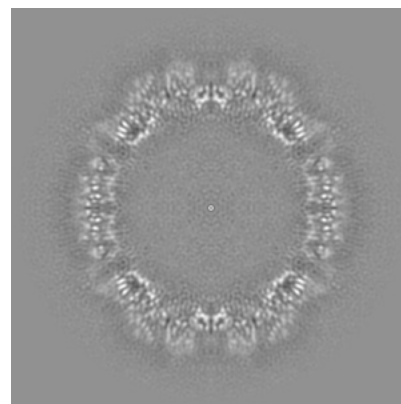
6.2.1 Primary map



X Index: 164



Y Index: 164

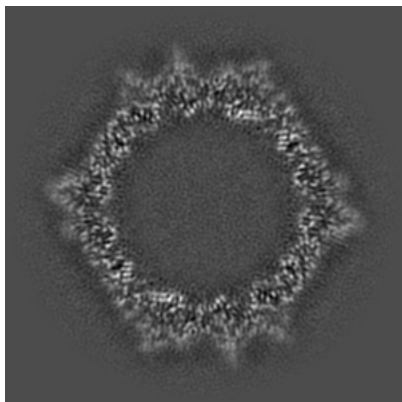


Z Index: 164

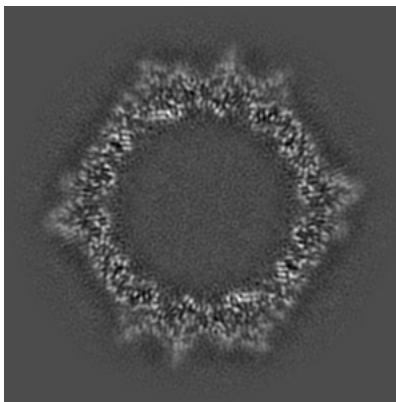
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

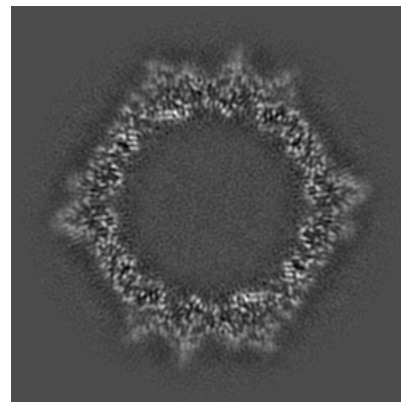
6.3.1 Primary map



X Index: 183



Y Index: 145

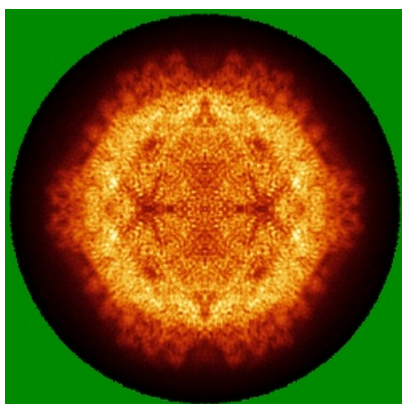


Z Index: 145

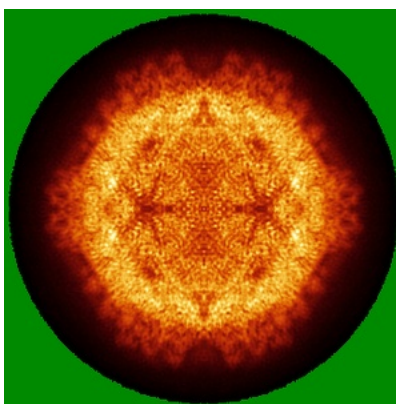
The images above show the largest variance slices of the map in three orthogonal directions.

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

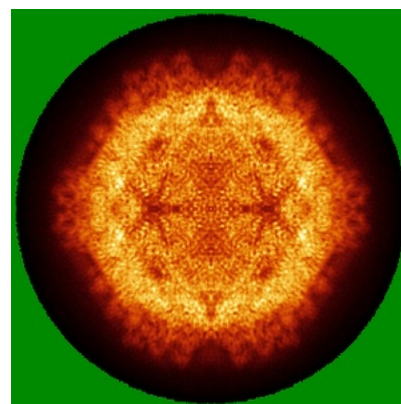
6.4.1 Primary map



X



Y

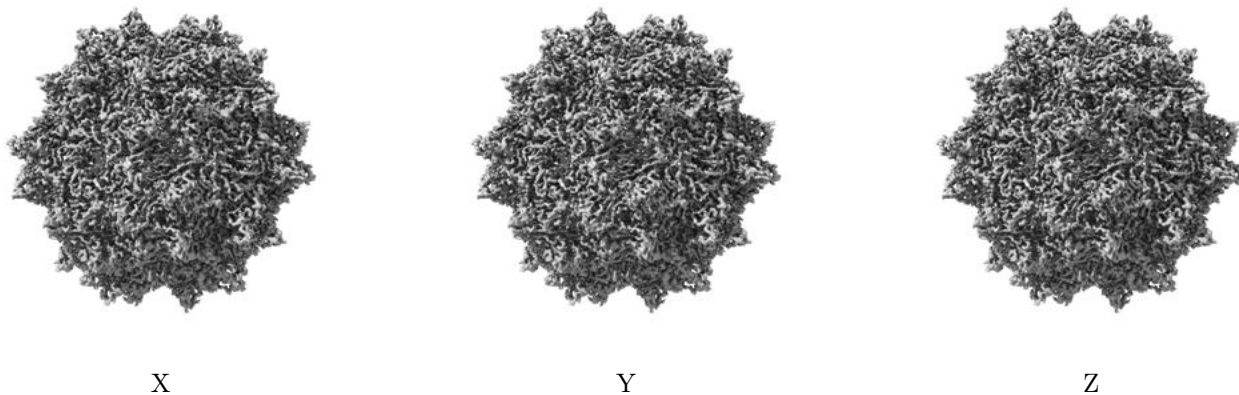


Z

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



The images above show the 3D surface view of the map at the recommended contour level 2.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

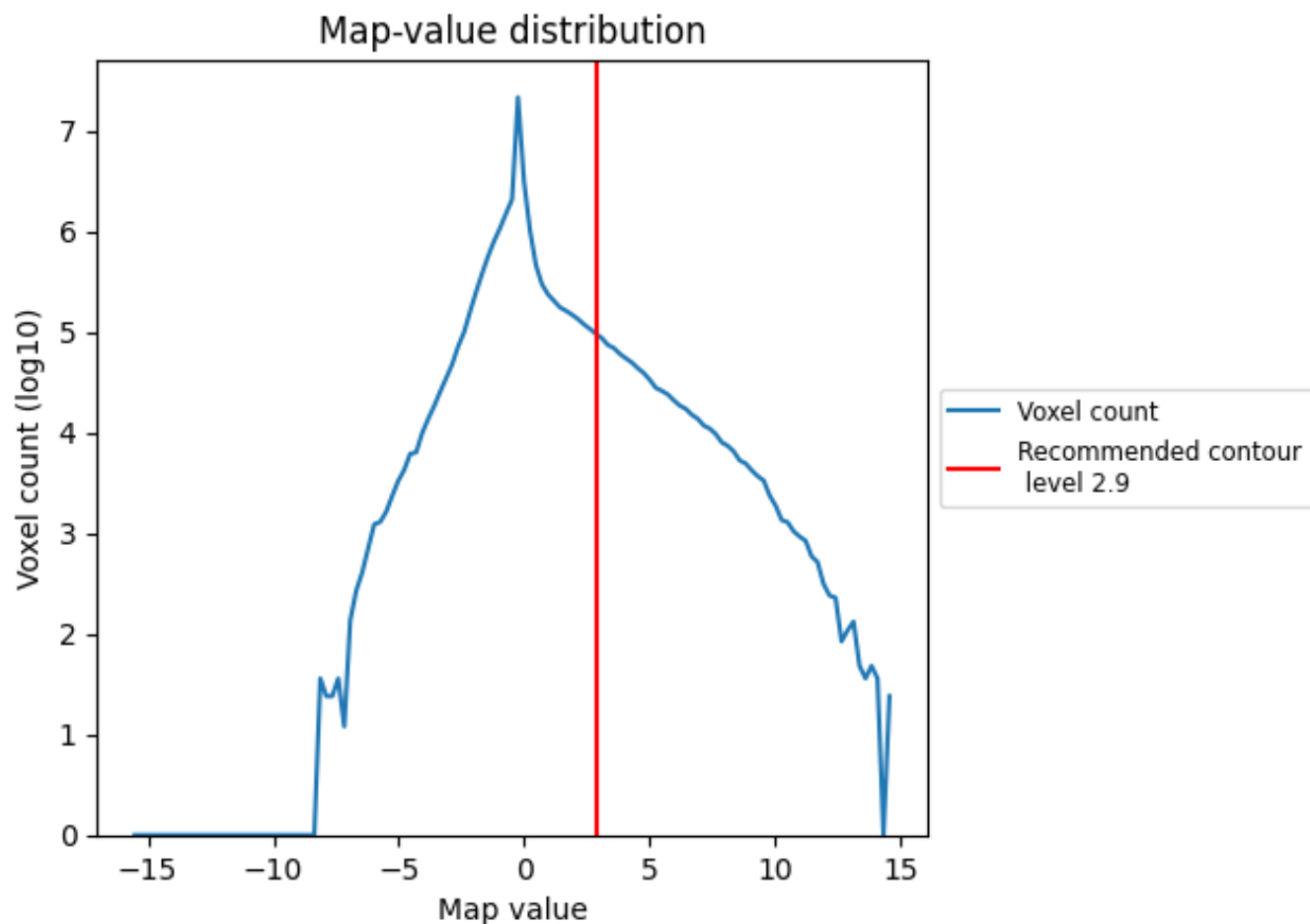
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

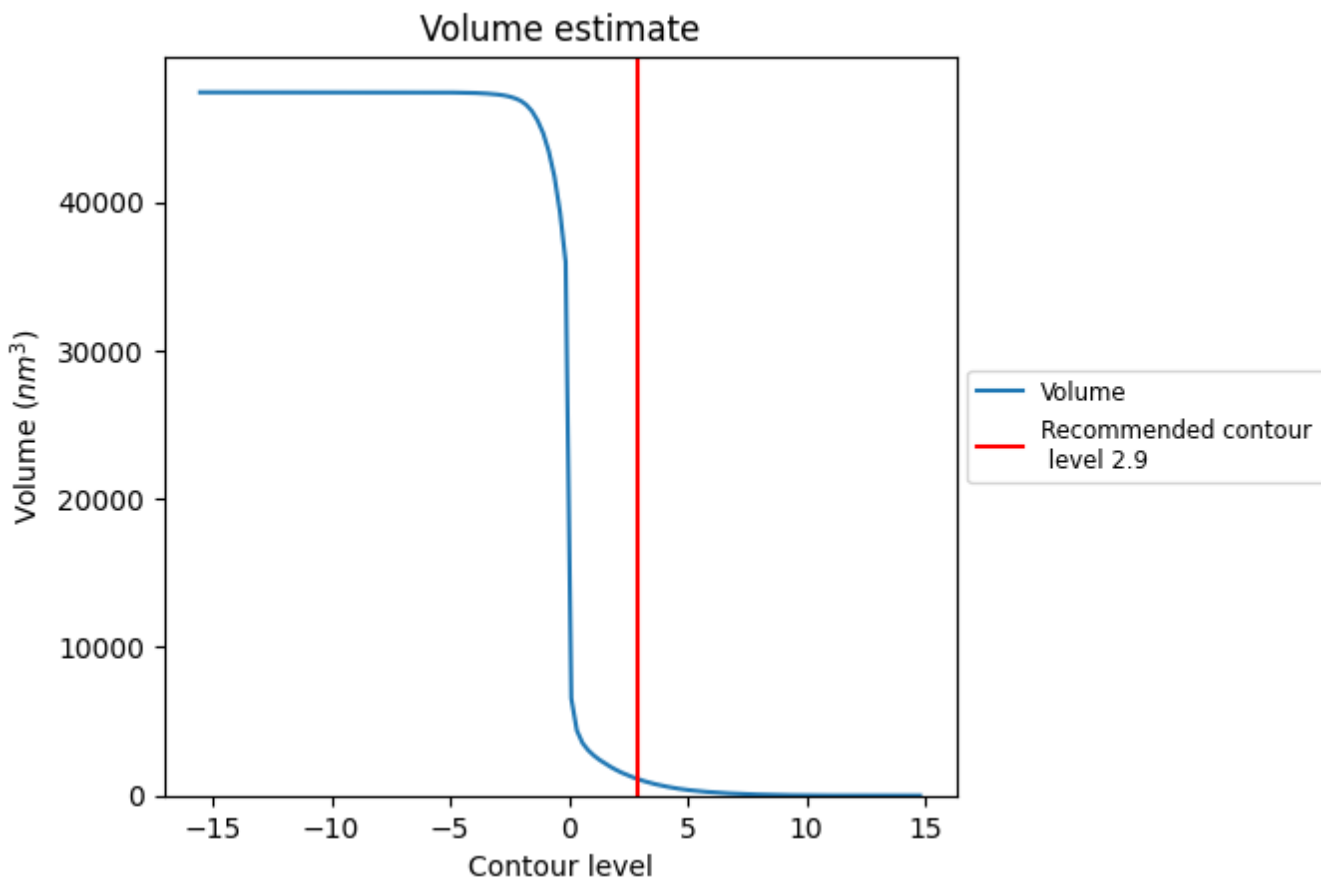
This section contains the results of statistical analysis of the map.

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.

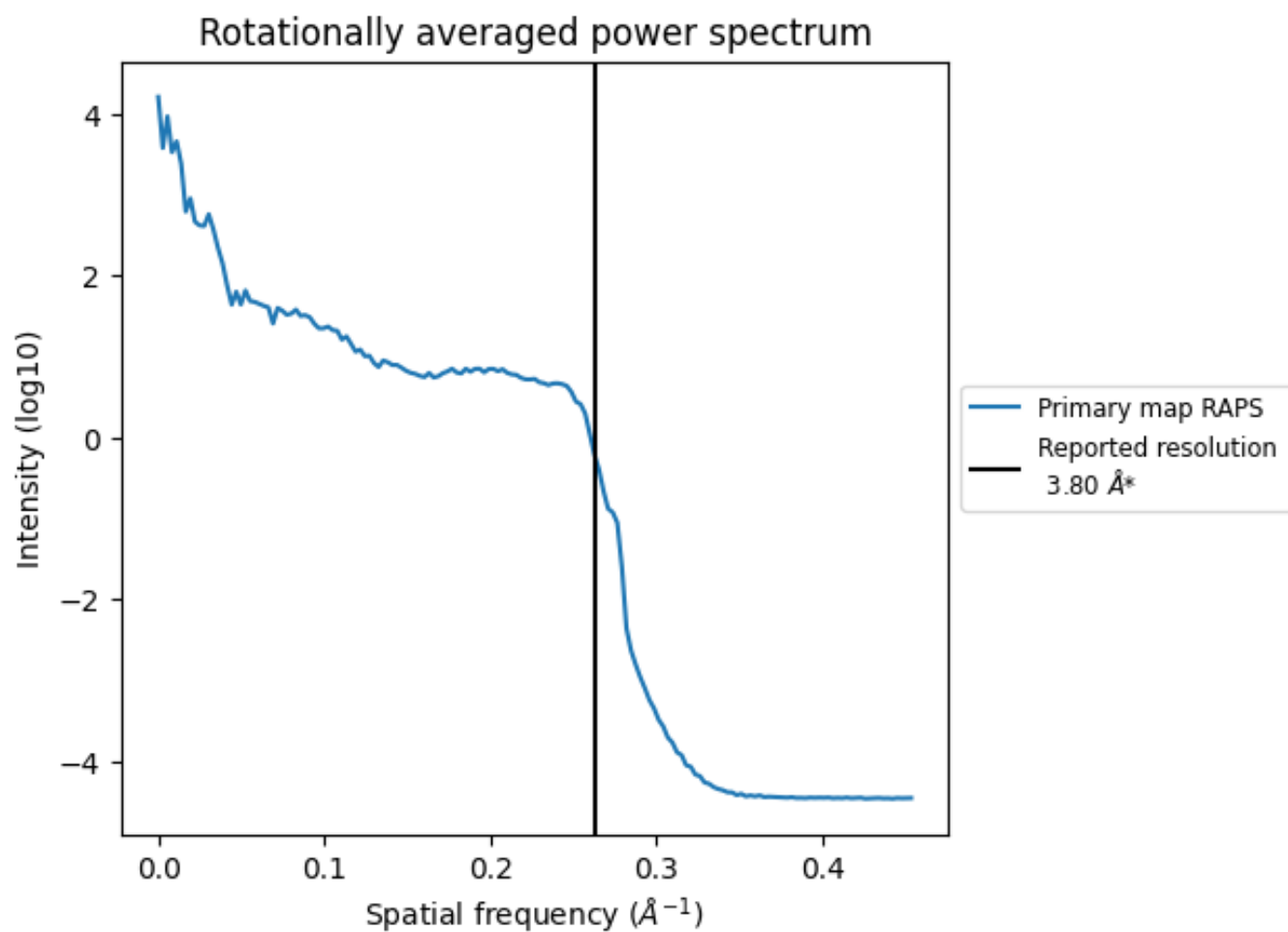
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1115 nm³; this corresponds to an approximate mass of 1007 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 0.263 Å⁻¹

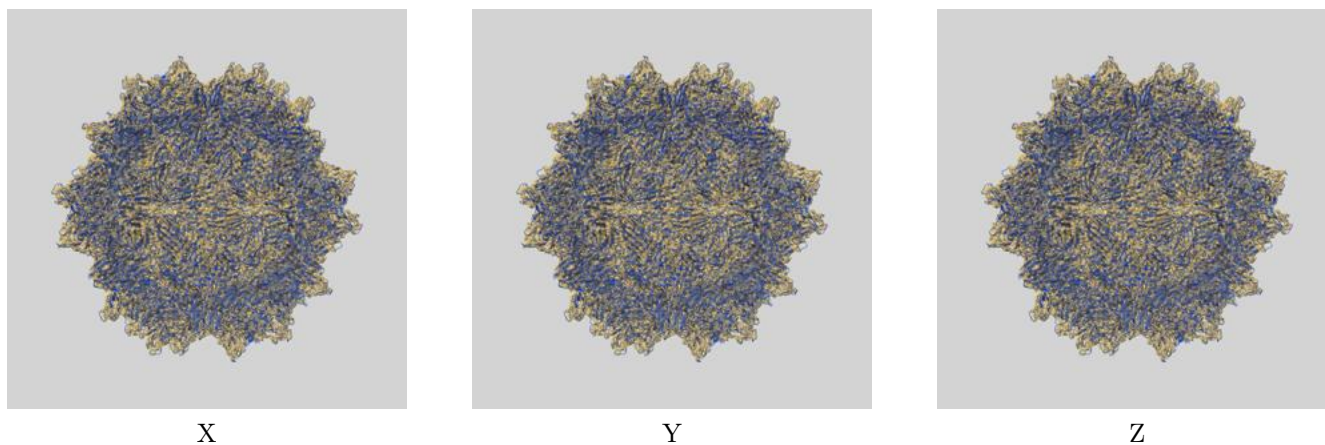
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

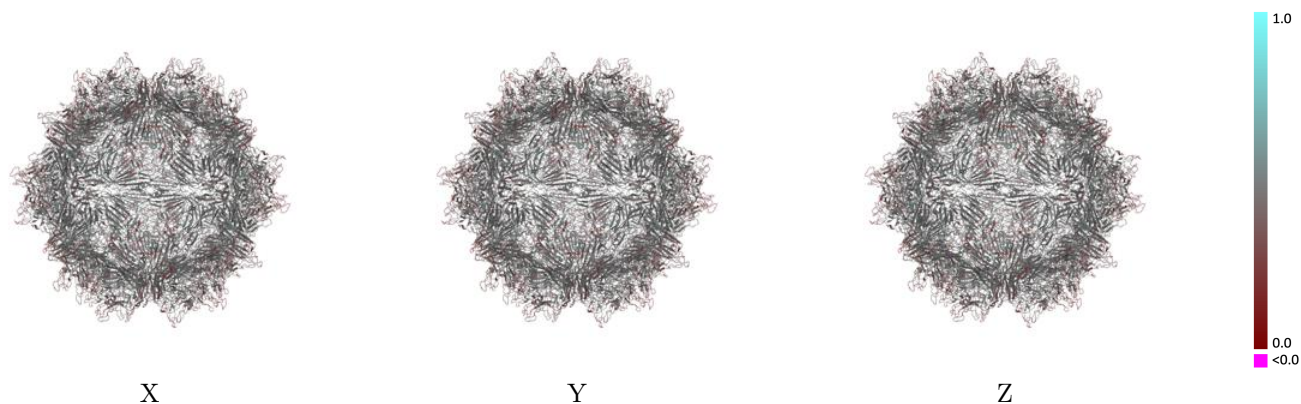
This section contains information regarding the fit between EMDB map EMD-8099 and PDB model 5IPI. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



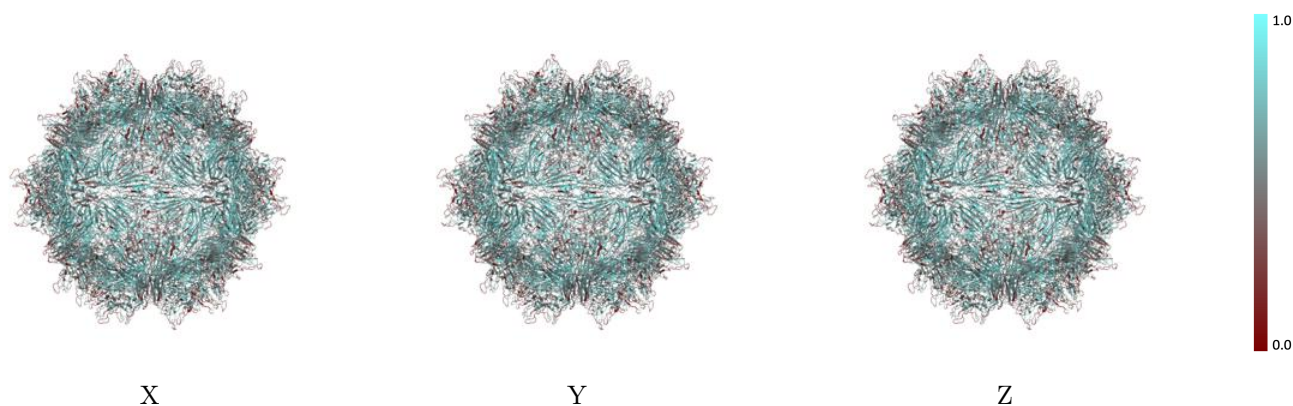
The images above show the 3D surface view of the map at the recommended contour level 2.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



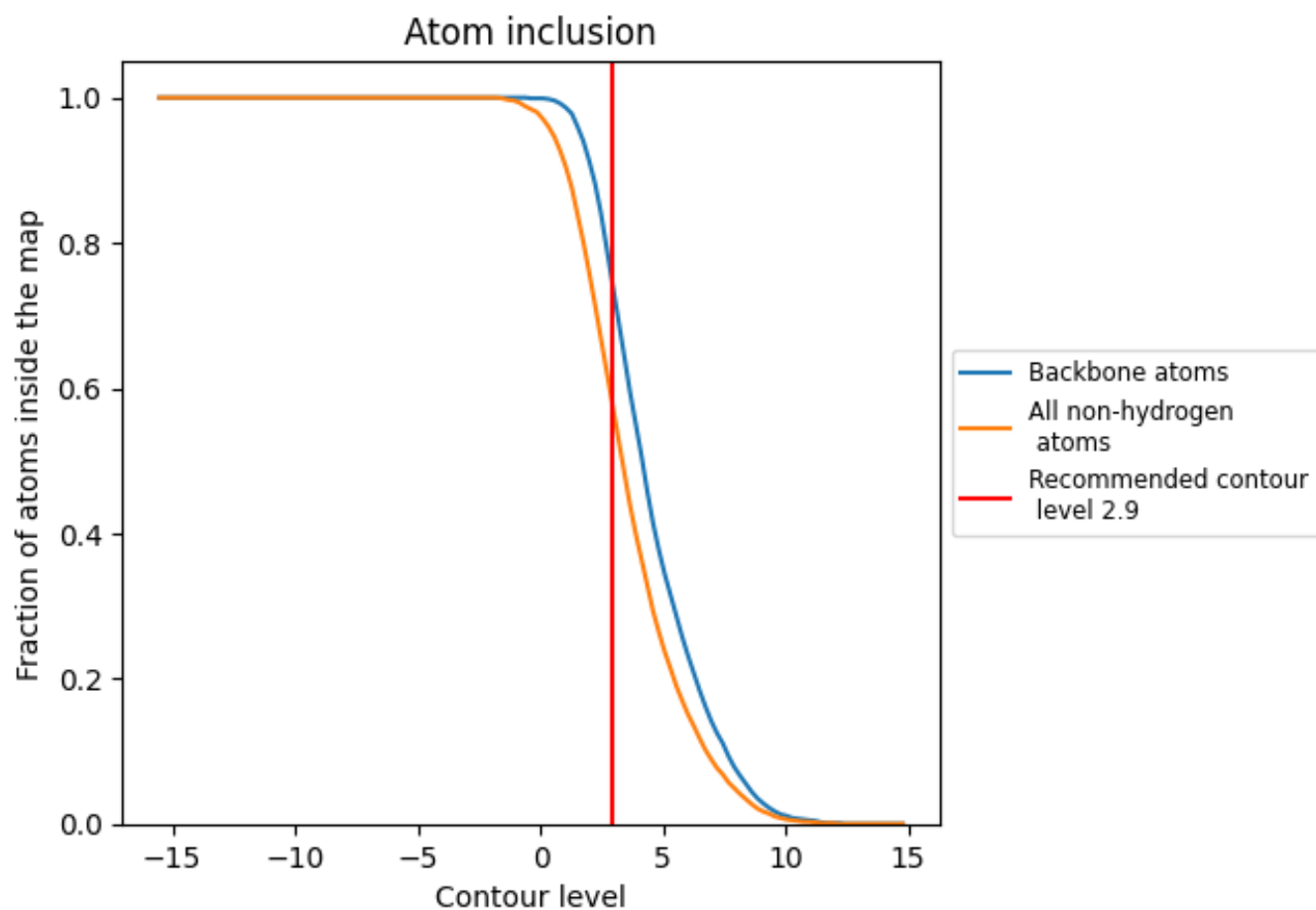
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.9).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































The table lists the average atom inclusion at the recommended contour level (2.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5850	 0.4410
1	 0.5860	 0.4430
2	 0.5850	 0.4410
3	 0.5860	 0.4400
4	 0.5840	 0.4400
5	 0.5840	 0.4420
6	 0.5840	 0.4420
7	 0.5860	 0.4420
8	 0.5860	 0.4410
A	 0.5860	 0.4420
B	 0.5840	 0.4410
C	 0.5860	 0.4410
D	 0.5830	 0.4410
E	 0.5860	 0.4420
F	 0.5850	 0.4410
G	 0.5860	 0.4420
H	 0.5840	 0.4410
I	 0.5860	 0.4410
J	 0.5860	 0.4410
K	 0.5840	 0.4420
L	 0.5850	 0.4410
M	 0.5860	 0.4410
N	 0.5840	 0.4400
O	 0.5860	 0.4400
P	 0.5840	 0.4410
Q	 0.5860	 0.4400
R	 0.5860	 0.4410
S	 0.5850	 0.4410
T	 0.5860	 0.4410
U	 0.5850	 0.4420
V	 0.5840	 0.4410
W	 0.5860	 0.4410
X	 0.5840	 0.4410
Y	 0.5850	 0.4400
Z	 0.5850	 0.4390



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Chain	Atom inclusion	Q-score
a	 0.5840	 0.4390
b	 0.5840	 0.4410
c	 0.5860	 0.4420
d	 0.5860	 0.4410
e	 0.5840	 0.4420
f	 0.5860	 0.4420
g	 0.5840	 0.4420
h	 0.5850	 0.4410
i	 0.5840	 0.4420
j	 0.5860	 0.4410
k	 0.5860	 0.4410
l	 0.5860	 0.4420
m	 0.5850	 0.4390
n	 0.5830	 0.4400
o	 0.5860	 0.4420
p	 0.5850	 0.4420
q	 0.5860	 0.4400
r	 0.5850	 0.4390
s	 0.5830	 0.4410
t	 0.5860	 0.4420
u	 0.5840	 0.4420
v	 0.5870	 0.4400
w	 0.5840	 0.4410
x	 0.5840	 0.4400
y	 0.5830	 0.4410
z	 0.5870	 0.4430