Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 11:58 AM EST

PDB ID	:	5IPK
EMDB ID	:	EMD-8100
Title	:	Structure of the R432A variant 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	:	3.70 Å(reported)

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

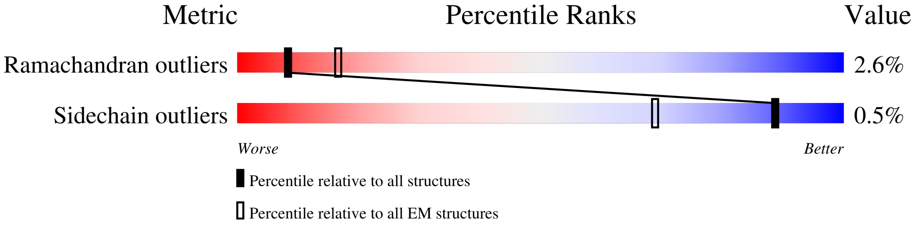
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

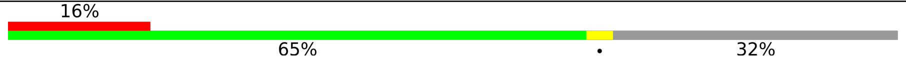
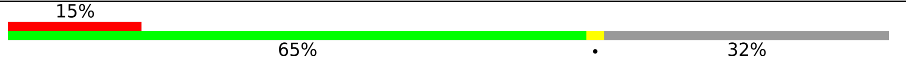
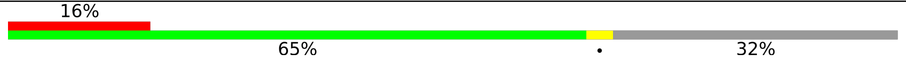
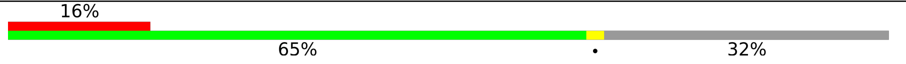
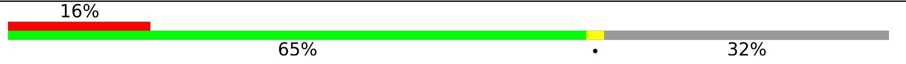
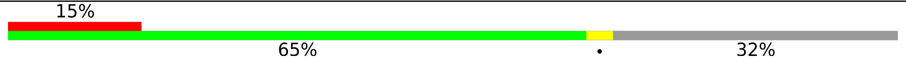
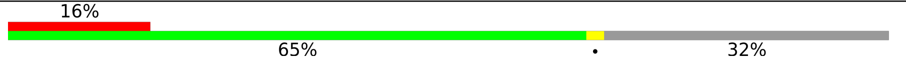
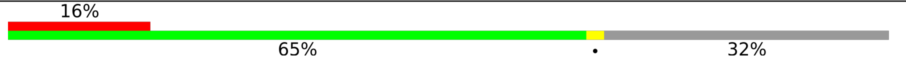
The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	1	735	
1	2	735	
1	3	735	
1	4	735	
1	5	735	
1	6	735	
1	7	735	
1	8	735	
1	A	735	

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Mol	Chain	Length	Quality of chain
1	B	735	16% 65% • 32%
1	C	735	16% 65% • 32%
1	D	735	16% 65% • 32%
1	E	735	15% 65% • 32%
1	F	735	16% 65% • 32%
1	G	735	16% 65% • 32%
1	H	735	16% 65% • 32%
1	I	735	16% 65% • 32%
1	J	735	15% 65% • 32%
1	K	735	16% 65% • 32%
1	L	735	16% 65% • 32%
1	M	735	15% 65% • 32%
1	N	735	16% 65% • 32%
1	O	735	15% 65% • 32%
1	P	735	16% 65% • 32%
1	Q	735	16% 65% • 32%
1	R	735	16% 65% • 32%
1	S	735	16% 65% • 32%
1	T	735	16% 65% • 32%
1	U	735	15% 65% • 32%
1	V	735	16% 65% • 32%
1	W	735	15% 65% • 32%
1	X	735	16% 65% • 32%
1	Y	735	15% 65% • 32%
1	Z	735	16% 65% • 32%

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Mol	Chain	Length	Quality of chain
1	a	735	16% 65% • 32%
1	b	735	16% 65% • 32%
1	c	735	16% 65% • 32%
1	d	735	16% 65% • 32%
1	e	735	16% 65% • 32%
1	f	735	15% 65% • 32%
1	g	735	16% 65% • 32%
1	h	735	15% 65% • 32%
1	i	735	16% 65% • 32%
1	j	735	15% 65% • 32%
1	k	735	15% 65% • 32%
1	l	735	16% 65% • 32%
1	m	735	16% 65% • 32%
1	n	735	16% 65% • 32%
1	o	735	16% 65% • 32%
1	p	735	15% 65% • 32%
1	q	735	15% 65% • 32%
1	r	735	16% 65% • 32%
1	s	735	16% 65% • 32%
1	t	735	16% 65% • 32%
1	u	735	16% 65% • 32%
1	v	735	15% 65% • 32%
1	w	735	16% 65% • 32%
1	x	735	16% 65% • 32%
1	y	735	16% 65% • 32%

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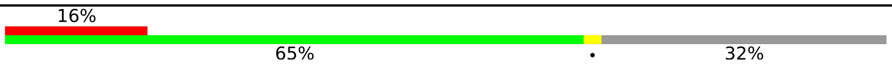
Mol	Chain	Length	Quality of chain
1	z	735	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 240540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	B	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	C	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	D	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	E	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	F	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	G	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	H	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	I	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	J	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	K	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	L	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	M	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	N	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	O	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	P	500	Total 4009	C 2528	N 697	O 773	S 11	0	0
1	Q	500	Total 4009	C 2528	N 697	O 773	S 11	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	R	500	Total C N O S 4009 2528 697 773 11	0	0
1	S	500	Total C N O S 4009 2528 697 773 11	0	0
1	T	500	Total C N O S 4009 2528 697 773 11	0	0
1	U	500	Total C N O S 4009 2528 697 773 11	0	0
1	V	500	Total C N O S 4009 2528 697 773 11	0	0
1	W	500	Total C N O S 4009 2528 697 773 11	0	0
1	X	500	Total C N O S 4009 2528 697 773 11	0	0
1	Y	500	Total C N O S 4009 2528 697 773 11	0	0
1	Z	500	Total C N O S 4009 2528 697 773 11	0	0
1	a	500	Total C N O S 4009 2528 697 773 11	0	0
1	b	500	Total C N O S 4009 2528 697 773 11	0	0
1	c	500	Total C N O S 4009 2528 697 773 11	0	0
1	d	500	Total C N O S 4009 2528 697 773 11	0	0
1	e	500	Total C N O S 4009 2528 697 773 11	0	0
1	f	500	Total C N O S 4009 2528 697 773 11	0	0
1	g	500	Total C N O S 4009 2528 697 773 11	0	0
1	h	500	Total C N O S 4009 2528 697 773 11	0	0
1	i	500	Total C N O S 4009 2528 697 773 11	0	0
1	j	500	Total C N O S 4009 2528 697 773 11	0	0
1	k	500	Total C N O S 4009 2528 697 773 11	0	0
1	l	500	Total C N O S 4009 2528 697 773 11	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	m	500	Total C N O S 4009 2528 697 773 11	0	0
1	n	500	Total C N O S 4009 2528 697 773 11	0	0
1	o	500	Total C N O S 4009 2528 697 773 11	0	0
1	p	500	Total C N O S 4009 2528 697 773 11	0	0
1	q	500	Total C N O S 4009 2528 697 773 11	0	0
1	r	500	Total C N O S 4009 2528 697 773 11	0	0
1	s	500	Total C N O S 4009 2528 697 773 11	0	0
1	t	500	Total C N O S 4009 2528 697 773 11	0	0
1	u	500	Total C N O S 4009 2528 697 773 11	0	0
1	v	500	Total C N O S 4009 2528 697 773 11	0	0
1	w	500	Total C N O S 4009 2528 697 773 11	0	0
1	x	500	Total C N O S 4009 2528 697 773 11	0	0
1	y	500	Total C N O S 4009 2528 697 773 11	0	0
1	z	500	Total C N O S 4009 2528 697 773 11	0	0
1	1	500	Total C N O S 4009 2528 697 773 11	0	0
1	2	500	Total C N O S 4009 2528 697 773 11	0	0
1	3	500	Total C N O S 4009 2528 697 773 11	0	0
1	4	500	Total C N O S 4009 2528 697 773 11	0	0
1	5	500	Total C N O S 4009 2528 697 773 11	0	0
1	6	500	Total C N O S 4009 2528 697 773 11	0	0
1	7	500	Total C N O S 4009 2528 697 773 11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	500	4009	2528	697	773	11	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	ALA	ARG	engineered mutation	UNP P03135
B	432	ALA	ARG	engineered mutation	UNP P03135
C	432	ALA	ARG	engineered mutation	UNP P03135
D	432	ALA	ARG	engineered mutation	UNP P03135
E	432	ALA	ARG	engineered mutation	UNP P03135
F	432	ALA	ARG	engineered mutation	UNP P03135
G	432	ALA	ARG	engineered mutation	UNP P03135
H	432	ALA	ARG	engineered mutation	UNP P03135
I	432	ALA	ARG	engineered mutation	UNP P03135
J	432	ALA	ARG	engineered mutation	UNP P03135
K	432	ALA	ARG	engineered mutation	UNP P03135
L	432	ALA	ARG	engineered mutation	UNP P03135
M	432	ALA	ARG	engineered mutation	UNP P03135
N	432	ALA	ARG	engineered mutation	UNP P03135
O	432	ALA	ARG	engineered mutation	UNP P03135
P	432	ALA	ARG	engineered mutation	UNP P03135
Q	432	ALA	ARG	engineered mutation	UNP P03135
R	432	ALA	ARG	engineered mutation	UNP P03135
S	432	ALA	ARG	engineered mutation	UNP P03135
T	432	ALA	ARG	engineered mutation	UNP P03135
U	432	ALA	ARG	engineered mutation	UNP P03135
V	432	ALA	ARG	engineered mutation	UNP P03135
W	432	ALA	ARG	engineered mutation	UNP P03135
X	432	ALA	ARG	engineered mutation	UNP P03135
Y	432	ALA	ARG	engineered mutation	UNP P03135
Z	432	ALA	ARG	engineered mutation	UNP P03135
a	432	ALA	ARG	engineered mutation	UNP P03135
b	432	ALA	ARG	engineered mutation	UNP P03135
c	432	ALA	ARG	engineered mutation	UNP P03135
d	432	ALA	ARG	engineered mutation	UNP P03135
e	432	ALA	ARG	engineered mutation	UNP P03135
f	432	ALA	ARG	engineered mutation	UNP P03135
g	432	ALA	ARG	engineered mutation	UNP P03135
h	432	ALA	ARG	engineered mutation	UNP P03135
i	432	ALA	ARG	engineered mutation	UNP P03135
j	432	ALA	ARG	engineered mutation	UNP P03135

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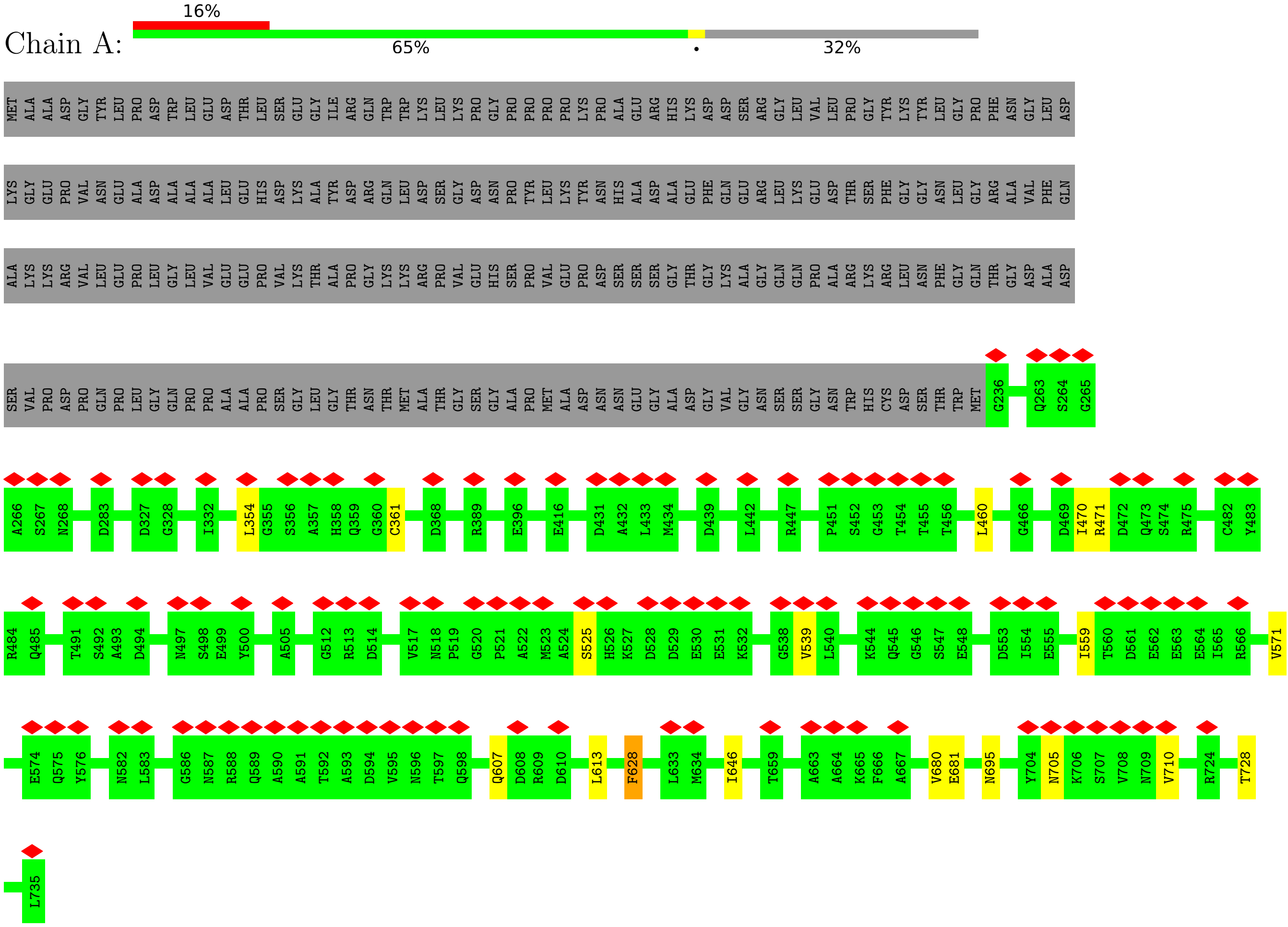
Chain	Residue	Modelled	Actual	Comment	Reference
k	432	ALA	ARG	engineered mutation	UNP P03135
l	432	ALA	ARG	engineered mutation	UNP P03135
m	432	ALA	ARG	engineered mutation	UNP P03135
n	432	ALA	ARG	engineered mutation	UNP P03135
o	432	ALA	ARG	engineered mutation	UNP P03135
p	432	ALA	ARG	engineered mutation	UNP P03135
q	432	ALA	ARG	engineered mutation	UNP P03135
r	432	ALA	ARG	engineered mutation	UNP P03135
s	432	ALA	ARG	engineered mutation	UNP P03135
t	432	ALA	ARG	engineered mutation	UNP P03135
u	432	ALA	ARG	engineered mutation	UNP P03135
v	432	ALA	ARG	engineered mutation	UNP P03135
w	432	ALA	ARG	engineered mutation	UNP P03135
x	432	ALA	ARG	engineered mutation	UNP P03135
y	432	ALA	ARG	engineered mutation	UNP P03135
z	432	ALA	ARG	engineered mutation	UNP P03135
1	432	ALA	ARG	engineered mutation	UNP P03135
2	432	ALA	ARG	engineered mutation	UNP P03135
3	432	ALA	ARG	engineered mutation	UNP P03135
4	432	ALA	ARG	engineered mutation	UNP P03135
5	432	ALA	ARG	engineered mutation	UNP P03135
6	432	ALA	ARG	engineered mutation	UNP P03135
7	432	ALA	ARG	engineered mutation	UNP P03135
8	432	ALA	ARG	engineered mutation	UNP P03135

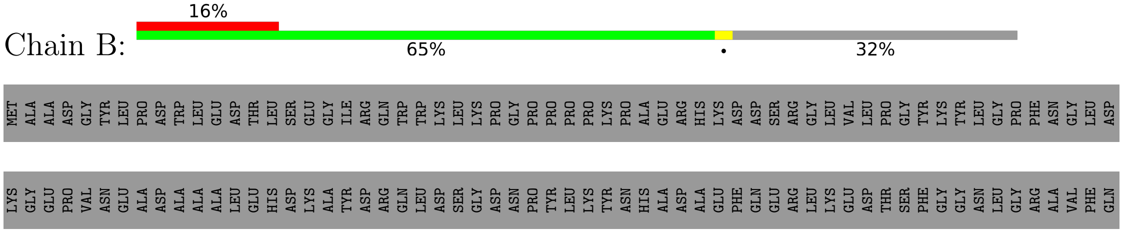
3 Residue-property plots ⓘ

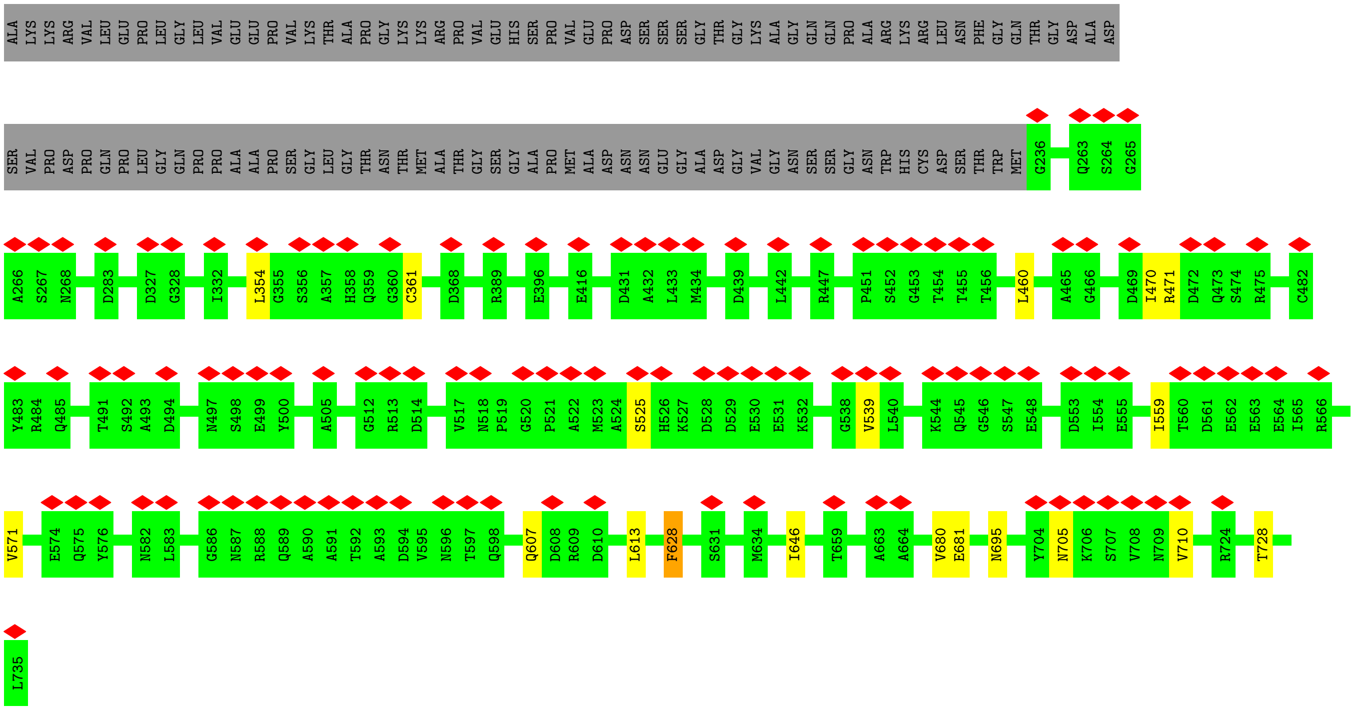
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Capsid protein VP1



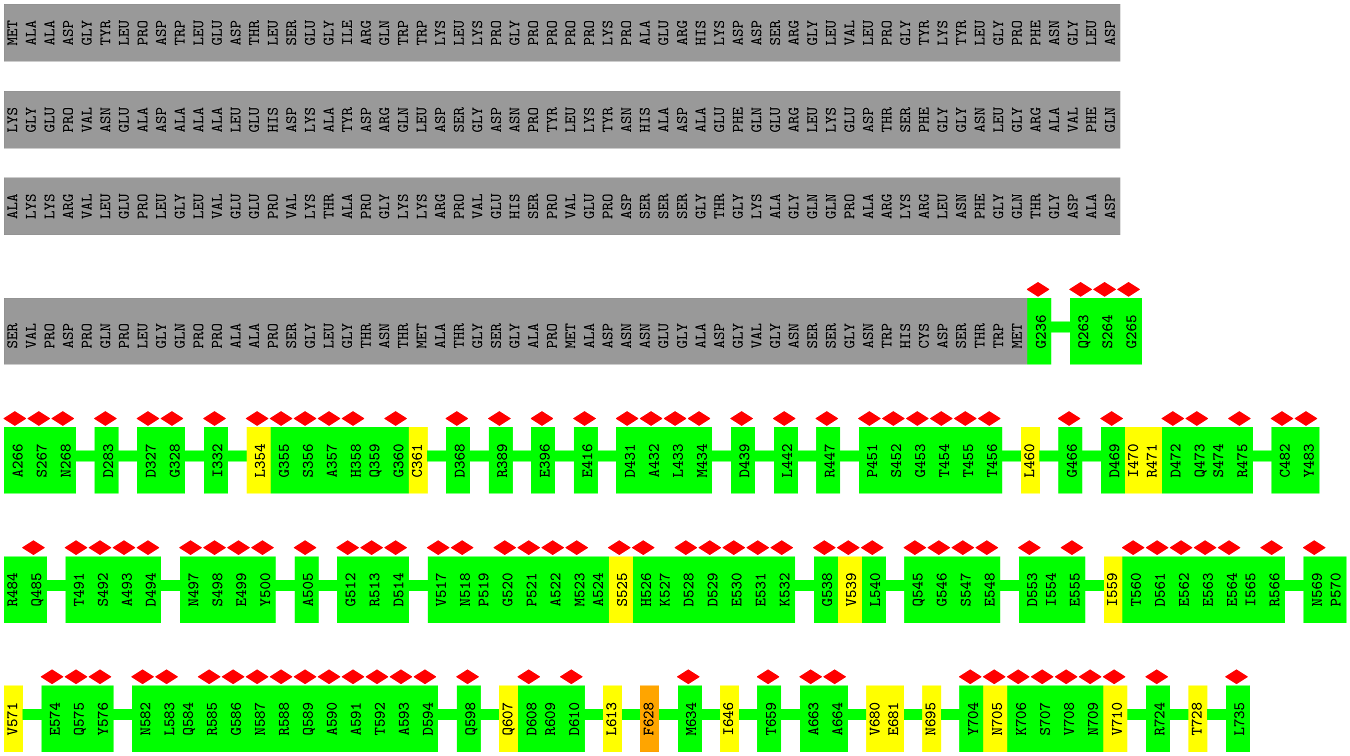
- Molecule 1: Capsid protein VP1





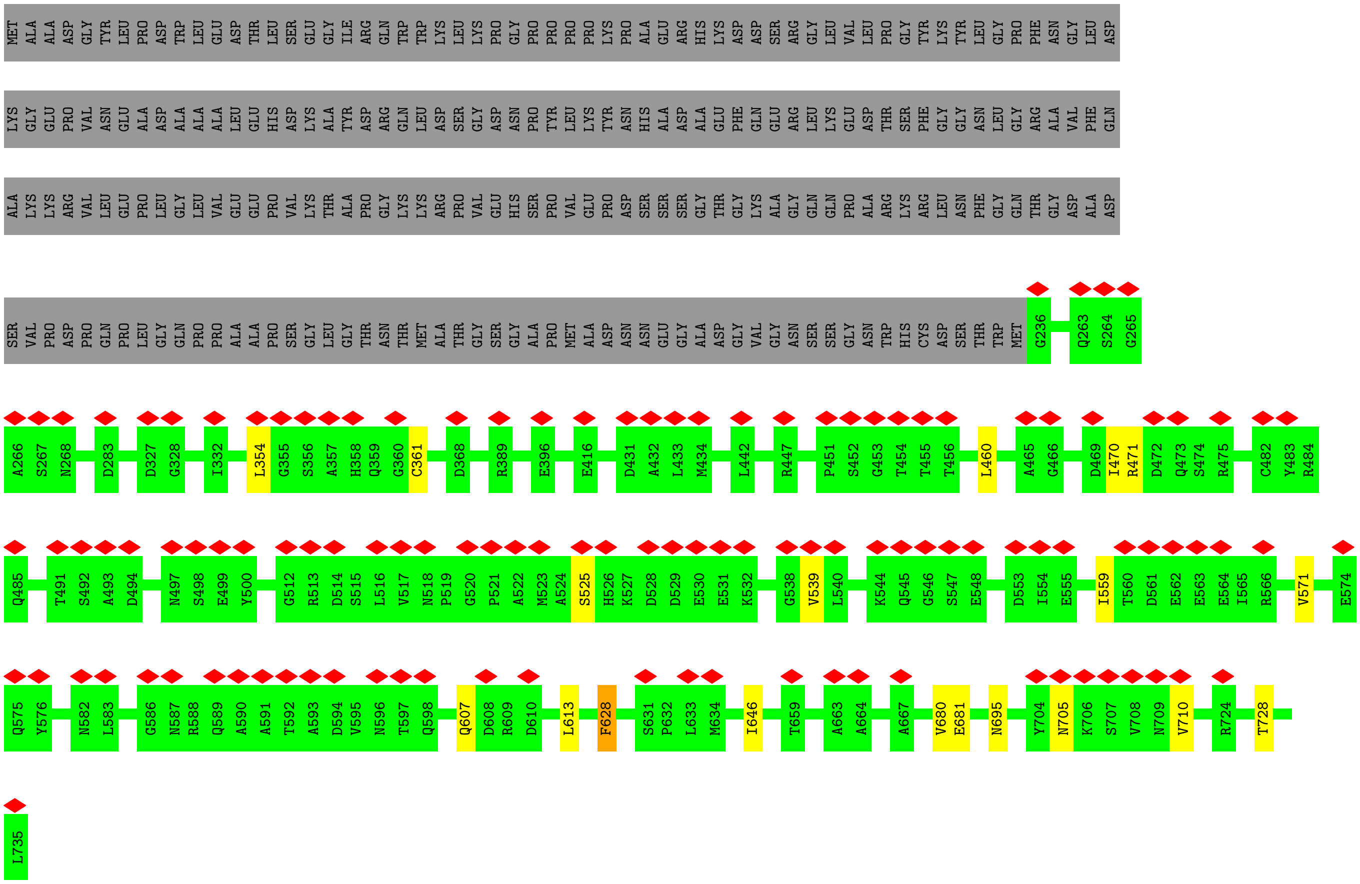
- Molecule 1: Capsid protein VP1

Chain C:

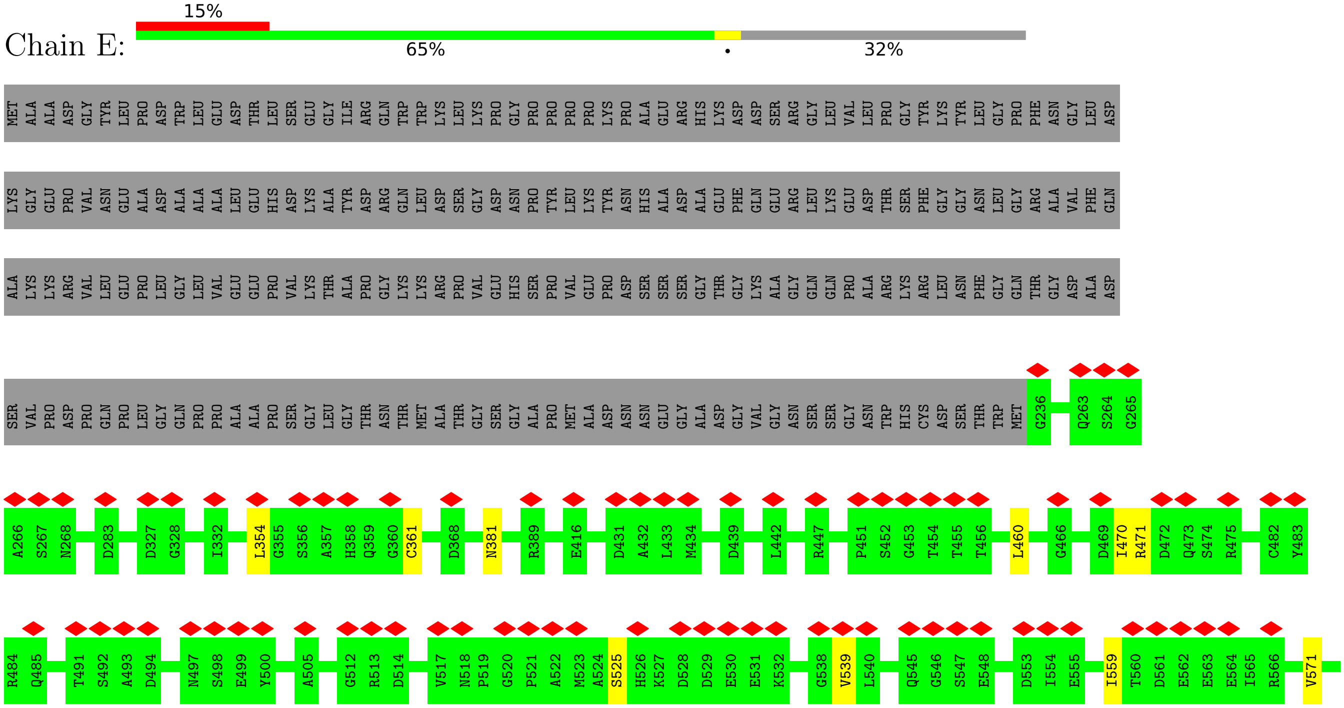


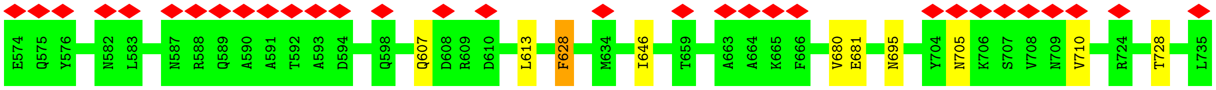
- Molecule 1: Capsid protein VP1

Chain D:



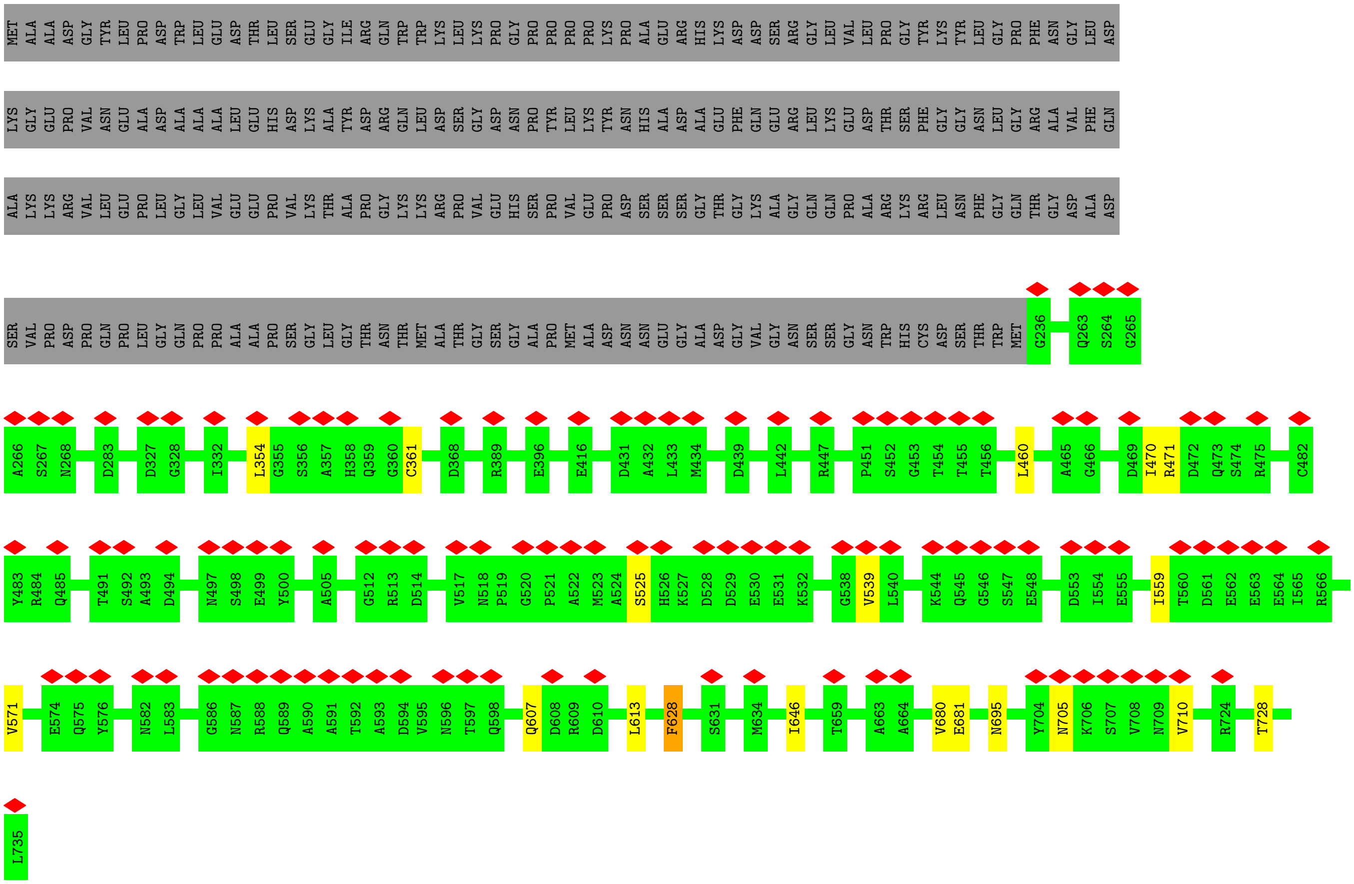
- Molecule 1: Capsid protein VP1





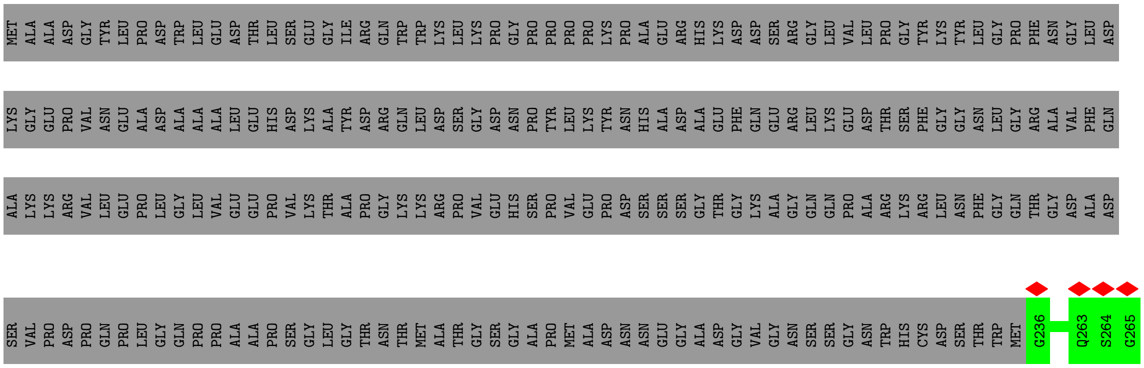
- Molecule 1: Capsid protein VP1

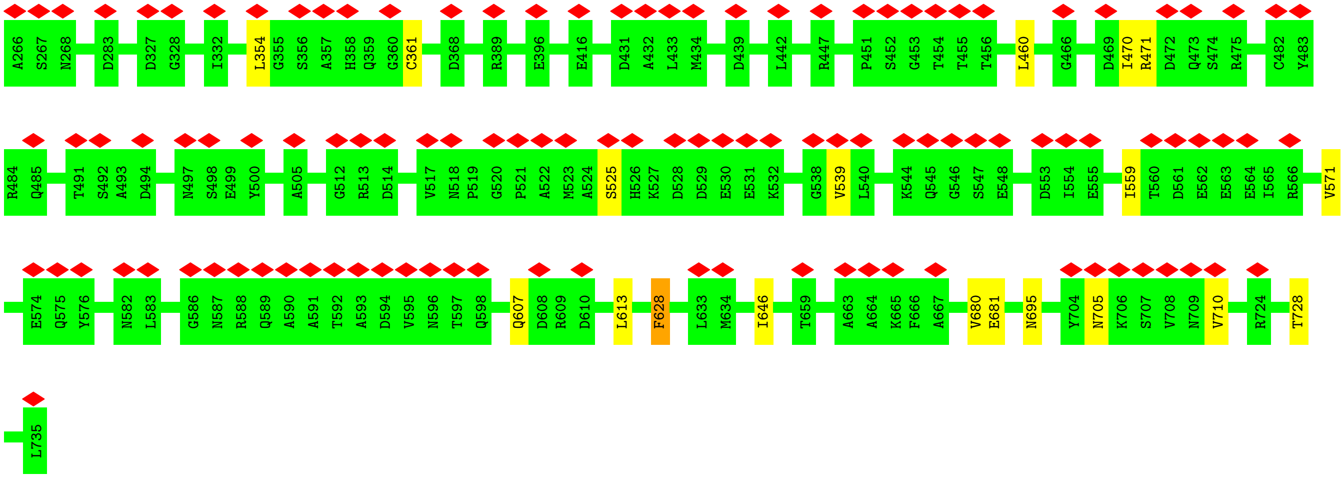
Chain F:



- Molecule 1: Capsid protein VP1

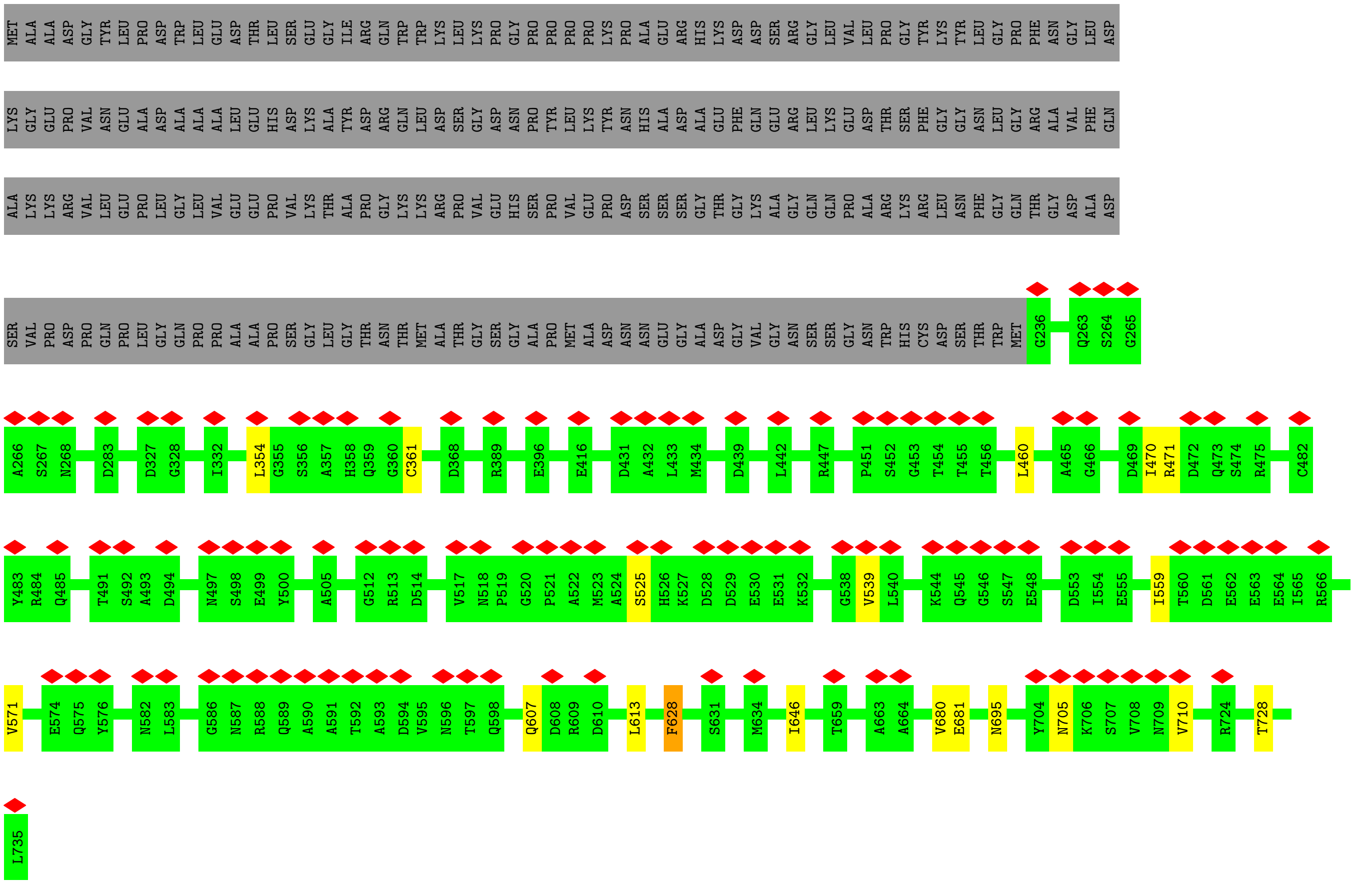
Chain G:





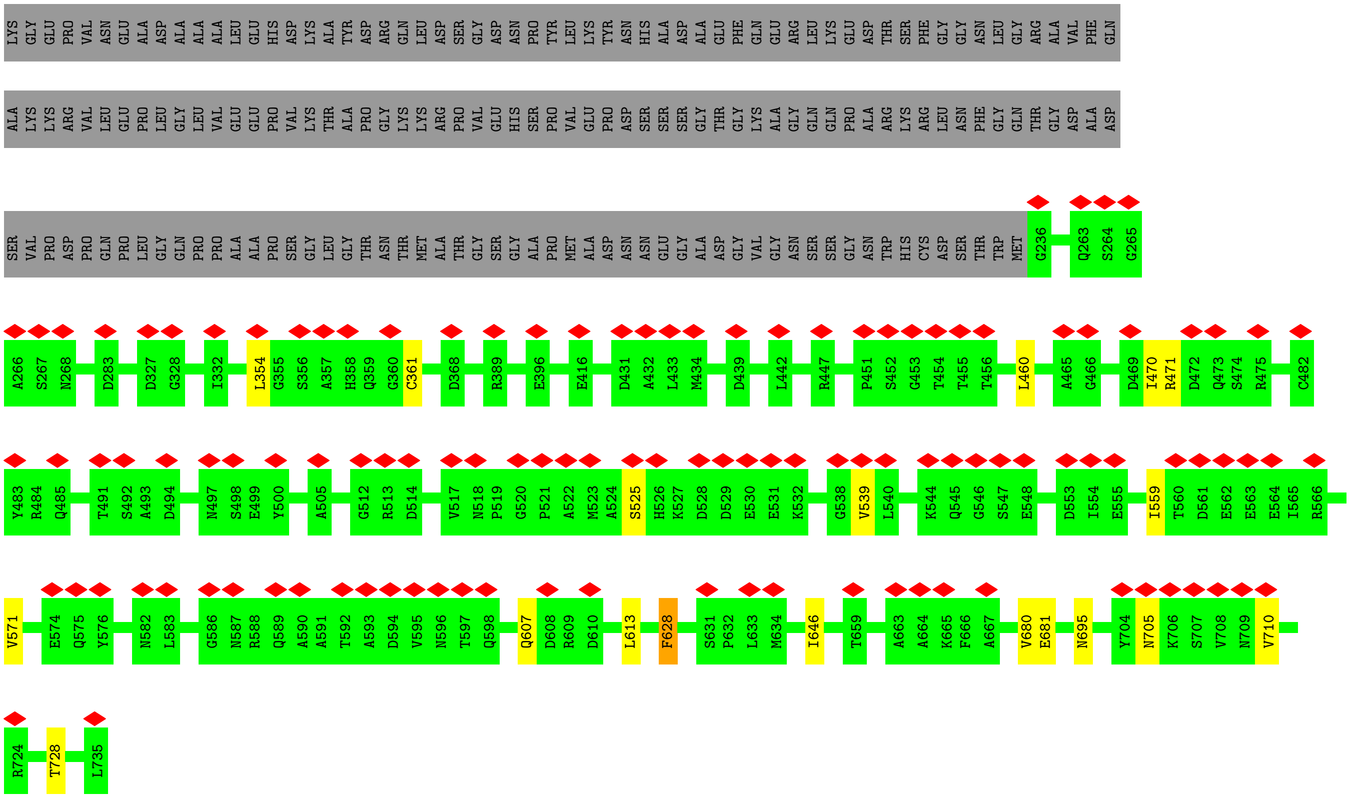
- Molecule 1: Capsid protein VP1

Chain H:



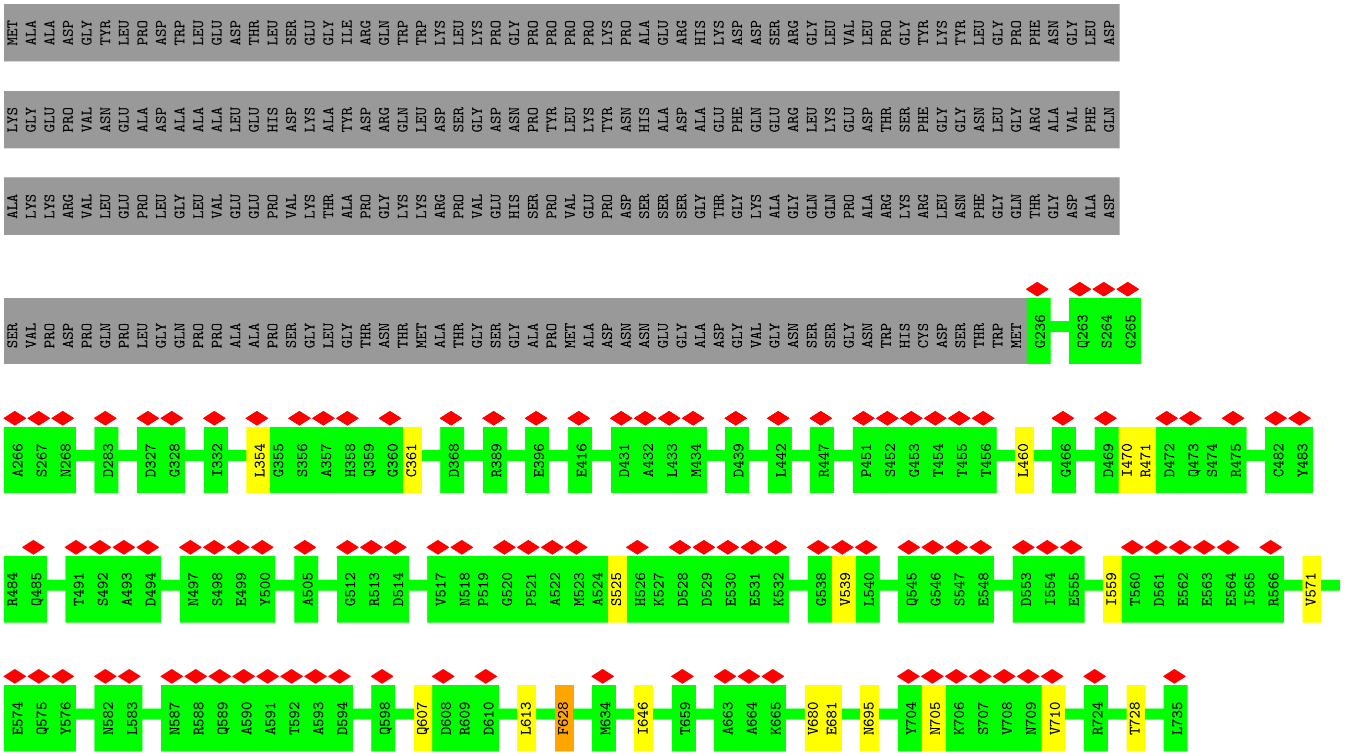
- Molecule 1: Capsid protein VP1

Chain I:



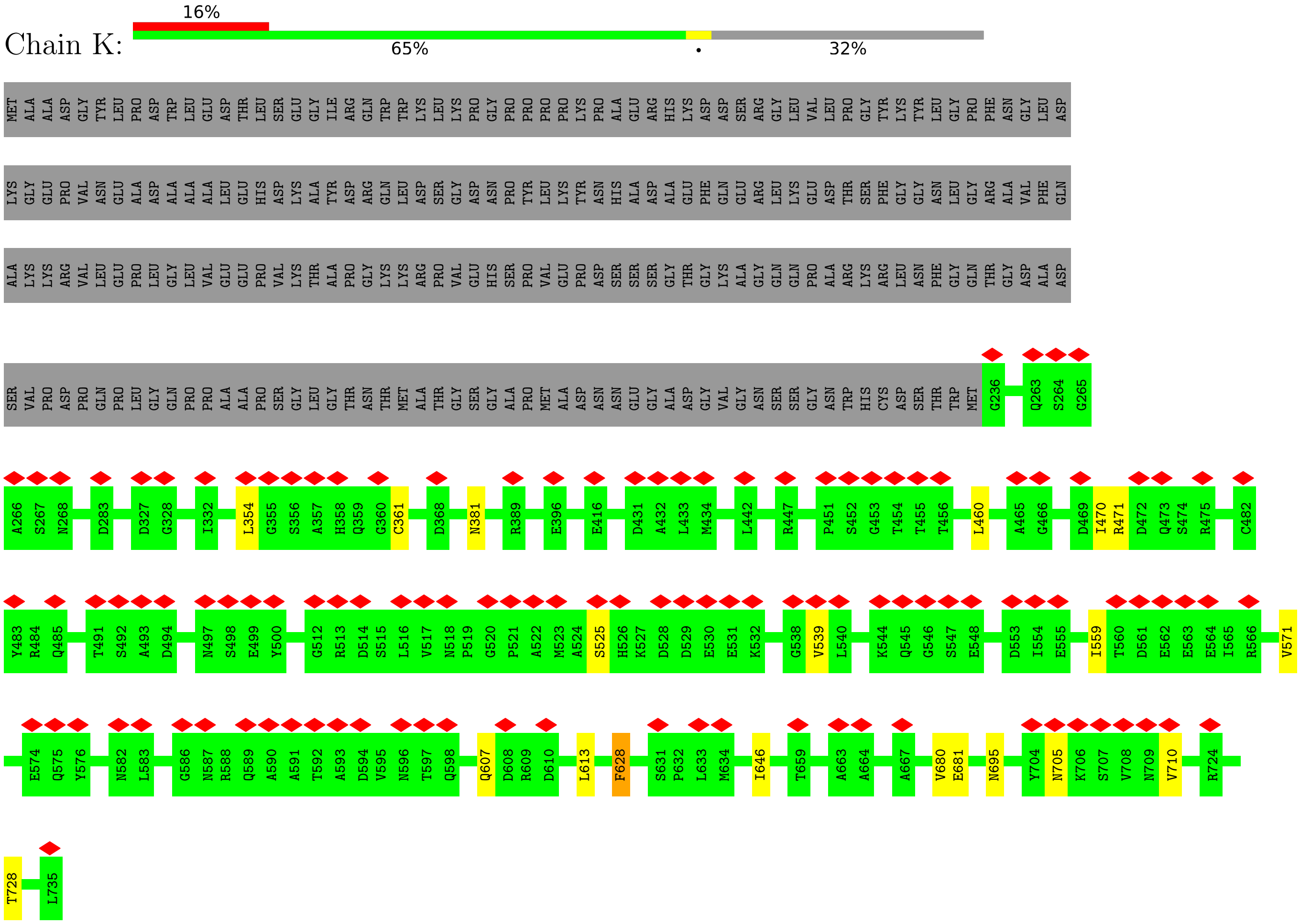
- Molecule 1: Capsid protein VP1

Chain J:



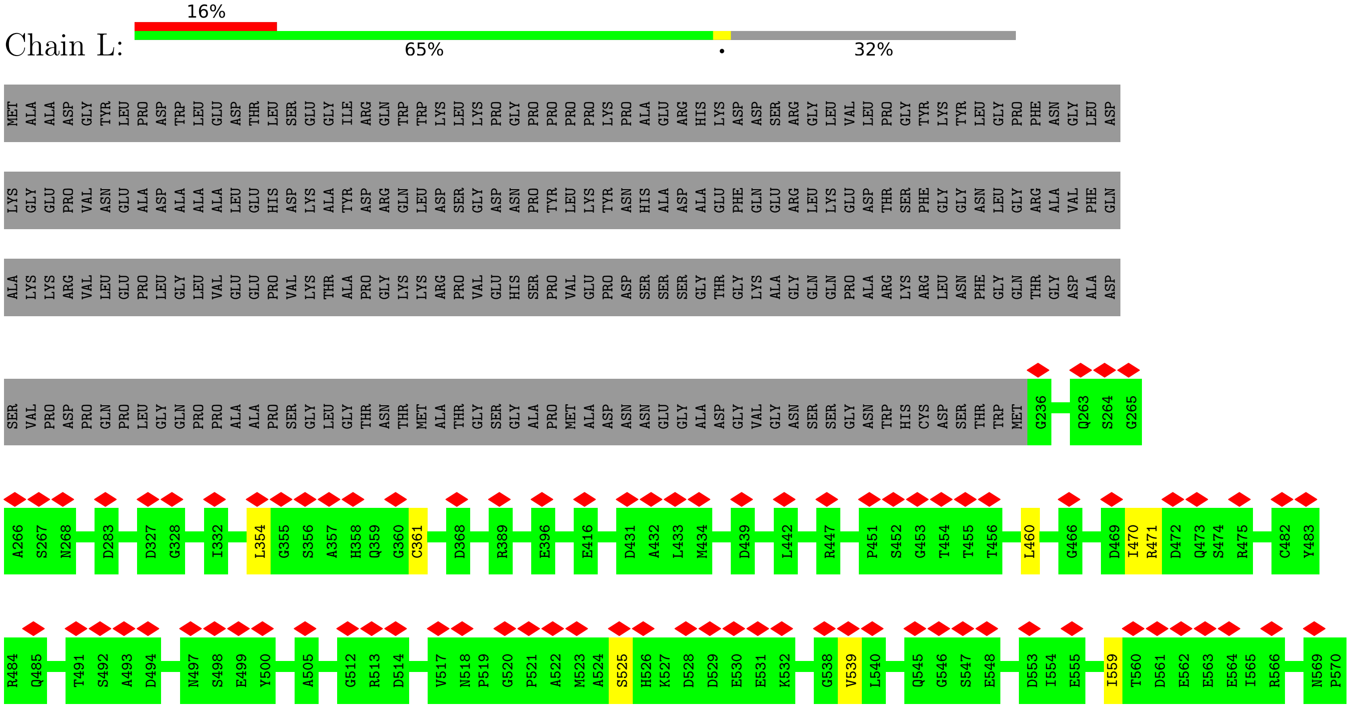
- Molecule 1: Capsid protein VP1

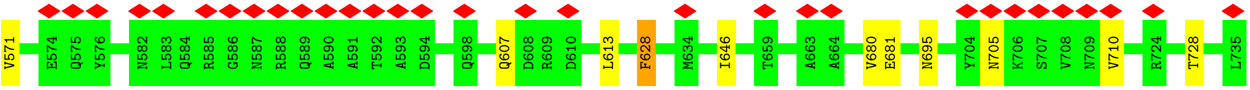
Chain K:



- Molecule 1: Capsid protein VP1

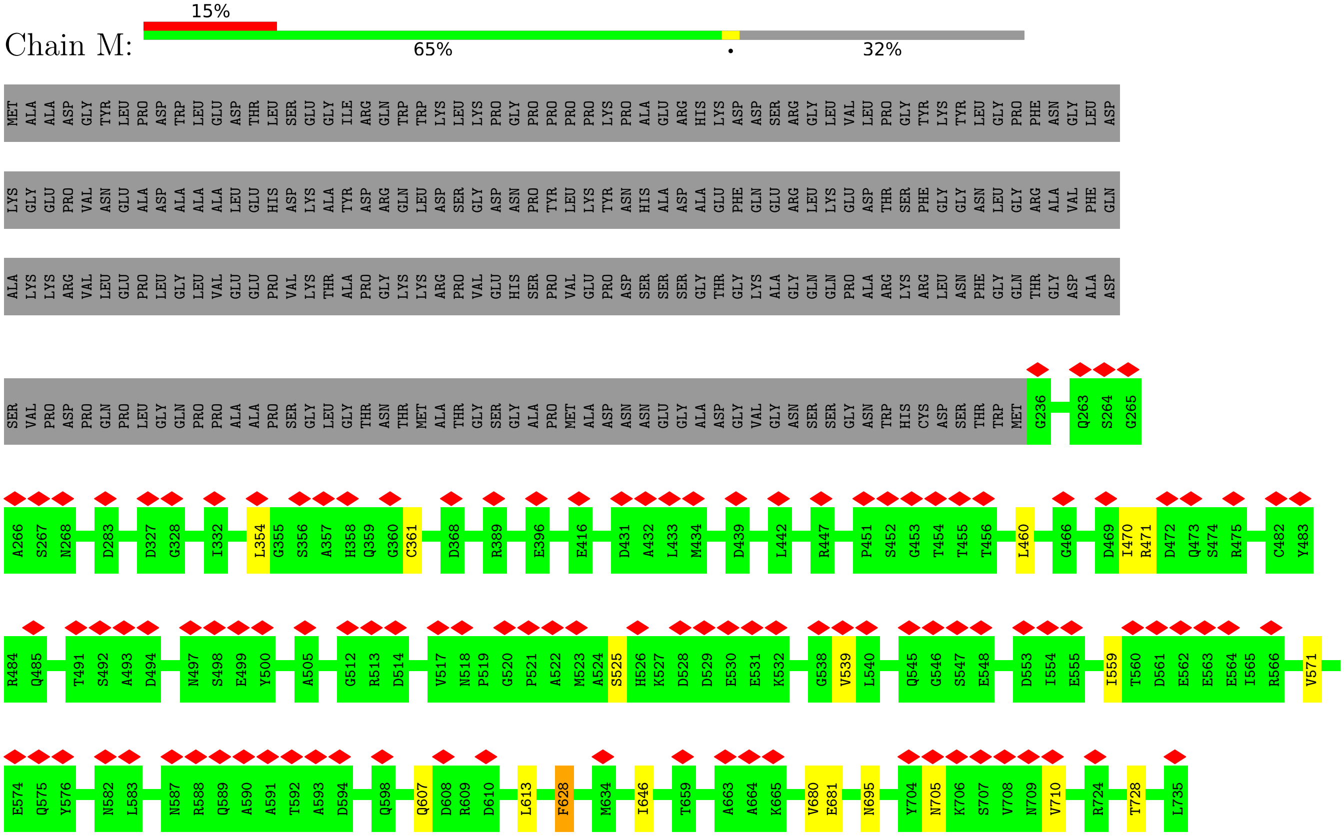
Chain L:





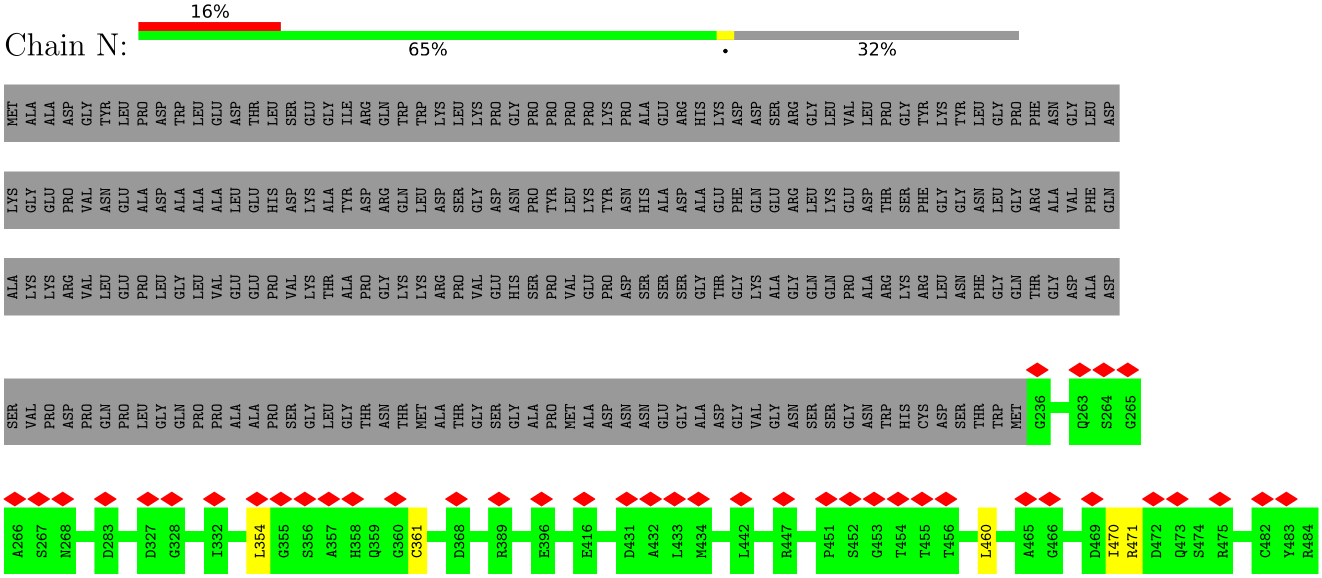
- Molecule 1: Capsid protein VP1

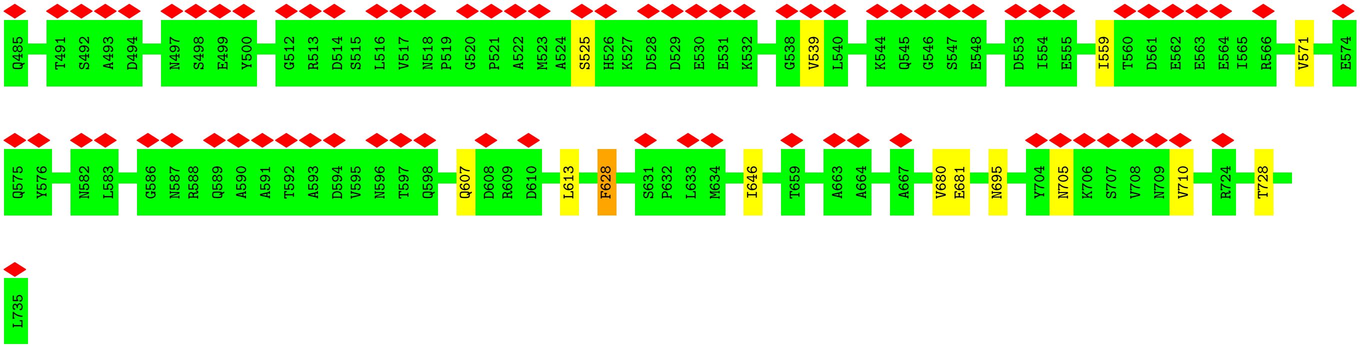
Chain M:



- Molecule 1: Capsid protein VP1

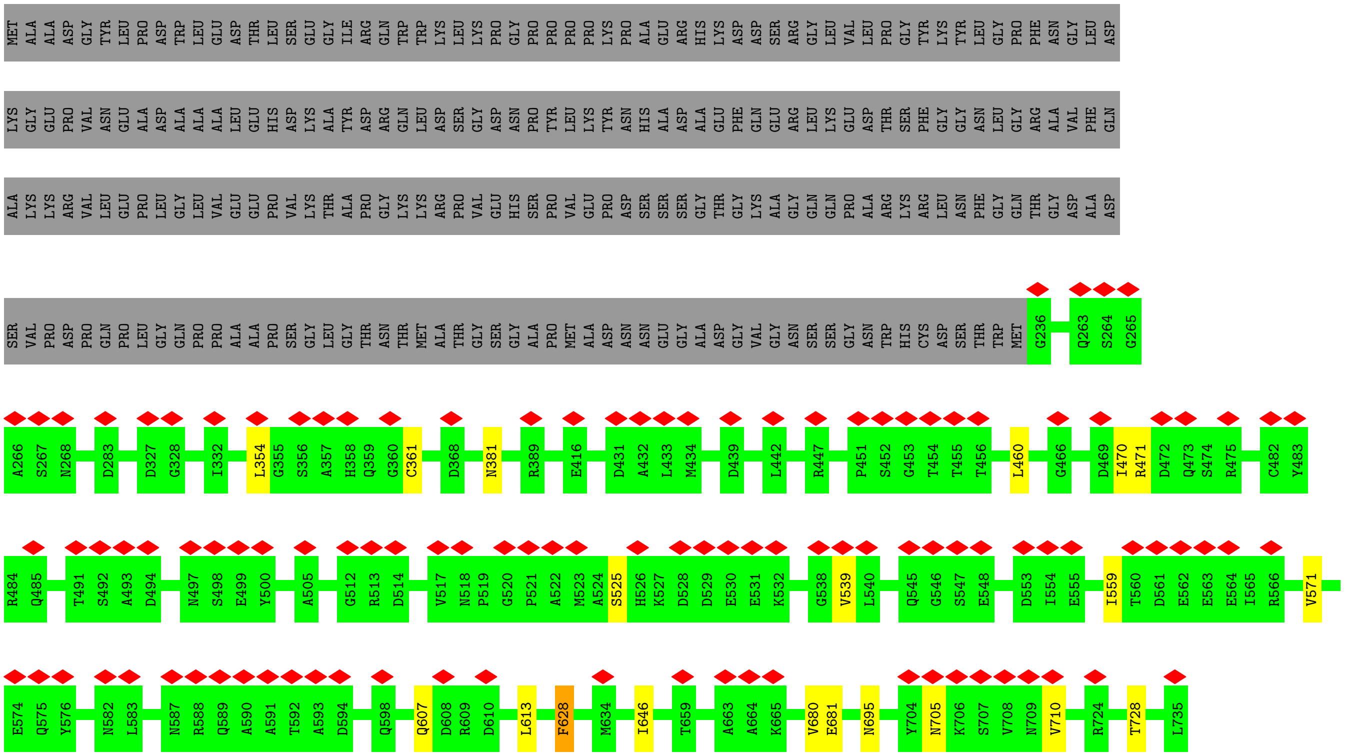
Chain N:





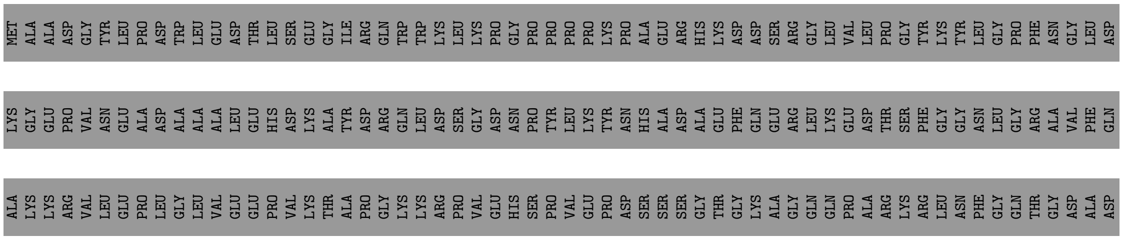
- Molecule 1: Capsid protein VP1

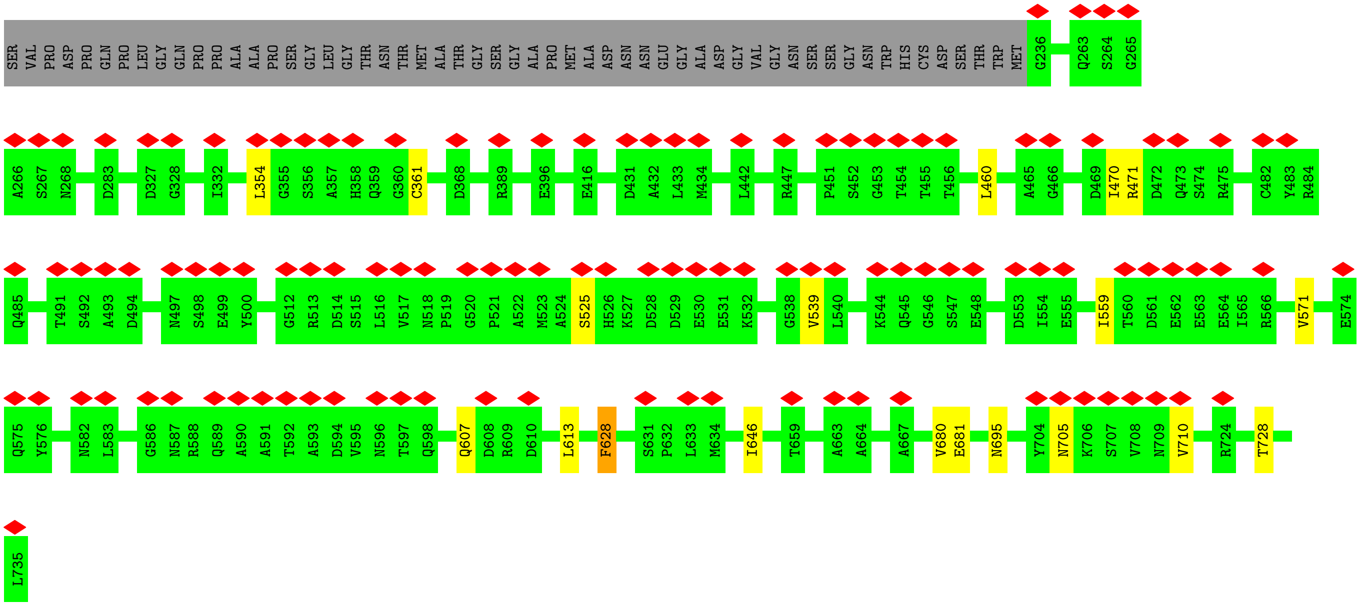
Chain O:



- Molecule 1: Capsid protein VP1

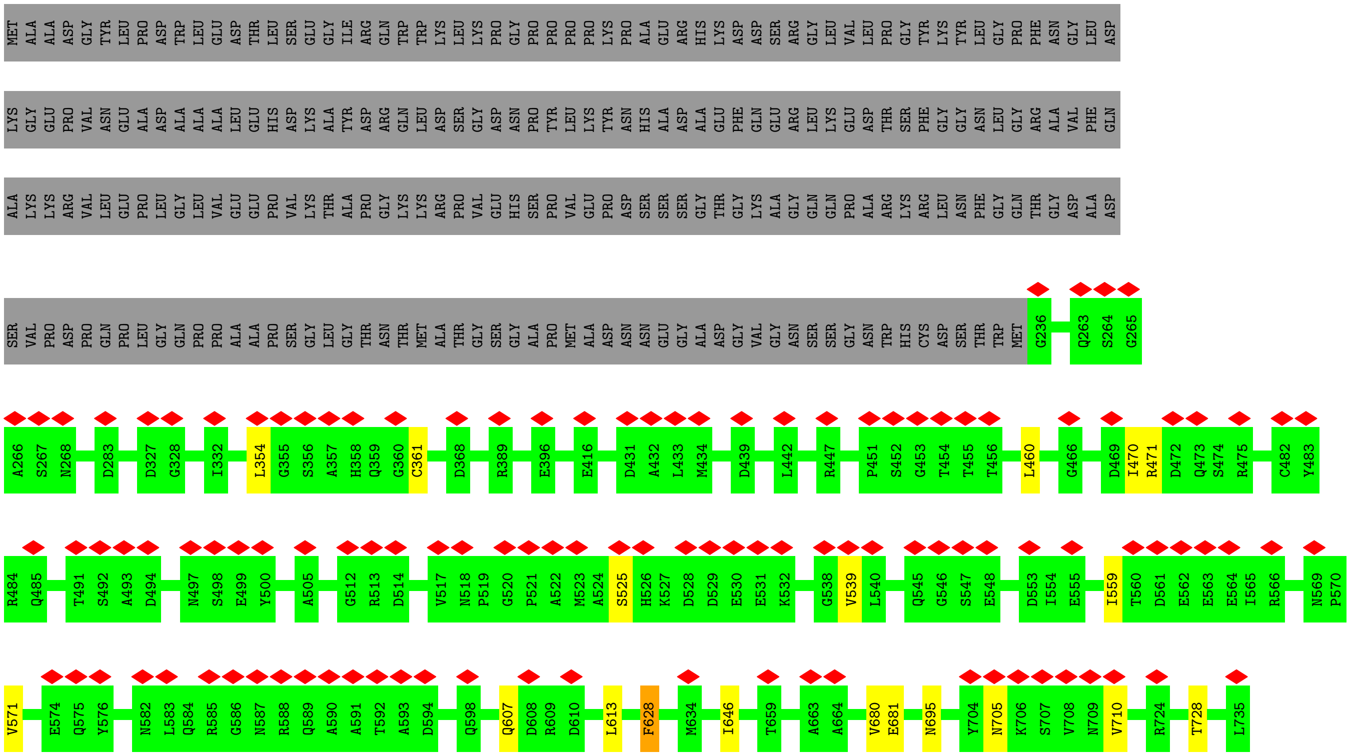
Chain P:





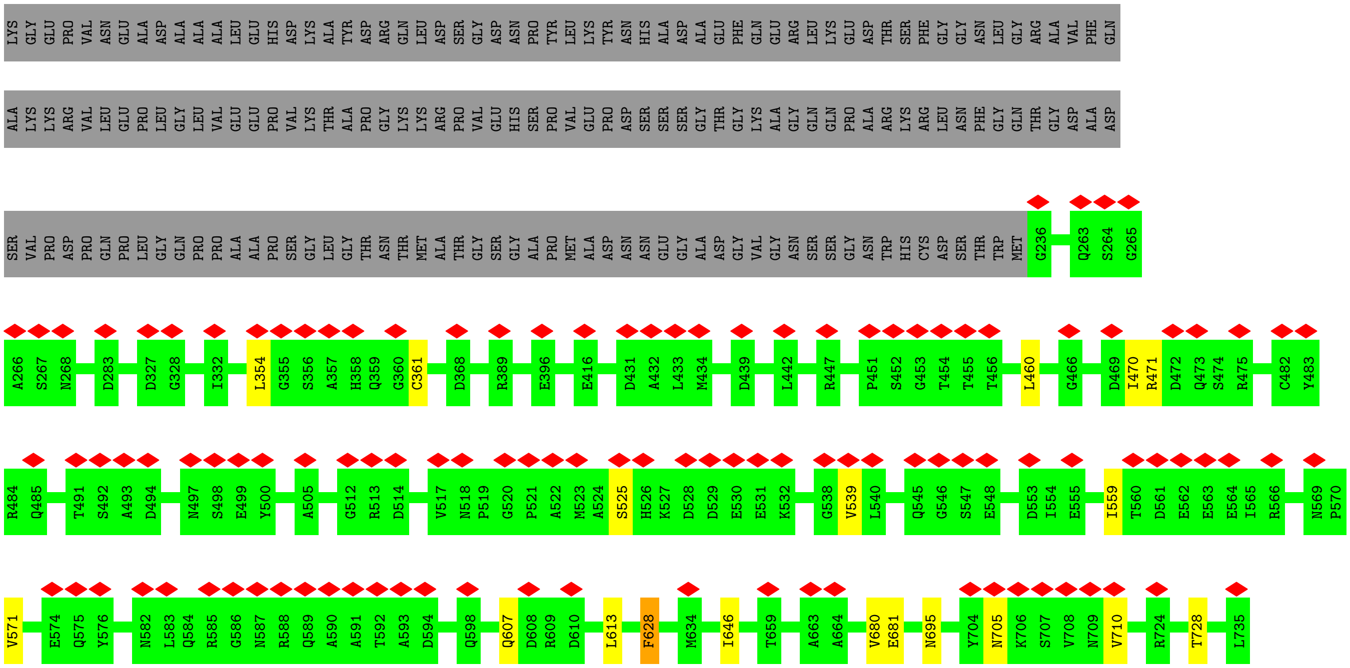
- Molecule 1: Capsid protein VP1

Chain Q:



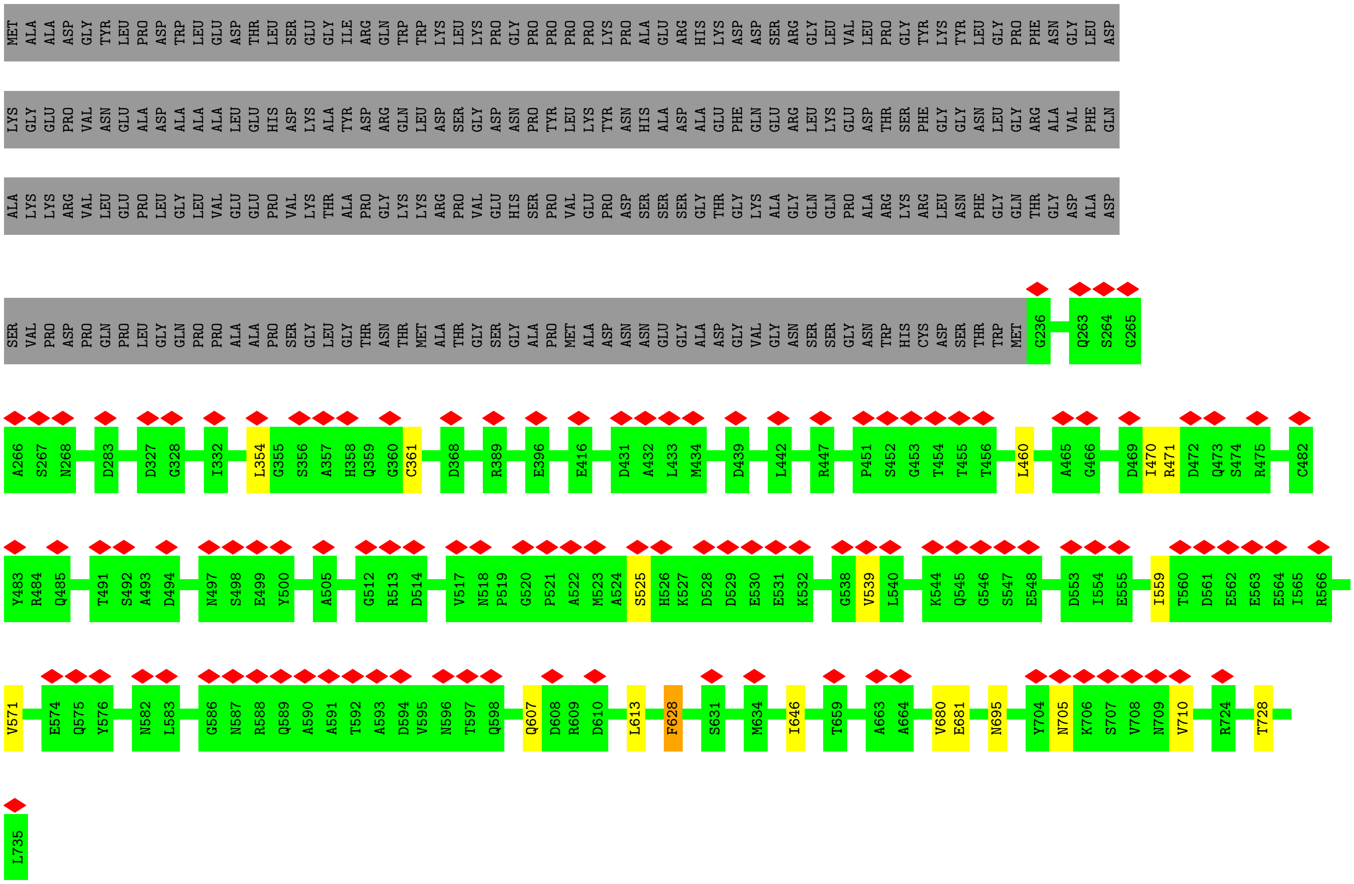
- Molecule 1: Capsid protein VP1

Chain R:

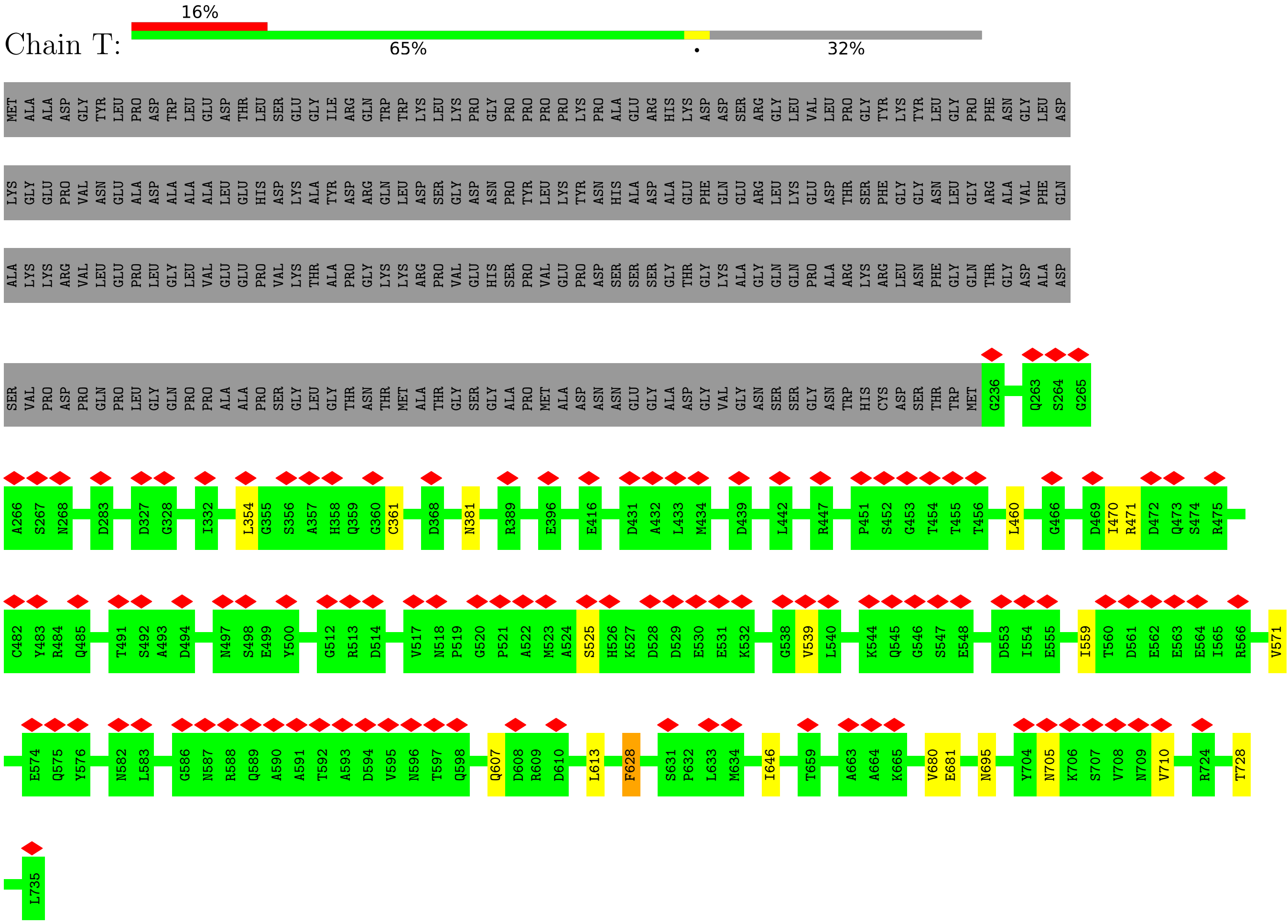


- Molecule 1: Capsid protein VP1

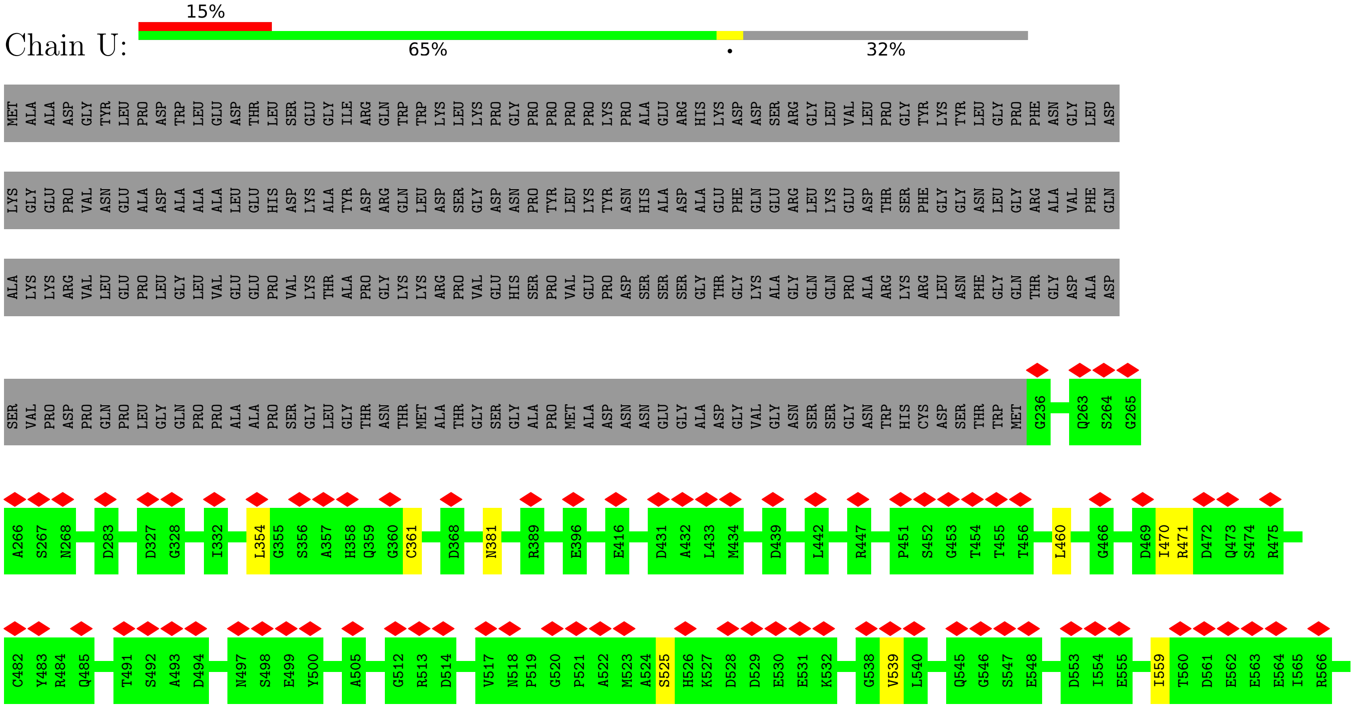
Chain S:

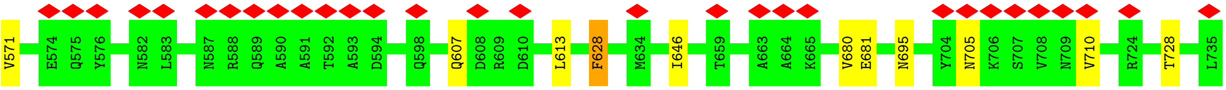


- Molecule 1: Capsid protein VP1



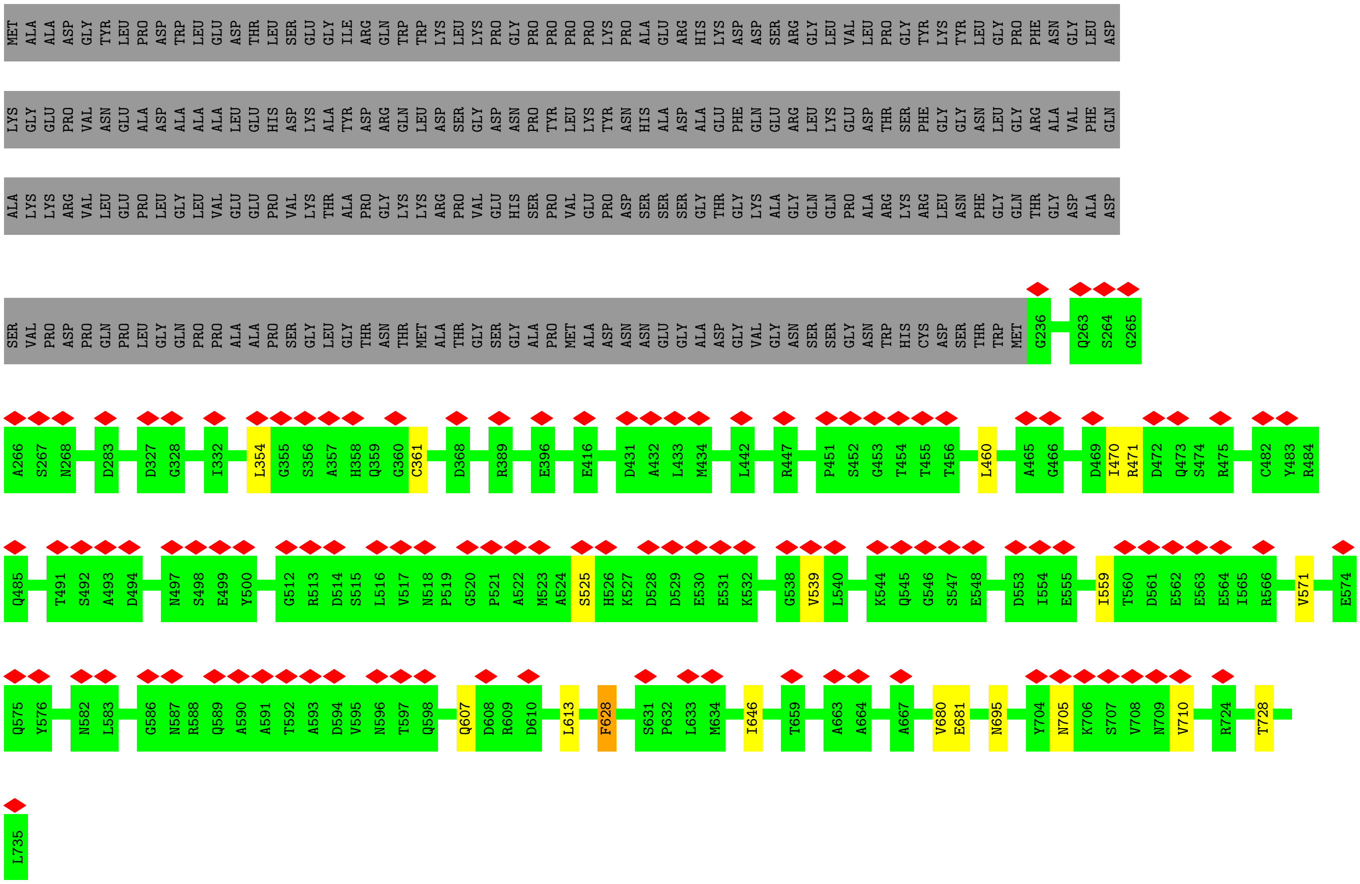
• Molecule 1: Capsid protein VP1





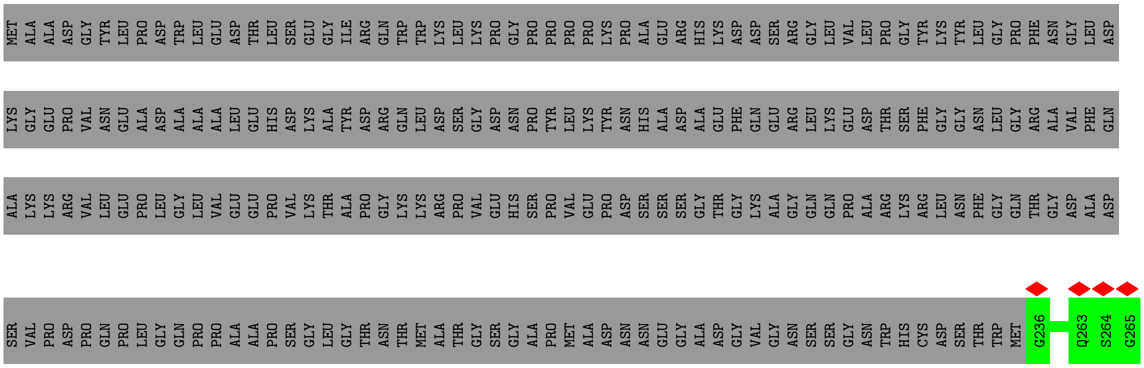
- Molecule 1: Capsid protein VP1

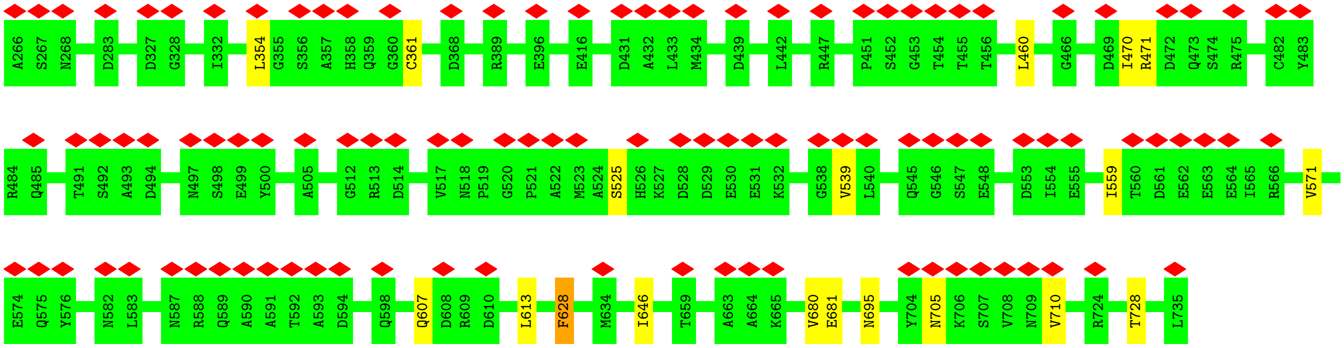
Chain V:



- Molecule 1: Capsid protein VP1

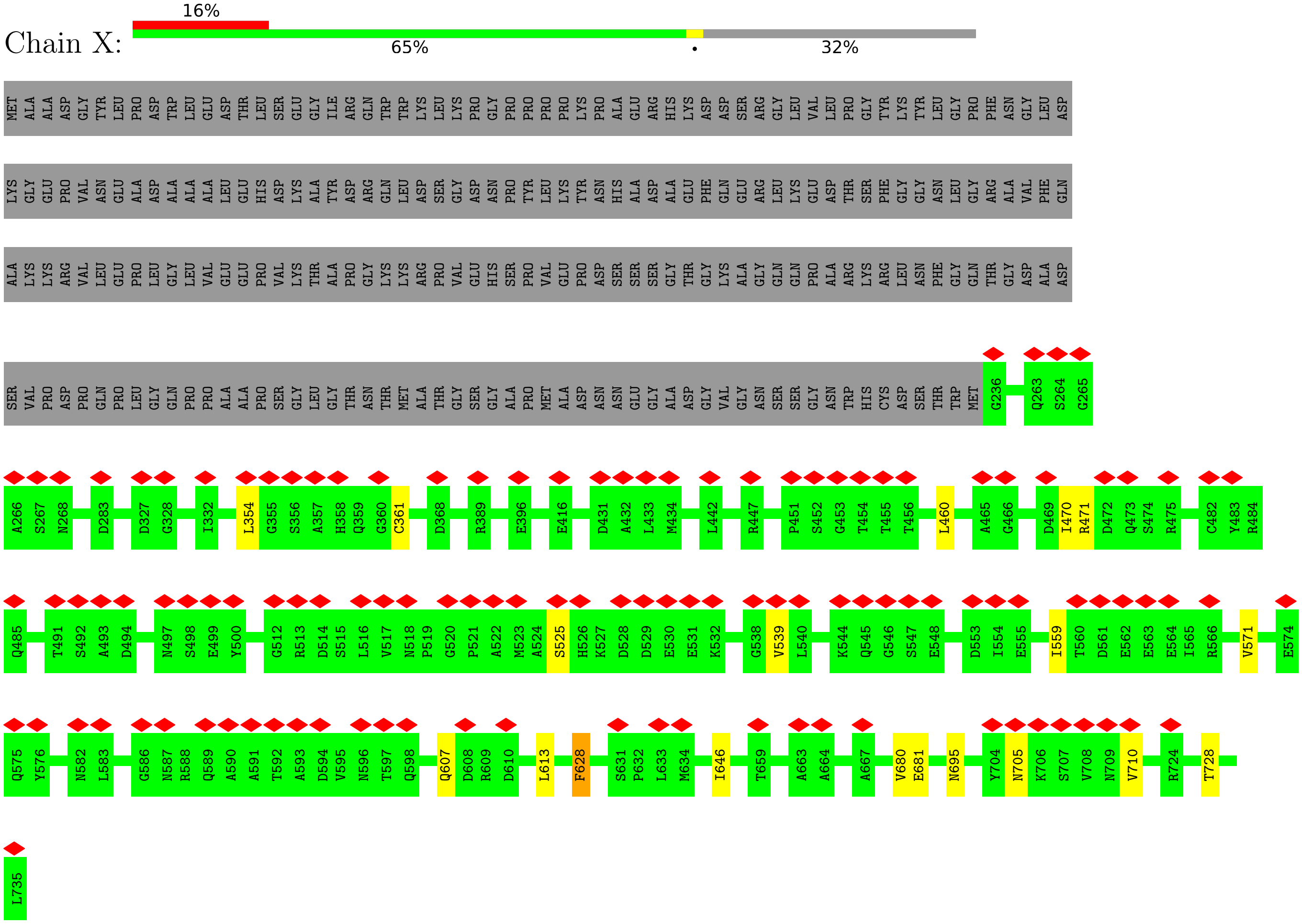
Chain W:





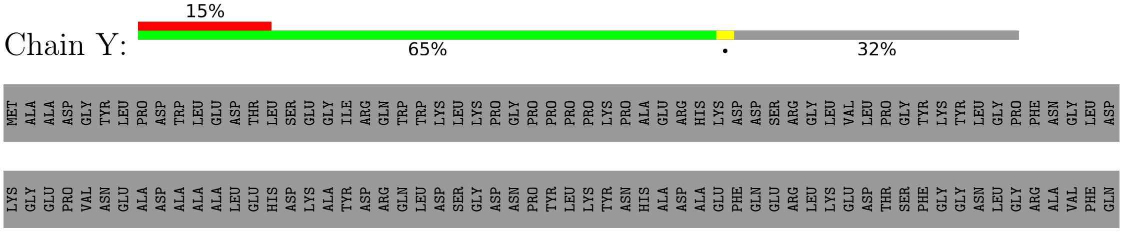
- Molecule 1: Capsid protein VP1

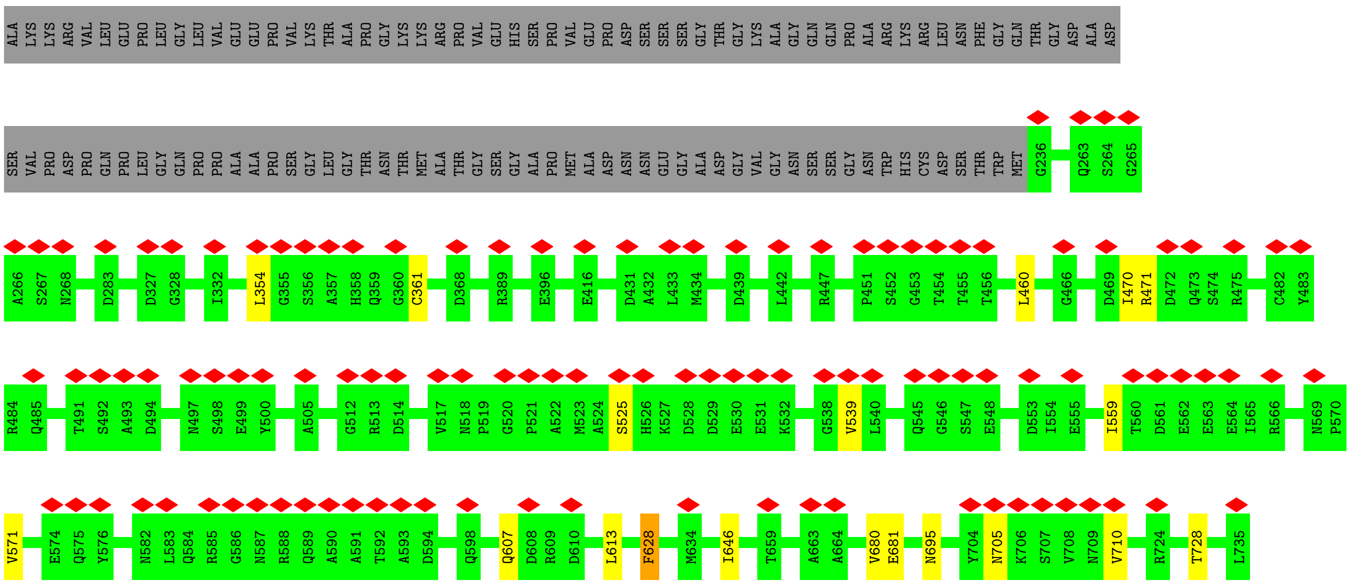
Chain X:



- Molecule 1: Capsid protein VP1

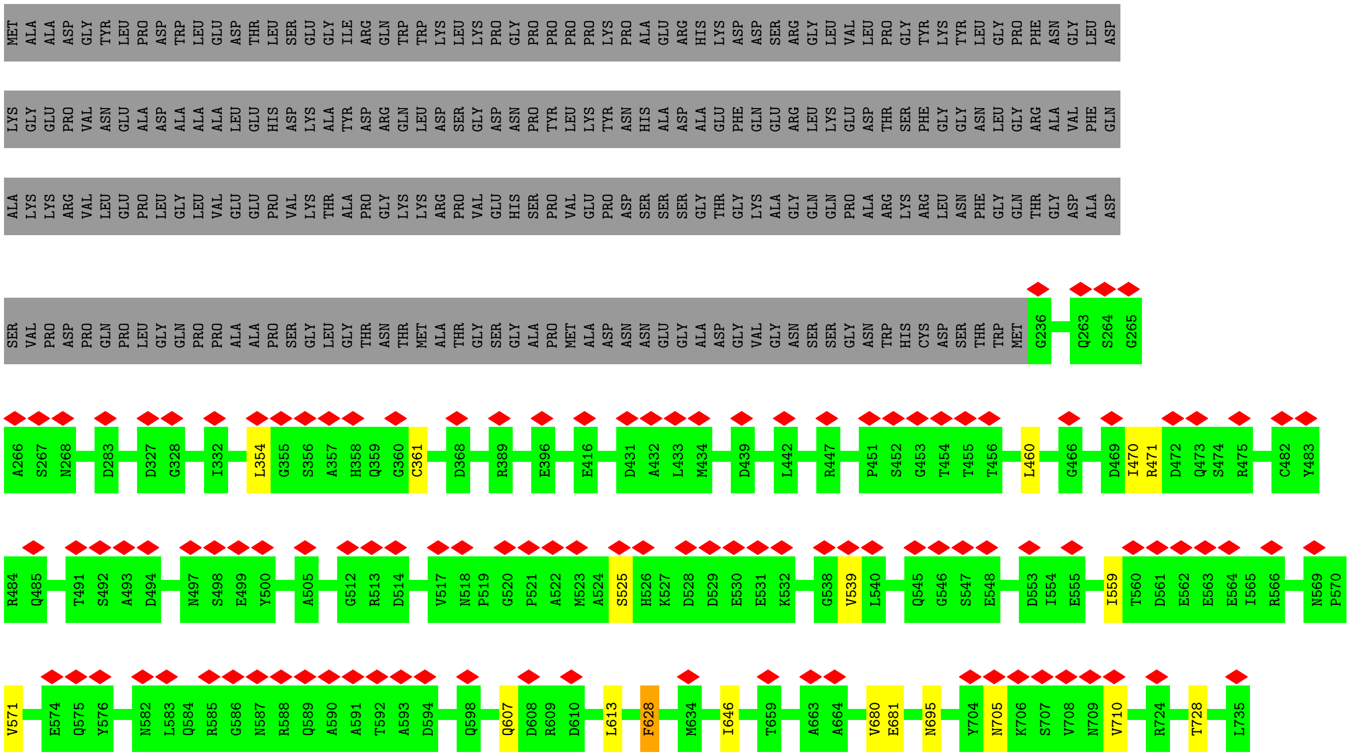
Chain Y:





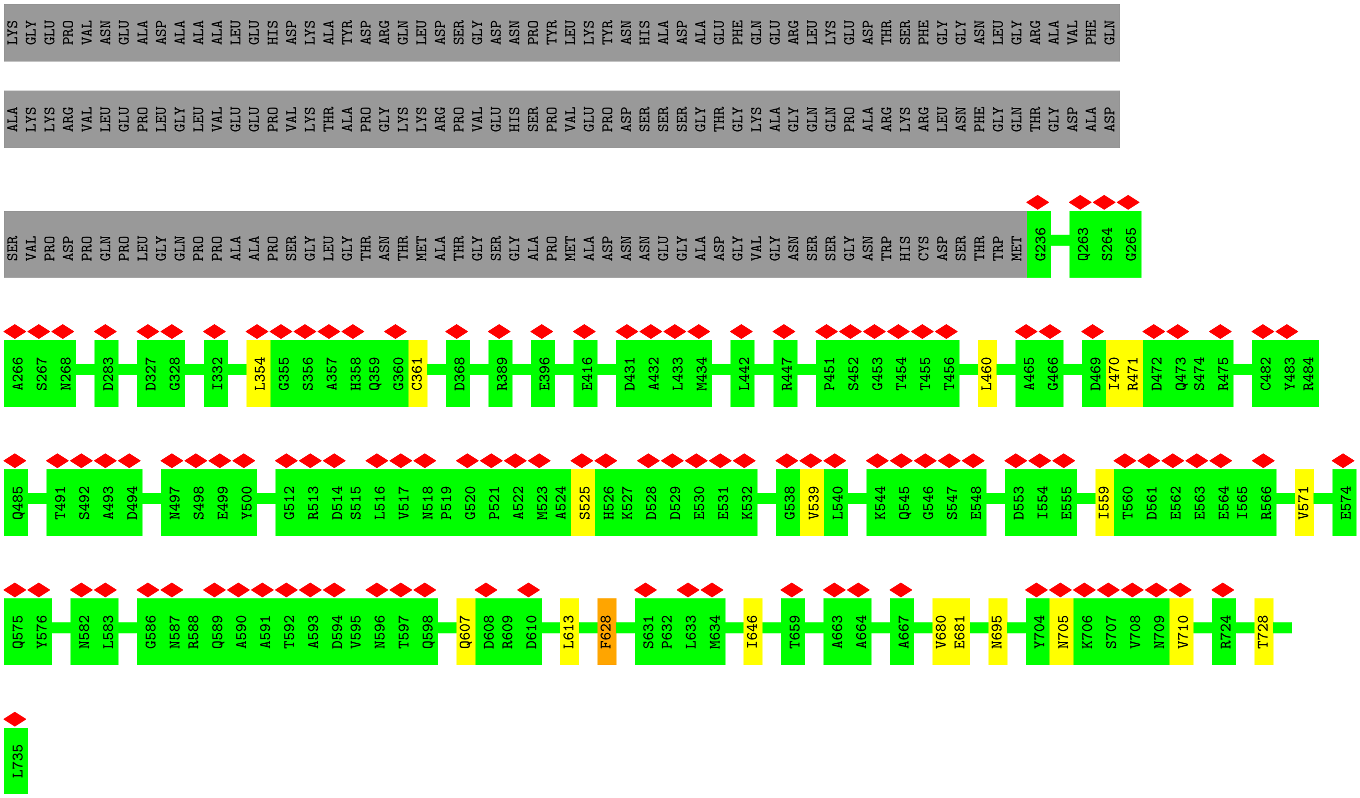
- Molecule 1: Capsid protein VP1

Chain Z:



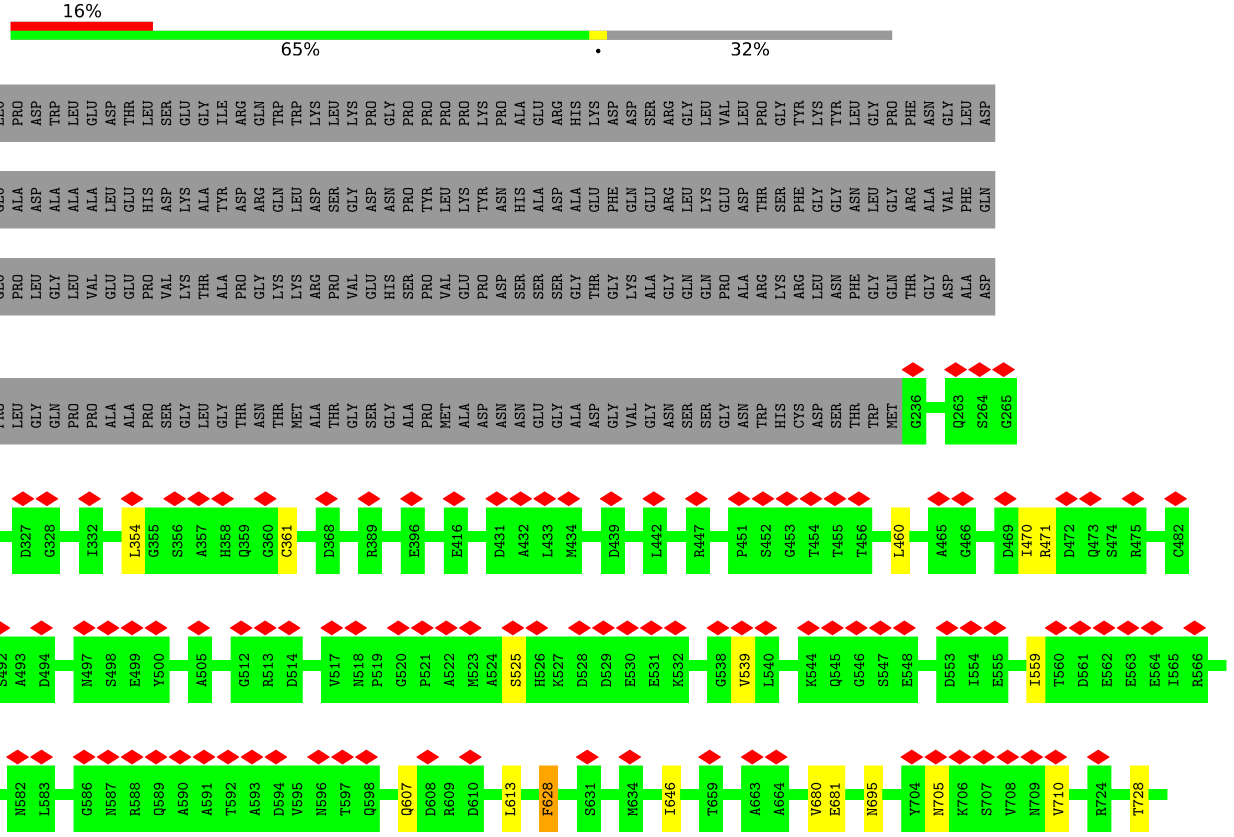
- Molecule 1: Capsid protein VP1

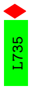
Chain a:



• Molecule 1: Capsid protein VP1

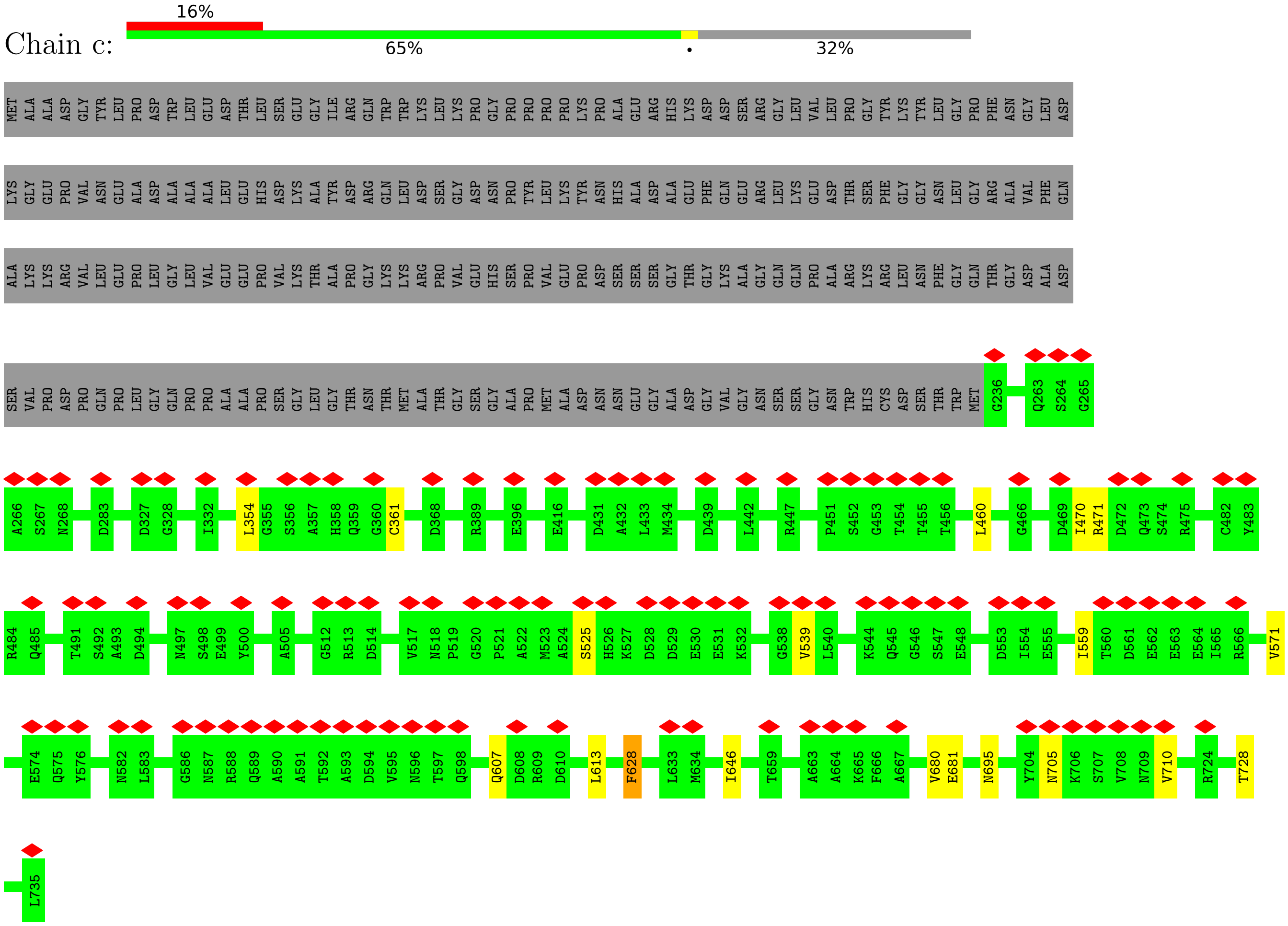
Chain b:





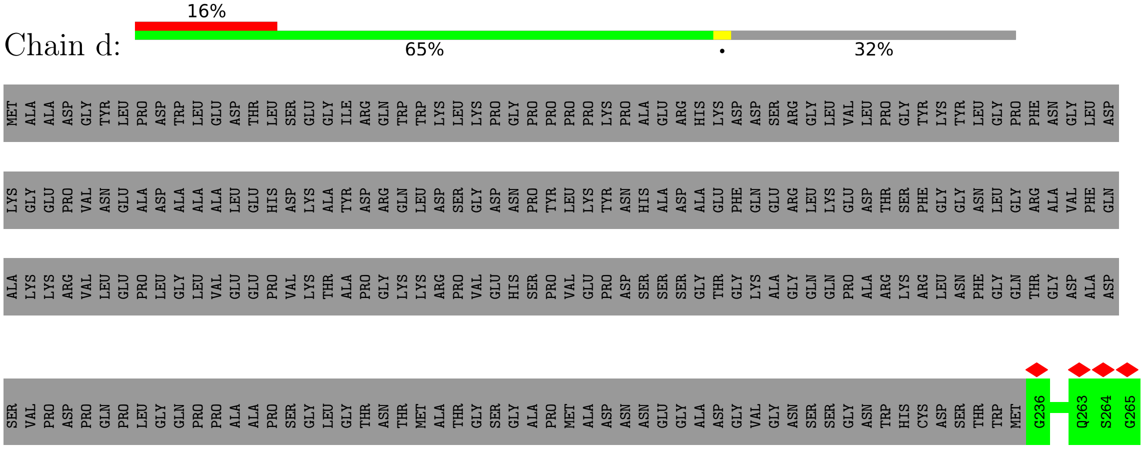
- Molecule 1: Capsid protein VP1

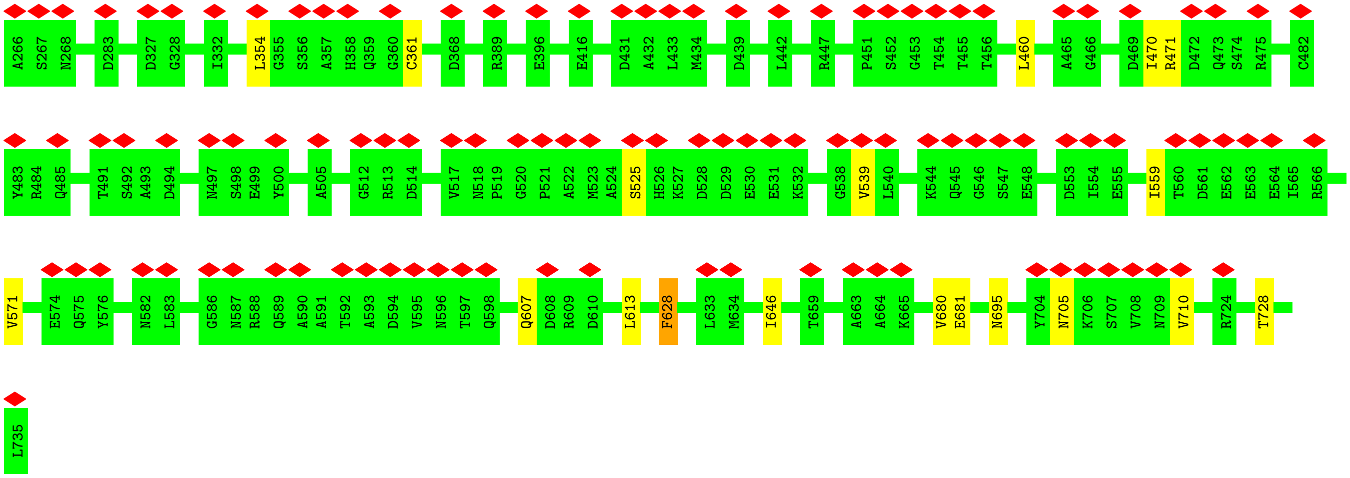
Chain c:



- Molecule 1: Capsid protein VP1

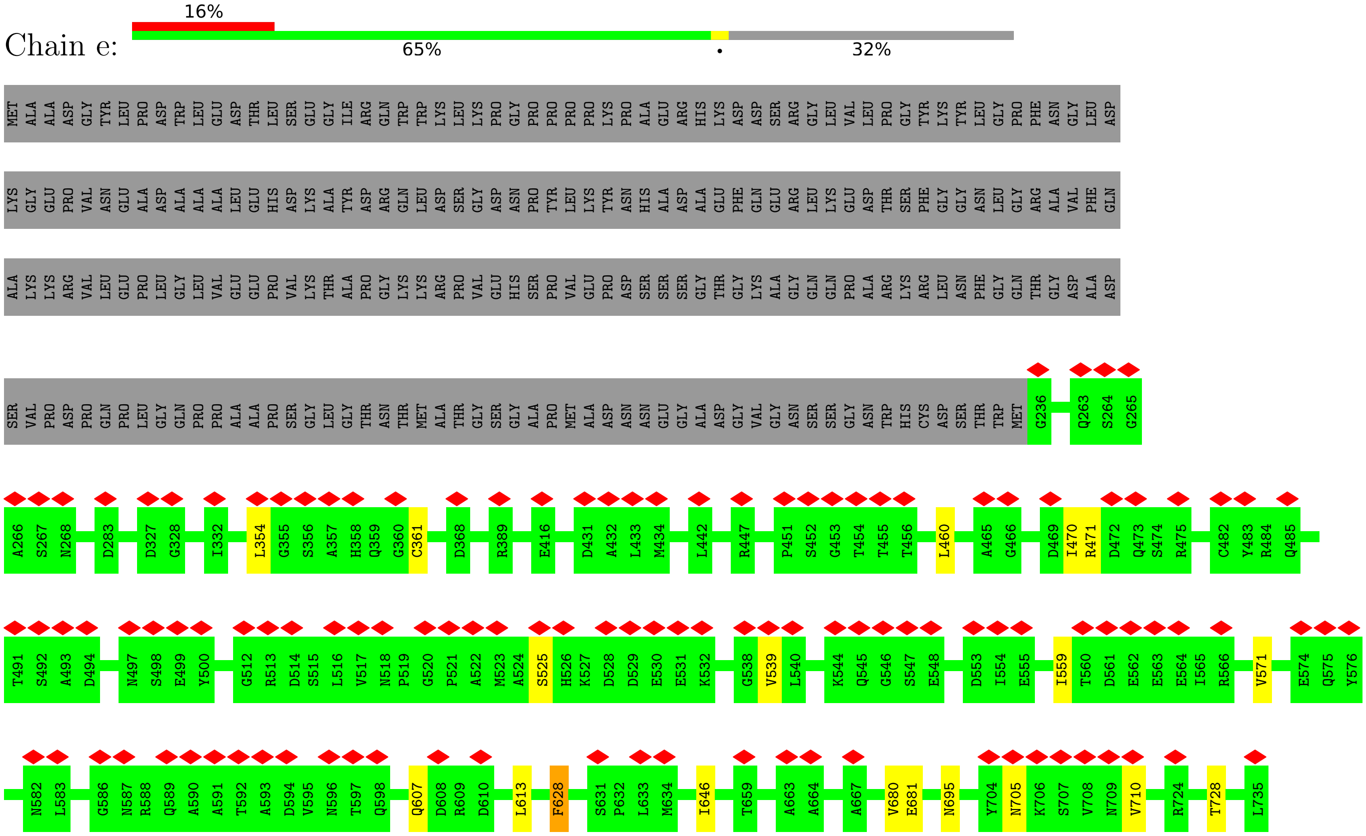
Chain d:





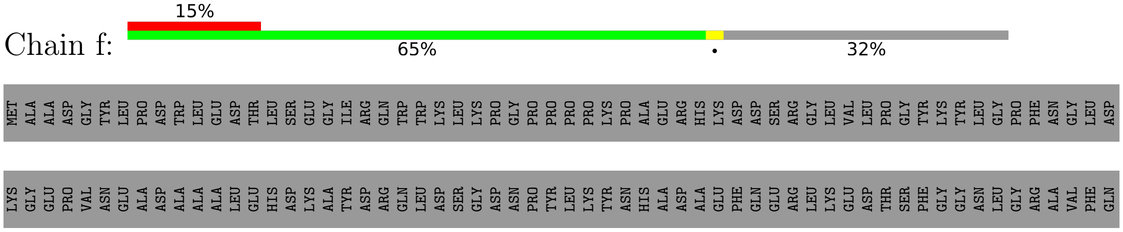
- Molecule 1: Capsid protein VP1

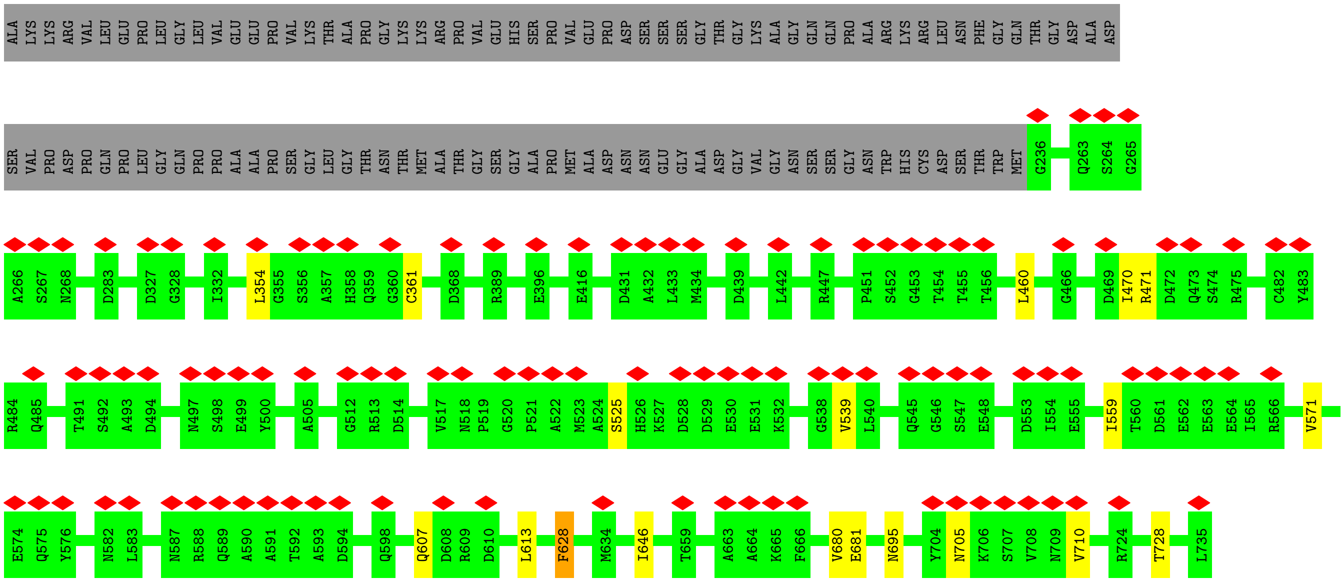
Chain e:



- Molecule 1: Capsid protein VP1

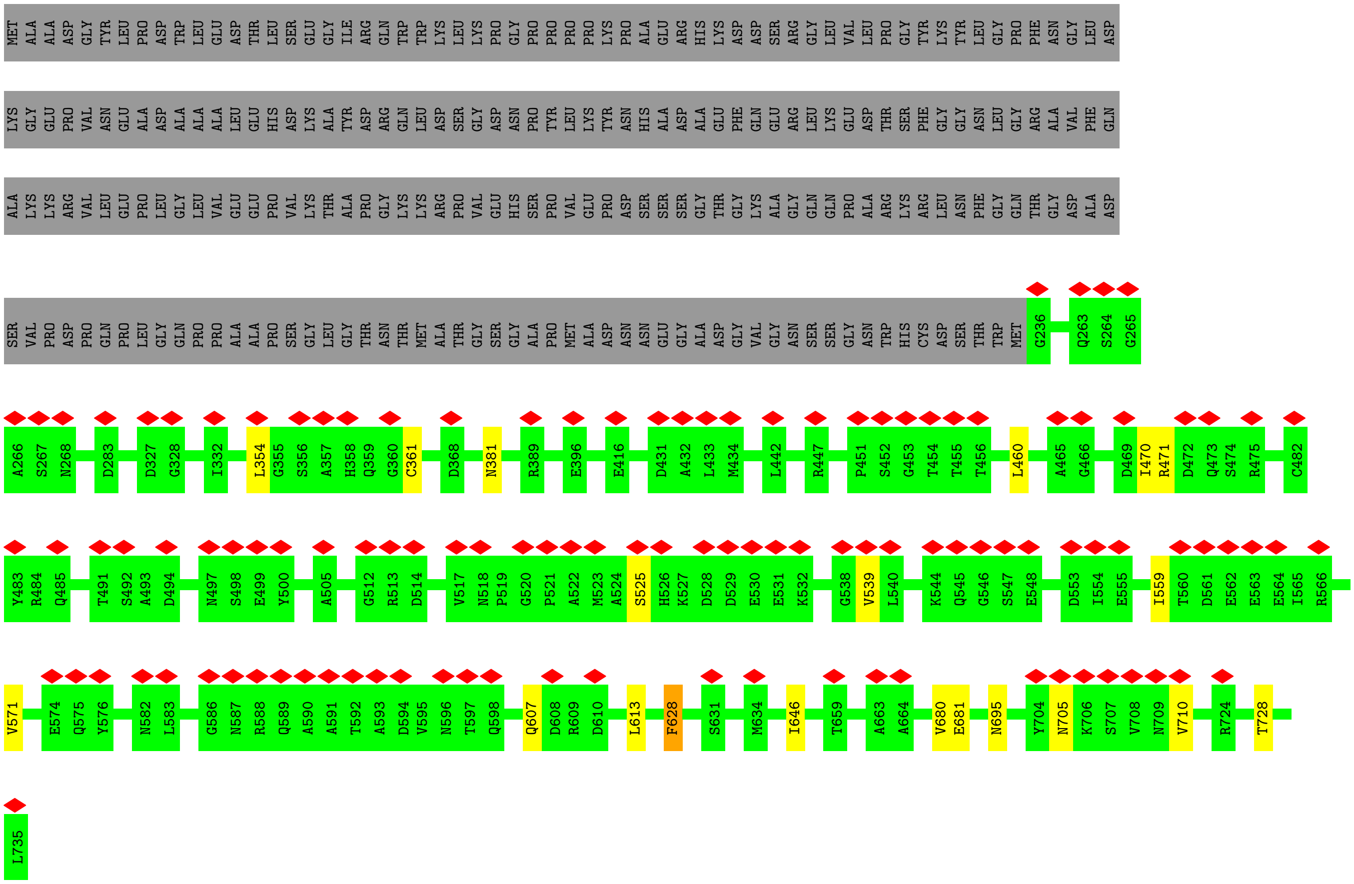
Chain f:





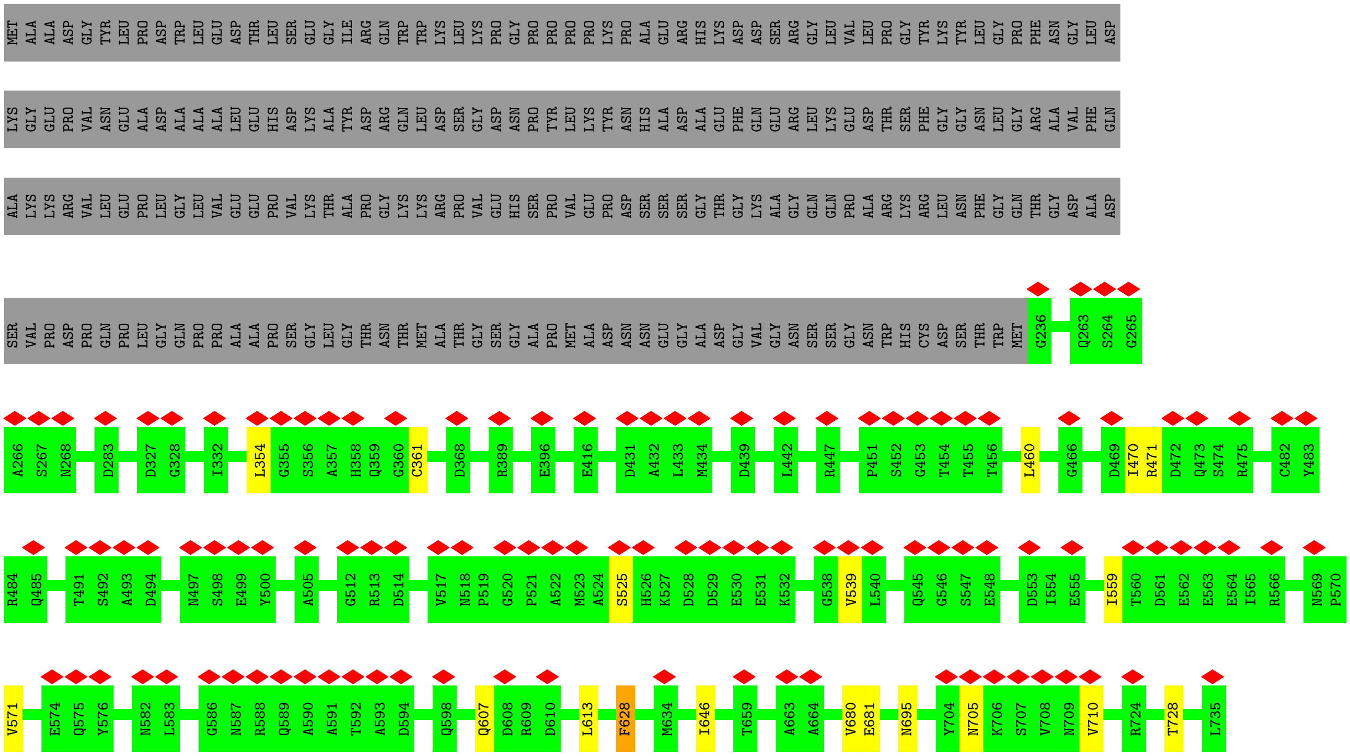
- Molecule 1: Capsid protein VP1

Chain g:



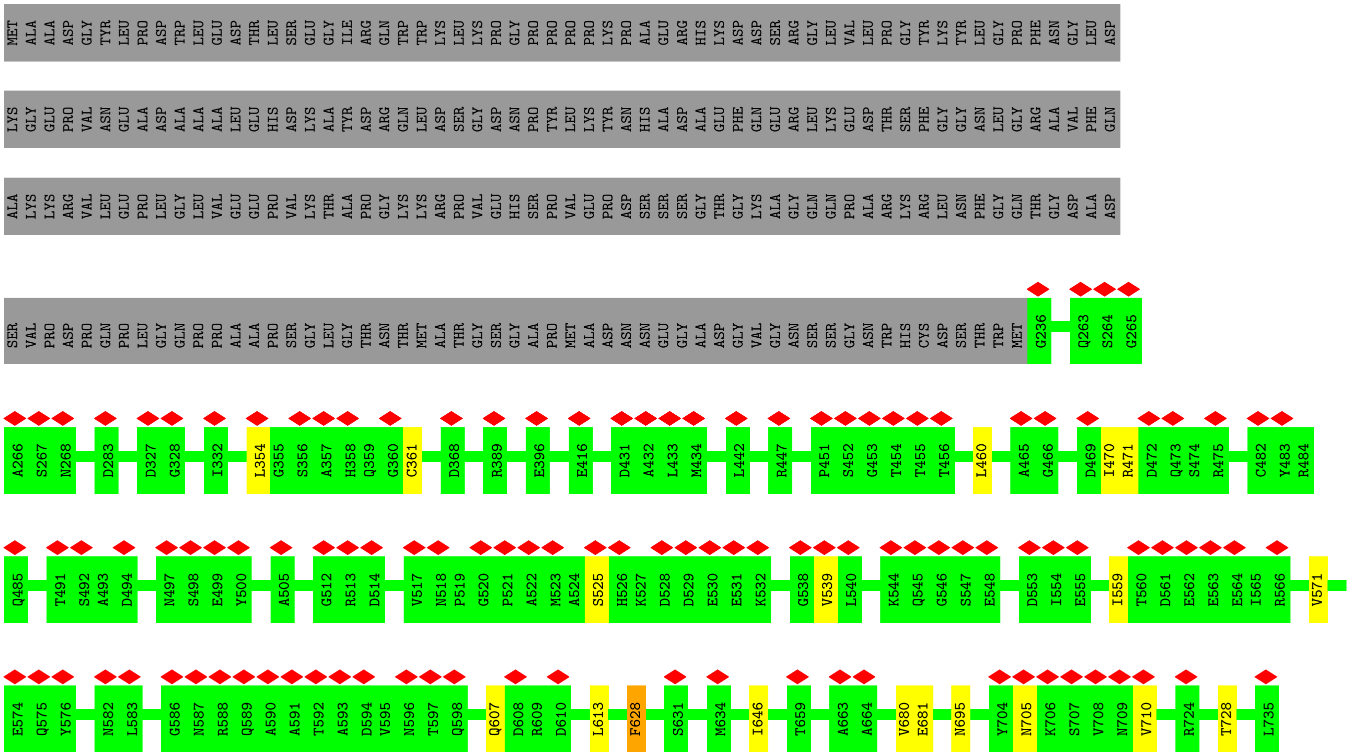
- Molecule 1: Capsid protein VP1

Chain h:



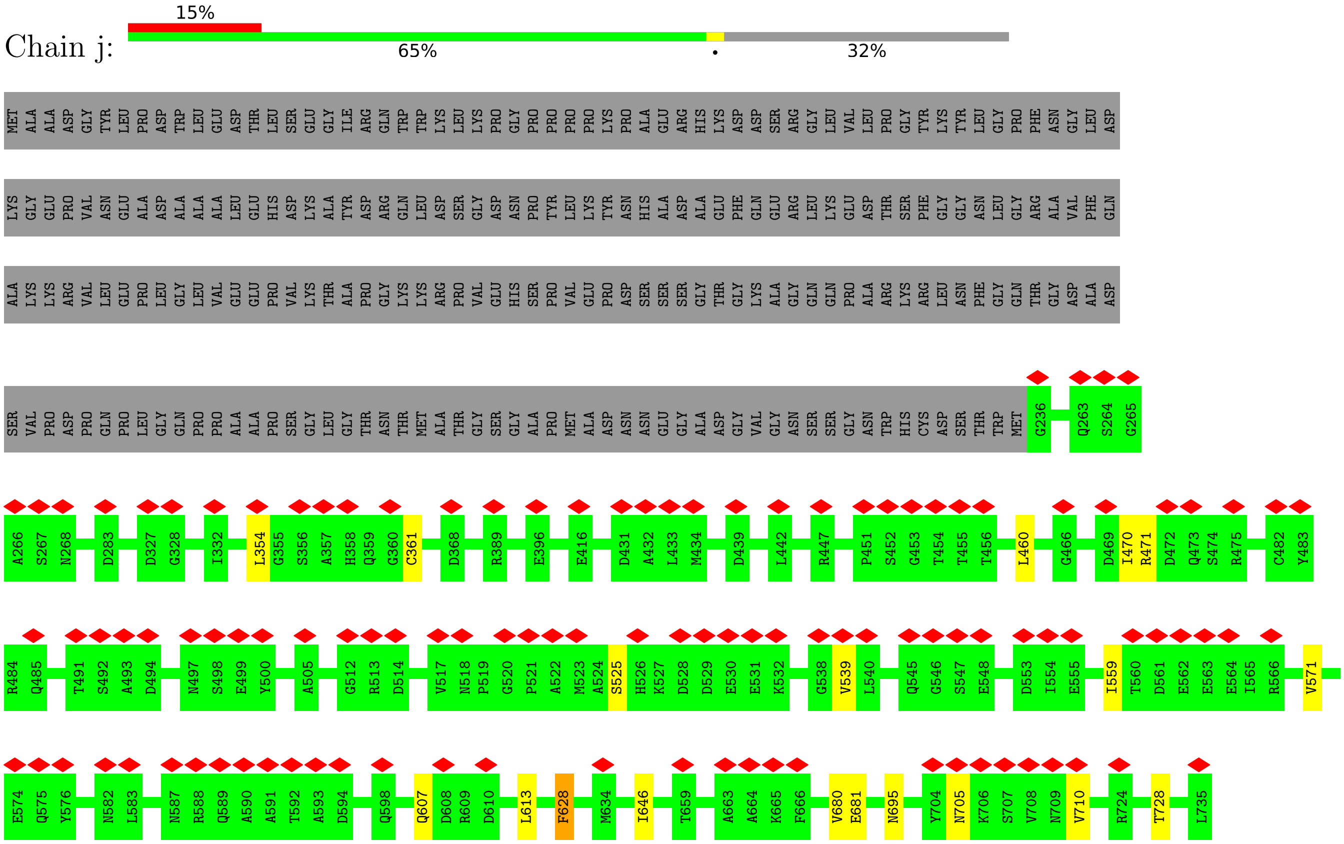
- Molecule 1: Capsid protein VP1

Chain i:



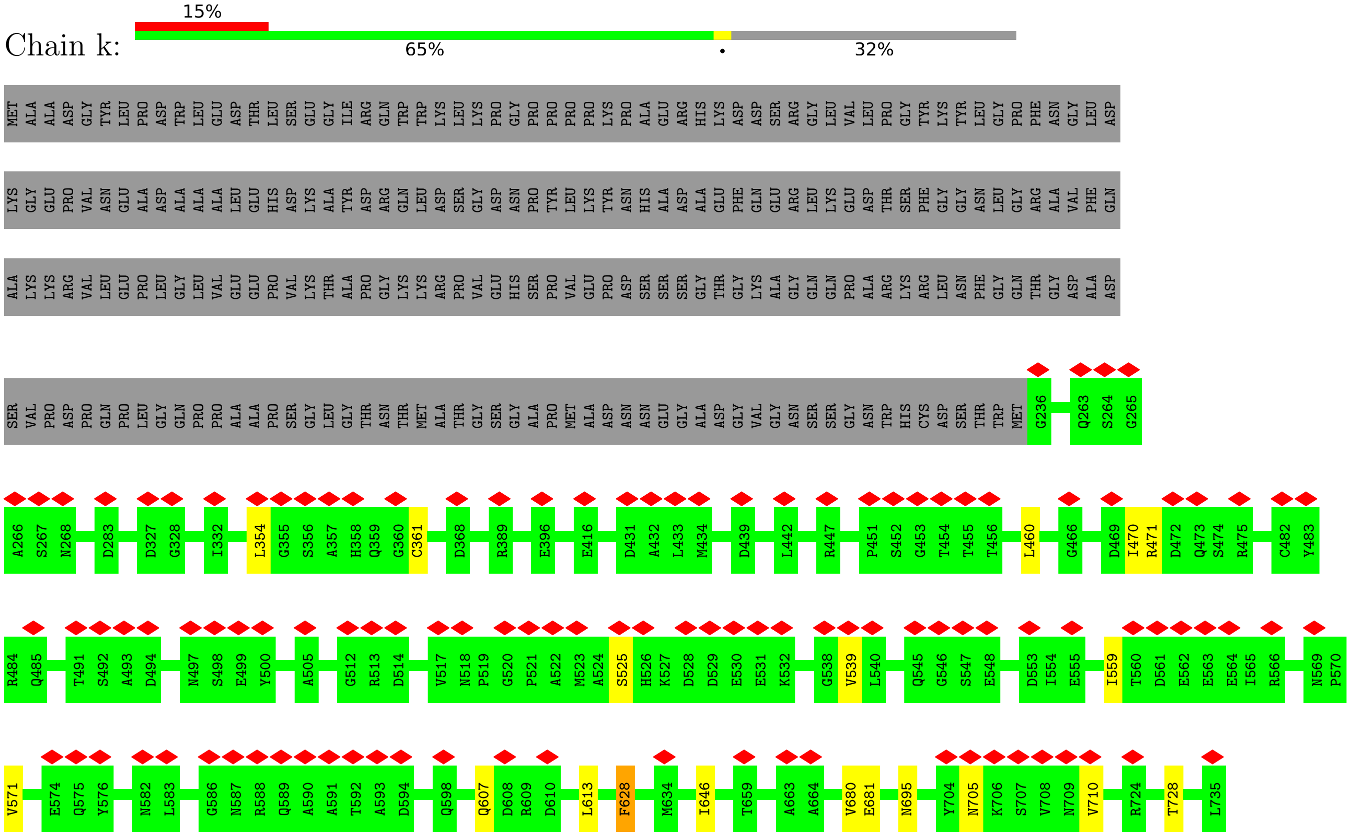
- Molecule 1: Capsid protein VP1

Chain j:

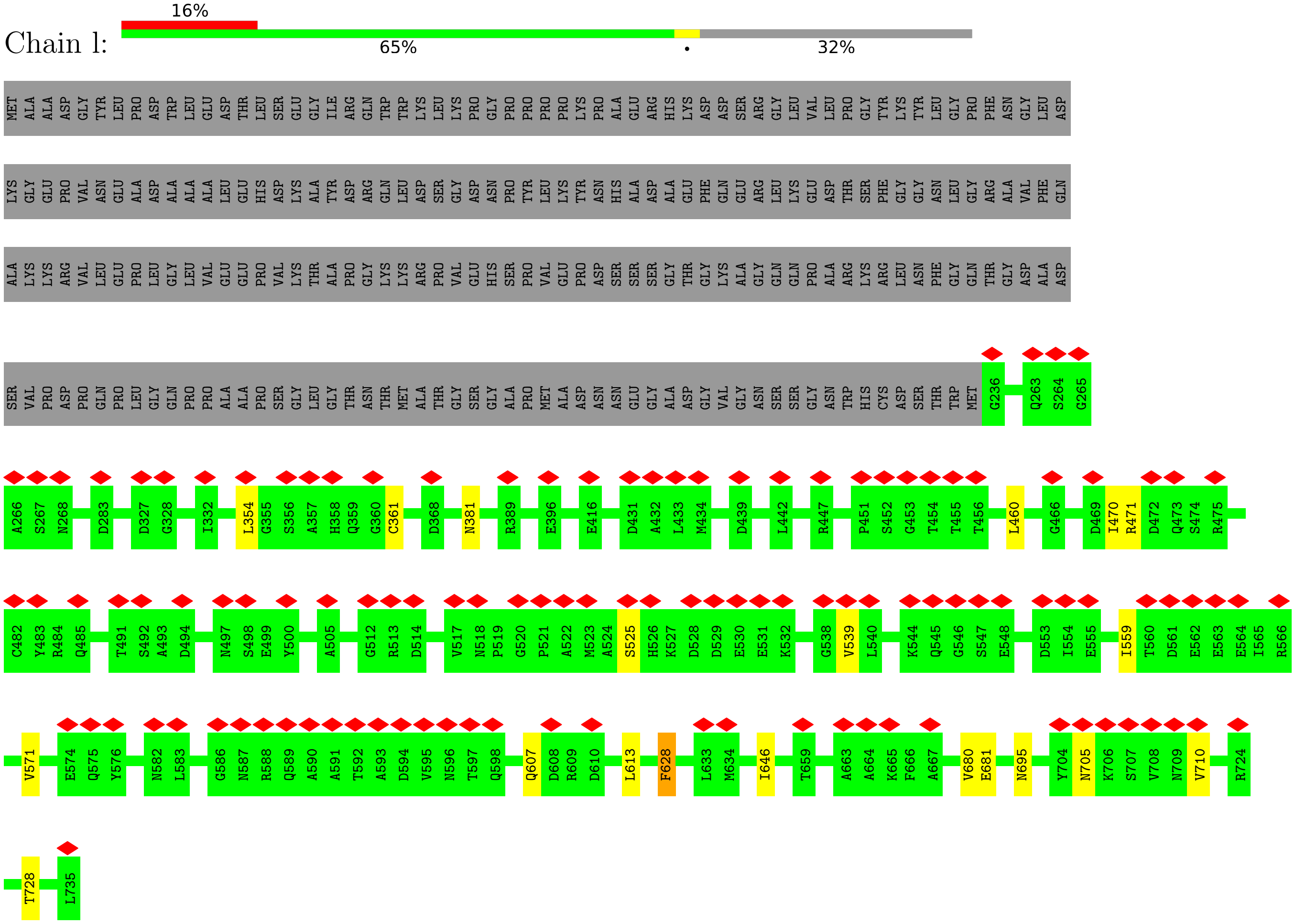


- Molecule 1: Capsid protein VP1

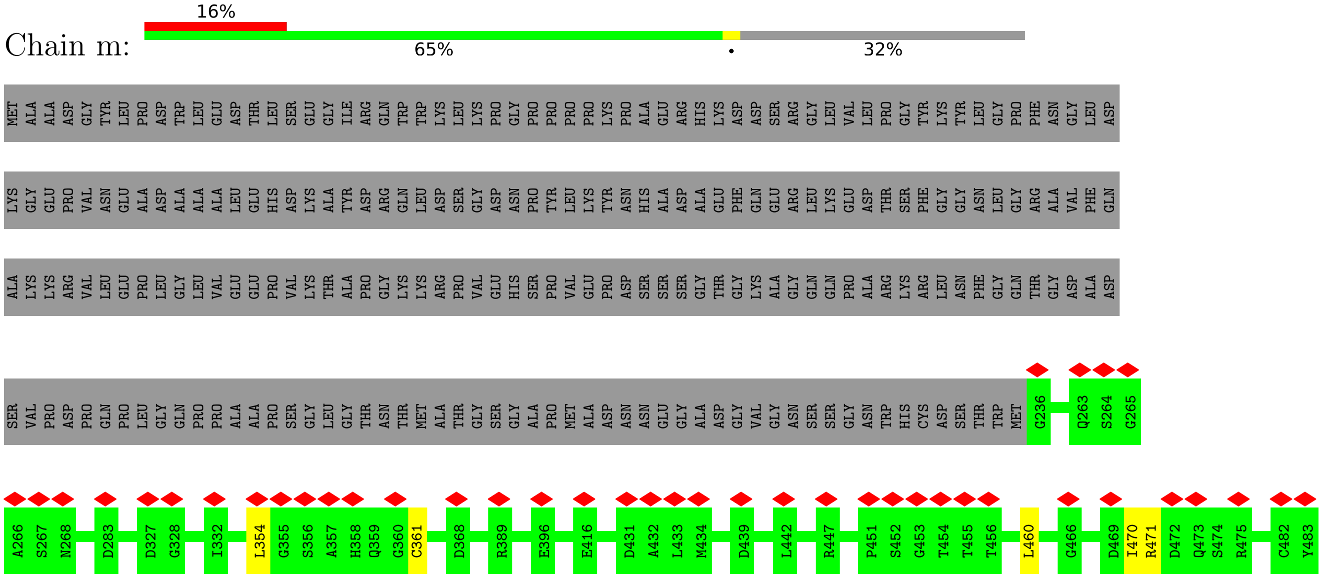
Chain k:

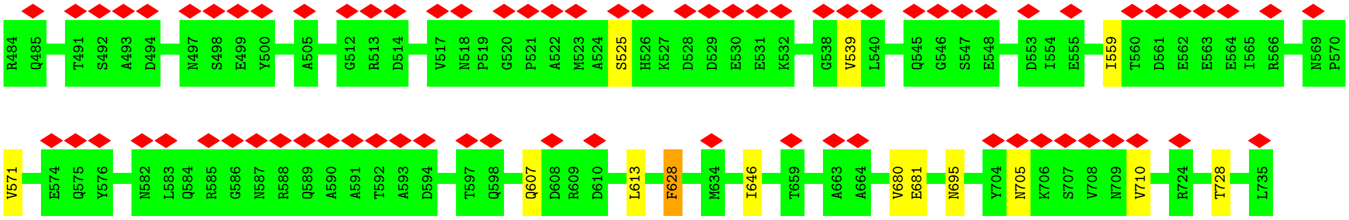


- Molecule 1: Capsid protein VP1



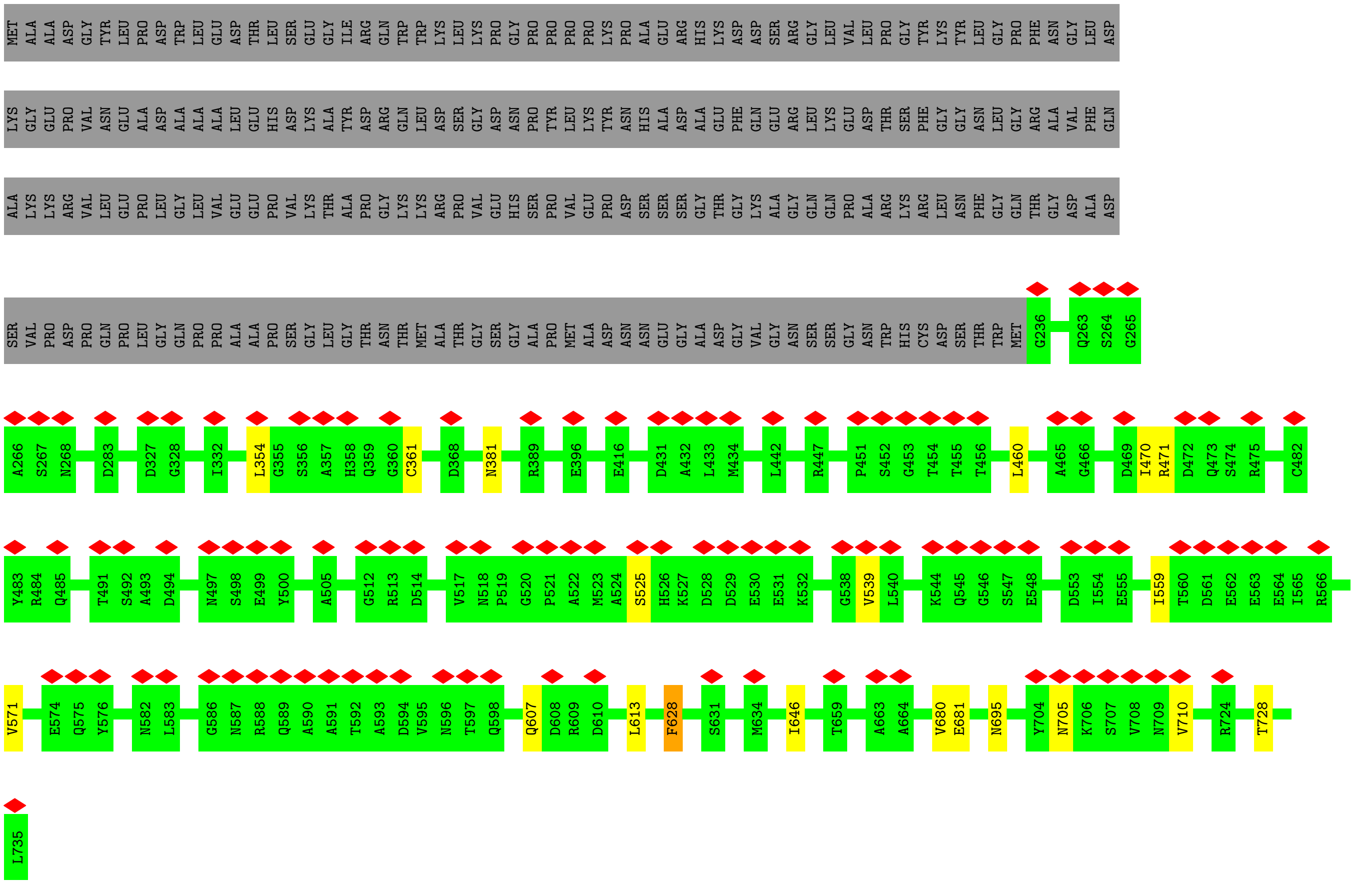
- Molecule 1: Capsid protein VP1





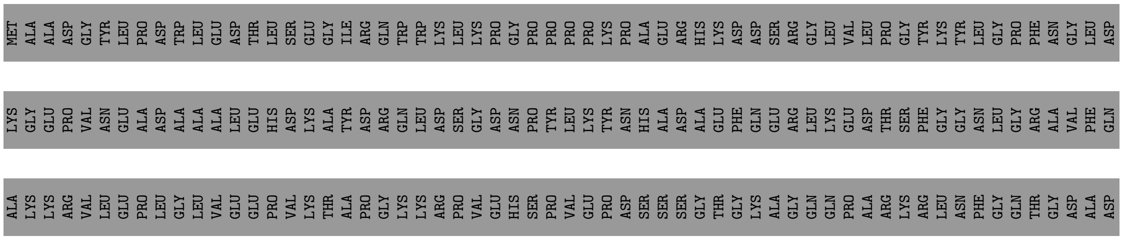
- Molecule 1: Capsid protein VP1

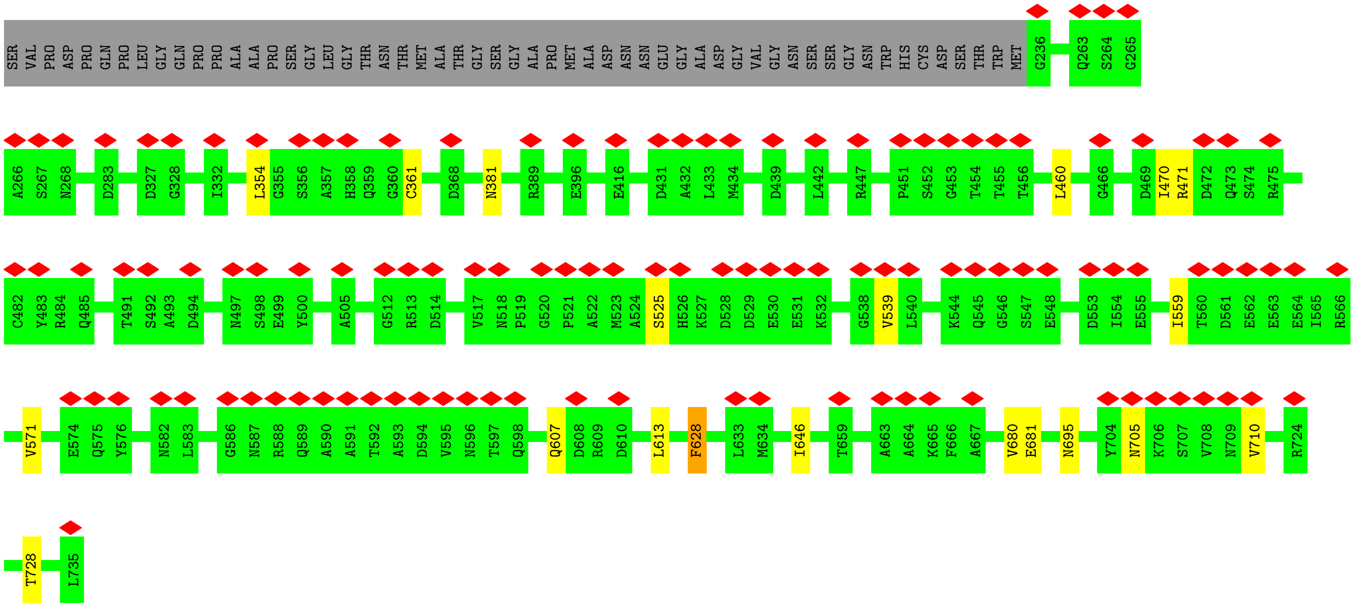
Chain n:



- Molecule 1: Capsid protein VP1

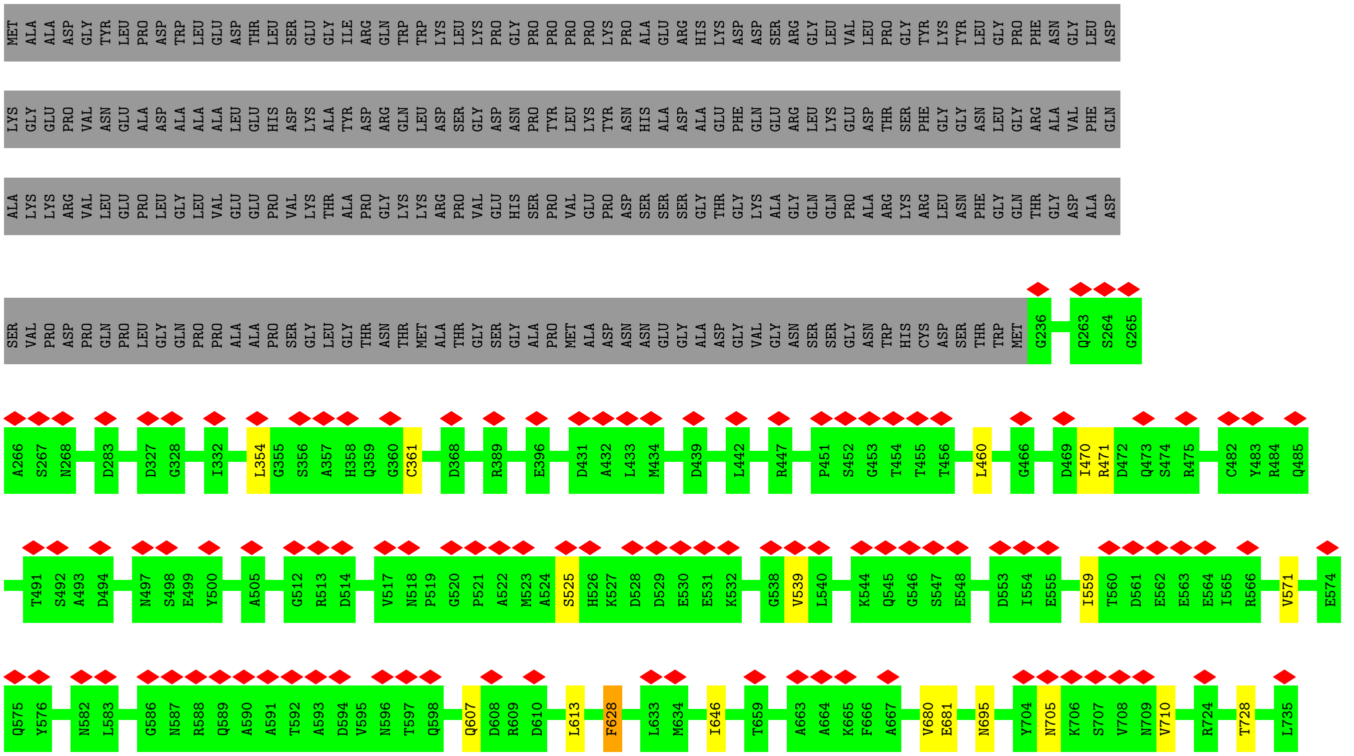
Chain o:





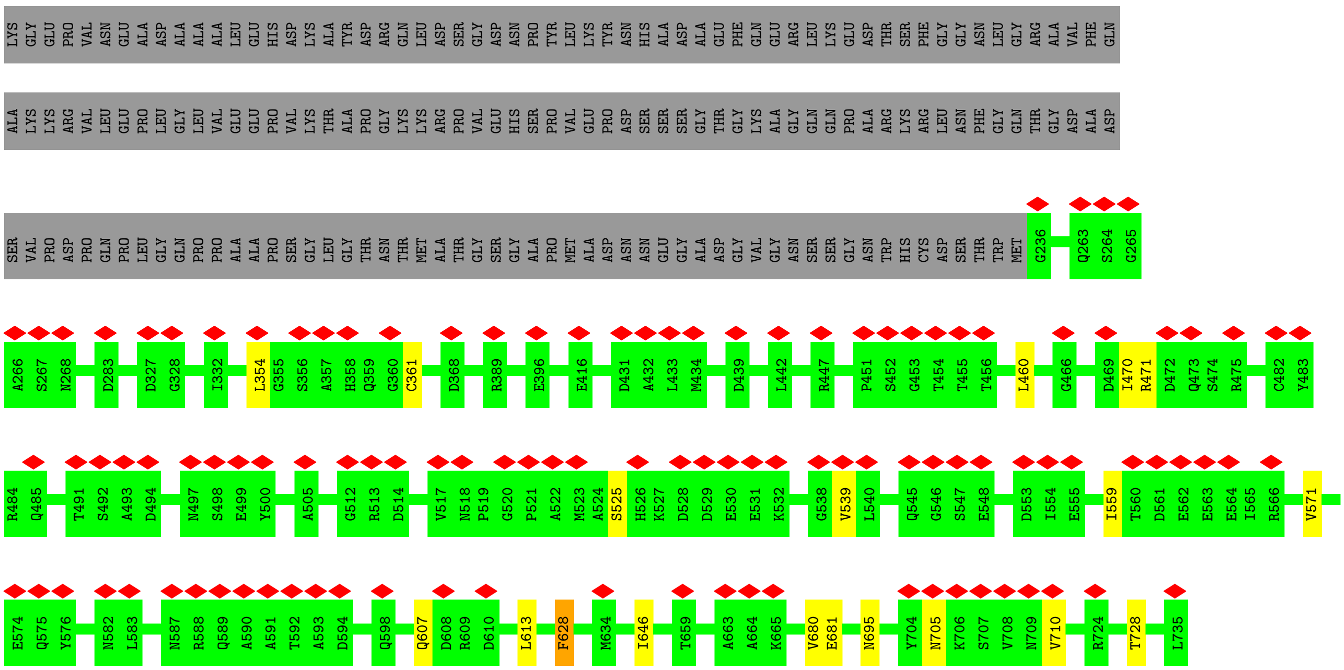
- Molecule 1: Capsid protein VP1

Chain p:



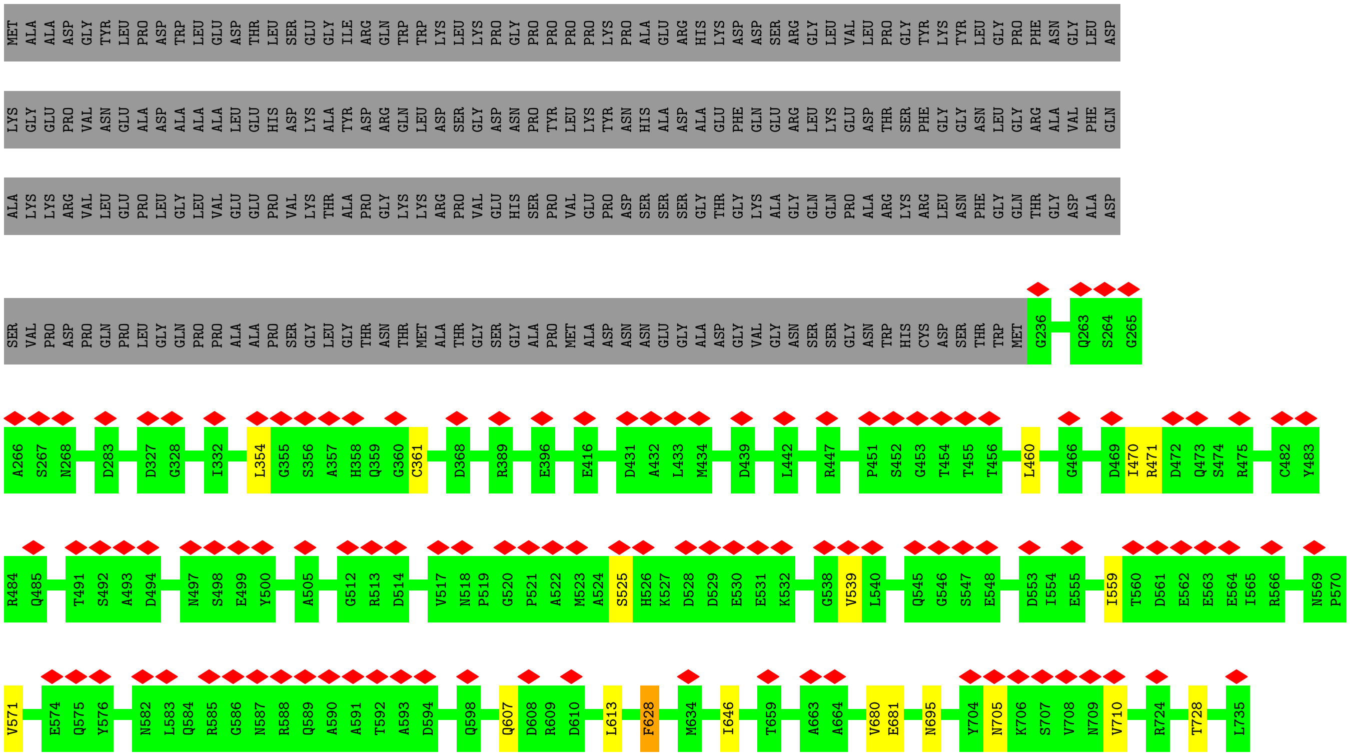
- Molecule 1: Capsid protein VP1

Chain q:



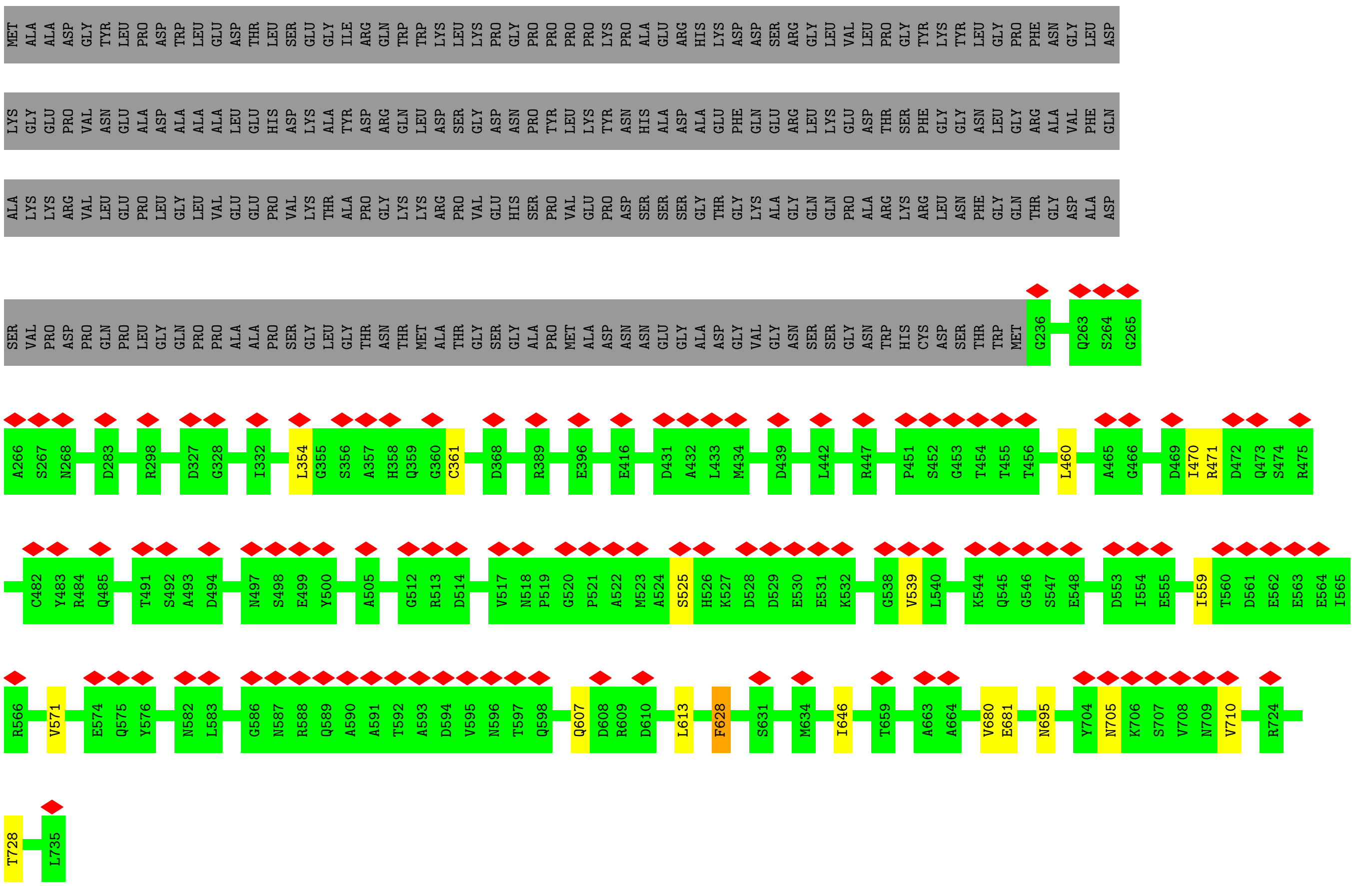
- Molecule 1: Capsid protein VP1

Chain r:

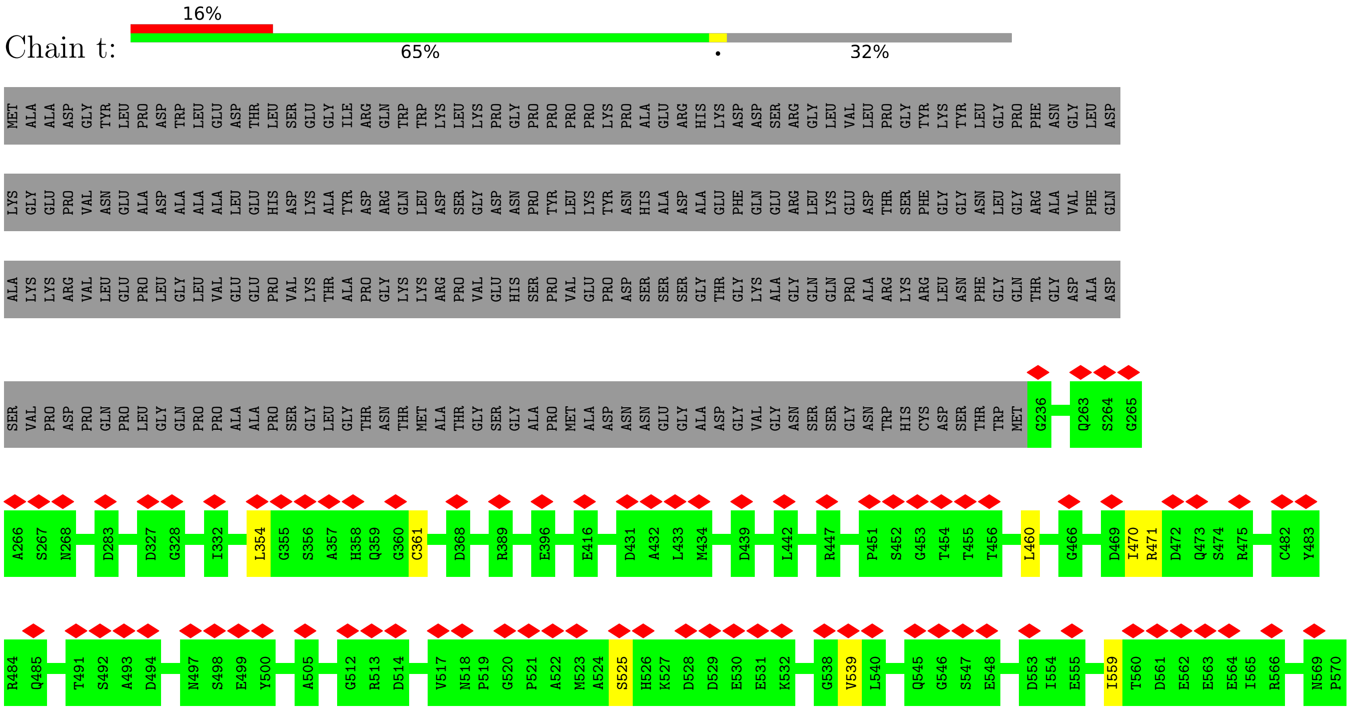


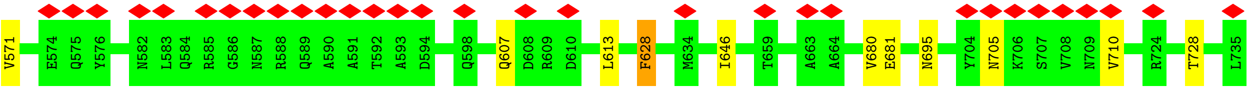
- Molecule 1: Capsid protein VP1

Chain s:

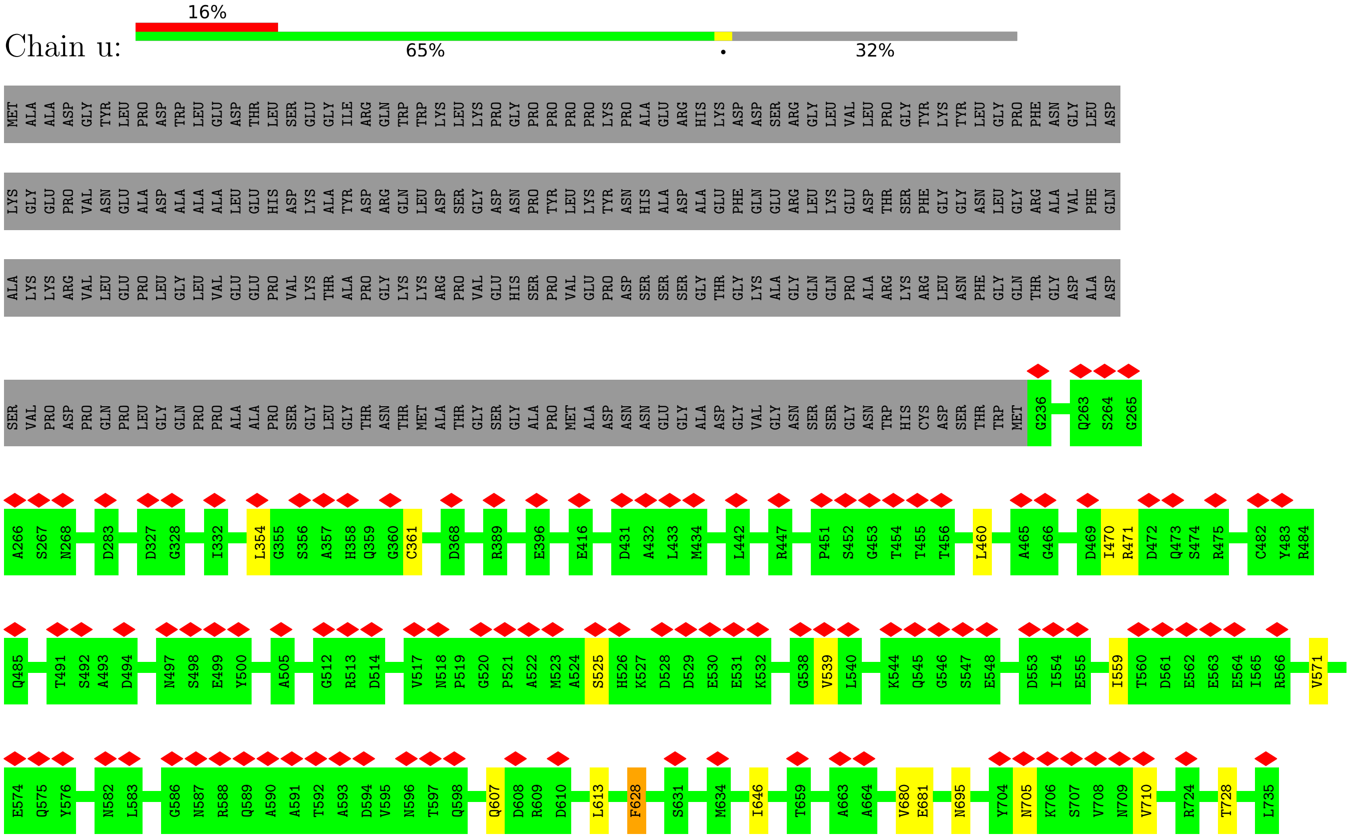


- Molecule 1: Capsid protein VP1

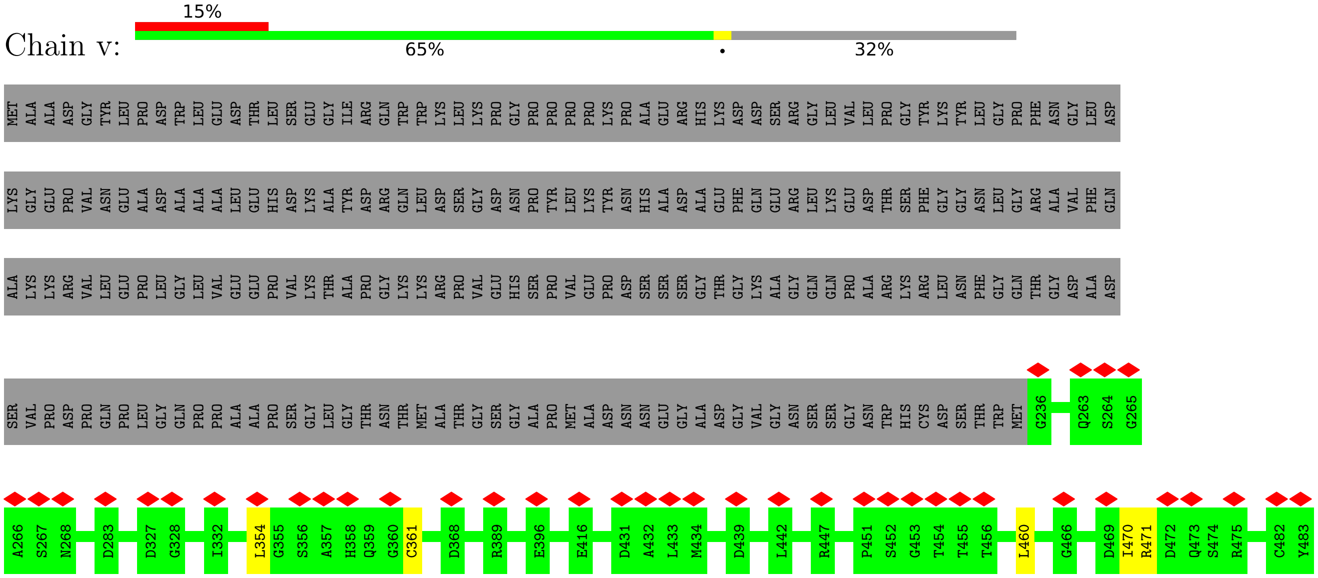


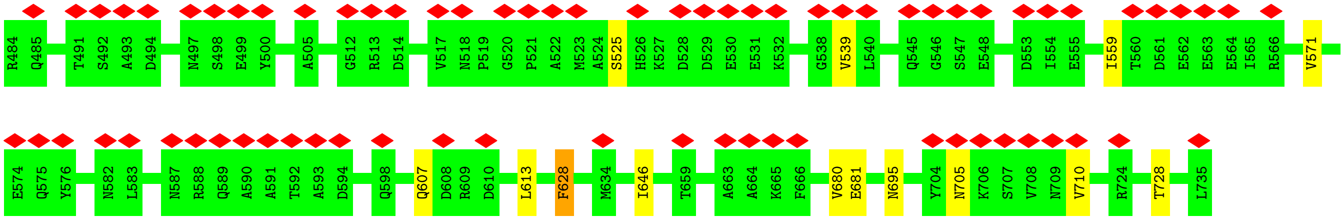


- Molecule 1: Capsid protein VP1



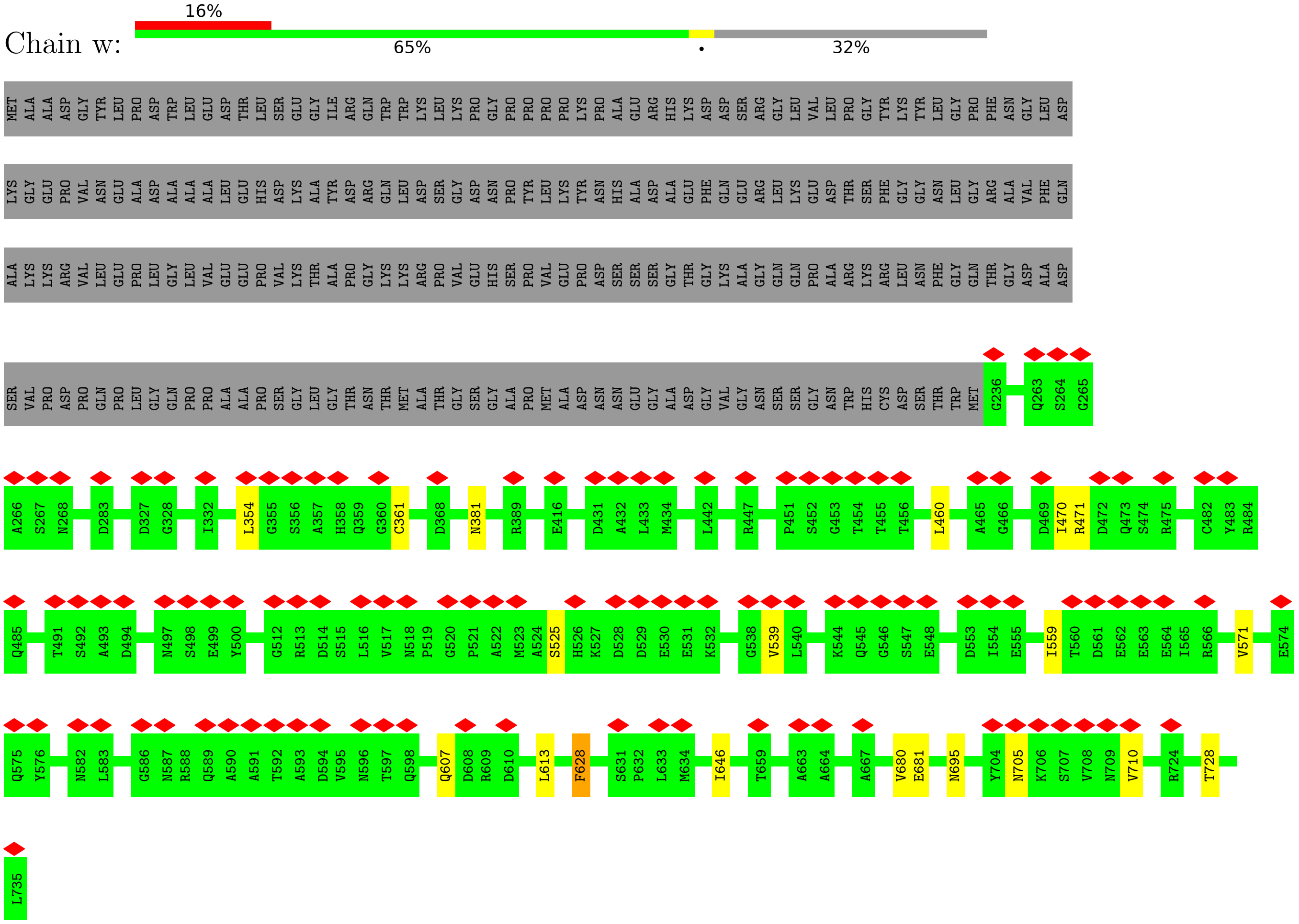
- Molecule 1: Capsid protein VP1





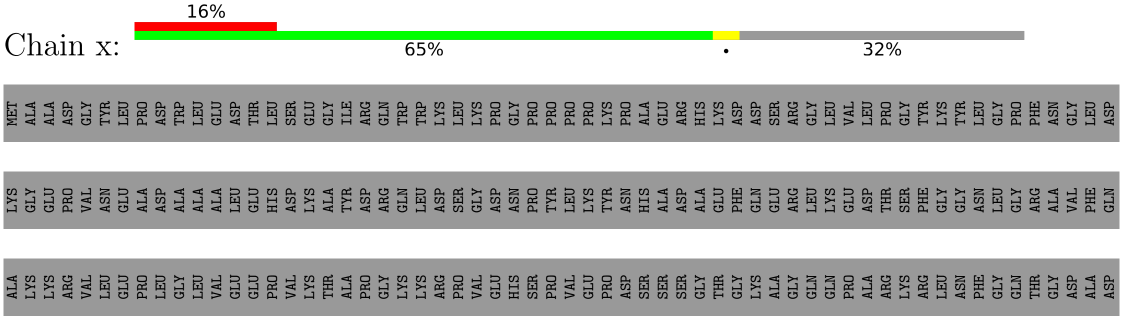
- Molecule 1: Capsid protein VP1

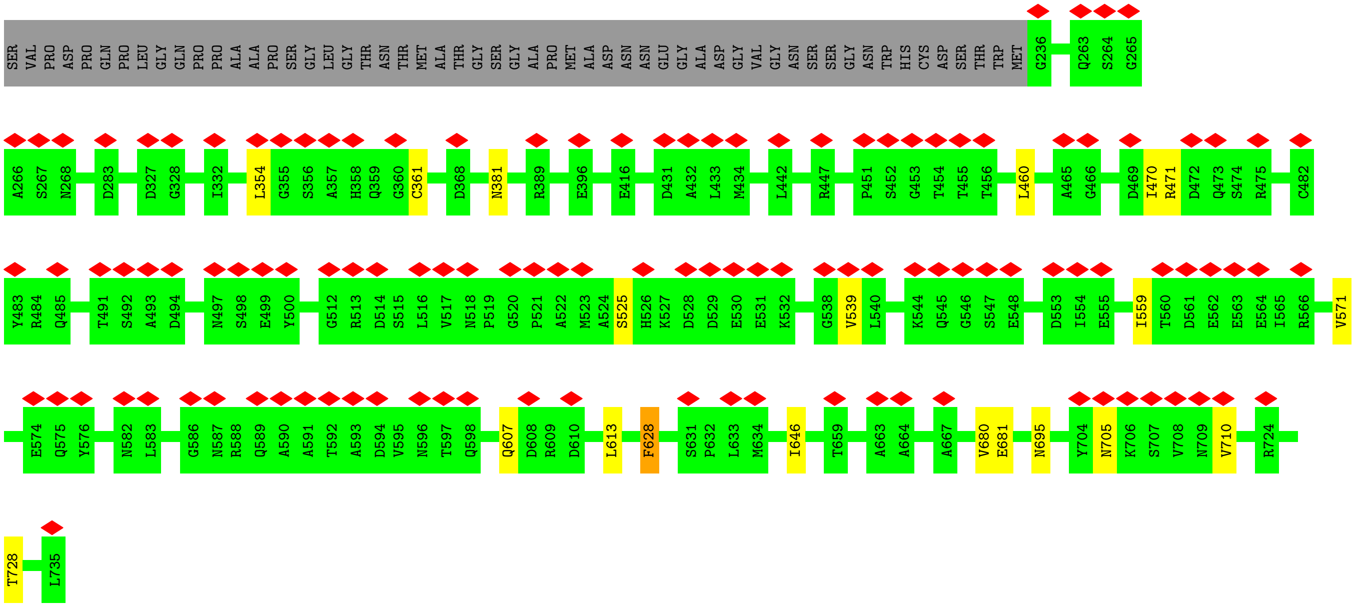
Chain w:



- Molecule 1: Capsid protein VP1

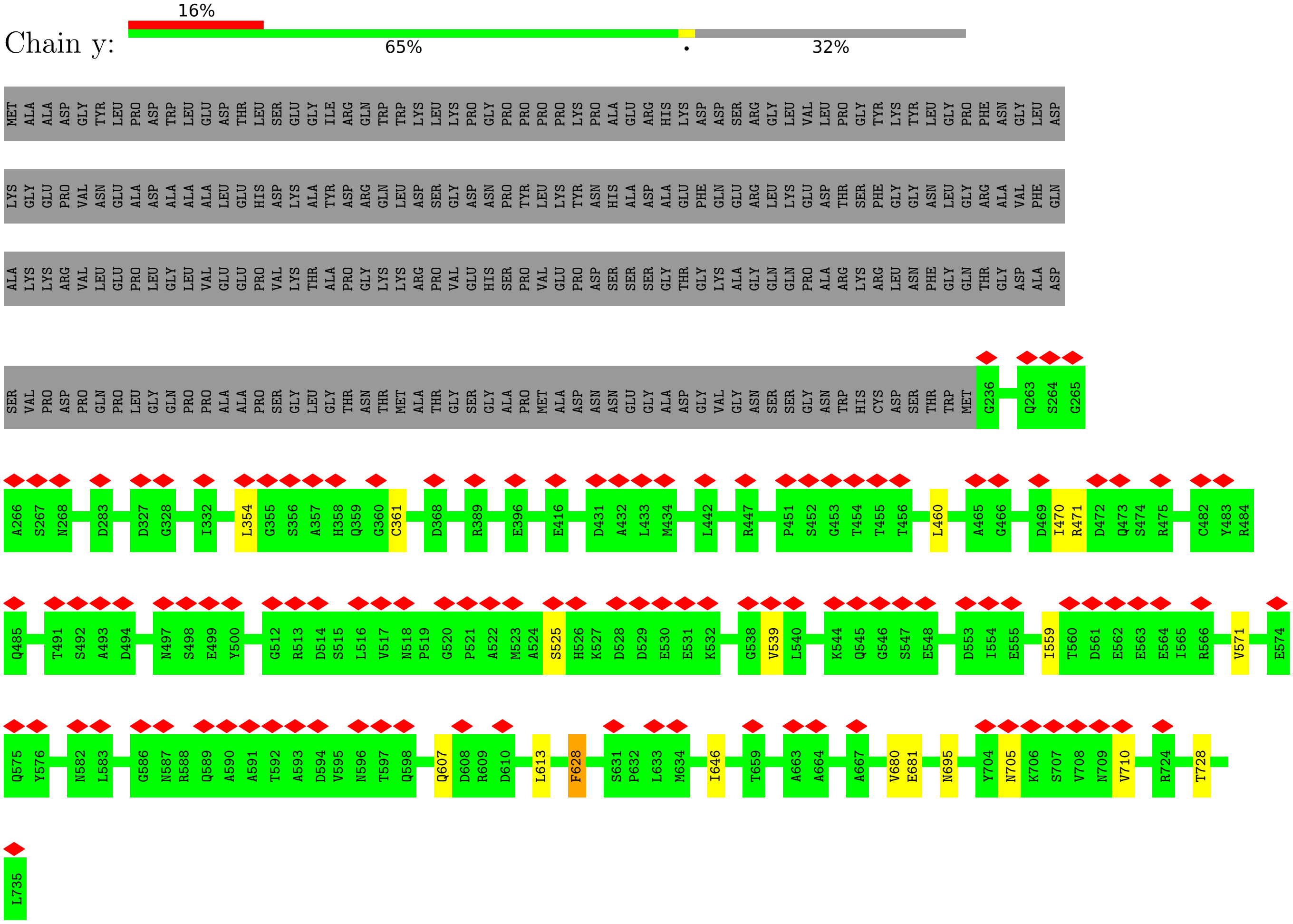
Chain x:



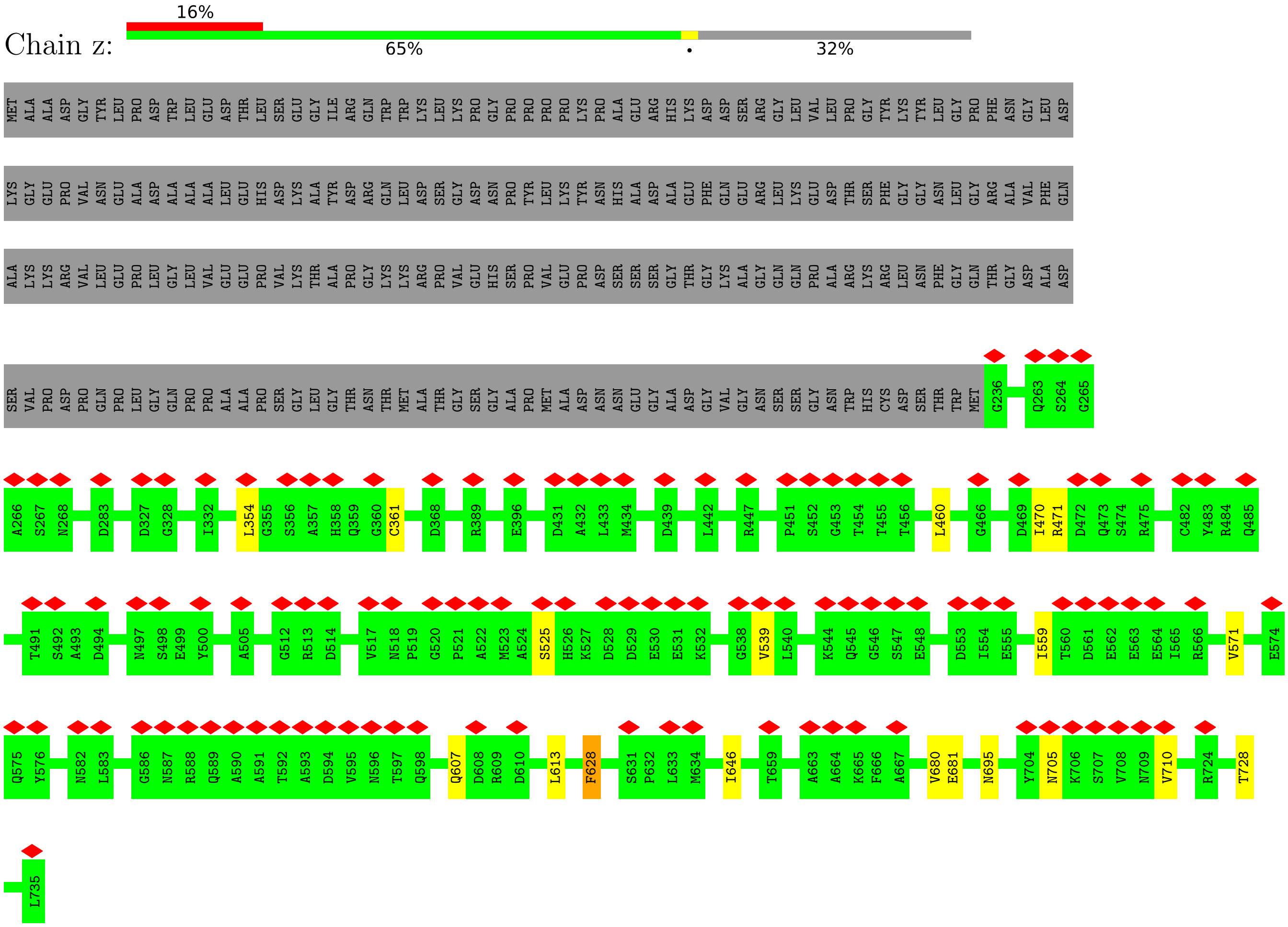


- Molecule 1: Capsid protein VP1

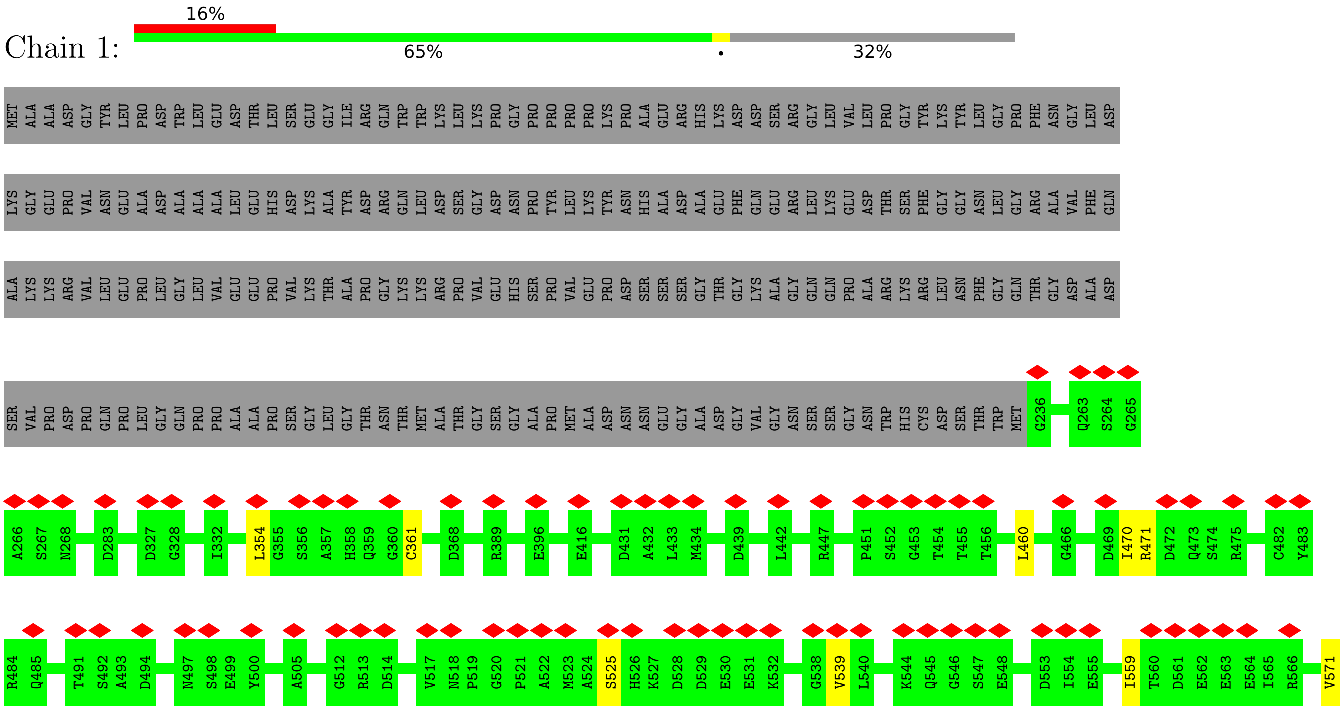
Chain y:

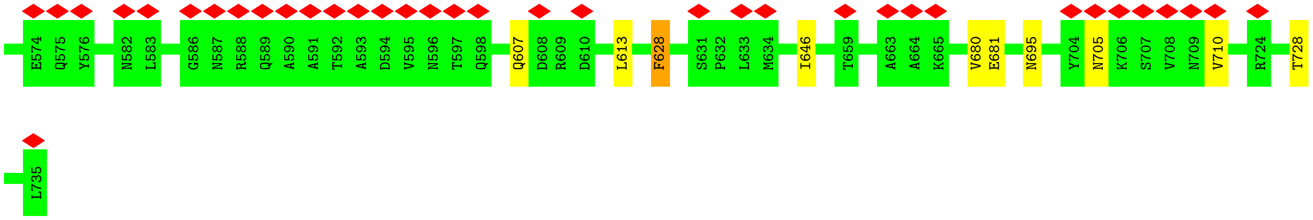


- Molecule 1: Capsid protein VP1



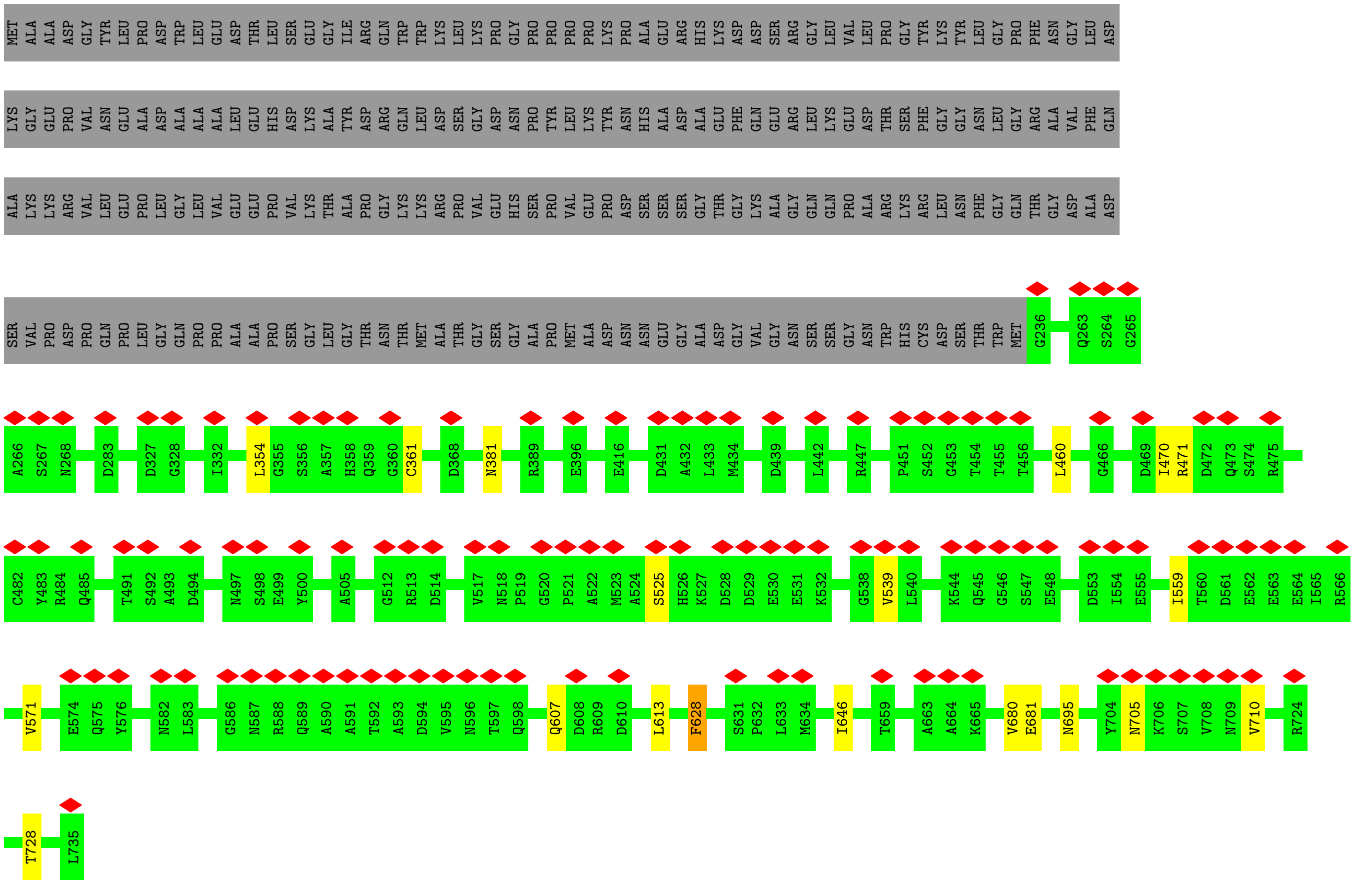
• Molecule 1: Capsid protein VP1





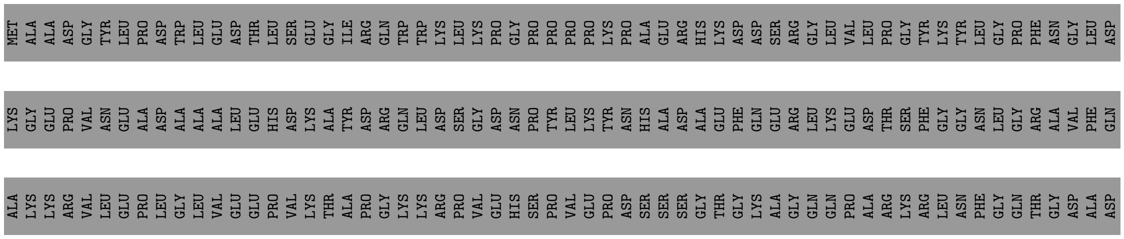
- Molecule 1: Capsid protein VP1

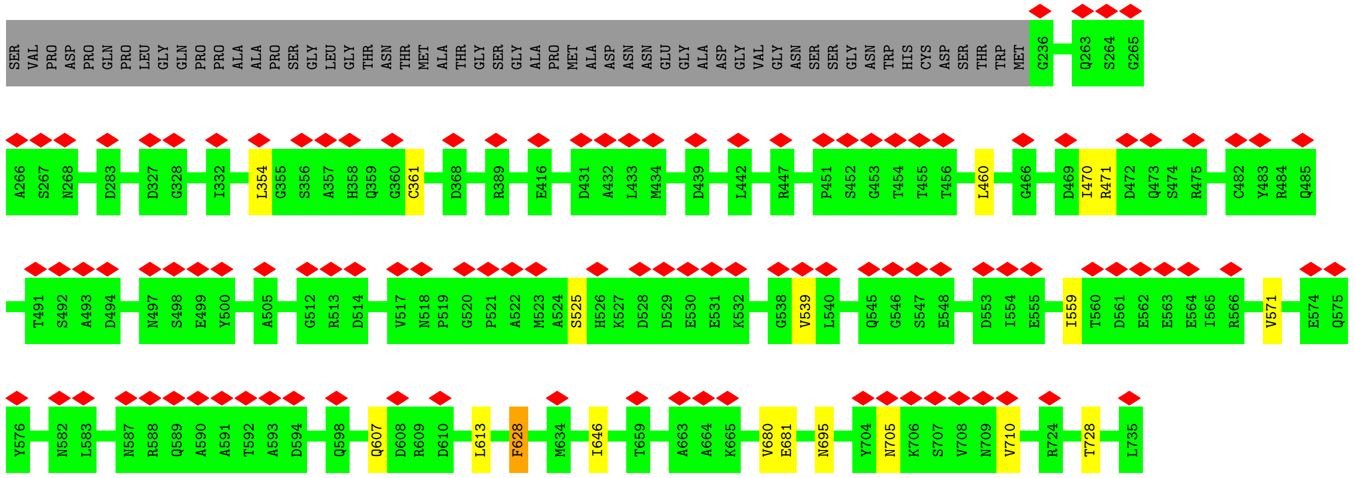
Chain 2:



- Molecule 1: Capsid protein VP1

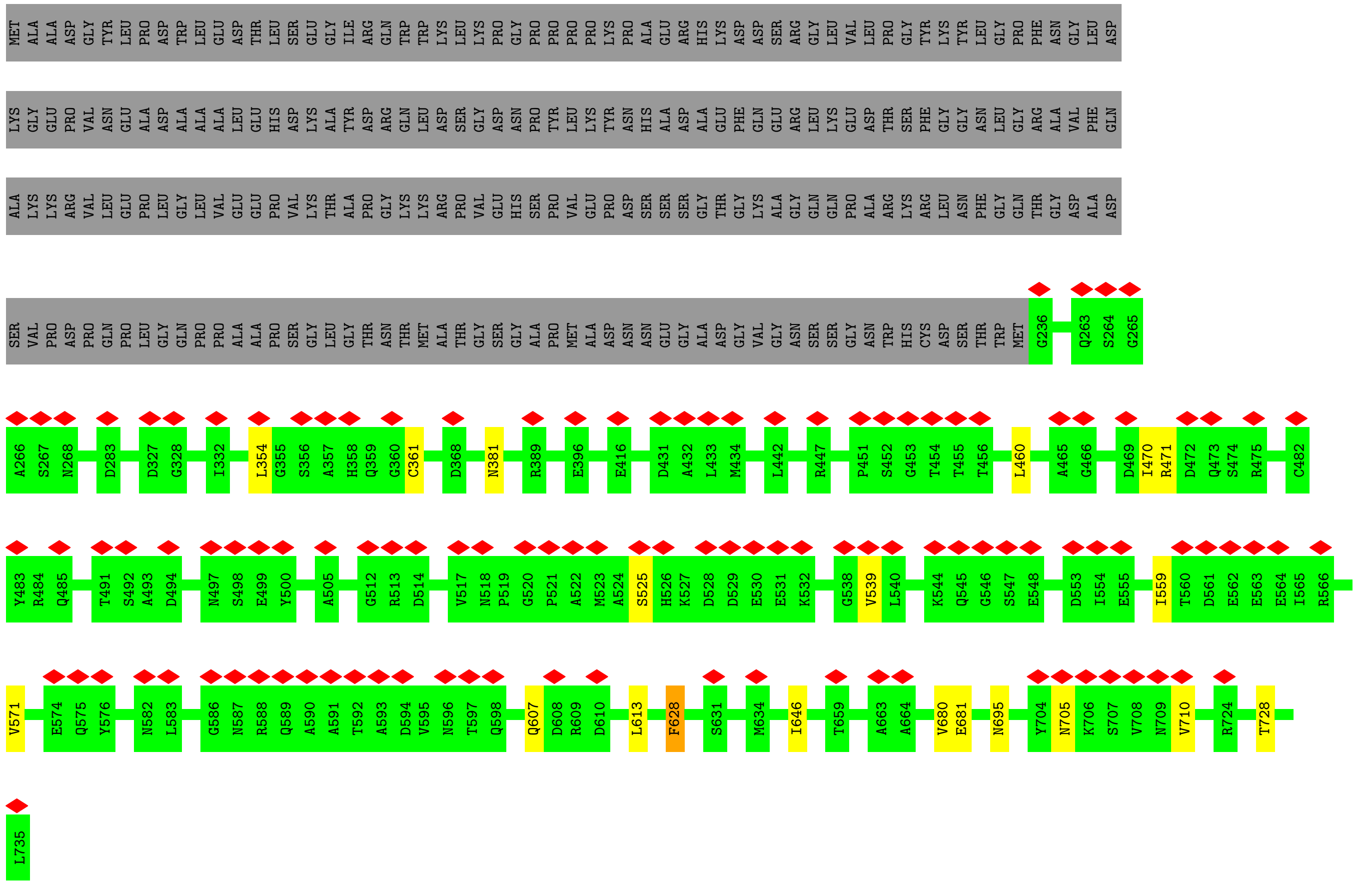
Chain 3:





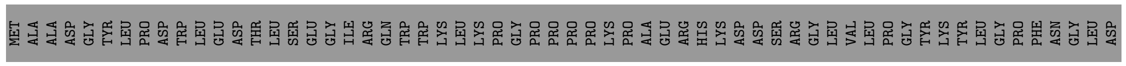
- Molecule 1: Capsid protein VP1

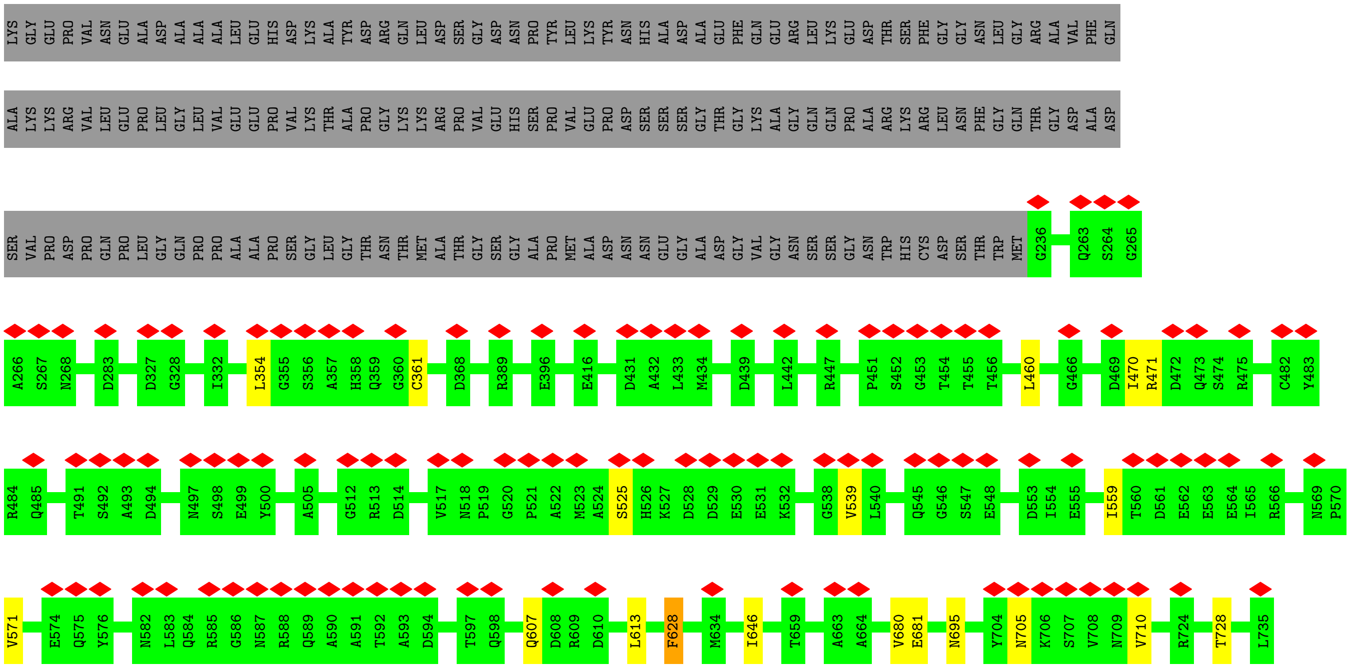
Chain 4:



- Molecule 1: Capsid protein VP1

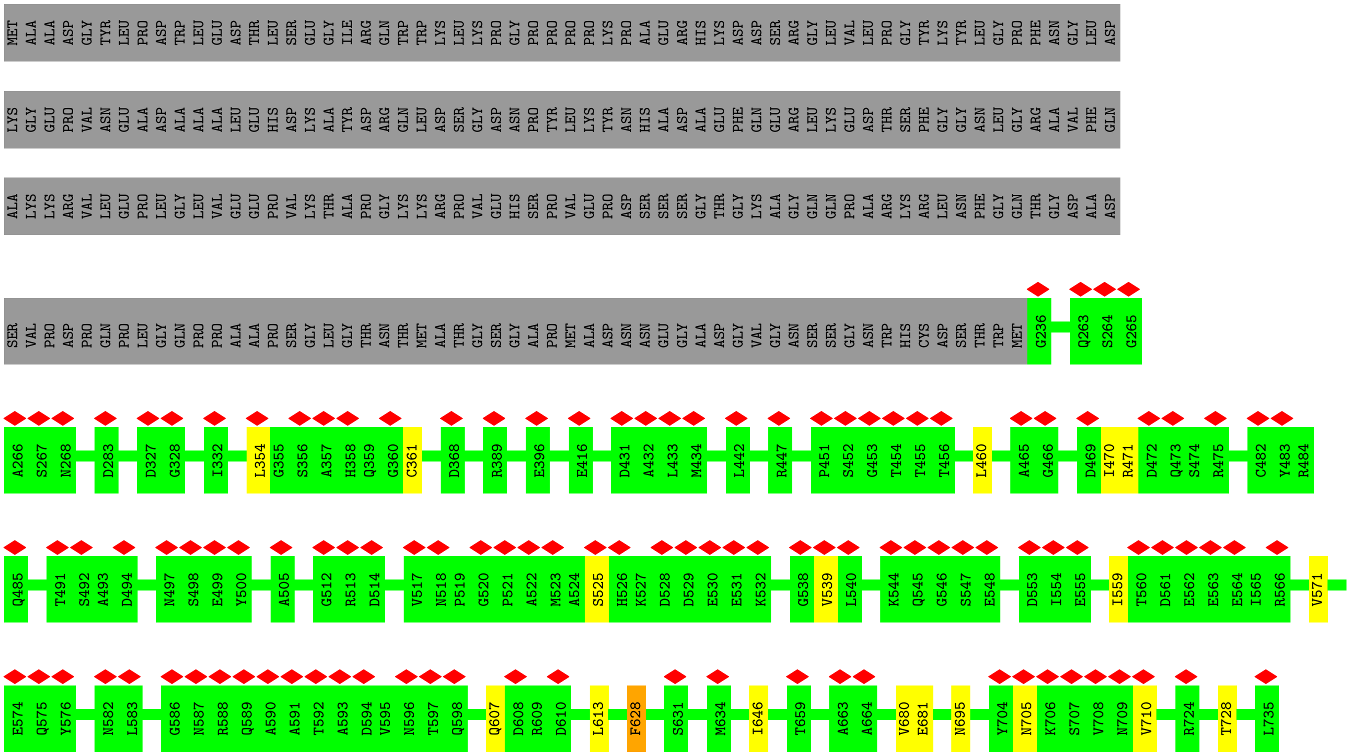
Chain 5:





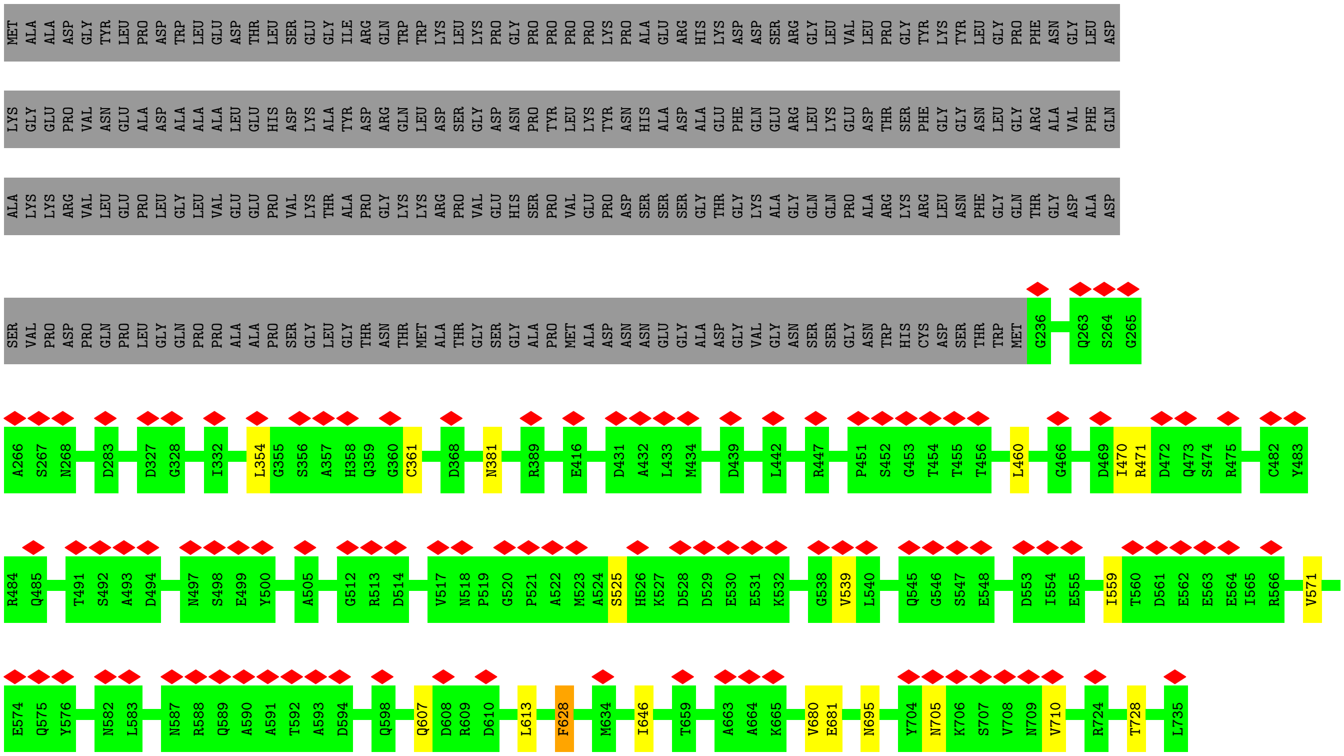
- Molecule 1: Capsid protein VP1

Chain 6:



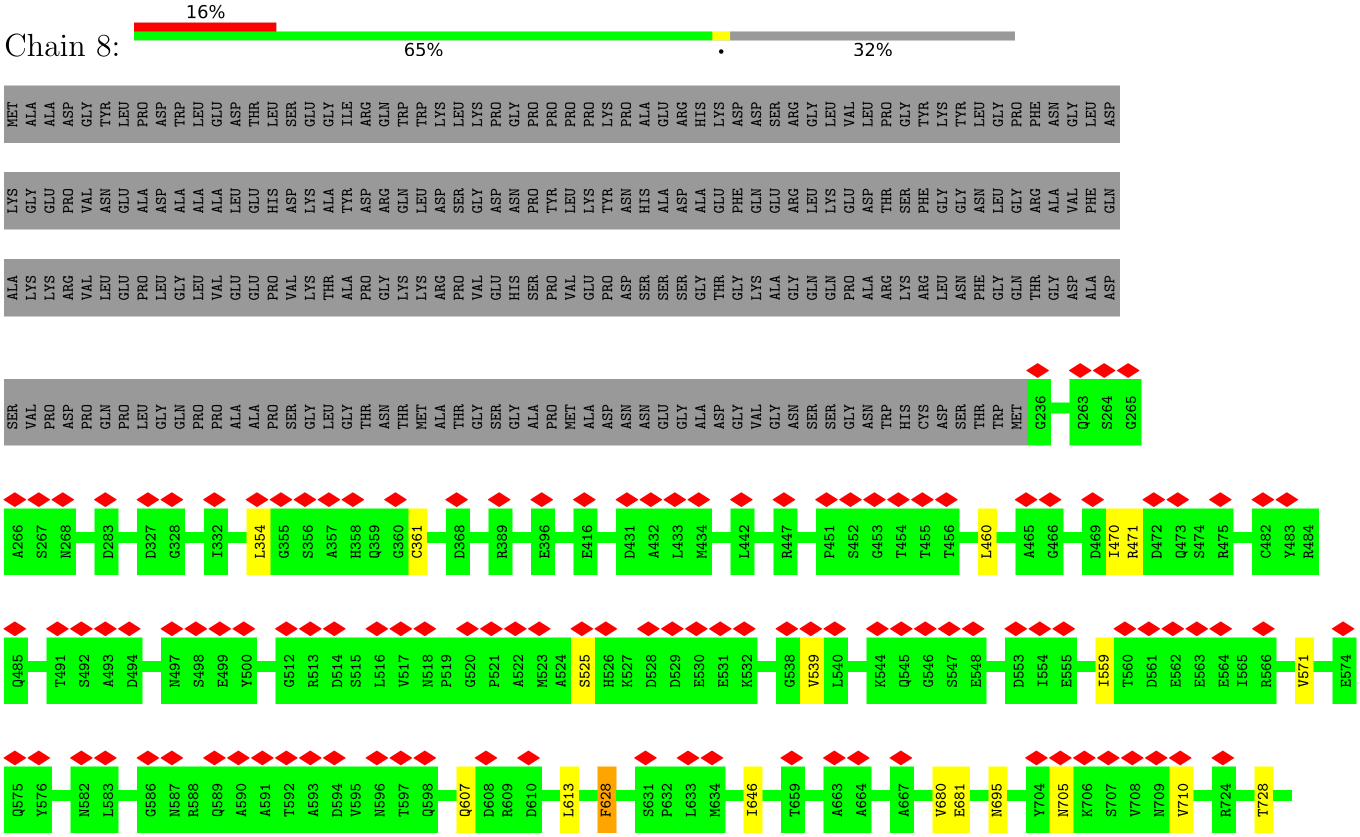
- Molecule 1: Capsid protein VP1

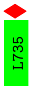
Chain 7:



- Molecule 1: Capsid protein VP1

Chain 8:




L735

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19457	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 $(e^-/\text{Å}^2)$	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	56924	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	14.966	Depositor
Minimum map value	-6.175	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.9	Depositor
Map size (Å)	361.9, 361.9, 361.9	wwPDB
Map dimensions	329, 329, 329	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.57	0/4127	0.68	0/5626
1	2	0.57	0/4127	0.68	0/5626
1	3	0.57	0/4127	0.68	0/5626
1	4	0.57	0/4127	0.68	0/5626
1	5	0.57	0/4127	0.68	0/5626
1	6	0.57	0/4127	0.68	0/5626
1	7	0.57	0/4127	0.68	0/5626
1	8	0.57	0/4127	0.68	0/5626
1	A	0.57	0/4127	0.68	0/5626
1	B	0.57	0/4127	0.68	0/5626
1	C	0.57	0/4127	0.68	0/5626
1	D	0.57	0/4127	0.68	0/5626
1	E	0.57	0/4127	0.68	0/5626
1	F	0.57	0/4127	0.68	0/5626
1	G	0.57	0/4127	0.68	0/5626
1	H	0.57	0/4127	0.68	0/5626
1	I	0.57	0/4127	0.68	0/5626
1	J	0.57	0/4127	0.68	0/5626
1	K	0.57	0/4127	0.68	0/5626
1	L	0.57	0/4127	0.68	0/5626
1	M	0.57	0/4127	0.68	0/5626
1	N	0.57	0/4127	0.68	0/5626
1	O	0.57	0/4127	0.68	0/5626
1	P	0.57	0/4127	0.68	0/5626
1	Q	0.57	0/4127	0.68	0/5626
1	R	0.57	0/4127	0.67	0/5626
1	S	0.57	0/4127	0.68	0/5626
1	T	0.57	0/4127	0.68	0/5626
1	U	0.57	0/4127	0.68	0/5626
1	V	0.57	0/4127	0.68	0/5626
1	W	0.57	0/4127	0.68	0/5626
1	X	0.57	0/4127	0.68	0/5626
1	Y	0.57	0/4127	0.68	0/5626
1	Z	0.57	0/4127	0.68	0/5626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.57	0/4127	0.68	0/5626
1	b	0.57	0/4127	0.68	0/5626
1	c	0.57	0/4127	0.68	0/5626
1	d	0.57	0/4127	0.68	0/5626
1	e	0.57	0/4127	0.68	0/5626
1	f	0.57	0/4127	0.68	0/5626
1	g	0.57	0/4127	0.68	0/5626
1	h	0.57	0/4127	0.68	0/5626
1	i	0.57	0/4127	0.68	0/5626
1	j	0.57	0/4127	0.68	0/5626
1	k	0.57	0/4127	0.68	0/5626
1	l	0.57	0/4127	0.68	0/5626
1	m	0.57	0/4127	0.68	0/5626
1	n	0.57	0/4127	0.68	0/5626
1	o	0.57	0/4127	0.68	0/5626
1	p	0.57	0/4127	0.68	0/5626
1	q	0.57	0/4127	0.68	0/5626
1	r	0.57	0/4127	0.68	0/5626
1	s	0.57	0/4127	0.68	0/5626
1	t	0.57	0/4127	0.68	0/5626
1	u	0.57	0/4127	0.68	0/5626
1	v	0.57	0/4127	0.68	0/5626
1	w	0.57	0/4127	0.68	0/5626
1	x	0.57	0/4127	0.68	0/5626
1	y	0.57	0/4127	0.68	0/5626
1	z	0.57	0/4127	0.68	0/5626
All	All	0.57	0/247620	0.68	0/337560

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	1	0	5
1	2	0	6
1	3	0	5
1	4	0	6
1	5	0	5
1	6	0	5
1	7	0	6
1	8	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
1	E	0	6
1	F	0	5
1	G	0	5
1	H	0	5
1	I	0	5
1	J	0	5
1	K	0	6
1	L	0	5
1	M	0	5
1	N	0	5
1	O	0	6
1	P	0	5
1	Q	0	5
1	R	0	5
1	S	0	5
1	T	0	6
1	U	0	6
1	V	0	5
1	W	0	5
1	X	0	5
1	Y	0	5
1	Z	0	5
1	a	0	5
1	b	0	5
1	c	0	5
1	d	0	5
1	e	0	5
1	f	0	5
1	g	0	6
1	h	0	5
1	i	0	5
1	j	0	5
1	k	0	5
1	l	0	6
1	m	0	5
1	n	0	6
1	o	0	6
1	p	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	5
1	r	0	5
1	s	0	5
1	t	0	5
1	u	0	5
1	v	0	5
1	w	0	6
1	x	0	6
1	y	0	5
1	z	0	5
All	All	0	314

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (314) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	354	LEU	Peptide
1	1	607	GLN	Peptide
1	1	628	PHE	Peptide
1	1	705	ASN	Peptide
1	1	728	THR	Peptide
1	2	354	LEU	Peptide
1	2	381	ASN	Peptide
1	2	607	GLN	Peptide
1	2	628	PHE	Peptide
1	2	705	ASN	Peptide
1	2	728	THR	Peptide
1	3	354	LEU	Peptide
1	3	607	GLN	Peptide
1	3	628	PHE	Peptide
1	3	705	ASN	Peptide
1	3	728	THR	Peptide
1	4	354	LEU	Peptide
1	4	381	ASN	Peptide
1	4	607	GLN	Peptide
1	4	628	PHE	Peptide
1	4	705	ASN	Peptide
1	4	728	THR	Peptide
1	5	354	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	5	607	GLN	Peptide
1	5	628	PHE	Peptide
1	5	705	ASN	Peptide
1	5	728	THR	Peptide
1	6	354	LEU	Peptide
1	6	607	GLN	Peptide
1	6	628	PHE	Peptide
1	6	705	ASN	Peptide
1	6	728	THR	Peptide
1	7	354	LEU	Peptide
1	7	381	ASN	Peptide
1	7	607	GLN	Peptide
1	7	628	PHE	Peptide
1	7	705	ASN	Peptide
1	7	728	THR	Peptide
1	8	354	LEU	Peptide
1	8	607	GLN	Peptide
1	8	628	PHE	Peptide
1	8	705	ASN	Peptide
1	8	728	THR	Peptide
1	A	354	LEU	Peptide
1	A	607	GLN	Peptide
1	A	628	PHE	Peptide
1	A	705	ASN	Peptide
1	A	728	THR	Peptide
1	B	354	LEU	Peptide
1	B	607	GLN	Peptide
1	B	628	PHE	Peptide
1	B	705	ASN	Peptide
1	B	728	THR	Peptide
1	C	354	LEU	Peptide
1	C	607	GLN	Peptide
1	C	628	PHE	Peptide
1	C	705	ASN	Peptide
1	C	728	THR	Peptide
1	D	354	LEU	Peptide
1	D	607	GLN	Peptide
1	D	628	PHE	Peptide
1	D	705	ASN	Peptide
1	D	728	THR	Peptide
1	E	354	LEU	Peptide
1	E	381	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	607	GLN	Peptide
1	E	628	PHE	Peptide
1	E	705	ASN	Peptide
1	E	728	THR	Peptide
1	F	354	LEU	Peptide
1	F	607	GLN	Peptide
1	F	628	PHE	Peptide
1	F	705	ASN	Peptide
1	F	728	THR	Peptide
1	G	354	LEU	Peptide
1	G	607	GLN	Peptide
1	G	628	PHE	Peptide
1	G	705	ASN	Peptide
1	G	728	THR	Peptide
1	H	354	LEU	Peptide
1	H	607	GLN	Peptide
1	H	628	PHE	Peptide
1	H	705	ASN	Peptide
1	H	728	THR	Peptide
1	I	354	LEU	Peptide
1	I	607	GLN	Peptide
1	I	628	PHE	Peptide
1	I	705	ASN	Peptide
1	I	728	THR	Peptide
1	J	354	LEU	Peptide
1	J	607	GLN	Peptide
1	J	628	PHE	Peptide
1	J	705	ASN	Peptide
1	J	728	THR	Peptide
1	K	354	LEU	Peptide
1	K	381	ASN	Peptide
1	K	607	GLN	Peptide
1	K	628	PHE	Peptide
1	K	705	ASN	Peptide
1	K	728	THR	Peptide
1	L	354	LEU	Peptide
1	L	607	GLN	Peptide
1	L	628	PHE	Peptide
1	L	705	ASN	Peptide
1	L	728	THR	Peptide
1	M	354	LEU	Peptide
1	M	607	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	M	628	PHE	Peptide
1	M	705	ASN	Peptide
1	M	728	THR	Peptide
1	N	354	LEU	Peptide
1	N	607	GLN	Peptide
1	N	628	PHE	Peptide
1	N	705	ASN	Peptide
1	N	728	THR	Peptide
1	O	354	LEU	Peptide
1	O	381	ASN	Peptide
1	O	607	GLN	Peptide
1	O	628	PHE	Peptide
1	O	705	ASN	Peptide
1	O	728	THR	Peptide
1	P	354	LEU	Peptide
1	P	607	GLN	Peptide
1	P	628	PHE	Peptide
1	P	705	ASN	Peptide
1	P	728	THR	Peptide
1	Q	354	LEU	Peptide
1	Q	607	GLN	Peptide
1	Q	628	PHE	Peptide
1	Q	705	ASN	Peptide
1	Q	728	THR	Peptide
1	R	354	LEU	Peptide
1	R	607	GLN	Peptide
1	R	628	PHE	Peptide
1	R	705	ASN	Peptide
1	R	728	THR	Peptide
1	S	354	LEU	Peptide
1	S	607	GLN	Peptide
1	S	628	PHE	Peptide
1	S	705	ASN	Peptide
1	S	728	THR	Peptide
1	T	354	LEU	Peptide
1	T	381	ASN	Peptide
1	T	607	GLN	Peptide
1	T	628	PHE	Peptide
1	T	705	ASN	Peptide
1	T	728	THR	Peptide
1	U	354	LEU	Peptide
1	U	381	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	U	607	GLN	Peptide
1	U	628	PHE	Peptide
1	U	705	ASN	Peptide
1	U	728	THR	Peptide
1	V	354	LEU	Peptide
1	V	607	GLN	Peptide
1	V	628	PHE	Peptide
1	V	705	ASN	Peptide
1	V	728	THR	Peptide
1	W	354	LEU	Peptide
1	W	607	GLN	Peptide
1	W	628	PHE	Peptide
1	W	705	ASN	Peptide
1	W	728	THR	Peptide
1	X	354	LEU	Peptide
1	X	607	GLN	Peptide
1	X	628	PHE	Peptide
1	X	705	ASN	Peptide
1	X	728	THR	Peptide
1	Y	354	LEU	Peptide
1	Y	607	GLN	Peptide
1	Y	628	PHE	Peptide
1	Y	705	ASN	Peptide
1	Y	728	THR	Peptide
1	Z	354	LEU	Peptide
1	Z	607	GLN	Peptide
1	Z	628	PHE	Peptide
1	Z	705	ASN	Peptide
1	Z	728	THR	Peptide
1	a	354	LEU	Peptide
1	a	607	GLN	Peptide
1	a	628	PHE	Peptide
1	a	705	ASN	Peptide
1	a	728	THR	Peptide
1	b	354	LEU	Peptide
1	b	607	GLN	Peptide
1	b	628	PHE	Peptide
1	b	705	ASN	Peptide
1	b	728	THR	Peptide
1	c	354	LEU	Peptide
1	c	607	GLN	Peptide
1	c	628	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	c	705	ASN	Peptide
1	c	728	THR	Peptide
1	d	354	LEU	Peptide
1	d	607	GLN	Peptide
1	d	628	PHE	Peptide
1	d	705	ASN	Peptide
1	d	728	THR	Peptide
1	e	354	LEU	Peptide
1	e	607	GLN	Peptide
1	e	628	PHE	Peptide
1	e	705	ASN	Peptide
1	e	728	THR	Peptide
1	f	354	LEU	Peptide
1	f	607	GLN	Peptide
1	f	628	PHE	Peptide
1	f	705	ASN	Peptide
1	f	728	THR	Peptide
1	g	354	LEU	Peptide
1	g	381	ASN	Peptide
1	g	607	GLN	Peptide
1	g	628	PHE	Peptide
1	g	705	ASN	Peptide
1	g	728	THR	Peptide
1	h	354	LEU	Peptide
1	h	607	GLN	Peptide
1	h	628	PHE	Peptide
1	h	705	ASN	Peptide
1	h	728	THR	Peptide
1	i	354	LEU	Peptide
1	i	607	GLN	Peptide
1	i	628	PHE	Peptide
1	i	705	ASN	Peptide
1	i	728	THR	Peptide
1	j	354	LEU	Peptide
1	j	607	GLN	Peptide
1	j	628	PHE	Peptide
1	j	705	ASN	Peptide
1	j	728	THR	Peptide
1	k	354	LEU	Peptide
1	k	607	GLN	Peptide
1	k	628	PHE	Peptide
1	k	705	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	k	728	THR	Peptide
1	l	354	LEU	Peptide
1	l	381	ASN	Peptide
1	l	607	GLN	Peptide
1	l	628	PHE	Peptide
1	l	705	ASN	Peptide
1	l	728	THR	Peptide
1	m	354	LEU	Peptide
1	m	607	GLN	Peptide
1	m	628	PHE	Peptide
1	m	705	ASN	Peptide
1	m	728	THR	Peptide
1	n	354	LEU	Peptide
1	n	381	ASN	Peptide
1	n	607	GLN	Peptide
1	n	628	PHE	Peptide
1	n	705	ASN	Peptide
1	n	728	THR	Peptide
1	o	354	LEU	Peptide
1	o	381	ASN	Peptide
1	o	607	GLN	Peptide
1	o	628	PHE	Peptide
1	o	705	ASN	Peptide
1	o	728	THR	Peptide
1	p	354	LEU	Peptide
1	p	607	GLN	Peptide
1	p	628	PHE	Peptide
1	p	705	ASN	Peptide
1	p	728	THR	Peptide
1	q	354	LEU	Peptide
1	q	607	GLN	Peptide
1	q	628	PHE	Peptide
1	q	705	ASN	Peptide
1	q	728	THR	Peptide
1	r	354	LEU	Peptide
1	r	607	GLN	Peptide
1	r	628	PHE	Peptide
1	r	705	ASN	Peptide
1	r	728	THR	Peptide
1	s	354	LEU	Peptide
1	s	607	GLN	Peptide
1	s	628	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	s	705	ASN	Peptide
1	s	728	THR	Peptide
1	t	354	LEU	Peptide
1	t	607	GLN	Peptide
1	t	628	PHE	Peptide
1	t	705	ASN	Peptide
1	t	728	THR	Peptide
1	u	354	LEU	Peptide
1	u	607	GLN	Peptide
1	u	628	PHE	Peptide
1	u	705	ASN	Peptide
1	u	728	THR	Peptide
1	v	354	LEU	Peptide
1	v	607	GLN	Peptide
1	v	628	PHE	Peptide
1	v	705	ASN	Peptide
1	v	728	THR	Peptide
1	w	354	LEU	Peptide
1	w	381	ASN	Peptide
1	w	607	GLN	Peptide
1	w	628	PHE	Peptide
1	w	705	ASN	Peptide
1	w	728	THR	Peptide
1	x	354	LEU	Peptide
1	x	381	ASN	Peptide
1	x	607	GLN	Peptide
1	x	628	PHE	Peptide
1	x	705	ASN	Peptide
1	x	728	THR	Peptide
1	y	354	LEU	Peptide
1	y	607	GLN	Peptide
1	y	628	PHE	Peptide
1	y	705	ASN	Peptide
1	y	728	THR	Peptide
1	z	354	LEU	Peptide
1	z	607	GLN	Peptide
1	z	628	PHE	Peptide
1	z	705	ASN	Peptide
1	z	728	THR	Peptide

5.2 Too-close contacts ⓘ

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

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	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	2	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	3	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	4	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	5	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	6	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	7	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	8	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	A	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	B	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	C	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	D	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	E	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	F	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	G	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	H	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	I	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	J	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	K	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	L	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	M	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	O	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	P	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	Q	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	R	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	S	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	T	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	U	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	V	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	W	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	X	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	Y	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	Z	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	a	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	b	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	c	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	d	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	e	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	f	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	g	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	h	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	i	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	j	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	k	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	l	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	m	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	n	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	o	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	p	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	q	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	r	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	s	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	t	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
1	u	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	v	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	w	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	x	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	y	498/735 (68%)	378 (76%)	107 (22%)	13 (3%)	5	34
1	z	498/735 (68%)	377 (76%)	108 (22%)	13 (3%)	5	34
All	All	29880/44100 (68%)	22656 (76%)	6444 (22%)	780 (3%)	8	34

All (780) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	680	VAL
1	B	680	VAL
1	C	680	VAL
1	D	680	VAL
1	E	680	VAL
1	F	680	VAL
1	G	680	VAL
1	H	680	VAL
1	I	680	VAL
1	J	680	VAL
1	K	680	VAL
1	L	680	VAL
1	M	680	VAL
1	N	680	VAL
1	O	680	VAL
1	P	680	VAL
1	Q	680	VAL
1	R	680	VAL
1	S	680	VAL
1	T	680	VAL
1	U	680	VAL
1	V	680	VAL
1	W	680	VAL
1	X	680	VAL
1	Y	680	VAL
1	Z	680	VAL

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Mol	Chain	Res	Type
1	a	680	VAL
1	b	680	VAL
1	c	680	VAL
1	d	680	VAL
1	e	680	VAL
1	f	680	VAL
1	g	680	VAL
1	h	680	VAL
1	i	680	VAL
1	j	680	VAL
1	k	680	VAL
1	l	680	VAL
1	m	680	VAL
1	n	680	VAL
1	o	680	VAL
1	p	680	VAL
1	q	680	VAL
1	r	680	VAL
1	s	680	VAL
1	t	680	VAL
1	u	680	VAL
1	v	680	VAL
1	w	680	VAL
1	x	680	VAL
1	y	680	VAL
1	z	680	VAL
1	1	680	VAL
1	2	680	VAL
1	3	680	VAL
1	4	680	VAL
1	5	680	VAL
1	6	680	VAL
1	7	680	VAL
1	8	680	VAL
1	A	470	ILE
1	A	471	ARG
1	A	525	SER
1	A	571	VAL
1	B	470	ILE
1	B	471	ARG
1	B	525	SER
1	B	571	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	C	470	ILE
1	C	471	ARG
1	C	525	SER
1	C	571	VAL
1	D	470	ILE
1	D	471	ARG
1	D	525	SER
1	D	571	VAL
1	E	470	ILE
1	E	471	ARG
1	E	525	SER
1	E	571	VAL
1	F	470	ILE
1	F	471	ARG
1	F	525	SER
1	F	571	VAL
1	G	470	ILE
1	G	471	ARG
1	G	525	SER
1	G	571	VAL
1	H	470	ILE
1	H	471	ARG
1	H	525	SER
1	H	571	VAL
1	I	470	ILE
1	I	471	ARG
1	I	525	SER
1	I	571	VAL
1	J	470	ILE
1	J	471	ARG
1	J	525	SER
1	J	571	VAL
1	K	470	ILE
1	K	471	ARG
1	K	525	SER
1	K	571	VAL
1	L	470	ILE
1	L	471	ARG
1	L	525	SER
1	L	571	VAL
1	M	470	ILE
1	M	471	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	525	SER
1	M	571	VAL
1	N	470	ILE
1	N	471	ARG
1	N	525	SER
1	N	571	VAL
1	O	470	ILE
1	O	471	ARG
1	O	525	SER
1	O	571	VAL
1	P	470	ILE
1	P	471	ARG
1	P	525	SER
1	P	571	VAL
1	Q	470	ILE
1	Q	471	ARG
1	Q	525	SER
1	Q	571	VAL
1	R	470	ILE
1	R	471	ARG
1	R	525	SER
1	R	571	VAL
1	S	470	ILE
1	S	471	ARG
1	S	525	SER
1	S	571	VAL
1	T	470	ILE
1	T	471	ARG
1	T	525	SER
1	T	571	VAL
1	U	470	ILE
1	U	471	ARG
1	U	525	SER
1	U	571	VAL
1	V	470	ILE
1	V	471	ARG
1	V	525	SER
1	V	571	VAL
1	W	470	ILE
1	W	471	ARG
1	W	525	SER
1	W	571	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	X	470	ILE
1	X	471	ARG
1	X	525	SER
1	X	571	VAL
1	Y	470	ILE
1	Y	471	ARG
1	Y	525	SER
1	Y	571	VAL
1	Z	470	ILE
1	Z	471	ARG
1	Z	525	SER
1	Z	571	VAL
1	a	470	ILE
1	a	471	ARG
1	a	525	SER
1	a	571	VAL
1	b	470	ILE
1	b	471	ARG
1	b	525	SER
1	b	571	VAL
1	c	470	ILE
1	c	471	ARG
1	c	525	SER
1	c	571	VAL
1	d	470	ILE
1	d	471	ARG
1	d	525	SER
1	d	571	VAL
1	e	470	ILE
1	e	471	ARG
1	e	525	SER
1	e	571	VAL
1	f	470	ILE
1	f	471	ARG
1	f	525	SER
1	f	571	VAL
1	g	470	ILE
1	g	471	ARG
1	g	525	SER
1	g	571	VAL
1	h	470	ILE
1	h	471	ARG

Continued on next page...

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Mol	Chain	Res	Type
1	h	525	SER
1	h	571	VAL
1	i	470	ILE
1	i	471	ARG
1	i	525	SER
1	i	571	VAL
1	j	470	ILE
1	j	471	ARG
1	j	525	SER
1	j	571	VAL
1	k	470	ILE
1	k	471	ARG
1	k	525	SER
1	k	571	VAL
1	l	470	ILE
1	l	471	ARG
1	l	525	SER
1	l	571	VAL
1	m	470	ILE
1	m	471	ARG
1	m	525	SER
1	m	571	VAL
1	n	470	ILE
1	n	471	ARG
1	n	525	SER
1	n	571	VAL
1	o	470	ILE
1	o	471	ARG
1	o	525	SER
1	o	571	VAL
1	p	470	ILE
1	p	471	ARG
1	p	525	SER
1	p	571	VAL
1	q	470	ILE
1	q	471	ARG
1	q	525	SER
1	q	571	VAL
1	r	470	ILE
1	r	471	ARG
1	r	525	SER
1	r	571	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	s	470	ILE
1	s	471	ARG
1	s	525	SER
1	s	571	VAL
1	t	470	ILE
1	t	471	ARG
1	t	525	SER
1	t	571	VAL
1	u	470	ILE
1	u	471	ARG
1	u	525	SER
1	u	571	VAL
1	v	470	ILE
1	v	471	ARG
1	v	525	SER
1	v	571	VAL
1	w	470	ILE
1	w	471	ARG
1	w	525	SER
1	w	571	VAL
1	x	470	ILE
1	x	471	ARG
1	x	525	SER
1	x	571	VAL
1	y	470	ILE
1	y	471	ARG
1	y	525	SER
1	y	571	VAL
1	z	470	ILE
1	z	471	ARG
1	z	525	SER
1	z	571	VAL
1	1	470	ILE
1	1	471	ARG
1	1	525	SER
1	1	571	VAL
1	2	470	ILE
1	2	471	ARG
1	2	525	SER
1	2	571	VAL
1	3	470	ILE
1	3	471	ARG

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Mol	Chain	Res	Type
1	3	525	SER
1	3	571	VAL
1	4	470	ILE
1	4	471	ARG
1	4	525	SER
1	4	571	VAL
1	5	470	ILE
1	5	471	ARG
1	5	525	SER
1	5	571	VAL
1	6	470	ILE
1	6	471	ARG
1	6	525	SER
1	6	571	VAL
1	7	470	ILE
1	7	471	ARG
1	7	525	SER
1	7	571	VAL
1	8	470	ILE
1	8	471	ARG
1	8	525	SER
1	8	571	VAL
1	A	539	VAL
1	B	539	VAL
1	C	539	VAL
1	D	539	VAL
1	E	539	VAL
1	F	539	VAL
1	G	539	VAL
1	H	539	VAL
1	I	539	VAL
1	J	539	VAL
1	K	539	VAL
1	L	539	VAL
1	M	539	VAL
1	N	539	VAL
1	O	539	VAL
1	P	539	VAL
1	Q	539	VAL
1	R	539	VAL
1	S	539	VAL
1	T	539	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	U	539	VAL
1	V	539	VAL
1	W	539	VAL
1	X	539	VAL
1	Y	539	VAL
1	Z	539	VAL
1	a	539	VAL
1	b	539	VAL
1	c	539	VAL
1	d	539	VAL
1	e	539	VAL
1	f	539	VAL
1	g	539	VAL
1	h	539	VAL
1	i	539	VAL
1	j	539	VAL
1	k	539	VAL
1	l	539	VAL
1	m	539	VAL
1	n	539	VAL
1	o	539	VAL
1	p	539	VAL
1	q	539	VAL
1	r	539	VAL
1	s	539	VAL
1	t	539	VAL
1	u	539	VAL
1	v	539	VAL
1	w	539	VAL
1	x	539	VAL
1	y	539	VAL
1	z	539	VAL
1	1	539	VAL
1	2	539	VAL
1	3	539	VAL
1	4	539	VAL
1	5	539	VAL
1	6	539	VAL
1	7	539	VAL
1	8	539	VAL
1	A	628	PHE
1	A	681	GLU

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Mol	Chain	Res	Type
1	B	628	PHE
1	B	681	GLU
1	C	628	PHE
1	C	681	GLU
1	D	628	PHE
1	D	681	GLU
1	E	628	PHE
1	E	681	GLU
1	F	628	PHE
1	F	681	GLU
1	G	628	PHE
1	G	681	GLU
1	H	628	PHE
1	H	681	GLU
1	I	628	PHE
1	I	681	GLU
1	J	628	PHE
1	J	681	GLU
1	K	628	PHE
1	K	681	GLU
1	L	628	PHE
1	L	681	GLU
1	M	628	PHE
1	M	681	GLU
1	N	628	PHE
1	N	681	GLU
1	O	628	PHE
1	O	681	GLU
1	P	628	PHE
1	P	681	GLU
1	Q	628	PHE
1	Q	681	GLU
1	R	628	PHE
1	R	681	GLU
1	S	628	PHE
1	S	681	GLU
1	T	628	PHE
1	T	681	GLU
1	U	628	PHE
1	U	681	GLU
1	V	628	PHE
1	V	681	GLU

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Mol	Chain	Res	Type
1	W	628	PHE
1	W	681	GLU
1	X	628	PHE
1	X	681	GLU
1	Y	628	PHE
1	Y	681	GLU
1	Z	628	PHE
1	Z	681	GLU
1	a	628	PHE
1	a	681	GLU
1	b	628	PHE
1	b	681	GLU
1	c	628	PHE
1	c	681	GLU
1	d	628	PHE
1	d	681	GLU
1	e	628	PHE
1	e	681	GLU
1	f	628	PHE
1	f	681	GLU
1	g	628	PHE
1	g	681	GLU
1	h	628	PHE
1	h	681	GLU
1	i	628	PHE
1	i	681	GLU
1	j	628	PHE
1	j	681	GLU
1	k	628	PHE
1	k	681	GLU
1	l	628	PHE
1	l	681	GLU
1	m	628	PHE
1	m	681	GLU
1	n	628	PHE
1	n	681	GLU
1	o	628	PHE
1	o	681	GLU
1	p	628	PHE
1	p	681	GLU
1	q	628	PHE
1	q	681	GLU

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Mol	Chain	Res	Type
1	r	628	PHE
1	r	681	GLU
1	s	628	PHE
1	s	681	GLU
1	t	628	PHE
1	t	681	GLU
1	u	628	PHE
1	u	681	GLU
1	v	628	PHE
1	v	681	GLU
1	w	628	PHE
1	w	681	GLU
1	x	628	PHE
1	x	681	GLU
1	y	628	PHE
1	y	681	GLU
1	z	628	PHE
1	z	681	GLU
1	1	628	PHE
1	1	681	GLU
1	2	628	PHE
1	2	681	GLU
1	3	628	PHE
1	3	681	GLU
1	4	628	PHE
1	4	681	GLU
1	5	628	PHE
1	5	681	GLU
1	6	628	PHE
1	6	681	GLU
1	7	628	PHE
1	7	681	GLU
1	8	628	PHE
1	8	681	GLU
1	A	361	CYS
1	A	559	ILE
1	A	695	ASN
1	B	361	CYS
1	B	559	ILE
1	B	695	ASN
1	C	361	CYS
1	C	559	ILE

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Mol	Chain	Res	Type
1	C	695	ASN
1	D	361	CYS
1	D	559	ILE
1	D	695	ASN
1	E	361	CYS
1	E	559	ILE
1	E	695	ASN
1	F	361	CYS
1	F	559	ILE
1	F	695	ASN
1	G	361	CYS
1	G	559	ILE
1	G	695	ASN
1	H	361	CYS
1	H	559	ILE
1	H	695	ASN
1	I	361	CYS
1	I	559	ILE
1	I	695	ASN
1	J	361	CYS
1	J	559	ILE
1	J	695	ASN
1	K	361	CYS
1	K	559	ILE
1	K	695	ASN
1	L	361	CYS
1	L	559	ILE
1	L	695	ASN
1	M	361	CYS
1	M	559	ILE
1	M	695	ASN
1	N	361	CYS
1	N	559	ILE
1	N	695	ASN
1	O	361	CYS
1	O	559	ILE
1	O	695	ASN
1	P	361	CYS
1	P	559	ILE
1	P	695	ASN
1	Q	361	CYS
1	Q	559	ILE

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Mol	Chain	Res	Type
1	Q	695	ASN
1	R	361	CYS
1	R	559	ILE
1	R	695	ASN
1	S	361	CYS
1	S	559	ILE
1	S	695	ASN
1	T	361	CYS
1	T	559	ILE
1	T	695	ASN
1	U	361	CYS
1	U	559	ILE
1	U	695	ASN
1	V	361	CYS
1	V	559	ILE
1	V	695	ASN
1	W	361	CYS
1	W	559	ILE
1	W	695	ASN
1	X	361	CYS
1	X	559	ILE
1	X	695	ASN
1	Y	361	CYS
1	Y	559	ILE
1	Y	695	ASN
1	Z	361	CYS
1	Z	559	ILE
1	Z	695	ASN
1	a	361	CYS
1	a	559	ILE
1	a	695	ASN
1	b	361	CYS
1	b	559	ILE
1	b	695	ASN
1	c	361	CYS
1	c	559	ILE
1	c	695	ASN
1	d	361	CYS
1	d	559	ILE
1	d	695	ASN
1	e	361	CYS
1	e	559	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	e	695	ASN
1	f	361	CYS
1	f	559	ILE
1	f	695	ASN
1	g	361	CYS
1	g	559	ILE
1	g	695	ASN
1	h	361	CYS
1	h	559	ILE
1	h	695	ASN
1	i	361	CYS
1	i	559	ILE
1	i	695	ASN
1	j	361	CYS
1	j	559	ILE
1	j	695	ASN
1	k	361	CYS
1	k	559	ILE
1	k	695	ASN
1	l	361	CYS
1	l	559	ILE
1	l	695	ASN
1	m	361	CYS
1	m	559	ILE
1	m	695	ASN
1	n	361	CYS
1	n	559	ILE
1	n	695	ASN
1	o	361	CYS
1	o	559	ILE
1	o	695	ASN
1	p	361	CYS
1	p	559	ILE
1	p	695	ASN
1	q	361	CYS
1	q	559	ILE
1	q	695	ASN
1	r	361	CYS
1	r	559	ILE
1	r	695	ASN
1	s	361	CYS
1	s	559	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	s	695	ASN
1	t	361	CYS
1	t	559	ILE
1	t	695	ASN
1	u	361	CYS
1	u	559	ILE
1	u	695	ASN
1	v	361	CYS
1	v	559	ILE
1	v	695	ASN
1	w	361	CYS
1	w	559	ILE
1	w	695	ASN
1	x	361	CYS
1	x	559	ILE
1	x	695	ASN
1	y	361	CYS
1	y	559	ILE
1	y	695	ASN
1	z	361	CYS
1	z	559	ILE
1	z	695	ASN
1	1	361	CYS
1	1	559	ILE
1	1	695	ASN
1	2	361	CYS
1	2	559	ILE
1	2	695	ASN
1	3	361	CYS
1	3	559	ILE
1	3	695	ASN
1	4	361	CYS
1	4	559	ILE
1	4	695	ASN
1	5	361	CYS
1	5	559	ILE
1	5	695	ASN
1	6	361	CYS
1	6	559	ILE
1	6	695	ASN
1	7	361	CYS
1	7	559	ILE

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Mol	Chain	Res	Type
1	7	695	ASN
1	8	361	CYS
1	8	559	ILE
1	8	695	ASN
1	A	710	VAL
1	B	710	VAL
1	C	710	VAL
1	D	710	VAL
1	E	710	VAL
1	F	710	VAL
1	G	710	VAL
1	H	710	VAL
1	I	710	VAL
1	J	710	VAL
1	K	710	VAL
1	L	710	VAL
1	M	710	VAL
1	N	710	VAL
1	O	710	VAL
1	P	710	VAL
1	Q	710	VAL
1	R	710	VAL
1	S	710	VAL
1	T	710	VAL
1	U	710	VAL
1	V	710	VAL
1	W	710	VAL
1	X	710	VAL
1	Y	710	VAL
1	Z	710	VAL
1	a	710	VAL
1	b	710	VAL
1	c	710	VAL
1	d	710	VAL
1	e	710	VAL
1	f	710	VAL
1	g	710	VAL
1	h	710	VAL
1	i	710	VAL
1	j	710	VAL
1	k	710	VAL
1	l	710	VAL

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Mol	Chain	Res	Type
1	m	710	VAL
1	n	710	VAL
1	o	710	VAL
1	p	710	VAL
1	q	710	VAL
1	r	710	VAL
1	s	710	VAL
1	t	710	VAL
1	u	710	VAL
1	v	710	VAL
1	w	710	VAL
1	x	710	VAL
1	y	710	VAL
1	z	710	VAL
1	1	710	VAL
1	2	710	VAL
1	3	710	VAL
1	4	710	VAL
1	5	710	VAL
1	6	710	VAL
1	7	710	VAL
1	8	710	VAL
1	A	646	ILE
1	B	646	ILE
1	C	646	ILE
1	D	646	ILE
1	E	646	ILE
1	F	646	ILE
1	G	646	ILE
1	H	646	ILE
1	I	646	ILE
1	J	646	ILE
1	K	646	ILE
1	L	646	ILE
1	M	646	ILE
1	N	646	ILE
1	O	646	ILE
1	P	646	ILE
1	Q	646	ILE
1	R	646	ILE
1	S	646	ILE
1	T	646	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	646	ILE
1	V	646	ILE
1	W	646	ILE
1	X	646	ILE
1	Y	646	ILE
1	Z	646	ILE
1	a	646	ILE
1	b	646	ILE
1	c	646	ILE
1	d	646	ILE
1	e	646	ILE
1	f	646	ILE
1	g	646	ILE
1	h	646	ILE
1	i	646	ILE
1	j	646	ILE
1	k	646	ILE
1	l	646	ILE
1	m	646	ILE
1	n	646	ILE
1	o	646	ILE
1	p	646	ILE
1	q	646	ILE
1	r	646	ILE
1	s	646	ILE
1	t	646	ILE
1	u	646	ILE
1	v	646	ILE
1	w	646	ILE
1	x	646	ILE
1	y	646	ILE
1	z	646	ILE
1	1	646	ILE
1	2	646	ILE
1	3	646	ILE
1	4	646	ILE
1	5	646	ILE
1	6	646	ILE
1	7	646	ILE
1	8	646	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	2	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	3	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	4	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	5	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	6	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	7	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	8	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	A	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	B	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	C	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	D	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	E	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	F	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	G	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	H	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	I	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	J	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	K	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	L	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	M	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	N	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	O	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	P	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	Q	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	R	444/629 (71%)	442 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	T	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	U	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	V	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	W	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	X	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	Y	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	Z	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	a	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	b	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	c	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	d	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	e	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	f	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	g	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	h	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	i	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	j	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	k	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	l	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	m	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	n	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	o	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	p	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	q	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	r	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	s	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	t	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	u	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	v	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	w	444/629 (71%)	442 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	y	444/629 (71%)	442 (100%)	2 (0%)	88	94
1	z	444/629 (71%)	442 (100%)	2 (0%)	88	94
All	All	26640/37740 (71%)	26520 (100%)	120 (0%)	89	94

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	460	LEU
1	A	613	LEU
1	B	460	LEU
1	B	613	LEU
1	C	460	LEU
1	C	613	LEU
1	D	460	LEU
1	D	613	LEU
1	E	460	LEU
1	E	613	LEU
1	F	460	LEU
1	F	613	LEU
1	G	460	LEU
1	G	613	LEU
1	H	460	LEU
1	H	613	LEU
1	I	460	LEU
1	I	613	LEU
1	J	460	LEU
1	J	613	LEU
1	K	460	LEU
1	K	613	LEU
1	L	460	LEU
1	L	613	LEU
1	M	460	LEU
1	M	613	LEU
1	N	460	LEU
1	N	613	LEU
1	O	460	LEU
1	O	613	LEU
1	P	460	LEU
1	P	613	LEU
1	Q	460	LEU

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Mol	Chain	Res	Type
1	Q	613	LEU
1	R	460	LEU
1	R	613	LEU
1	S	460	LEU
1	S	613	LEU
1	T	460	LEU
1	T	613	LEU
1	U	460	LEU
1	U	613	LEU
1	V	460	LEU
1	V	613	LEU
1	W	460	LEU
1	W	613	LEU
1	X	460	LEU
1	X	613	LEU
1	Y	460	LEU
1	Y	613	LEU
1	Z	460	LEU
1	Z	613	LEU
1	a	460	LEU
1	a	613	LEU
1	b	460	LEU
1	b	613	LEU
1	c	460	LEU
1	c	613	LEU
1	d	460	LEU
1	d	613	LEU
1	e	460	LEU
1	e	613	LEU
1	f	460	LEU
1	f	613	LEU
1	g	460	LEU
1	g	613	LEU
1	h	460	LEU
1	h	613	LEU
1	i	460	LEU
1	i	613	LEU
1	j	460	LEU
1	j	613	LEU
1	k	460	LEU
1	k	613	LEU
1	l	460	LEU

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Mol	Chain	Res	Type
1	l	613	LEU
1	m	460	LEU
1	m	613	LEU
1	n	460	LEU
1	n	613	LEU
1	o	460	LEU
1	o	613	LEU
1	p	460	LEU
1	p	613	LEU
1	q	460	LEU
1	q	613	LEU
1	r	460	LEU
1	r	613	LEU
1	s	460	LEU
1	s	613	LEU
1	t	460	LEU
1	t	613	LEU
1	u	460	LEU
1	u	613	LEU
1	v	460	LEU
1	v	613	LEU
1	w	460	LEU
1	w	613	LEU
1	x	460	LEU
1	x	613	LEU
1	y	460	LEU
1	y	613	LEU
1	z	460	LEU
1	z	613	LEU
1	1	460	LEU
1	1	613	LEU
1	2	460	LEU
1	2	613	LEU
1	3	460	LEU
1	3	613	LEU
1	4	460	LEU
1	4	613	LEU
1	5	460	LEU
1	5	613	LEU
1	6	460	LEU
1	6	613	LEU
1	7	460	LEU

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Mol	Chain	Res	Type
1	7	613	LEU
1	8	460	LEU
1	8	613	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (558) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	382	ASN
1	A	440	GLN
1	A	461	GLN
1	A	473	GLN
1	A	589	GLN
1	A	598	GLN
1	A	607	GLN
1	A	656	ASN
1	A	690	ASN
1	B	253	ASN
1	B	382	ASN
1	B	440	GLN
1	B	461	GLN
1	B	473	GLN
1	B	589	GLN
1	B	598	GLN
1	B	607	GLN
1	B	656	ASN
1	B	690	ASN
1	C	253	ASN
1	C	382	ASN
1	C	440	GLN
1	C	461	GLN
1	C	473	GLN
1	C	589	GLN
1	C	598	GLN
1	C	607	GLN
1	C	656	ASN
1	C	690	ASN
1	D	253	ASN
1	D	382	ASN
1	D	440	GLN
1	D	461	GLN
1	D	473	GLN

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Mol	Chain	Res	Type
1	D	598	GLN
1	D	607	GLN
1	D	656	ASN
1	D	690	ASN
1	E	253	ASN
1	E	382	ASN
1	E	440	GLN
1	E	461	GLN
1	E	473	GLN
1	E	589	GLN
1	E	598	GLN
1	E	607	GLN
1	E	656	ASN
1	F	253	ASN
1	F	382	ASN
1	F	440	GLN
1	F	461	GLN
1	F	473	GLN
1	F	589	GLN
1	F	598	GLN
1	F	607	GLN
1	F	656	ASN
1	G	253	ASN
1	G	382	ASN
1	G	440	GLN
1	G	461	GLN
1	G	473	GLN
1	G	589	GLN
1	G	598	GLN
1	G	607	GLN
1	G	656	ASN
1	H	253	ASN
1	H	382	ASN
1	H	440	GLN
1	H	461	GLN
1	H	473	GLN
1	H	589	GLN
1	H	598	GLN
1	H	607	GLN
1	H	656	ASN
1	I	253	ASN
1	I	382	ASN

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Mol	Chain	Res	Type
1	I	440	GLN
1	I	461	GLN
1	I	473	GLN
1	I	589	GLN
1	I	607	GLN
1	I	656	ASN
1	J	253	ASN
1	J	382	ASN
1	J	440	GLN
1	J	461	GLN
1	J	473	GLN
1	J	589	GLN
1	J	598	GLN
1	J	607	GLN
1	J	656	ASN
1	J	690	ASN
1	K	253	ASN
1	K	382	ASN
1	K	440	GLN
1	K	461	GLN
1	K	473	GLN
1	K	589	GLN
1	K	598	GLN
1	K	607	GLN
1	K	656	ASN
1	K	690	ASN
1	L	253	ASN
1	L	382	ASN
1	L	440	GLN
1	L	461	GLN
1	L	473	GLN
1	L	589	GLN
1	L	598	GLN
1	L	607	GLN
1	L	656	ASN
1	L	690	ASN
1	M	253	ASN
1	M	382	ASN
1	M	440	GLN
1	M	461	GLN
1	M	473	GLN
1	M	589	GLN

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Mol	Chain	Res	Type
1	M	598	GLN
1	M	607	GLN
1	M	656	ASN
1	M	690	ASN
1	N	253	ASN
1	N	382	ASN
1	N	440	GLN
1	N	461	GLN
1	N	473	GLN
1	N	589	GLN
1	N	598	GLN
1	N	607	GLN
1	N	656	ASN
1	O	253	ASN
1	O	382	ASN
1	O	440	GLN
1	O	461	GLN
1	O	473	GLN
1	O	589	GLN
1	O	598	GLN
1	O	607	GLN
1	O	656	ASN
1	P	253	ASN
1	P	382	ASN
1	P	440	GLN
1	P	461	GLN
1	P	473	GLN
1	P	589	GLN
1	P	598	GLN
1	P	607	GLN
1	P	656	ASN
1	Q	253	ASN
1	Q	382	ASN
1	Q	440	GLN
1	Q	461	GLN
1	Q	473	GLN
1	Q	589	GLN
1	Q	598	GLN
1	Q	607	GLN
1	Q	656	ASN
1	Q	690	ASN
1	R	253	ASN

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Mol	Chain	Res	Type
1	R	255	HIS
1	R	382	ASN
1	R	440	GLN
1	R	461	GLN
1	R	473	GLN
1	R	589	GLN
1	R	598	GLN
1	R	607	GLN
1	R	656	ASN
1	S	253	ASN
1	S	382	ASN
1	S	440	GLN
1	S	461	GLN
1	S	473	GLN
1	S	589	GLN
1	S	598	GLN
1	S	607	GLN
1	S	656	ASN
1	T	253	ASN
1	T	382	ASN
1	T	440	GLN
1	T	461	GLN
1	T	473	GLN
1	T	589	GLN
1	T	598	GLN
1	T	607	GLN
1	T	656	ASN
1	U	253	ASN
1	U	382	ASN
1	U	440	GLN
1	U	461	GLN
1	U	473	GLN
1	U	589	GLN
1	U	598	GLN
1	U	607	GLN
1	U	656	ASN
1	U	690	ASN
1	V	253	ASN
1	V	382	ASN
1	V	440	GLN
1	V	461	GLN
1	V	473	GLN

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Mol	Chain	Res	Type
1	V	589	GLN
1	V	598	GLN
1	V	607	GLN
1	V	656	ASN
1	V	690	ASN
1	W	253	ASN
1	W	382	ASN
1	W	440	GLN
1	W	461	GLN
1	W	473	GLN
1	W	589	GLN
1	W	598	GLN
1	W	607	GLN
1	W	656	ASN
1	X	253	ASN
1	X	382	ASN
1	X	440	GLN
1	X	461	GLN
1	X	473	GLN
1	X	589	GLN
1	X	607	GLN
1	X	656	ASN
1	Y	253	ASN
1	Y	382	ASN
1	Y	440	GLN
1	Y	461	GLN
1	Y	473	GLN
1	Y	589	GLN
1	Y	598	GLN
1	Y	607	GLN
1	Y	656	ASN
1	Z	253	ASN
1	Z	255	HIS
1	Z	382	ASN
1	Z	440	GLN
1	Z	461	GLN
1	Z	473	GLN
1	Z	589	GLN
1	Z	607	GLN
1	Z	656	ASN
1	a	253	ASN
1	a	259	GLN

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Mol	Chain	Res	Type
1	a	382	ASN
1	a	440	GLN
1	a	461	GLN
1	a	473	GLN
1	a	589	GLN
1	a	598	GLN
1	a	607	GLN
1	a	656	ASN
1	b	253	ASN
1	b	382	ASN
1	b	440	GLN
1	b	461	GLN
1	b	473	GLN
1	b	589	GLN
1	b	598	GLN
1	b	607	GLN
1	b	656	ASN
1	b	690	ASN
1	c	253	ASN
1	c	382	ASN
1	c	440	GLN
1	c	461	GLN
1	c	473	GLN
1	c	589	GLN
1	c	598	GLN
1	c	607	GLN
1	c	656	ASN
1	d	253	ASN
1	d	382	ASN
1	d	440	GLN
1	d	473	GLN
1	d	589	GLN
1	d	598	GLN
1	d	607	GLN
1	d	656	ASN
1	d	690	ASN
1	e	253	ASN
1	e	382	ASN
1	e	440	GLN
1	e	461	GLN
1	e	473	GLN
1	e	589	GLN

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Mol	Chain	Res	Type
1	e	598	GLN
1	e	607	GLN
1	e	656	ASN
1	e	690	ASN
1	f	253	ASN
1	f	382	ASN
1	f	440	GLN
1	f	461	GLN
1	f	473	GLN
1	f	589	GLN
1	f	598	GLN
1	f	607	GLN
1	f	656	ASN
1	g	253	ASN
1	g	382	ASN
1	g	440	GLN
1	g	461	GLN
1	g	473	GLN
1	g	589	GLN
1	g	607	GLN
1	g	656	ASN
1	g	690	ASN
1	h	253	ASN
1	h	382	ASN
1	h	440	GLN
1	h	461	GLN
1	h	473	GLN
1	h	589	GLN
1	h	598	GLN
1	h	607	GLN
1	h	656	ASN
1	h	690	ASN
1	i	253	ASN
1	i	382	ASN
1	i	440	GLN
1	i	461	GLN
1	i	473	GLN
1	i	589	GLN
1	i	607	GLN
1	i	656	ASN
1	i	690	ASN
1	j	253	ASN

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Mol	Chain	Res	Type
1	j	382	ASN
1	j	440	GLN
1	j	461	GLN
1	j	473	GLN
1	j	589	GLN
1	j	598	GLN
1	j	607	GLN
1	j	656	ASN
1	k	253	ASN
1	k	382	ASN
1	k	440	GLN
1	k	461	GLN
1	k	473	GLN
1	k	589	GLN
1	k	598	GLN
1	k	607	GLN
1	k	656	ASN
1	k	690	ASN
1	l	253	ASN
1	l	255	HIS
1	l	382	ASN
1	l	440	GLN
1	l	461	GLN
1	l	473	GLN
1	l	589	GLN
1	l	598	GLN
1	l	607	GLN
1	l	656	ASN
1	l	690	ASN
1	m	253	ASN
1	m	255	HIS
1	m	382	ASN
1	m	440	GLN
1	m	461	GLN
1	m	473	GLN
1	m	589	GLN
1	m	598	GLN
1	m	607	GLN
1	m	656	ASN
1	n	253	ASN
1	n	382	ASN
1	n	440	GLN

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Mol	Chain	Res	Type
1	n	461	GLN
1	n	473	GLN
1	n	589	GLN
1	n	598	GLN
1	n	607	GLN
1	n	656	ASN
1	o	253	ASN
1	o	382	ASN
1	o	440	GLN
1	o	461	GLN
1	o	473	GLN
1	o	589	GLN
1	o	598	GLN
1	o	607	GLN
1	o	656	ASN
1	o	690	ASN
1	p	253	ASN
1	p	382	ASN
1	p	440	GLN
1	p	461	GLN
1	p	473	GLN
1	p	589	GLN
1	p	598	GLN
1	p	607	GLN
1	p	656	ASN
1	q	253	ASN
1	q	259	GLN
1	q	440	GLN
1	q	461	GLN
1	q	473	GLN
1	q	589	GLN
1	q	598	GLN
1	q	607	GLN
1	q	656	ASN
1	r	253	ASN
1	r	382	ASN
1	r	440	GLN
1	r	461	GLN
1	r	473	GLN
1	r	589	GLN
1	r	607	GLN
1	r	656	ASN

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Mol	Chain	Res	Type
1	s	253	ASN
1	s	382	ASN
1	s	440	GLN
1	s	473	GLN
1	s	589	GLN
1	s	598	GLN
1	s	607	GLN
1	s	656	ASN
1	t	253	ASN
1	t	255	HIS
1	t	382	ASN
1	t	440	GLN
1	t	461	GLN
1	t	473	GLN
1	t	589	GLN
1	t	598	GLN
1	t	607	GLN
1	t	656	ASN
1	u	253	ASN
1	u	382	ASN
1	u	440	GLN
1	u	461	GLN
1	u	473	GLN
1	u	589	GLN
1	u	598	GLN
1	u	607	GLN
1	u	656	ASN
1	v	253	ASN
1	v	382	ASN
1	v	440	GLN
1	v	461	GLN
1	v	473	GLN
1	v	589	GLN
1	v	598	GLN
1	v	607	GLN
1	v	656	ASN
1	w	253	ASN
1	w	382	ASN
1	w	440	GLN
1	w	461	GLN
1	w	473	GLN
1	w	589	GLN

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Mol	Chain	Res	Type
1	w	598	GLN
1	w	607	GLN
1	w	656	ASN
1	w	690	ASN
1	x	253	ASN
1	x	382	ASN
1	x	440	GLN
1	x	461	GLN
1	x	473	GLN
1	x	589	GLN
1	x	607	GLN
1	x	656	ASN
1	y	253	ASN
1	y	382	ASN
1	y	440	GLN
1	y	461	GLN
1	y	473	GLN
1	y	589	GLN
1	y	598	GLN
1	y	607	GLN
1	y	656	ASN
1	z	253	ASN
1	z	382	ASN
1	z	440	GLN
1	z	461	GLN
1	z	473	GLN
1	z	589	GLN
1	z	598	GLN
1	z	607	GLN
1	z	656	ASN
1	z	690	ASN
1	1	253	ASN
1	1	382	ASN
1	1	440	GLN
1	1	461	GLN
1	1	473	GLN
1	1	589	GLN
1	1	598	GLN
1	1	607	GLN
1	1	656	ASN
1	2	253	ASN
1	2	382	ASN

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Mol	Chain	Res	Type
1	2	440	GLN
1	2	473	GLN
1	2	589	GLN
1	2	598	GLN
1	2	607	GLN
1	2	656	ASN
1	2	690	ASN
1	3	253	ASN
1	3	382	ASN
1	3	440	GLN
1	3	461	GLN
1	3	473	GLN
1	3	589	GLN
1	3	598	GLN
1	3	607	GLN
1	3	656	ASN
1	4	253	ASN
1	4	382	ASN
1	4	440	GLN
1	4	461	GLN
1	4	473	GLN
1	4	589	GLN
1	4	598	GLN
1	4	607	GLN
1	4	656	ASN
1	5	253	ASN
1	5	382	ASN
1	5	440	GLN
1	5	461	GLN
1	5	473	GLN
1	5	589	GLN
1	5	598	GLN
1	5	607	GLN
1	5	656	ASN
1	5	690	ASN
1	6	253	ASN
1	6	382	ASN
1	6	440	GLN
1	6	461	GLN
1	6	473	GLN
1	6	589	GLN
1	6	598	GLN

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Mol	Chain	Res	Type
1	6	607	GLN
1	6	656	ASN
1	7	253	ASN
1	7	382	ASN
1	7	440	GLN
1	7	461	GLN
1	7	473	GLN
1	7	589	GLN
1	7	598	GLN
1	7	607	GLN
1	7	656	ASN
1	8	253	ASN
1	8	382	ASN
1	8	440	GLN
1	8	461	GLN
1	8	473	GLN
1	8	589	GLN
1	8	607	GLN
1	8	656	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

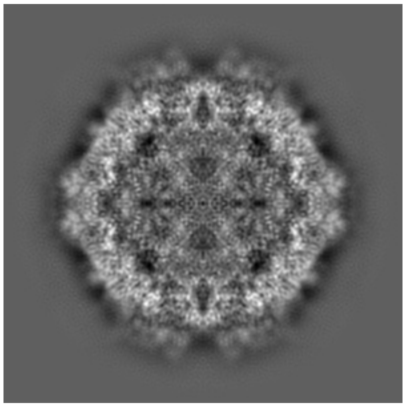
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8100. These allow visual inspection of the internal detail of the map and identification of artifacts.

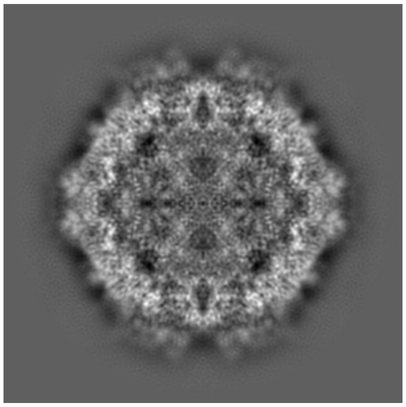
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

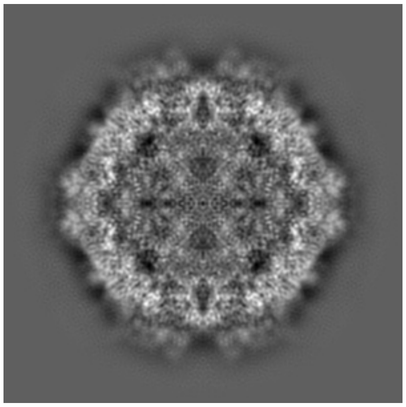
6.1.1 Primary map



X



Y

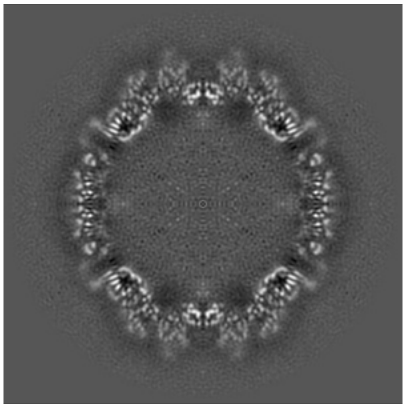


Z

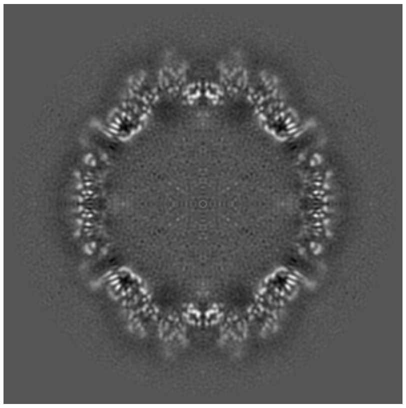
The images above show the map projected in three orthogonal directions.

6.2 Central slices

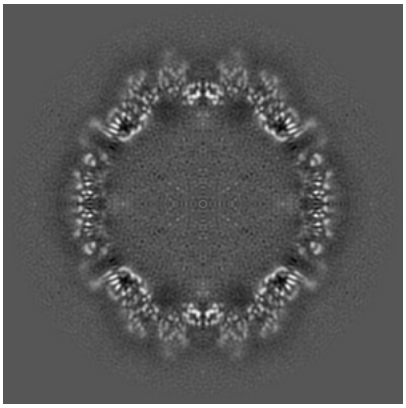
6.2.1 Primary map



X Index: 164



Y Index: 164

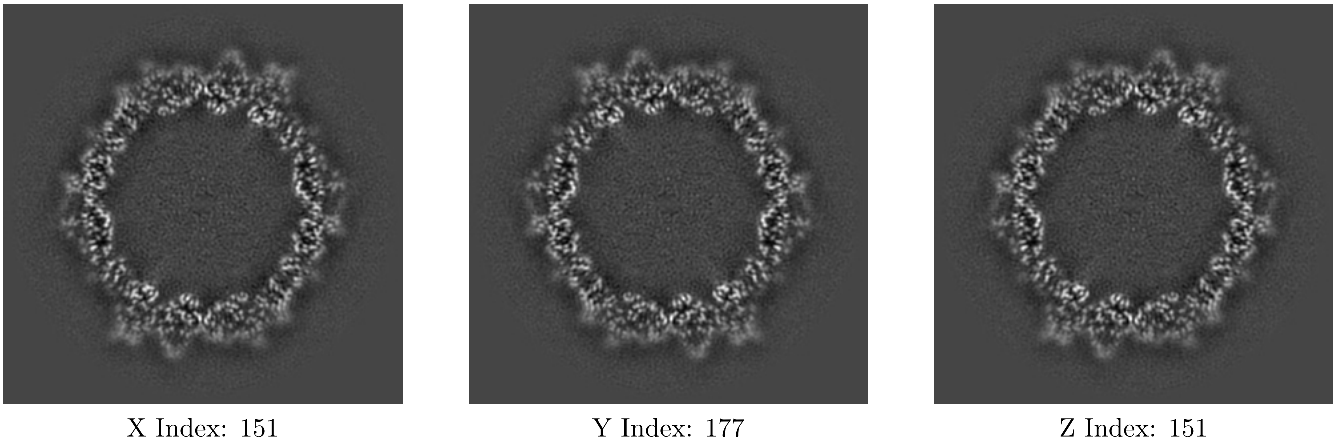


Z Index: 164

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

6.3 Largest variance slices ⓘ

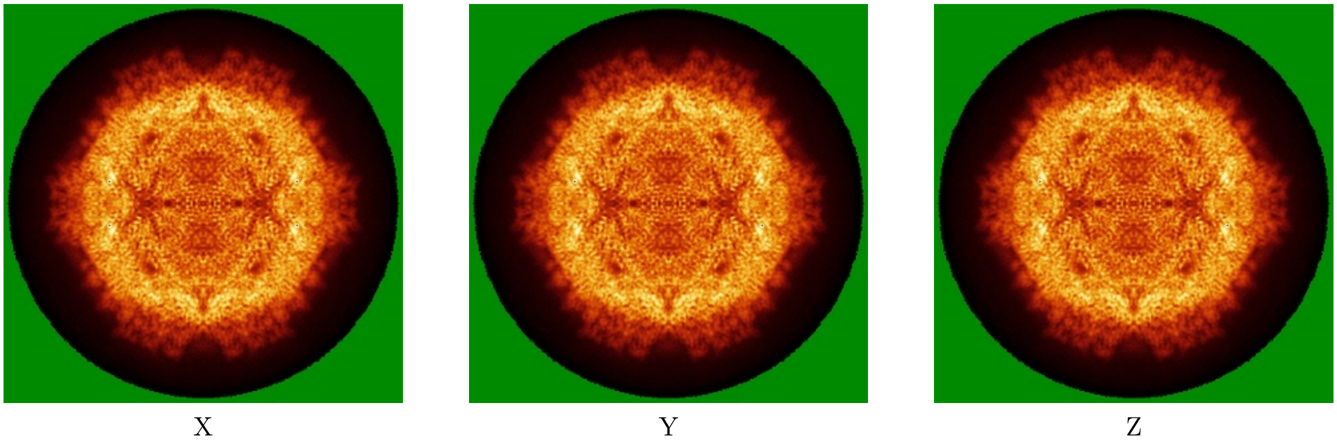
6.3.1 Primary map



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

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

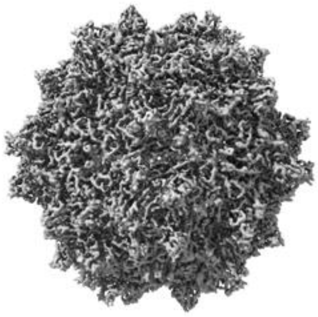
6.4.1 Primary map



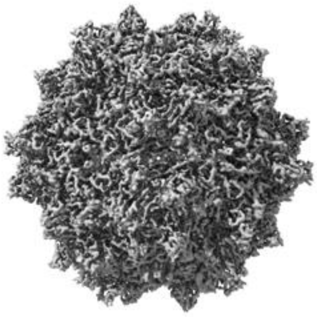
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

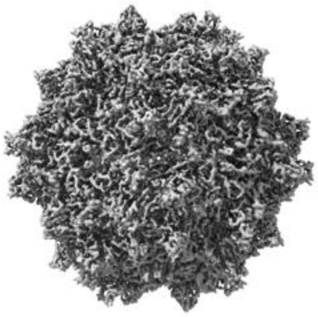
6.5.1 Primary map



X



Y



Z

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.

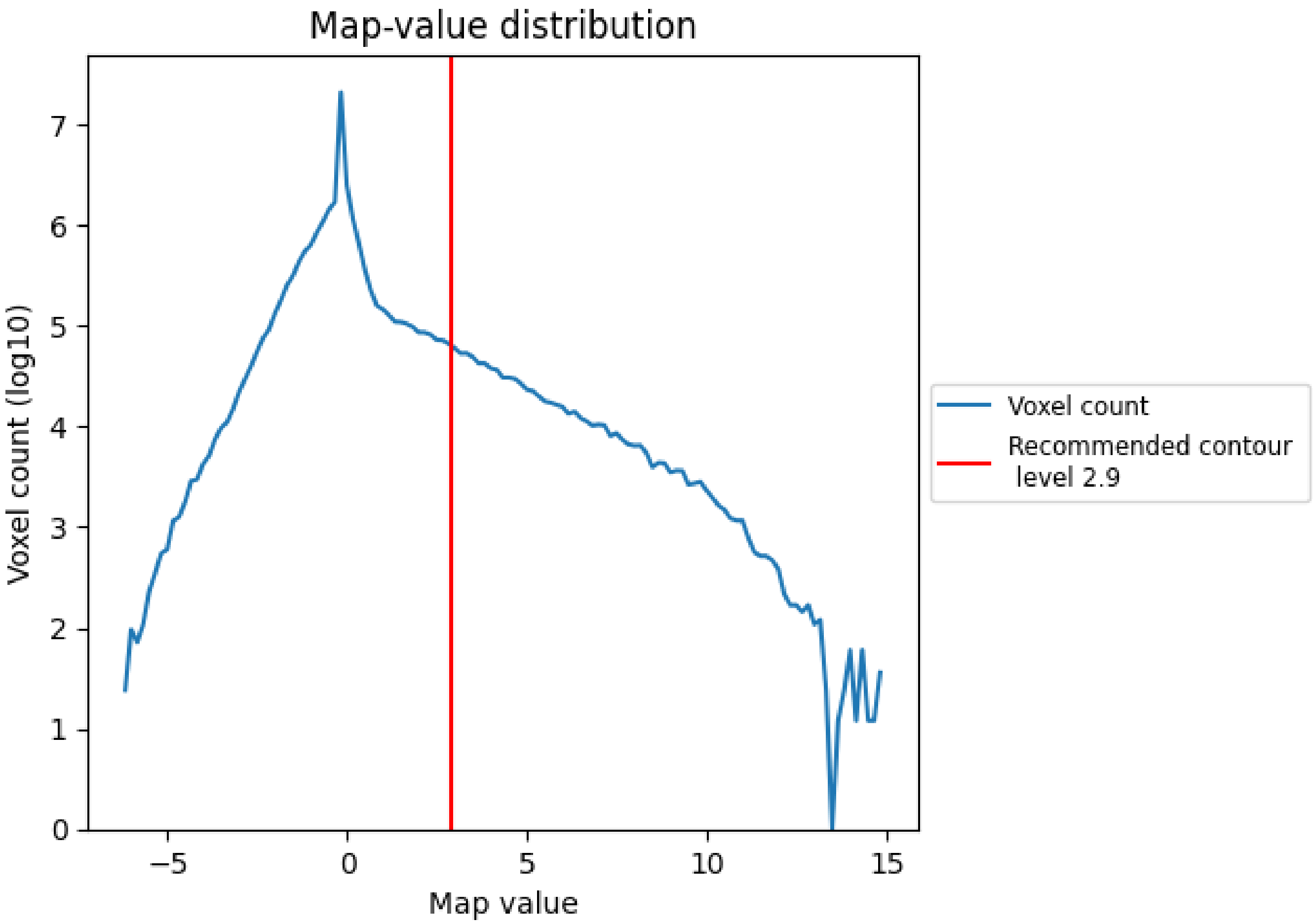
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

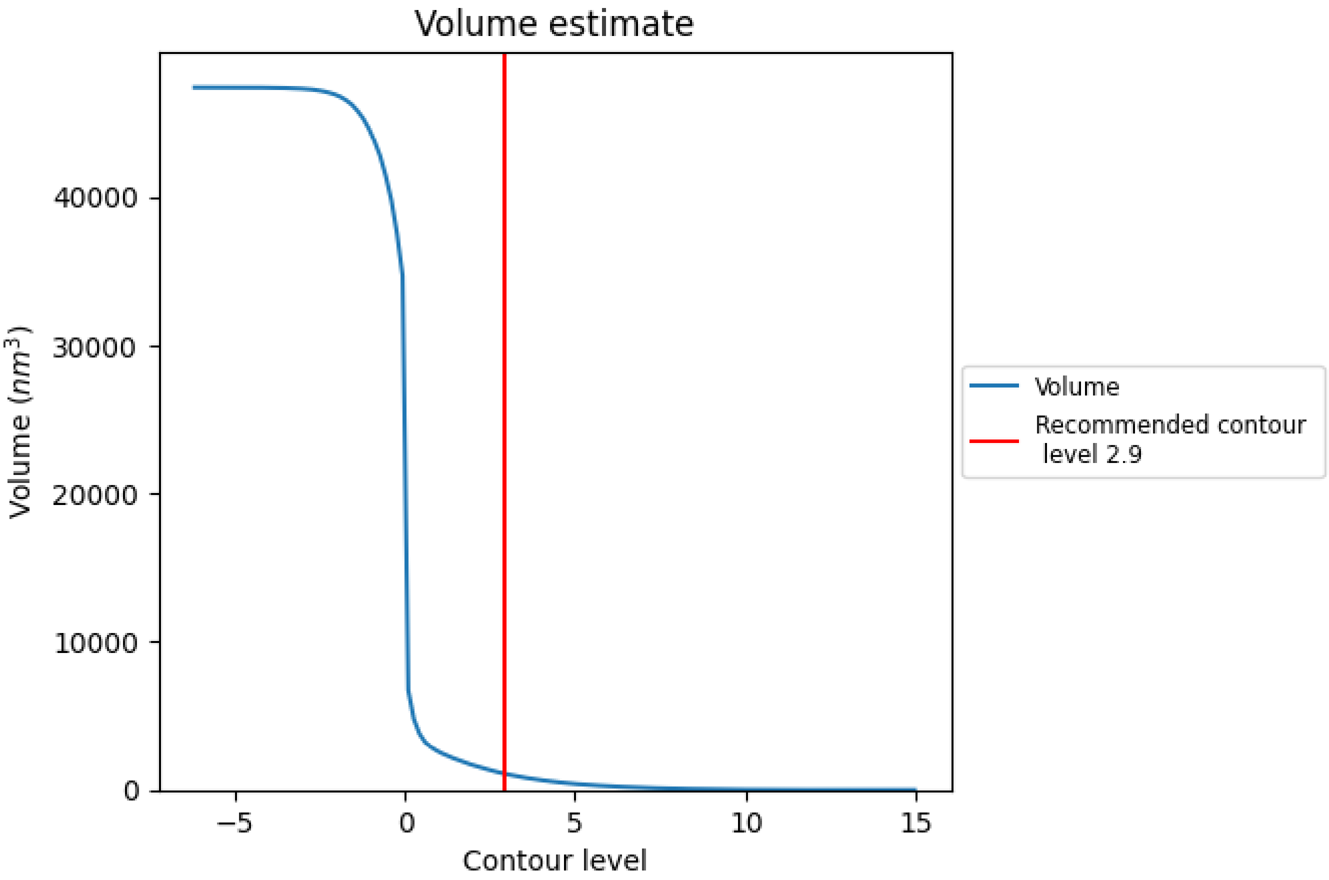
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

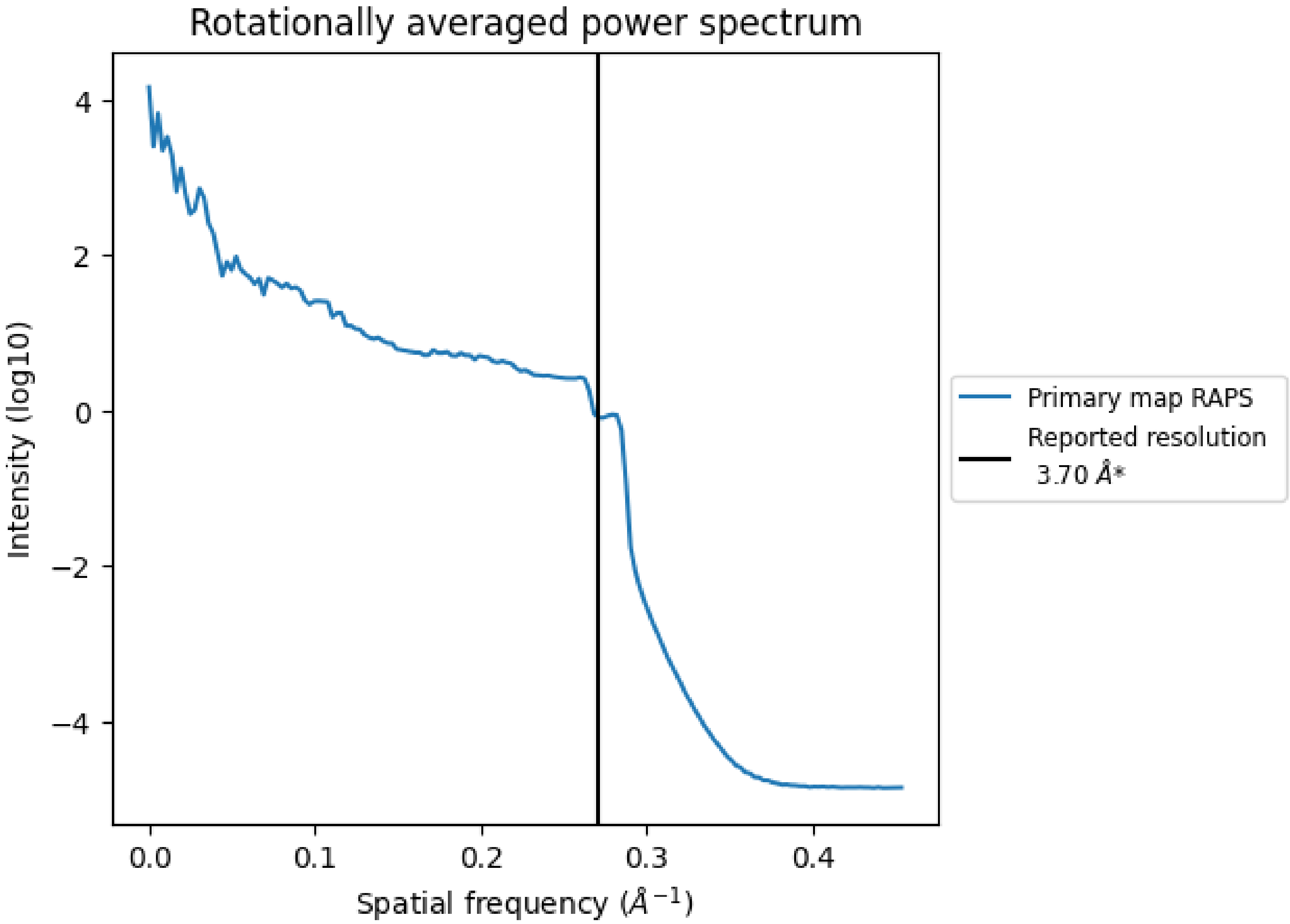
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1108 nm^3; this corresponds to an approximate mass of 1001 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

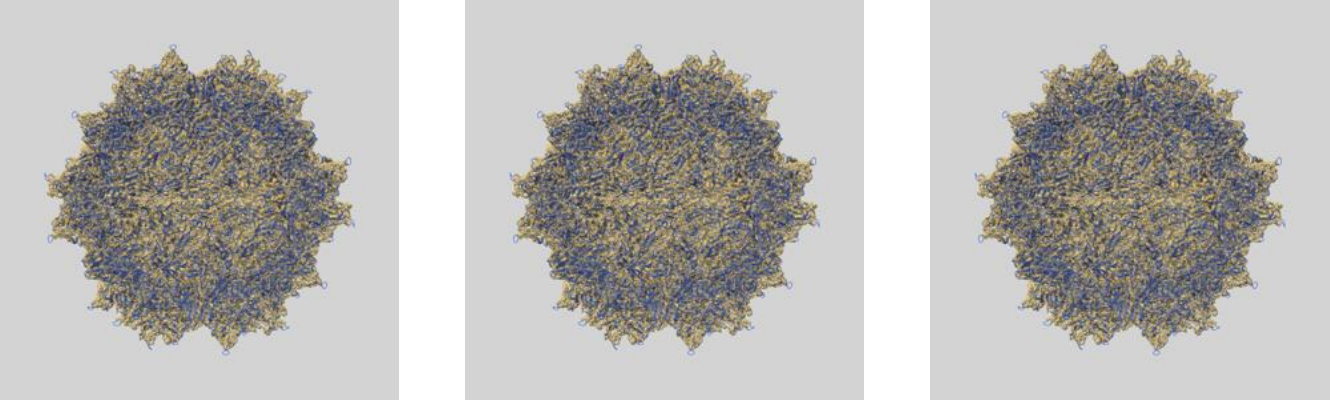
8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-8100 and PDB model 5IPK. Per-residue inclusion information can be found in section 3 on page 11.

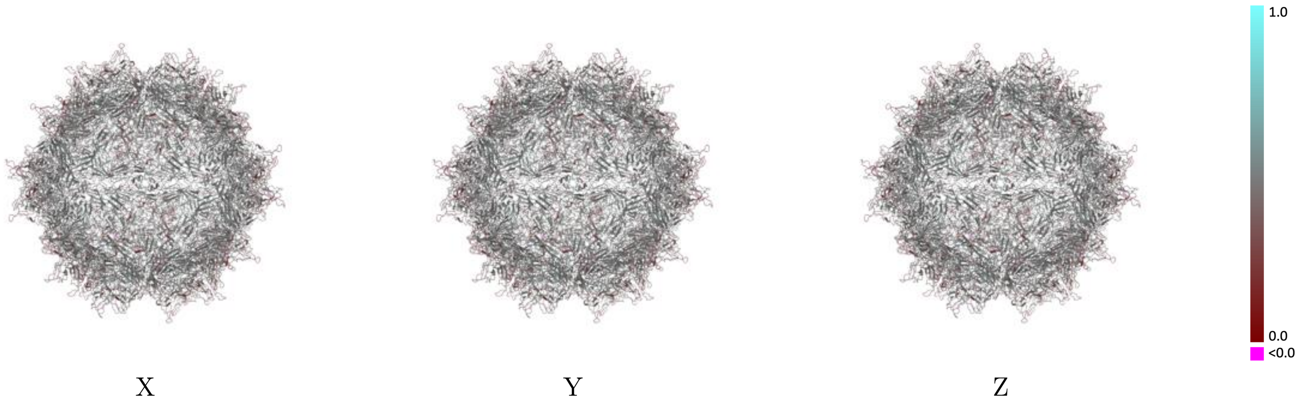
9.1 Map-model overlay ⓘ



X Y Z

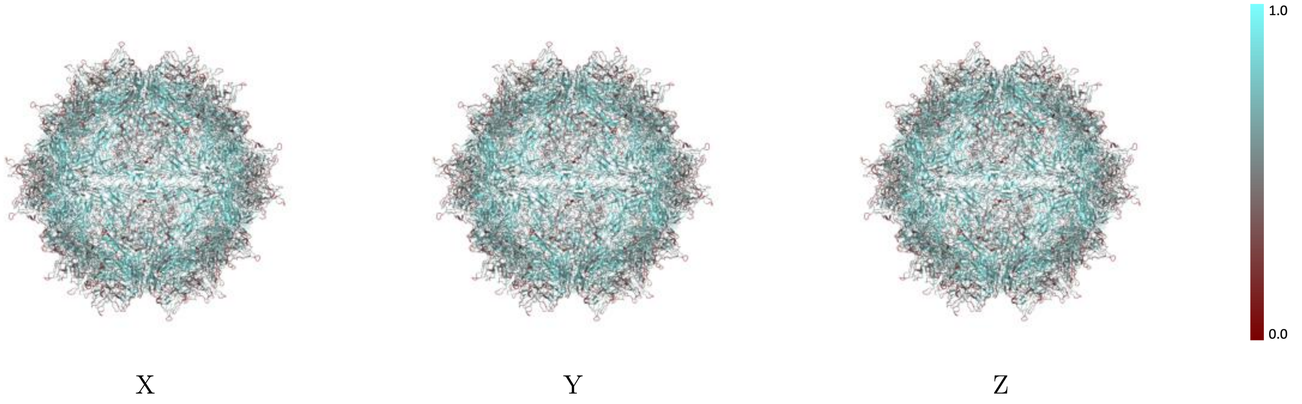
The images above show the 3D surface view of the map at the recommended contour level 2.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



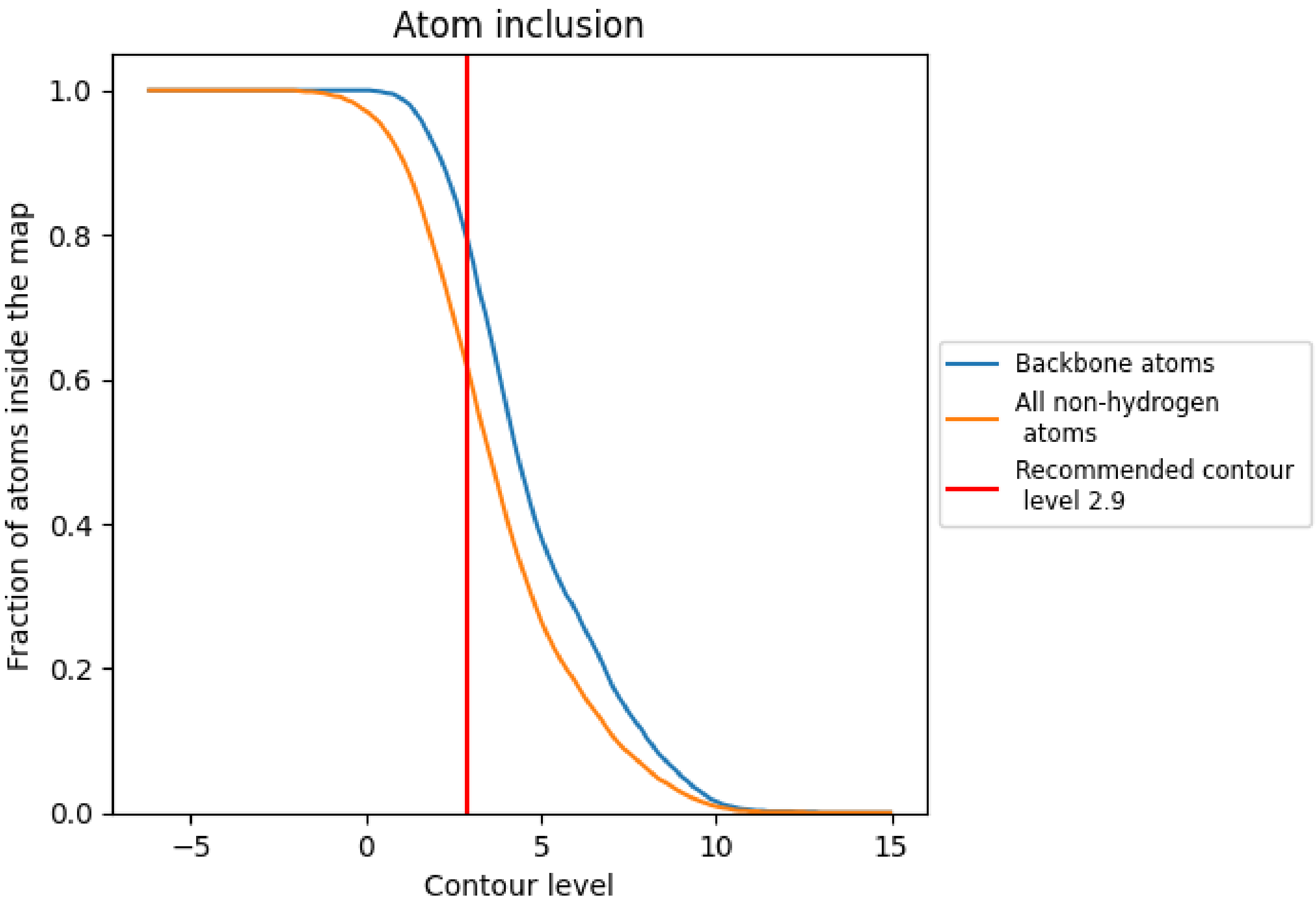
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



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 ⓘ



At the recommended contour level, 79% of all backbone atoms, 62% 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	0.6160	0.4490
1	0.6190	0.4500
2	0.6190	0.4490
3	0.6190	0.4480
4	0.6130	0.4490
5	0.6140	0.4490
6	0.6130	0.4490
7	0.6190	0.4500
8	0.6160	0.4490
A	0.6180	0.4490
B	0.6120	0.4490
C	0.6140	0.4490
D	0.6160	0.4500
E	0.6190	0.4490
F	0.6120	0.4480
G	0.6180	0.4500
H	0.6130	0.4480
I	0.6180	0.4480
J	0.6190	0.4480
K	0.6160	0.4500
L	0.6140	0.4480
M	0.6190	0.4490
N	0.6160	0.4490
O	0.6190	0.4490
P	0.6160	0.4500
Q	0.6140	0.4500
R	0.6140	0.4500
S	0.6130	0.4490
T	0.6200	0.4480
U	0.6190	0.4500
V	0.6170	0.4490
W	0.6190	0.4490
X	0.6160	0.4500
Y	0.6140	0.4490
Z	0.6140	0.4460

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Chain	Atom inclusion	Q-score
a	0.6160	0.4480
b	0.6130	0.4490
c	0.6180	0.4490
d	0.6190	0.4480
e	0.6170	0.4490
f	0.6190	0.4500
g	0.6130	0.4500
h	0.6130	0.4500
i	0.6130	0.4490
j	0.6180	0.4490
k	0.6130	0.4490
l	0.6180	0.4490
m	0.6140	0.4470
n	0.6130	0.4470
o	0.6180	0.4500
p	0.6170	0.4490
q	0.6190	0.4480
r	0.6140	0.4480
s	0.6110	0.4460
t	0.6140	0.4490
u	0.6130	0.4490
v	0.6190	0.4490
w	0.6170	0.4480
x	0.6170	0.4490
y	0.6160	0.4490
z	0.6180	0.4500