



## wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 01:42 AM EDT

PDB ID : 6BX1 / pdb\_00006bx1  
EMDB ID : EMD-7302  
Title : Atomic resolution structure of human bufavirus 3  
Authors : Mietzsch, M.; Agbandje-McKenna, M.  
Deposited on : 2017-12-15  
Resolution : 3.25 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

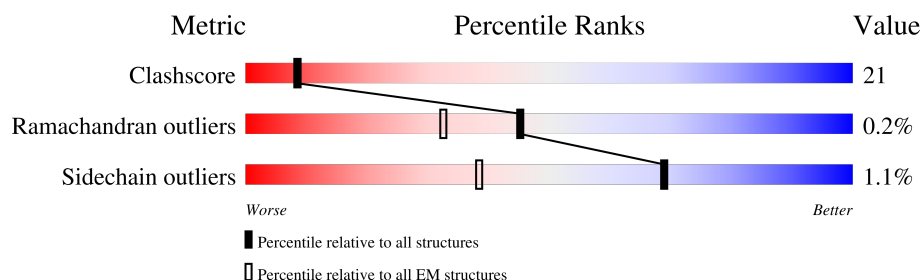
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.25 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	540	59% 39% .
1	1	540	59% 39% .
1	2	540	59% 39% .
1	3	540	59% 39% .
1	4	540	59% 39% .
1	5	540	59% 39% .
1	6	540	59% 38% .
1	7	540	59% 39% .


























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Mol	Chain	Length	Quality of chain
1	A	540	 59% 38% .
1	B	540	 58% 39% .
1	C	540	 59% 38% .
1	D	540	 59% 39% .
1	E	540	 60% 38% .
1	F	540	 59% 39% .
1	G	540	 60% 38% .
1	H	540	 59% 39% .
1	I	540	 59% 39% .
1	J	540	 59% 39% .
1	K	540	 59% 39% .
1	L	540	 59% 39% .
1	M	540	 59% 39% .
1	N	540	 59% 39% .
1	O	540	 59% 39% .
1	P	540	 58% 39% .
1	Q	540	 59% 39% .
1	R	540	 59% 39% .
1	S	540	 59% 39% .
1	T	540	 59% 39% .
1	U	540	 58% 39% .
1	V	540	 59% 38% .
1	W	540	 59% 38% .
1	X	540	 59% 39% .
1	Y	540	 59% 39% .



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Mol	Chain	Length	Quality of chain
1	Z	540	 59% 39% .
1	a	540	 59% 38% .
1	b	540	 59% 39% .
1	c	540	 59% 39% .
1	d	540	 59% 39% .
1	e	540	 59% 39% .
1	f	540	 59% 38% .
1	g	540	 58% 39% .
1	h	540	 59% 39% .
1	i	540	 59% 39% .
1	j	540	 58% 39% .
1	k	540	 59% 39% .
1	l	540	 60% 38% .
1	m	540	 59% 39% .
1	n	540	 59% 39% .
1	o	540	 59% 38% .
1	p	540	 59% 39% .
1	q	540	 59% 39% .
1	r	540	 59% 38% .
1	s	540	 60% 38% .
1	t	540	 59% 39% .
1	u	540	 59% 38% .
1	v	540	 59% 39% .
1	w	540	 59% 39% .
1	x	540	 59% 39% .

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Mol	Chain	Length	Quality of chain
1	y	540	 59%39%•
1	z	540	 59%38%•

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 261180 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	B	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	C	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	D	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	E	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	F	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	G	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	H	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	I	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	J	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	K	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	L	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	M	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	N	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	O	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	P	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		
1	Q	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	S	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	T	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	U	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	V	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	W	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	X	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	Y	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	Z	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	0	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	1	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	2	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	3	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	4	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	5	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	a	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	b	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	c	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	d	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	e	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	f	540	Total 4353	C 2752	N 758	O 828	S 15	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	h	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	i	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	j	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	k	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	l	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	m	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	n	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	o	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	p	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	q	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	r	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	s	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	t	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	u	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	v	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	w	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	x	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	y	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	z	540	Total 4353	C 2752	N 758	O 828	S 15	0	0
1	6	540	Total 4353	C 2752	N 758	O 828	S 15	0	0

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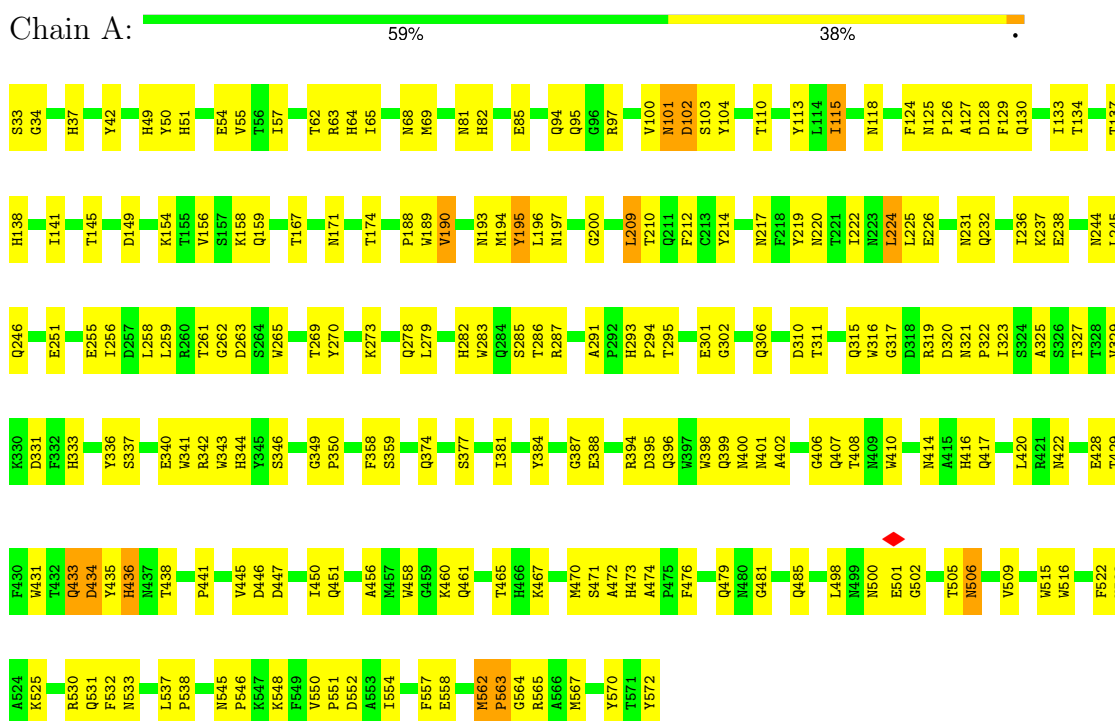
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	540	Total	C	N	O	S	0	0
			4353	2752	758	828	15		

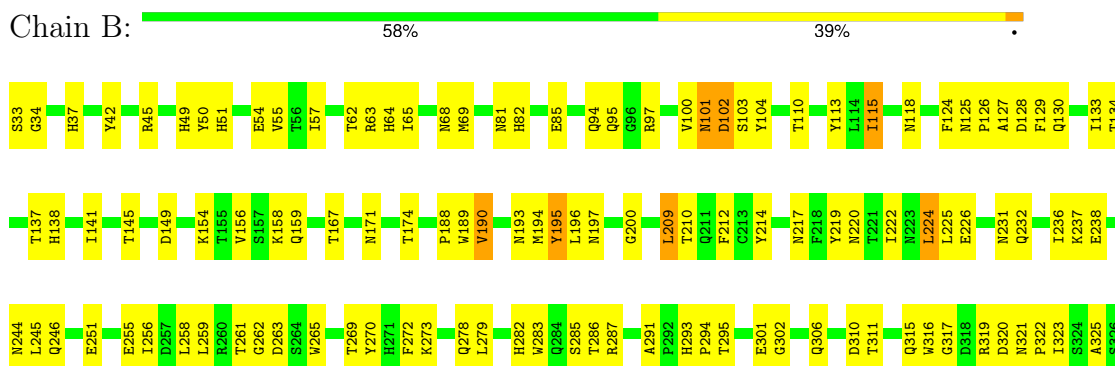
### 3 Residue-property plots

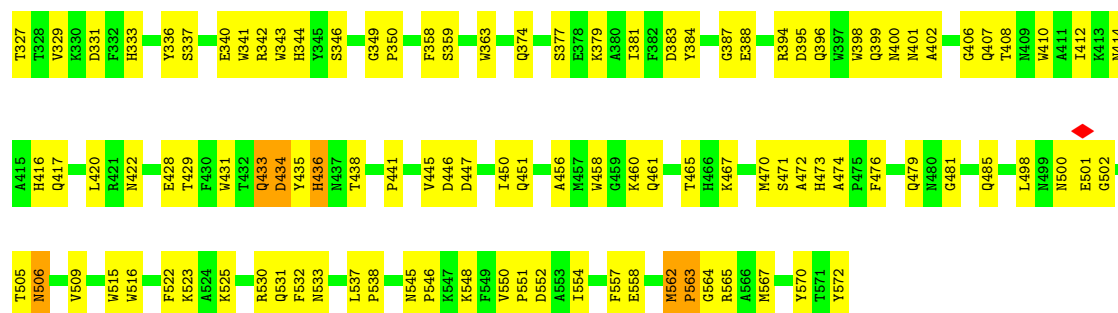
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: VP2



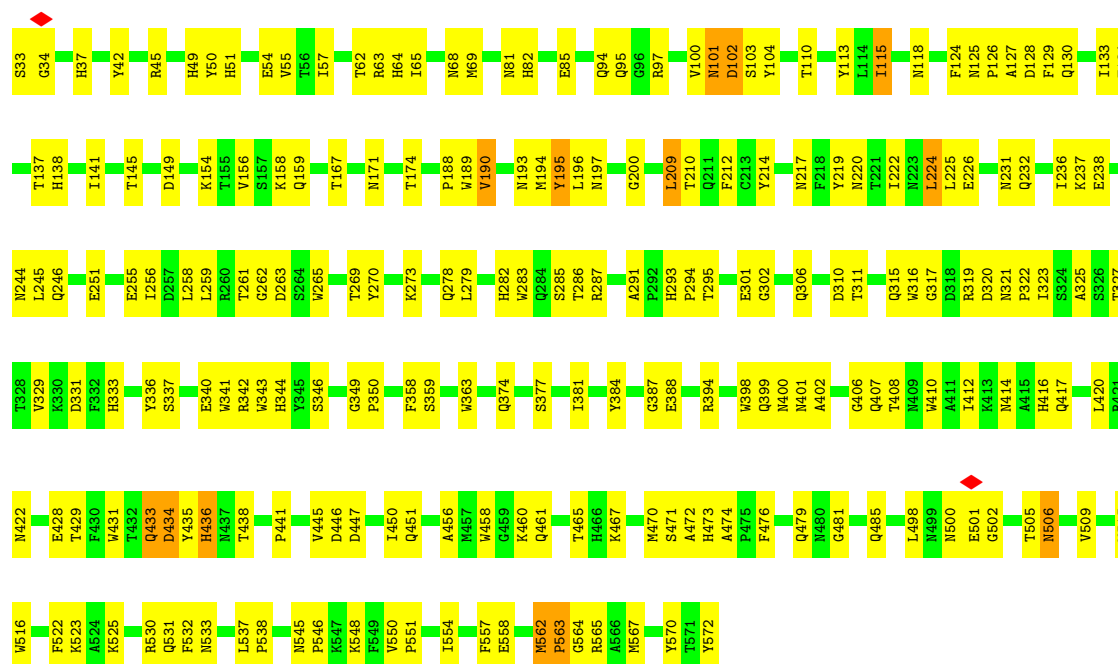
#### • Molecule 1: VP2





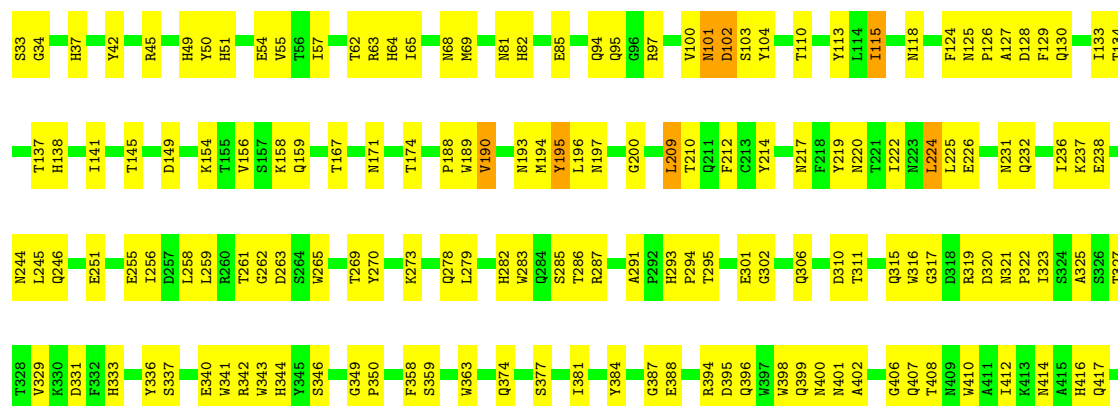
• Molecule 1: VP2

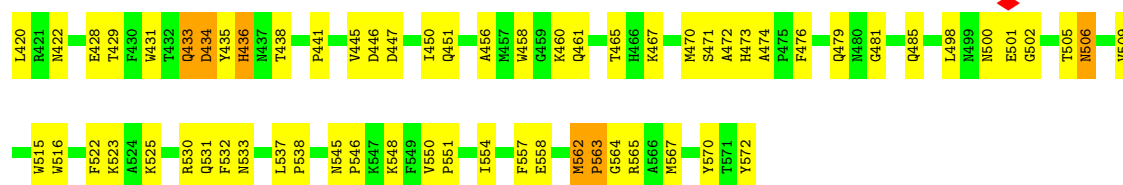
Chain C: 59% 38%



• Molecule 1: VP2

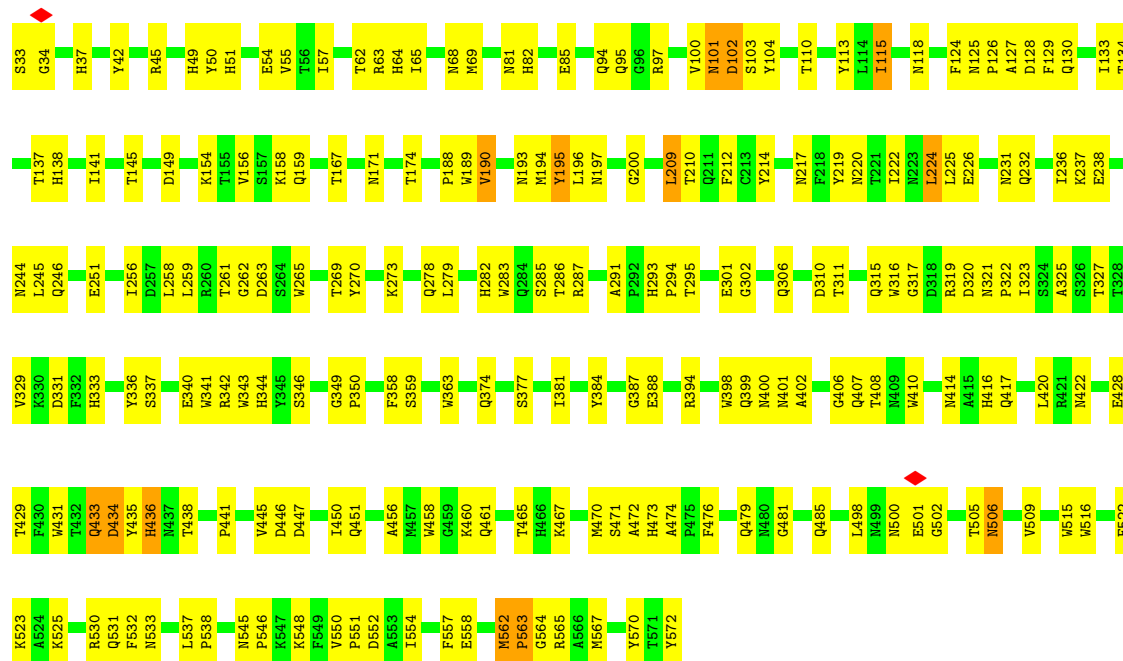
Chain D: 59% 39%





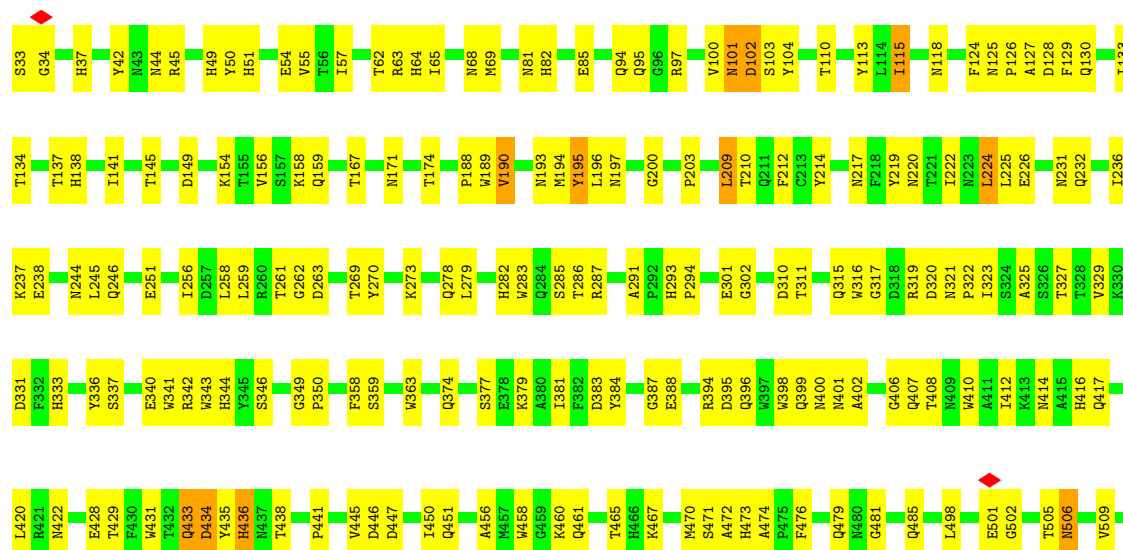
• Molecule 1: VP2

Chain E: 60% 38%



• Molecule 1: VP2

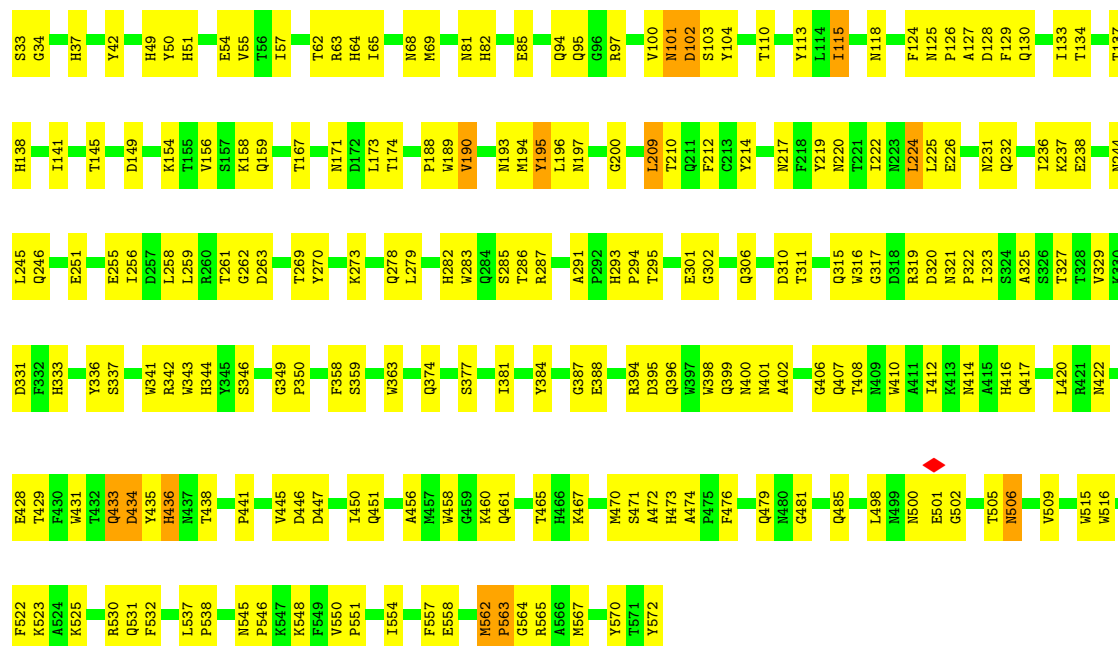
Chain F: 59% 39%





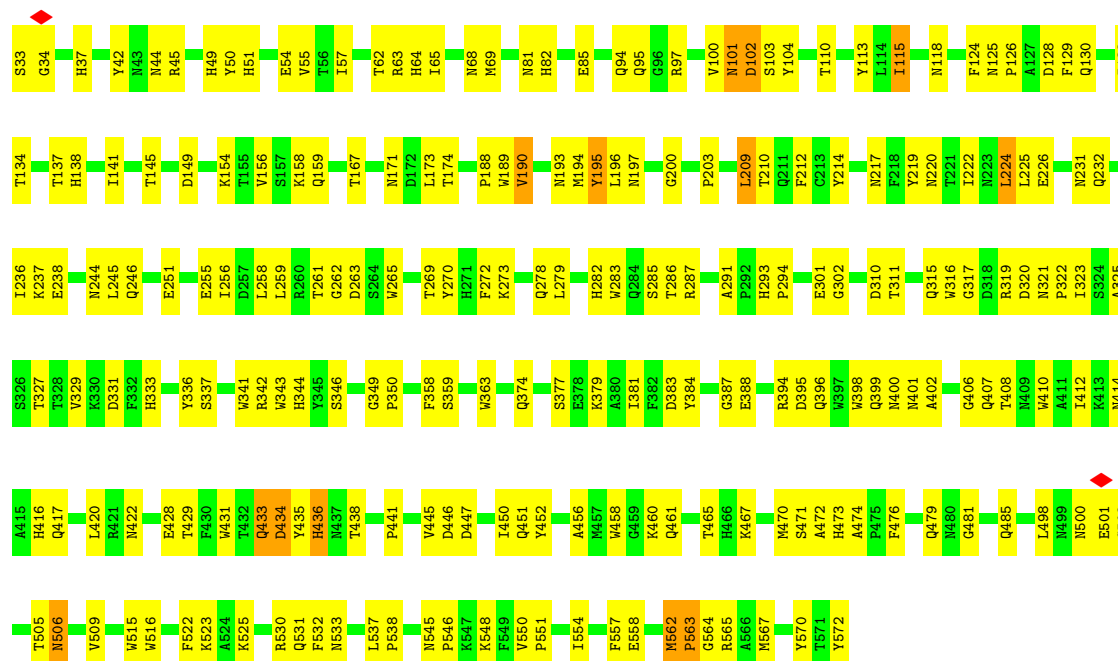
### • Molecule 1: VP2

Chain G: 60% 38%

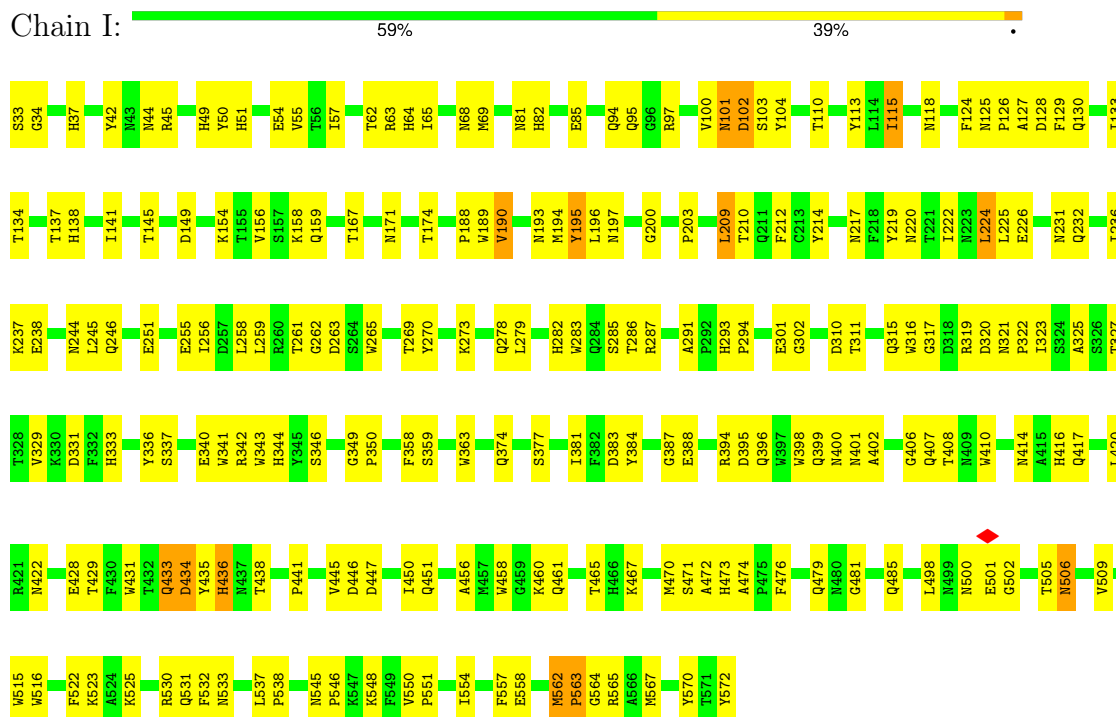


### • Molecule 1: VP2

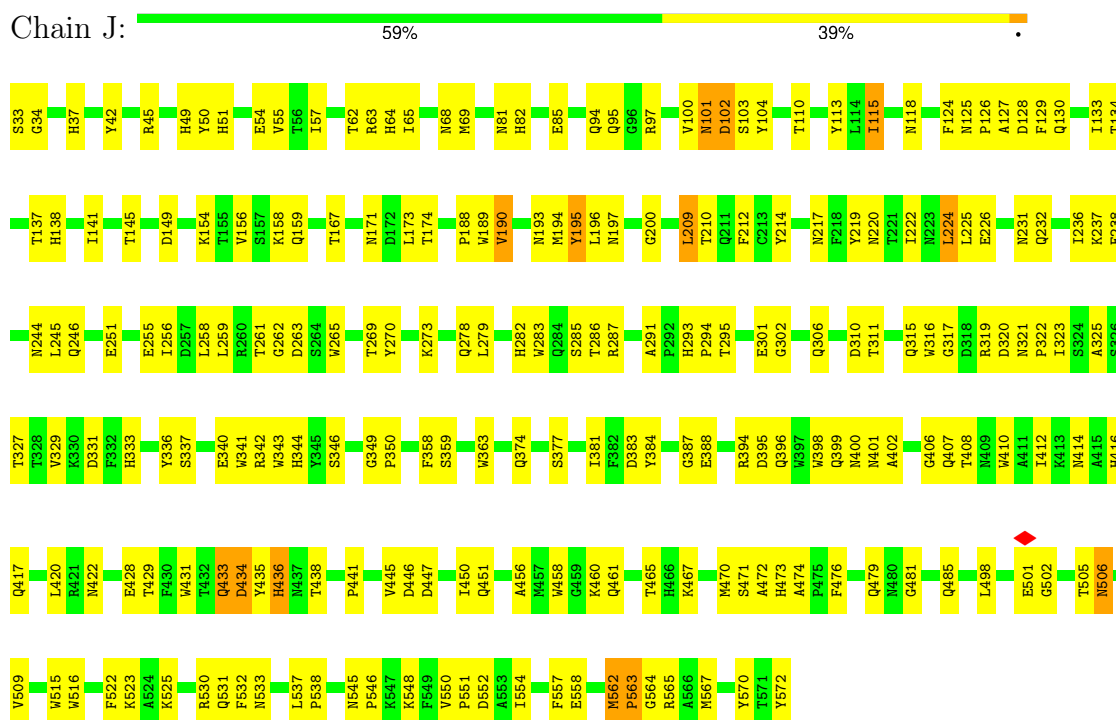
Chain H: 59% 39%



- Molecule 1: VP2

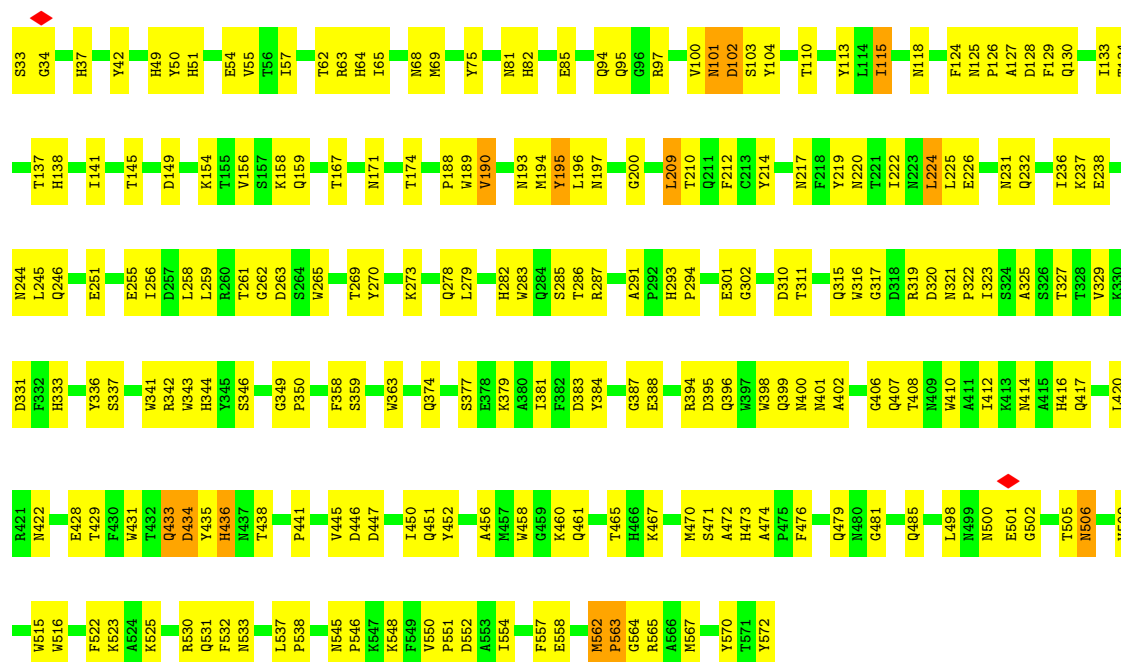


- Molecule 1: VP2



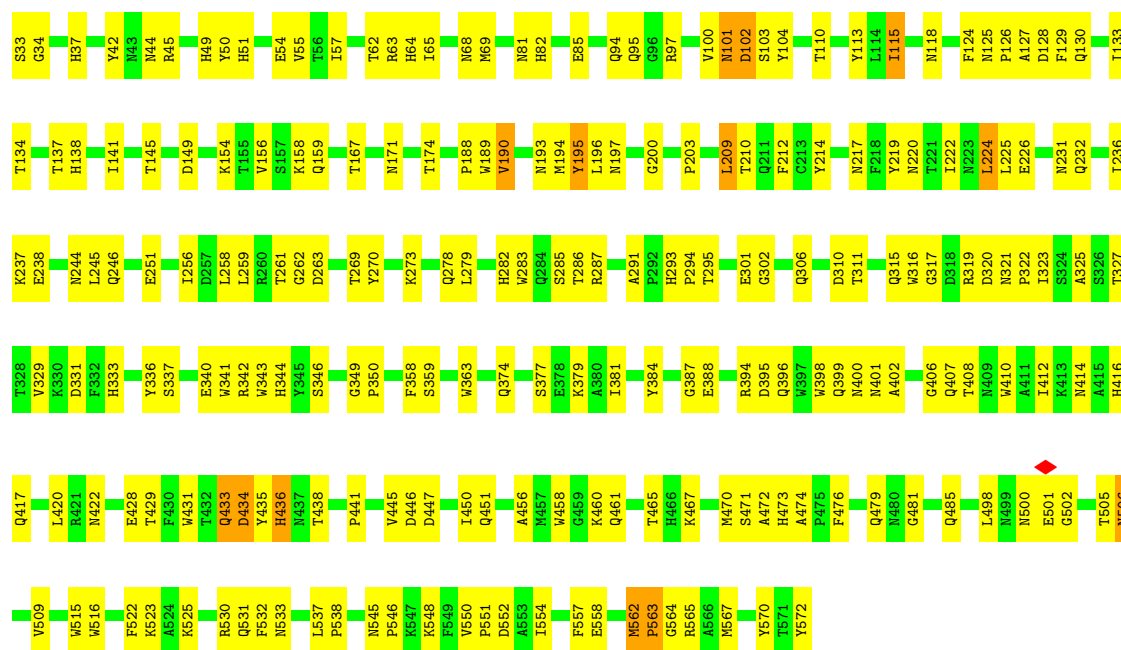
- Molecule 1: VP2





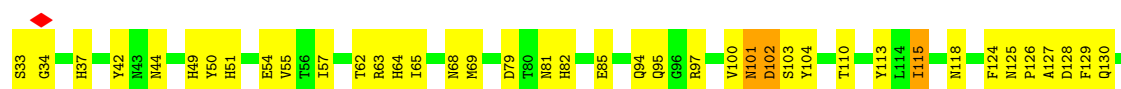
• Molecule 1: VP2

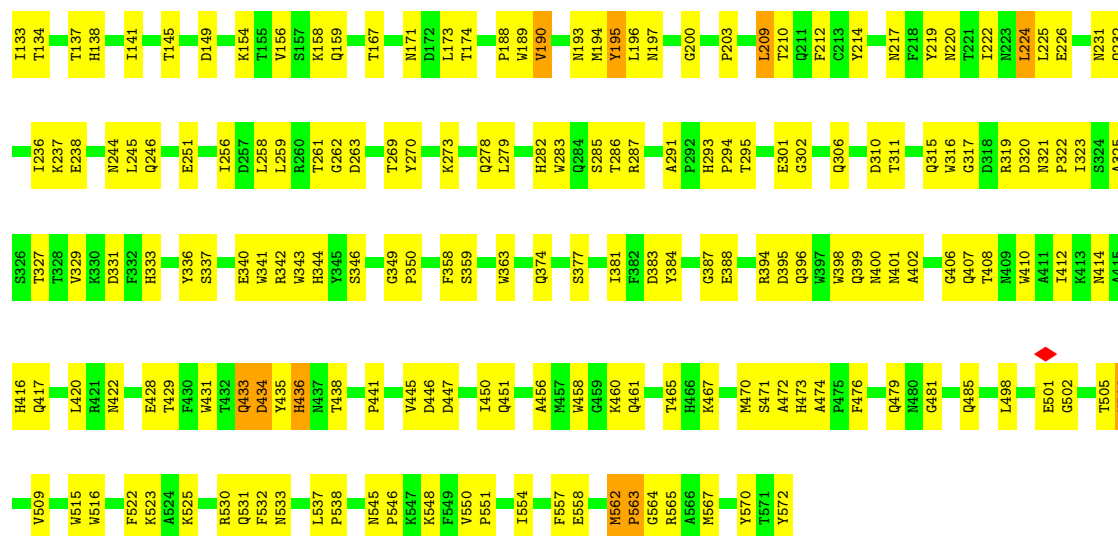
Chain L: 59% 39%



• Molecule 1: VP2

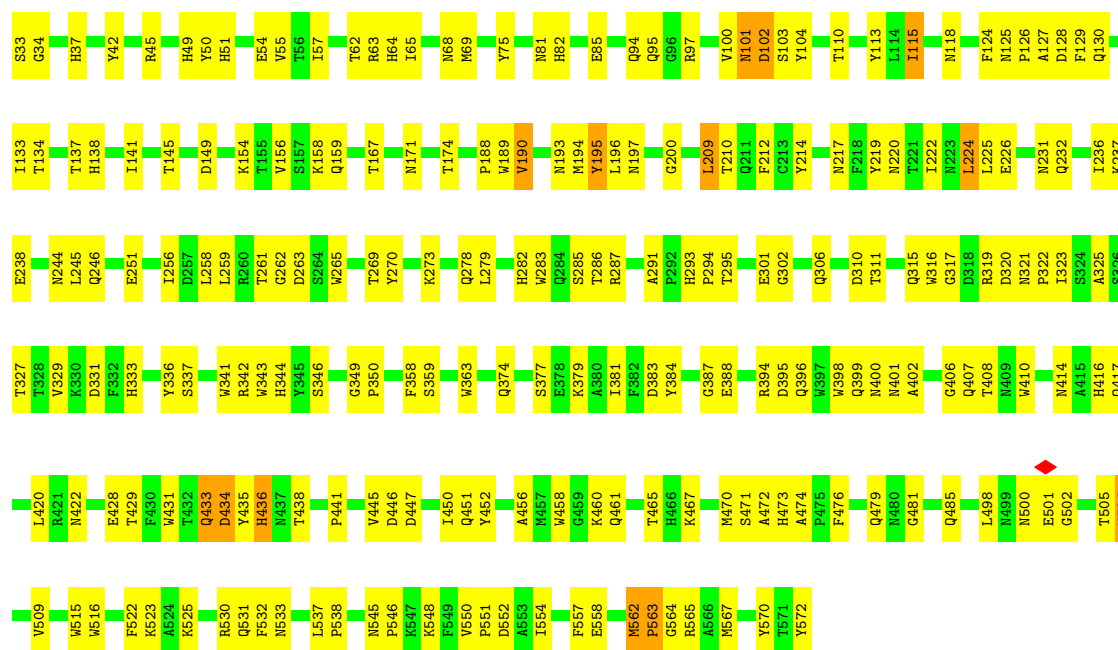
Chain M: 59% 39%





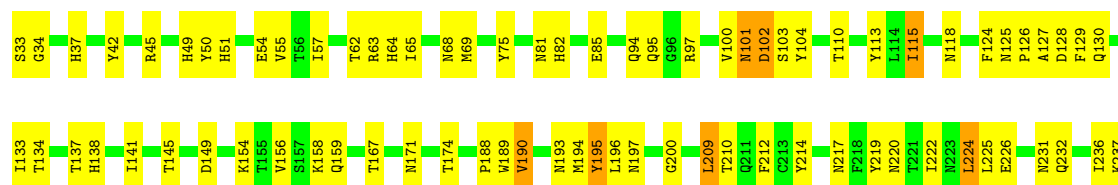
• Molecule 1: VP2

Chain N: 59% 39%



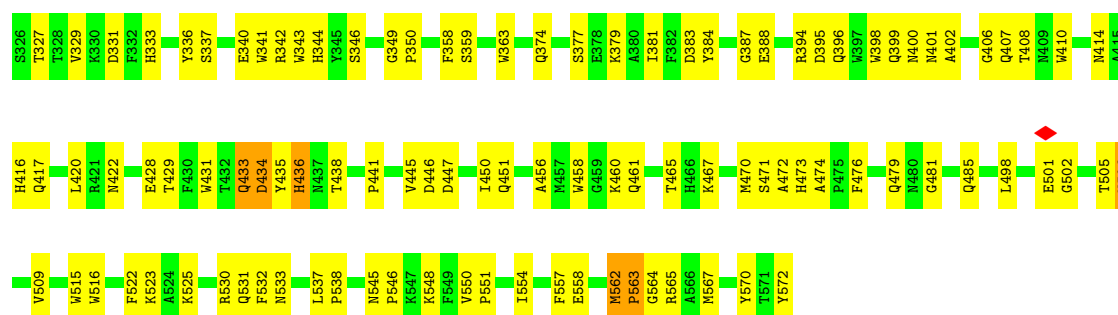
• Molecule 1: VP2

Chain O: 59% 39%

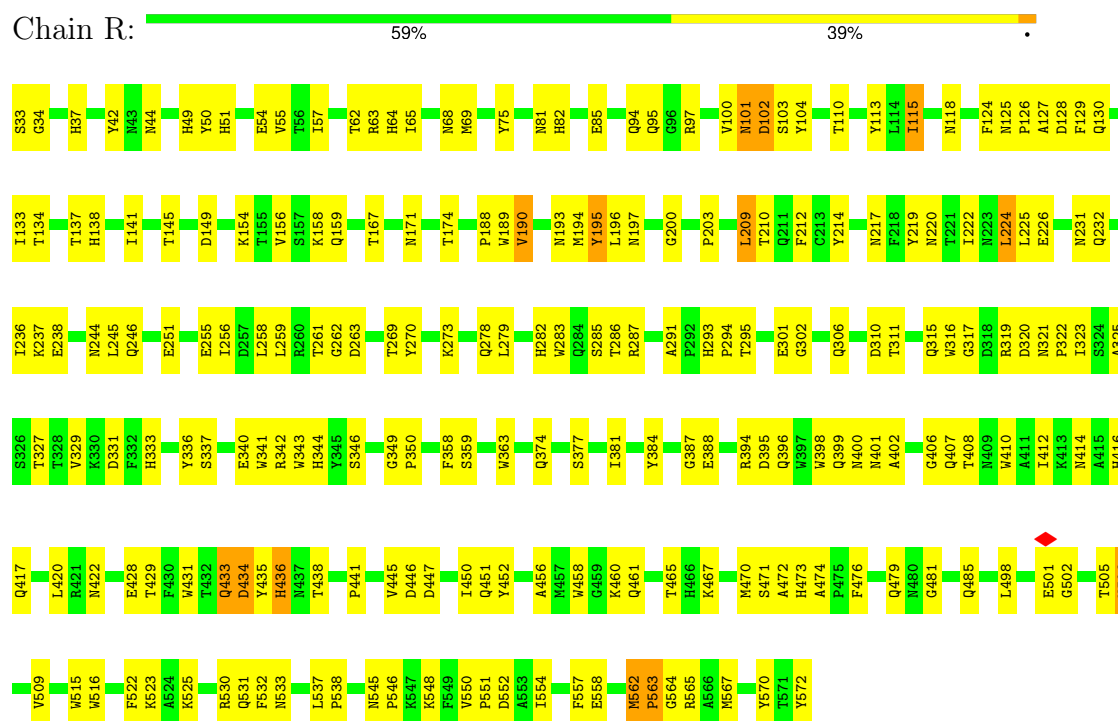




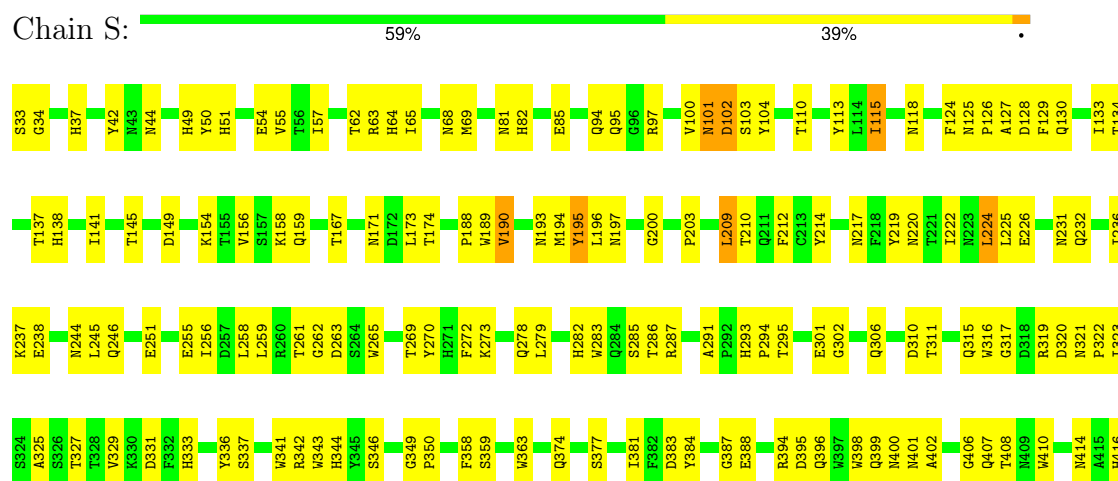


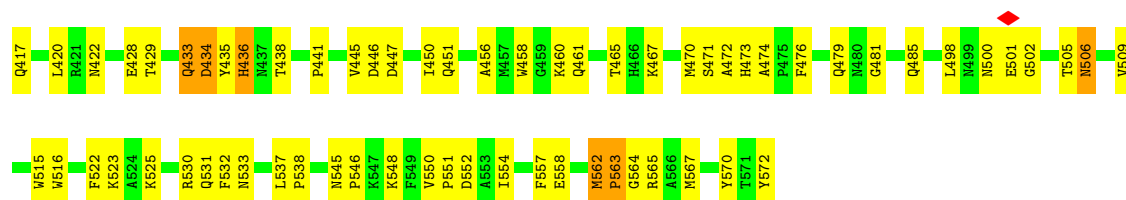


• Molecule 1: VP2



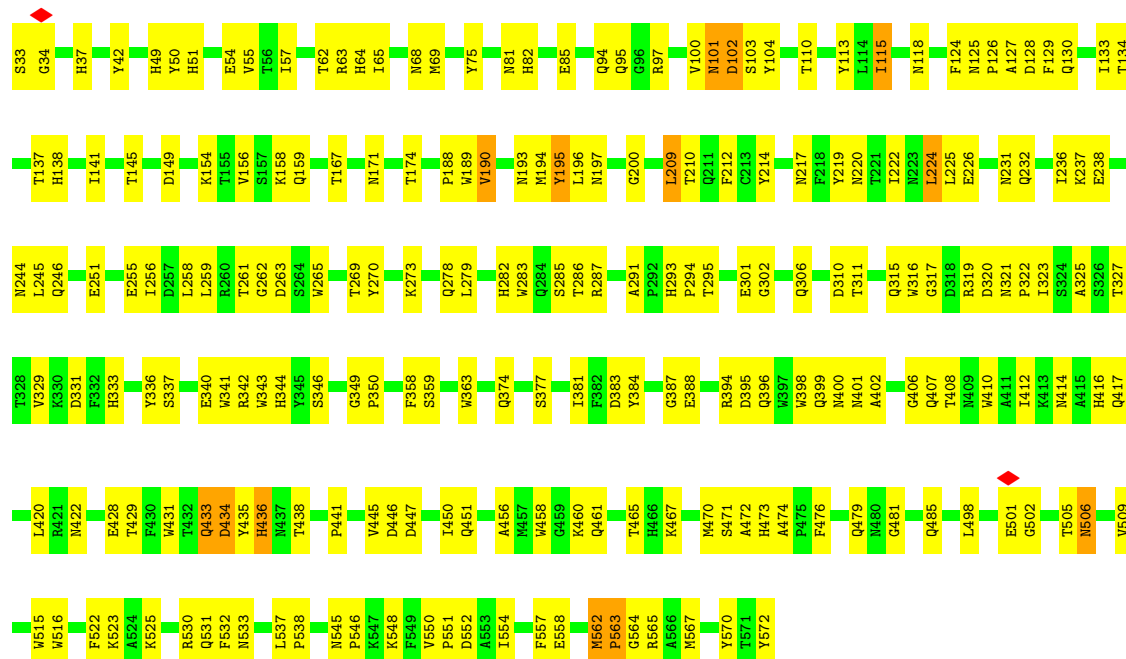
• Molecule 1: VP2





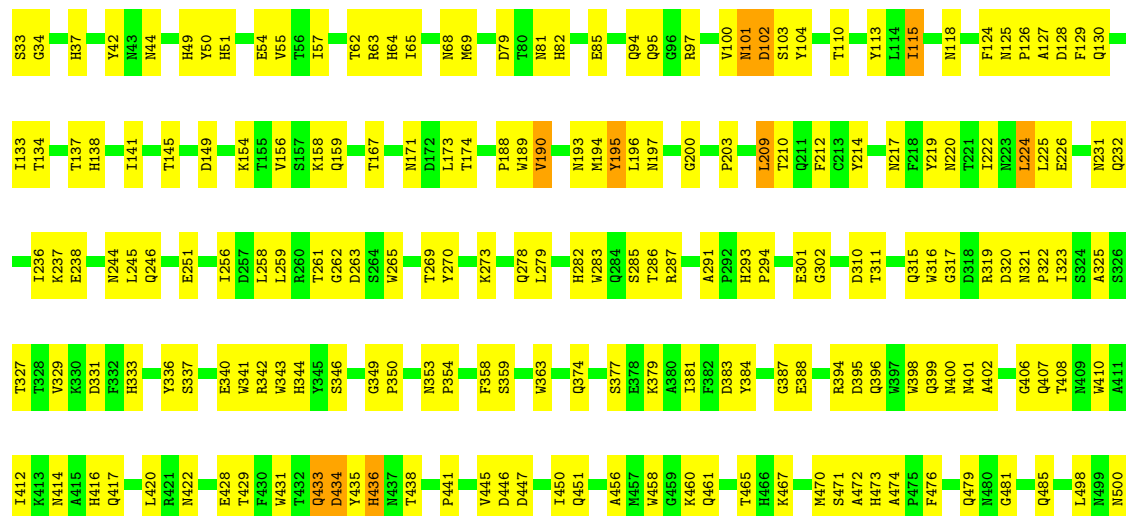
• Molecule 1: VP2

Chain T: 59% 39%



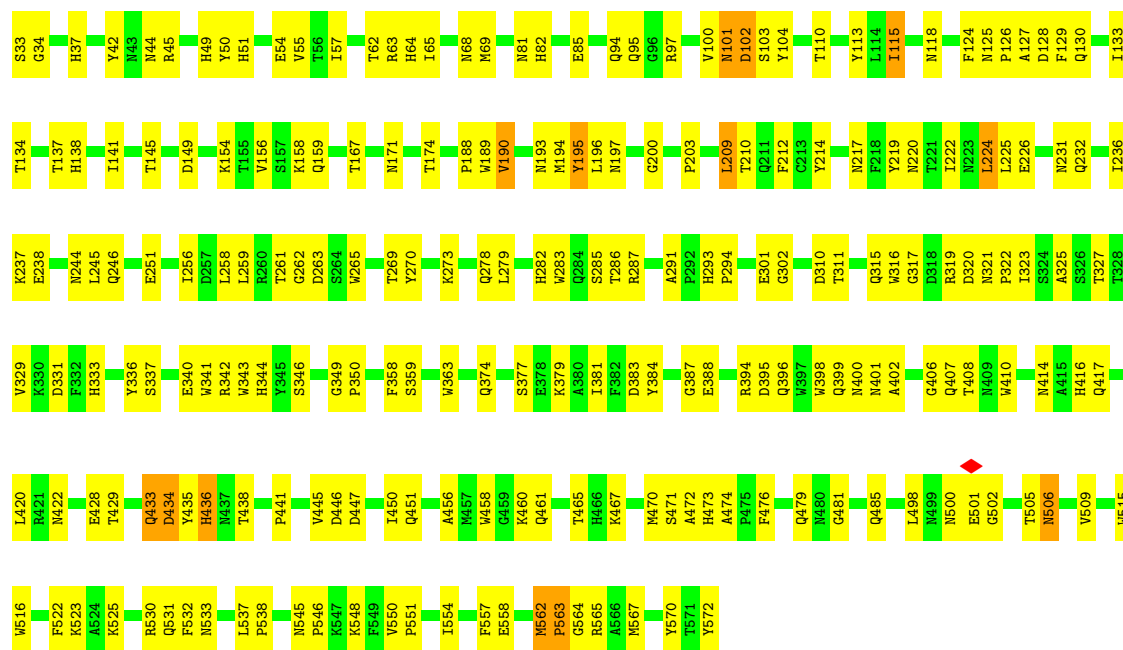
• Molecule 1: VP2

Chain U: 58% 39%

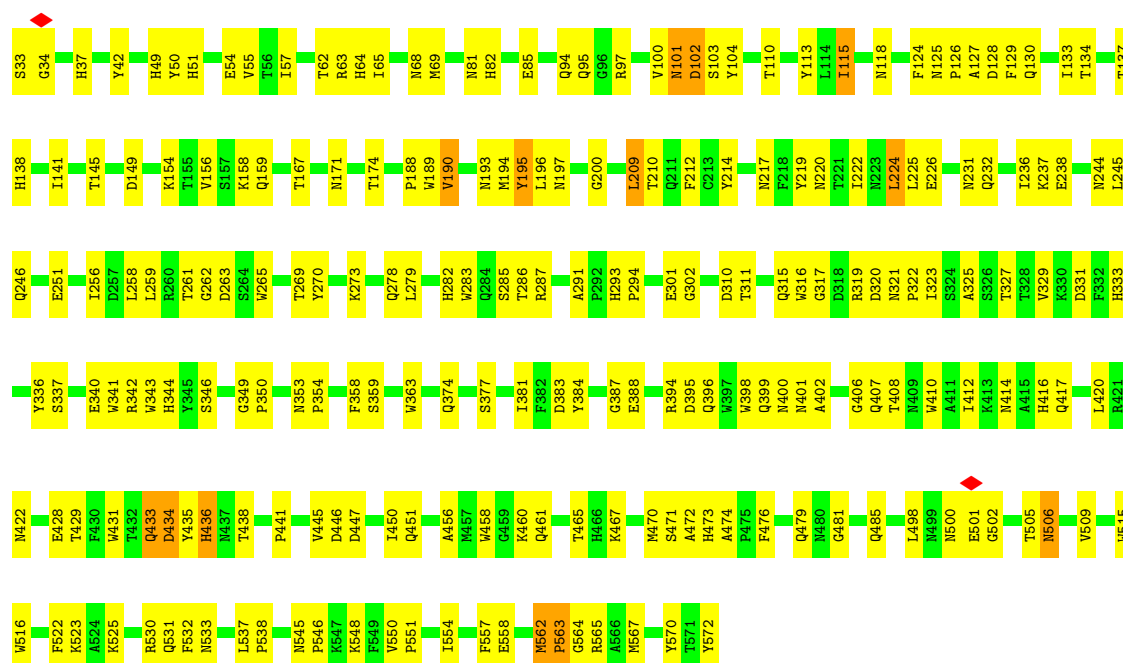




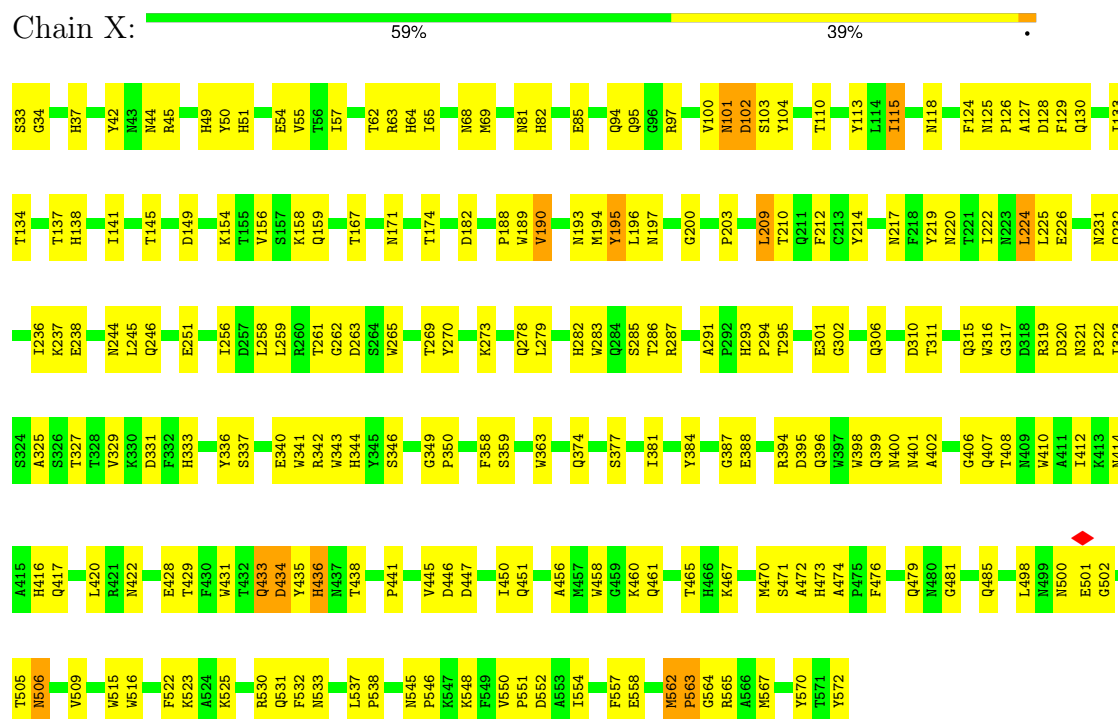
• Molecule 1: VP2



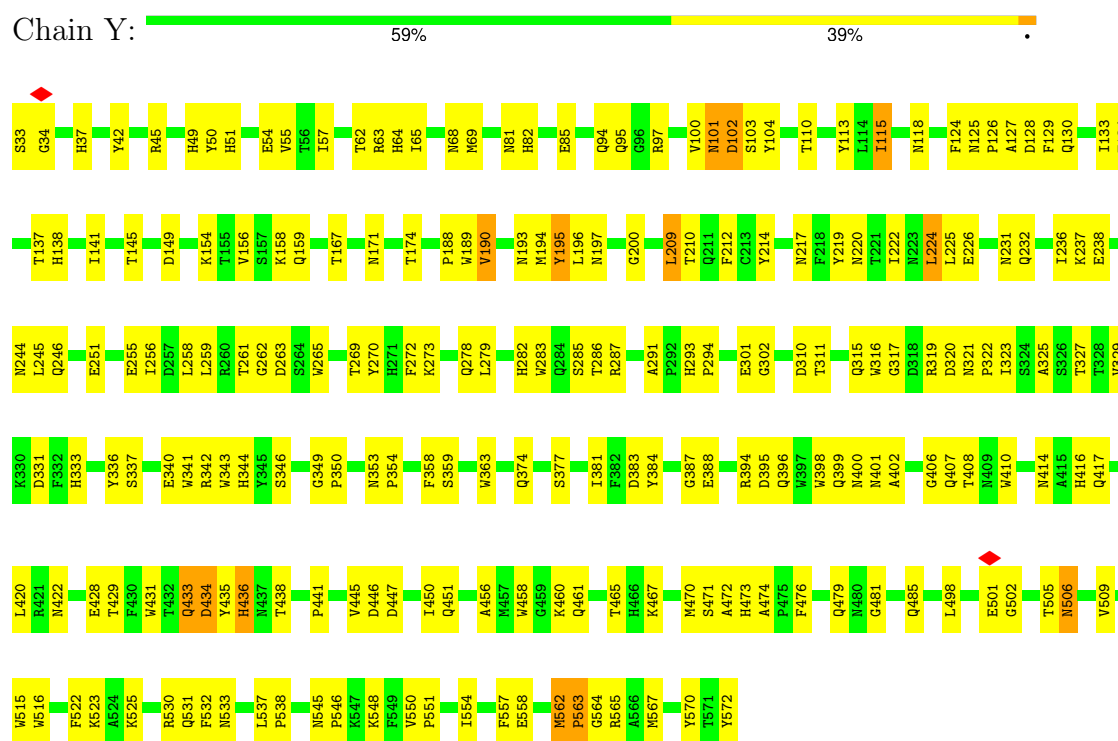
• Molecule 1: VP2



## ● Molecule 1: VP2

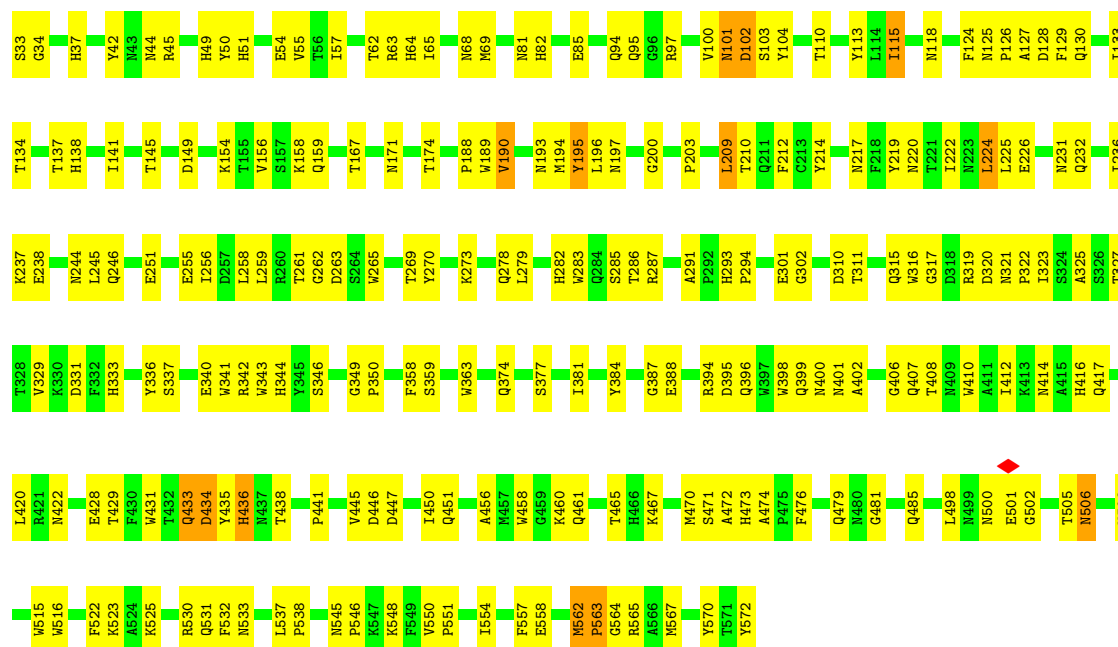


## ● Molecule 1: VP2



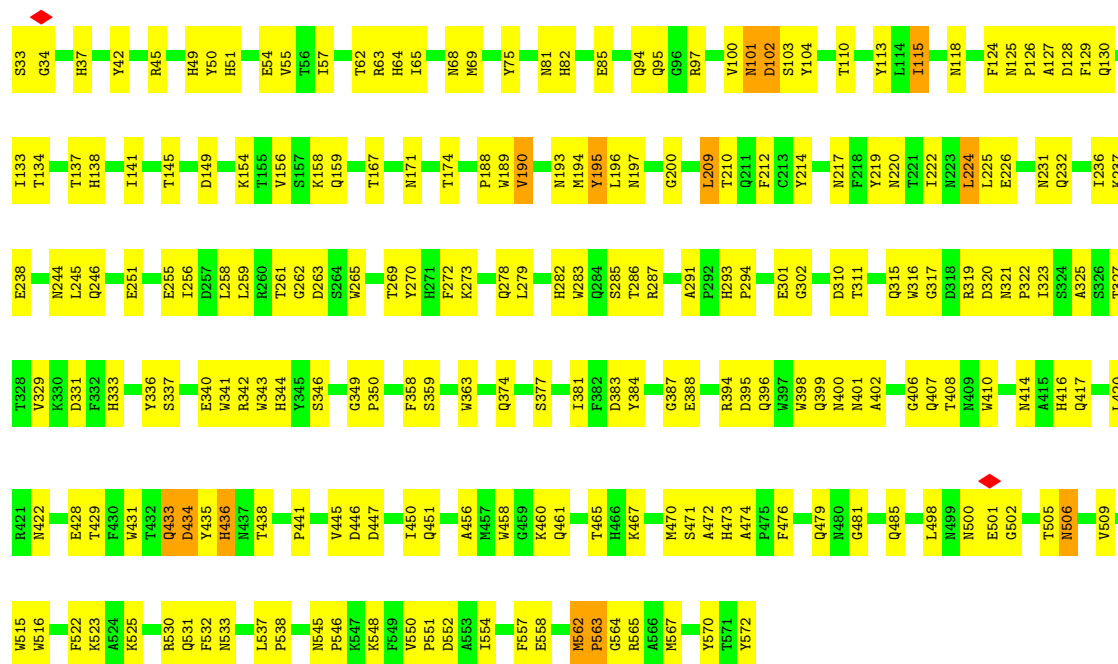
## ● Molecule 1: VP2





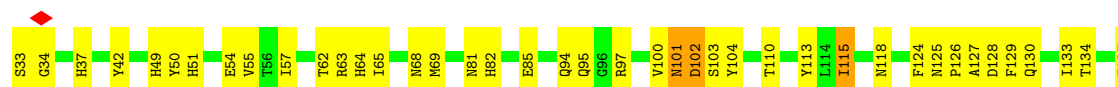
• Molecule 1: VP2

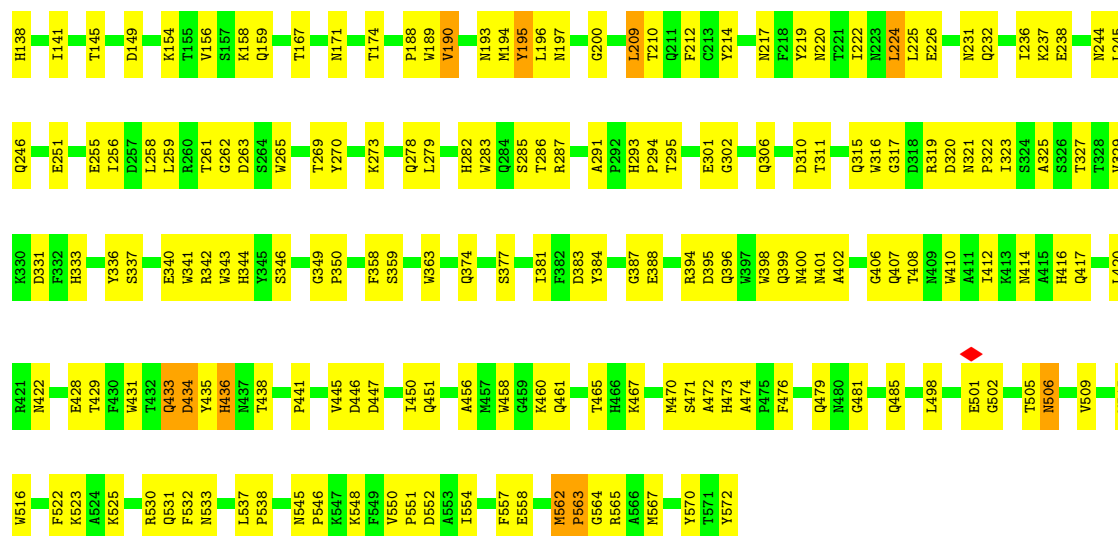
Chain 0: 59% 39%



• Molecule 1: VP2

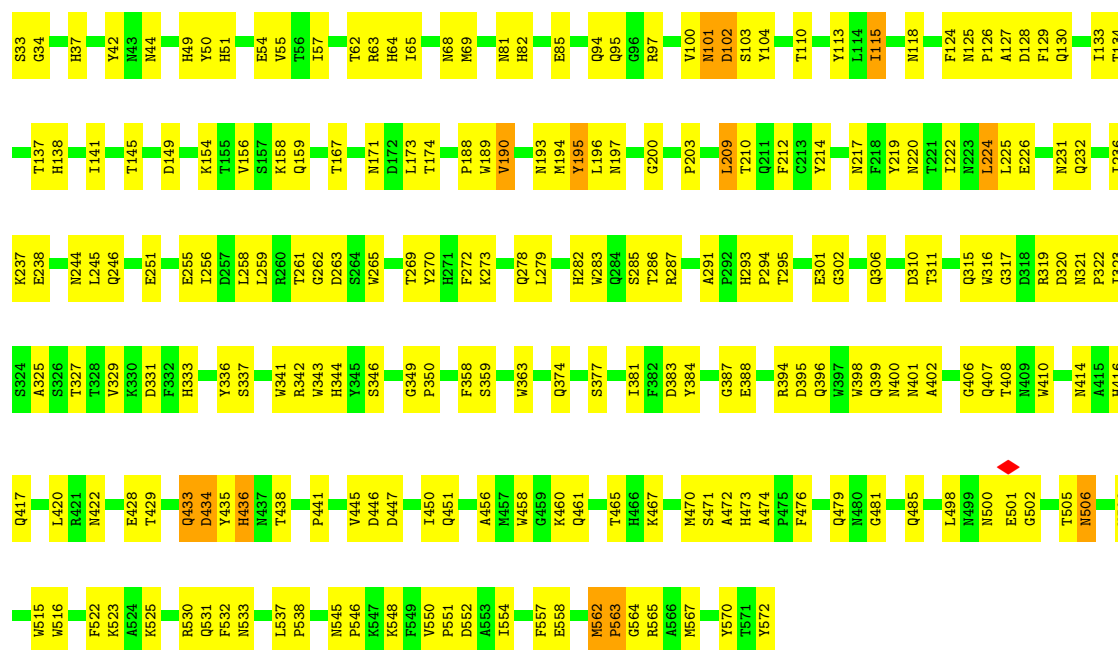
Chain 1: 59% 39%





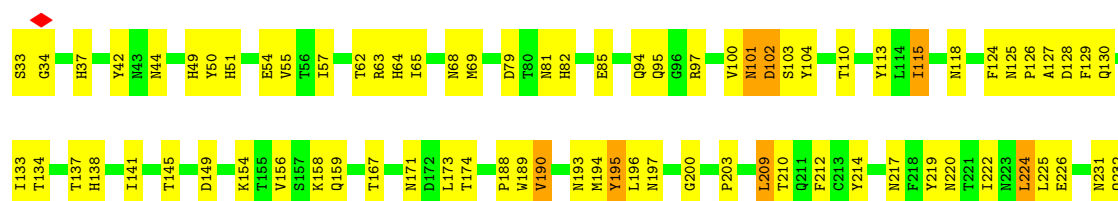
• Molecule 1: VP2

Chain 2: 59% 39% .



• Molecule 1: VP2

Chain 3: 59% 39% .

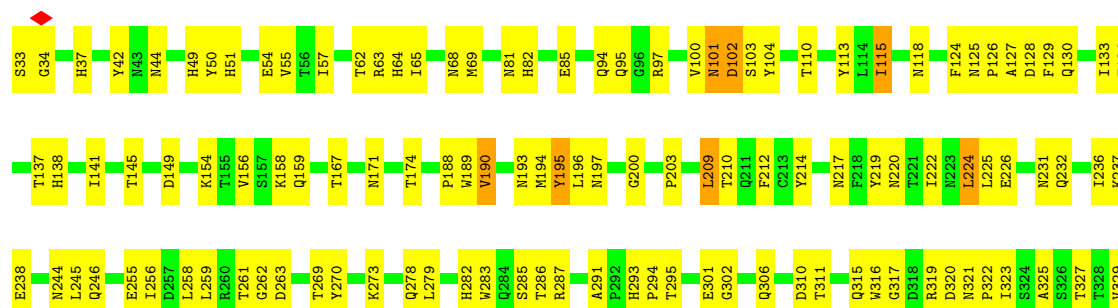


- Molecule 1: VP2

Chain 4:  59% 39%

- Molecule 1: VP2

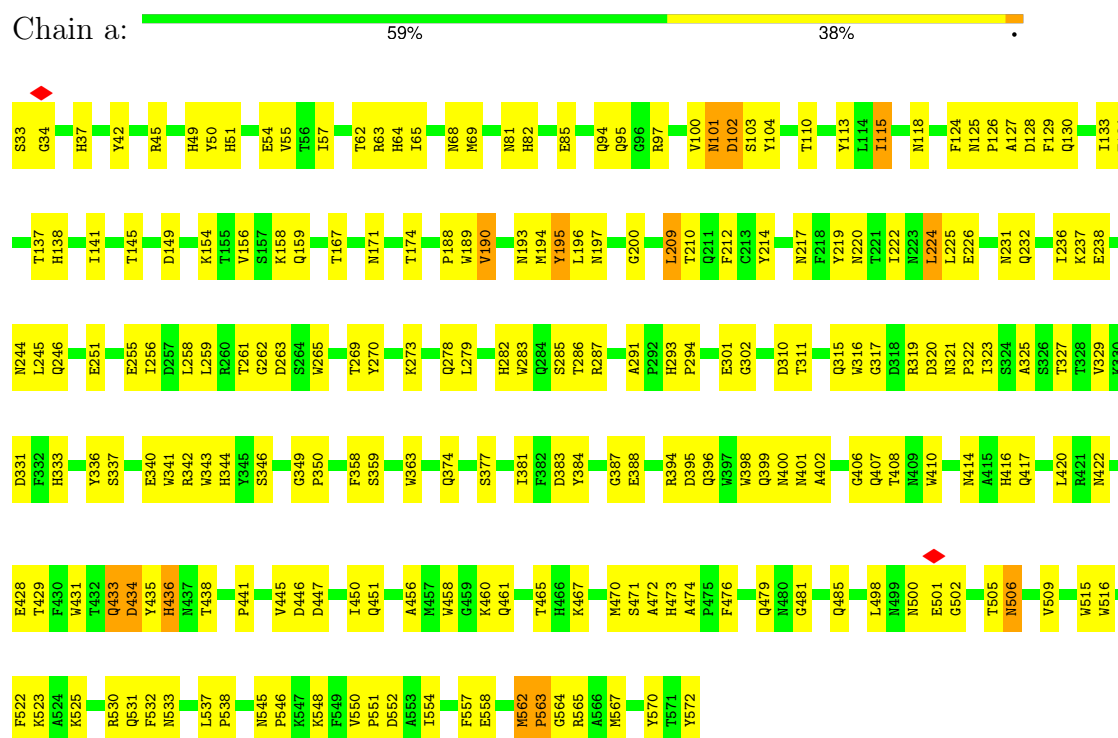
Chain 5:  59% 39%



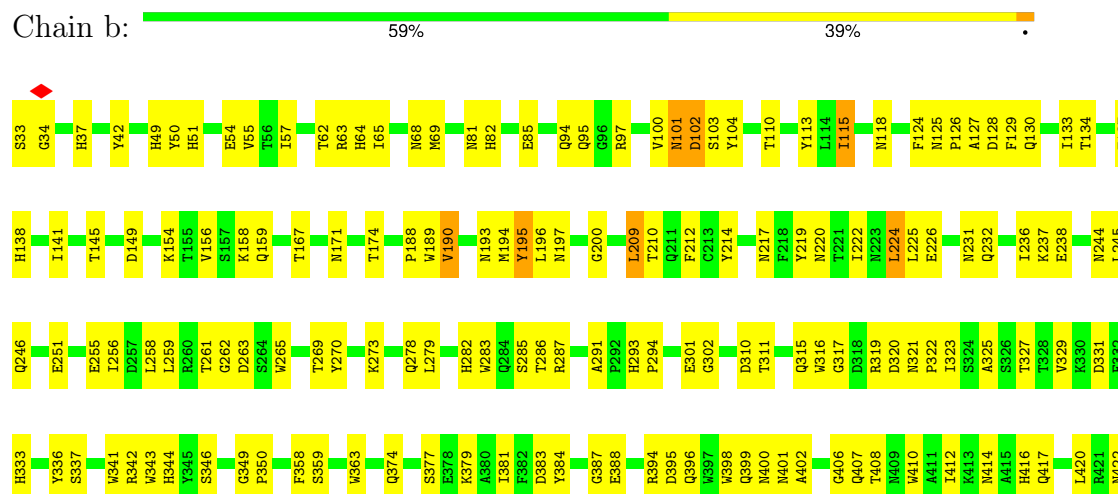




• Molecule 1: VP2



• Molecule 1: VP2

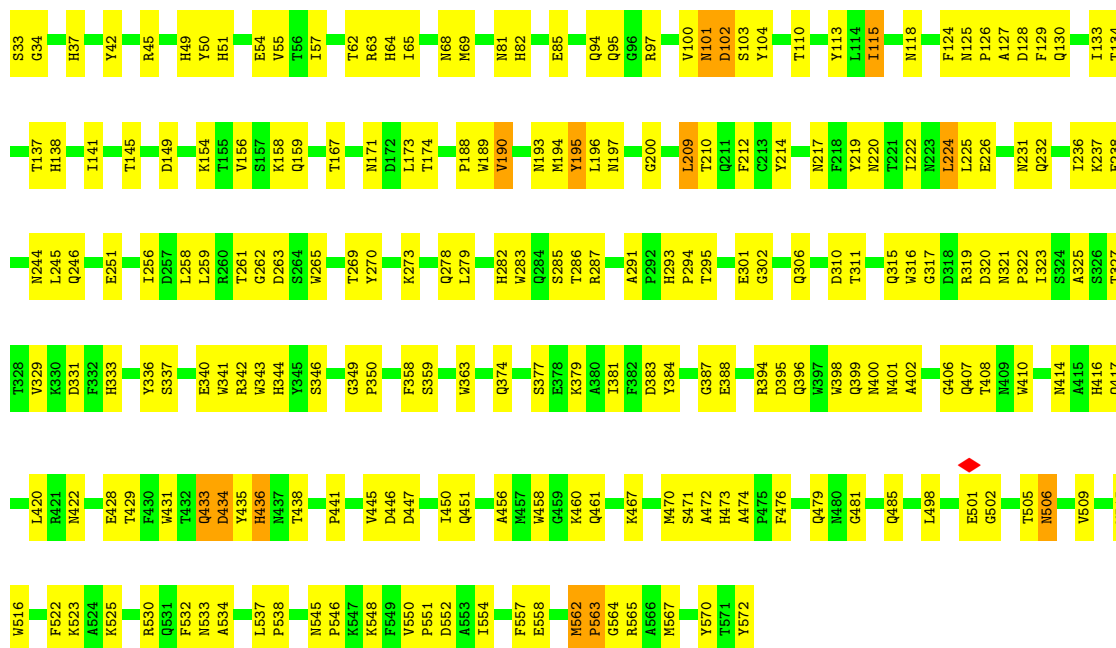






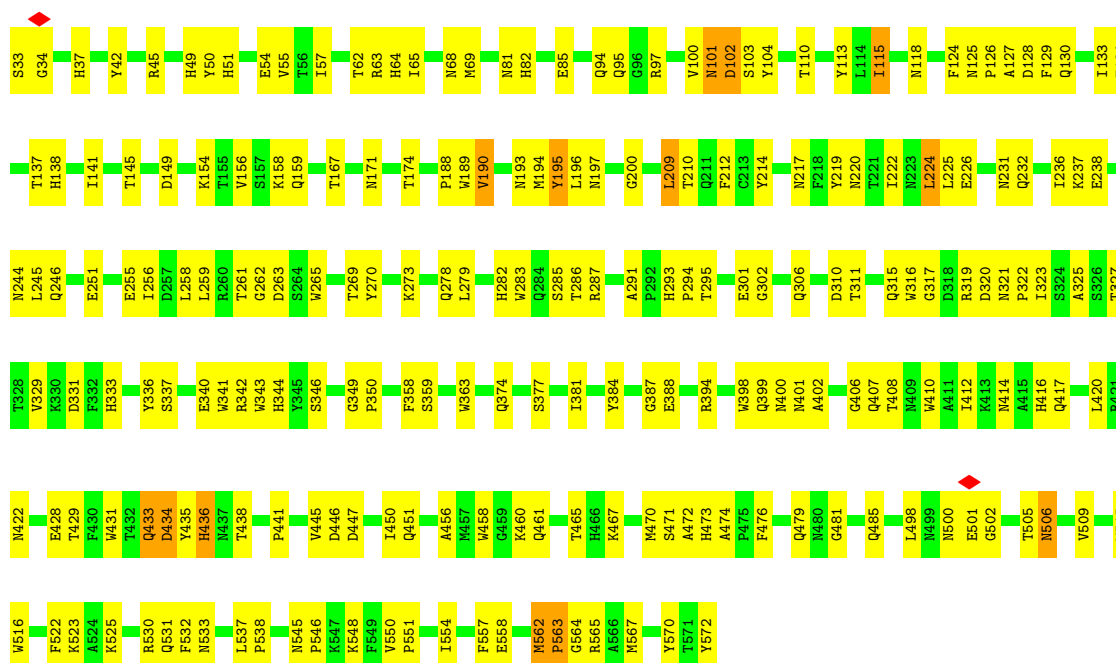
• Molecule 1: VP2

Chain e: 59% 39%

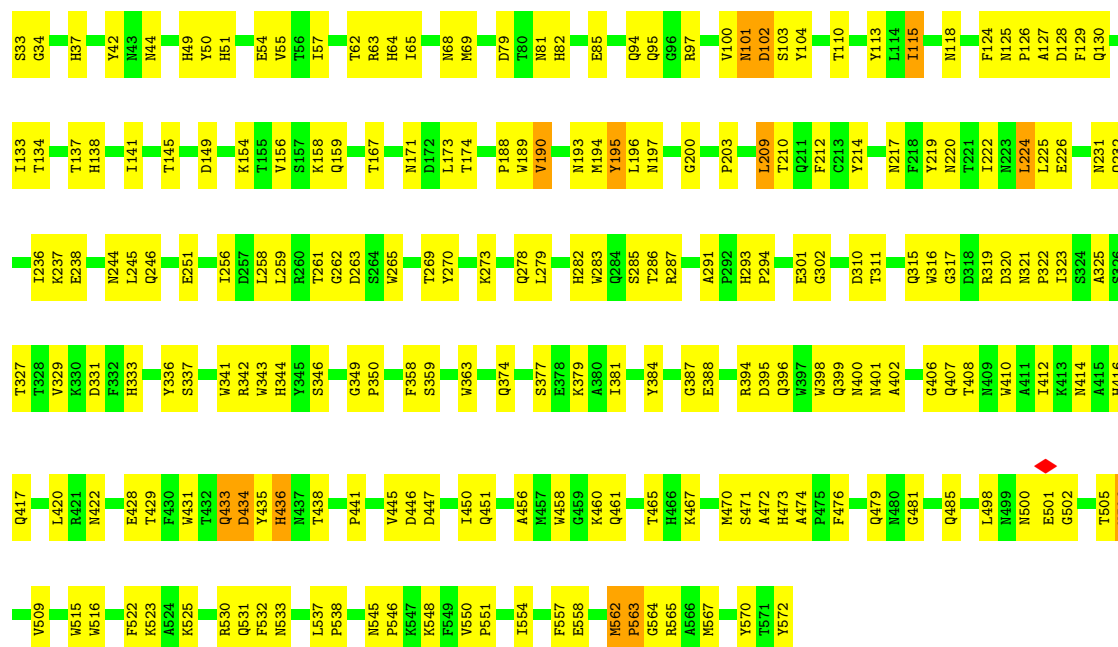


• Molecule 1: VP2

Chain f: 59% 38%

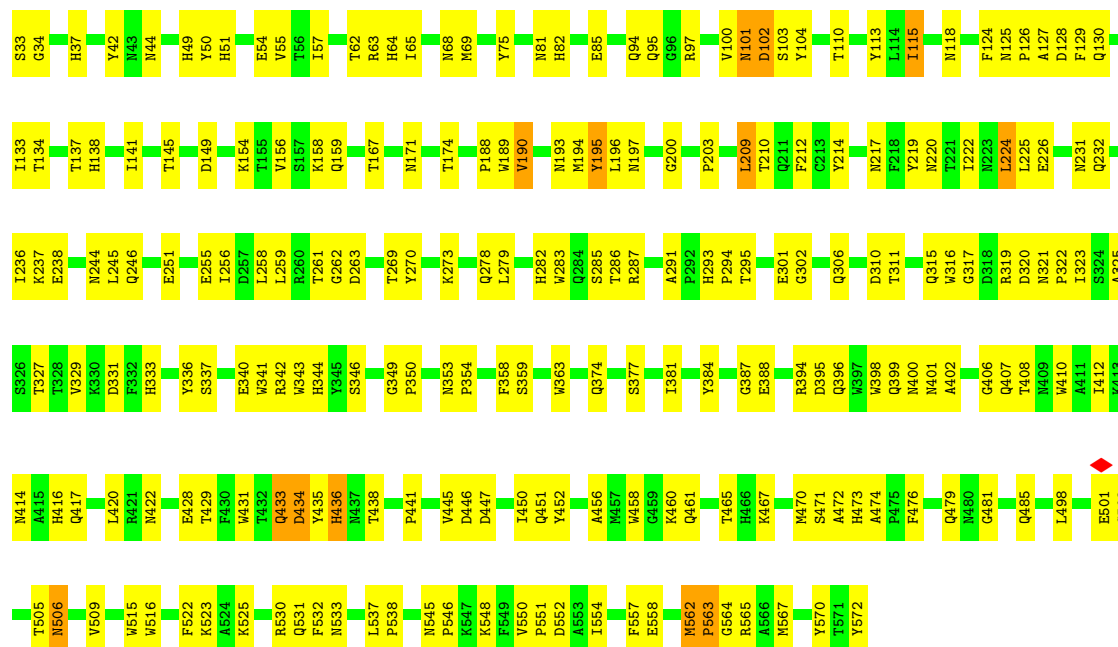






• Molecule 1: VP2

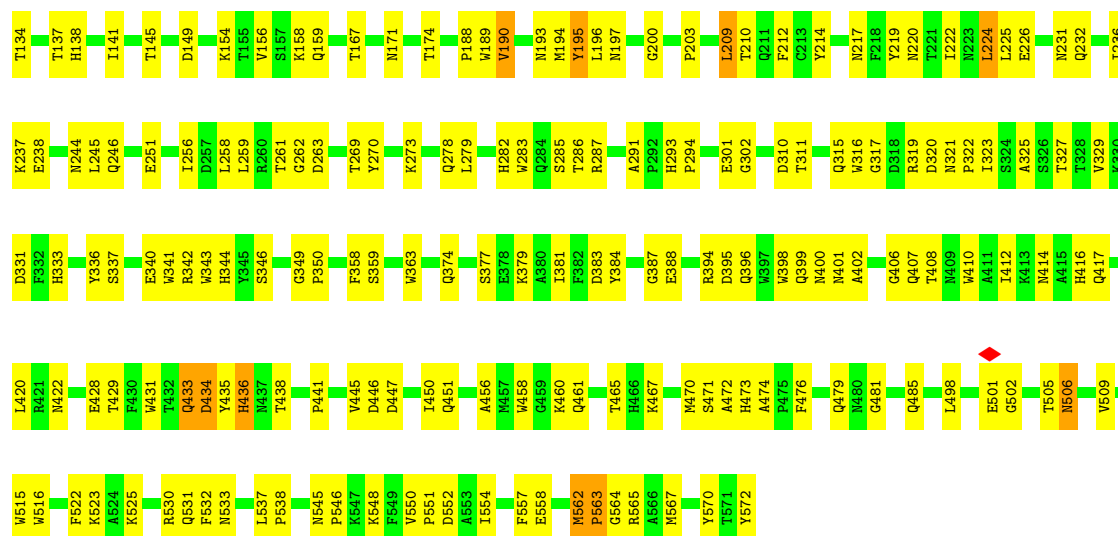
Chain j: 58% 39%



• Molecule 1: VP2

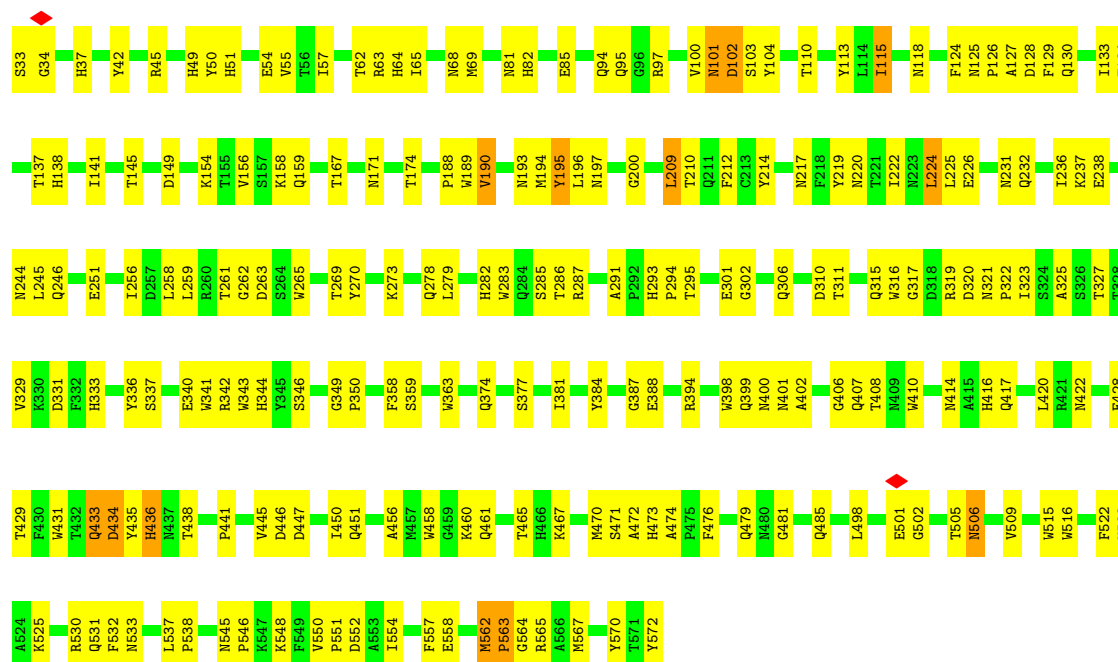
Chain k: 59% 39%





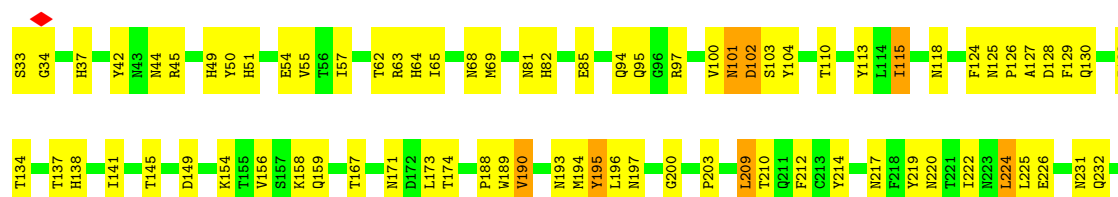
• Molecule 1: VP2

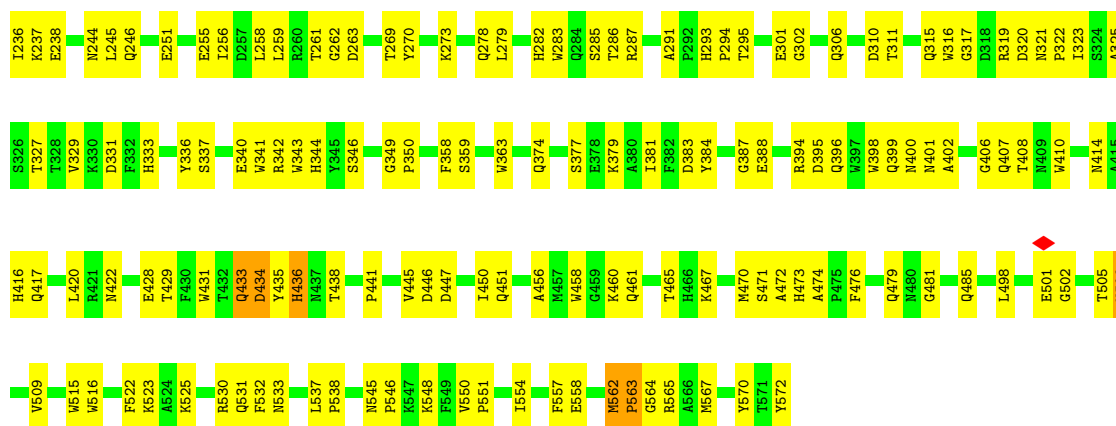
Chain l: 60% 38%



• Molecule 1: VP2

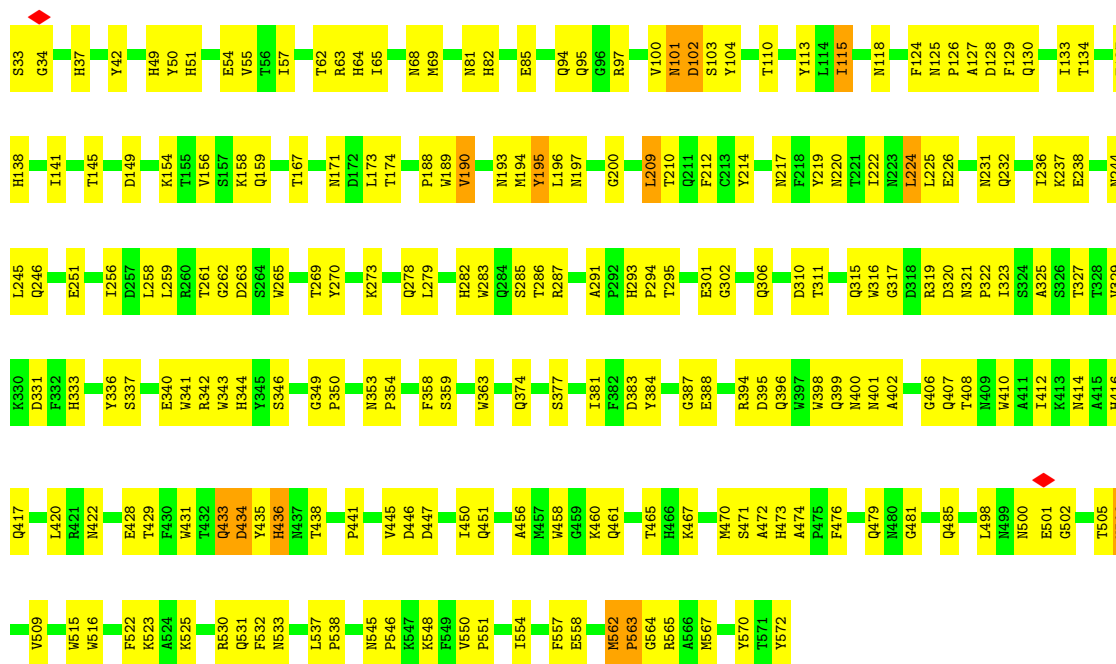
Chain m: 59% 39%





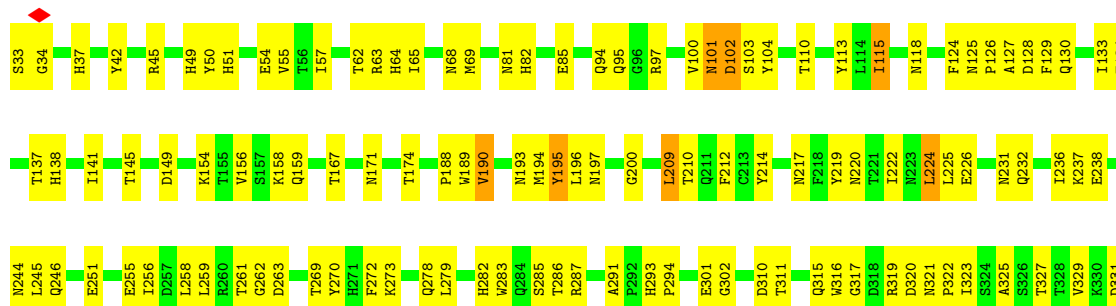
### • Molecule 1: VP2

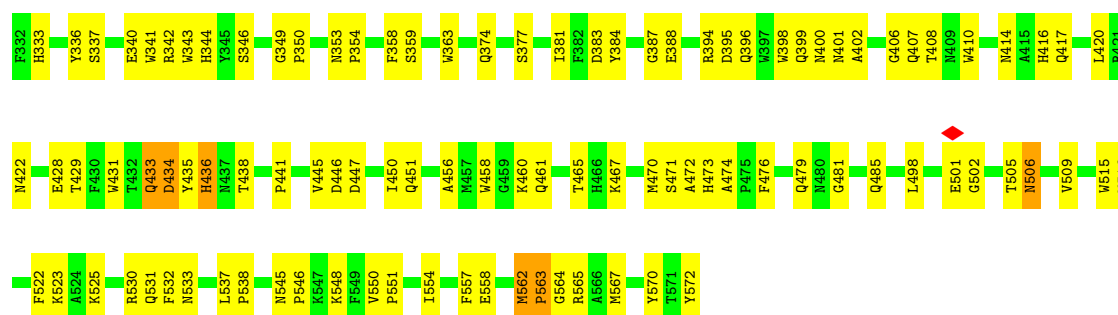
Chain n: 59% 39%



### • Molecule 1: VP2

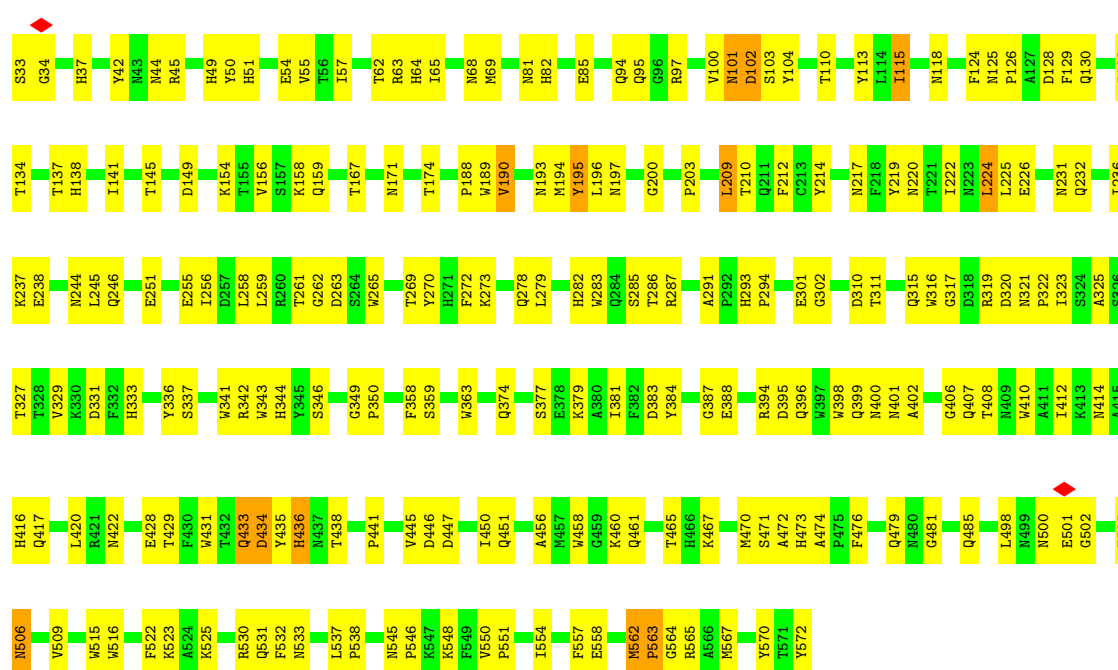
Chain o: 59% 38%





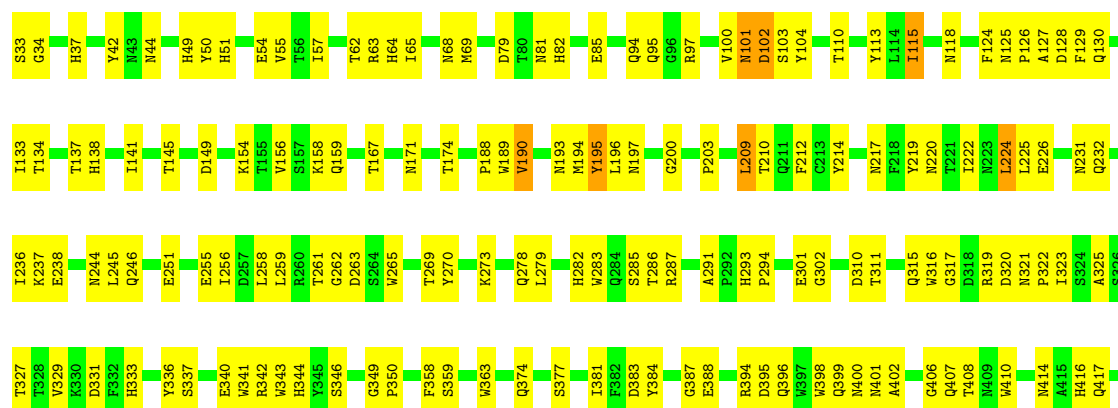
• Molecule 1: VP2

Chain p: 59% 39%



• Molecule 1: VP2

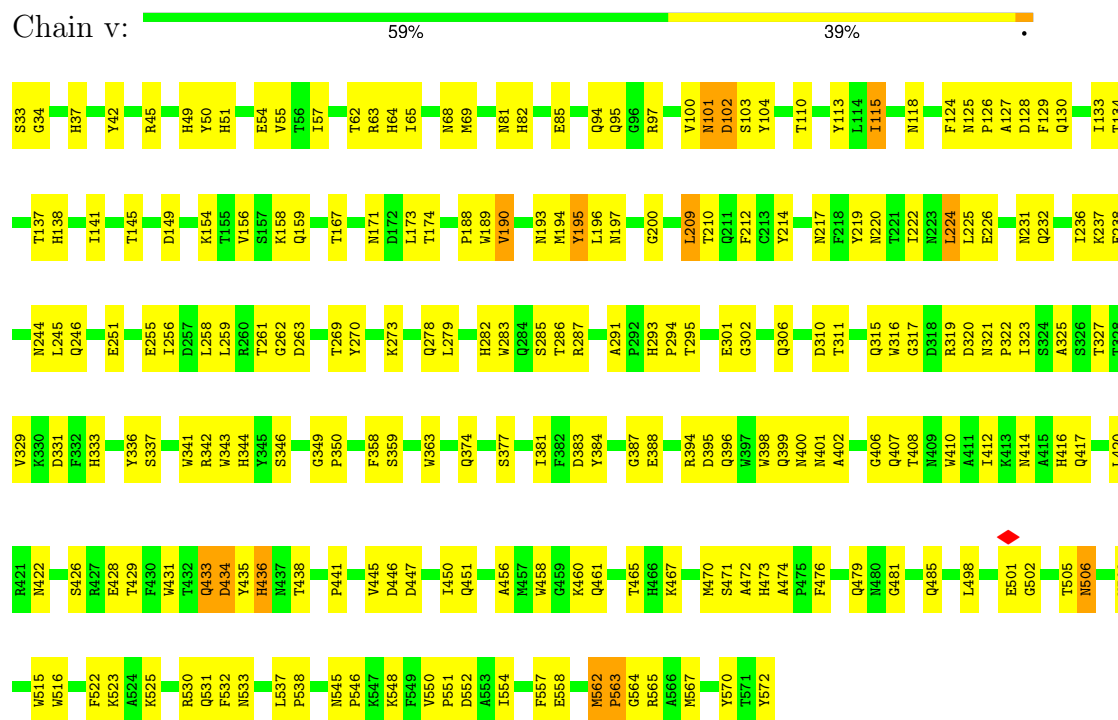
Chain q: 59% 39%



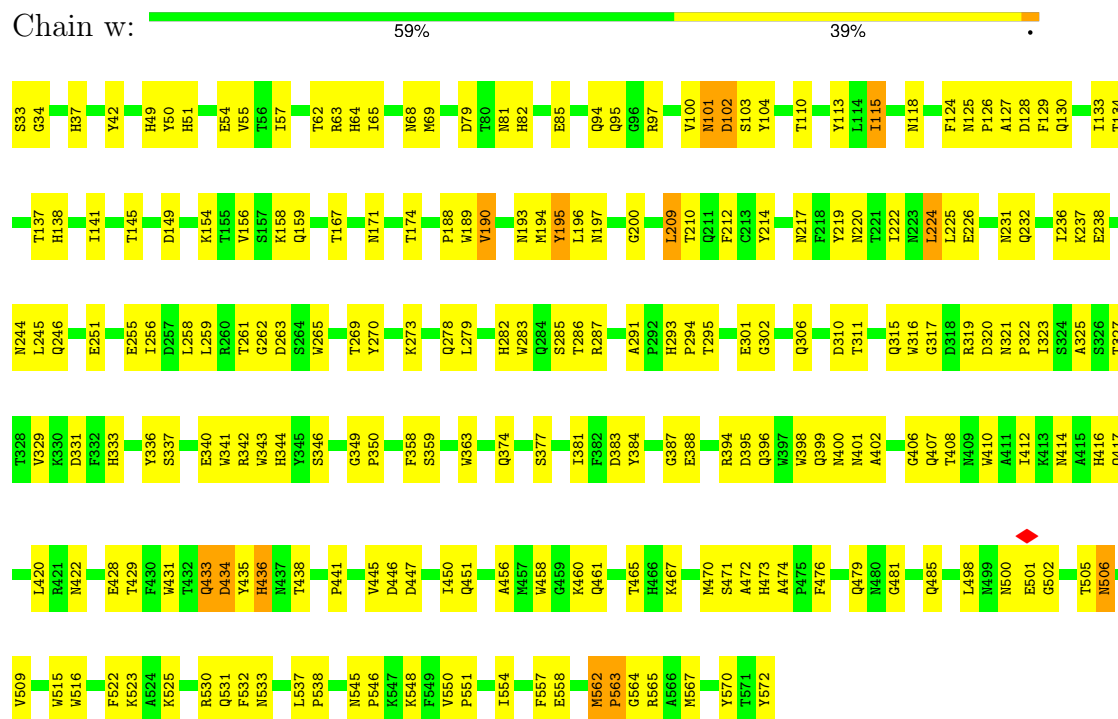






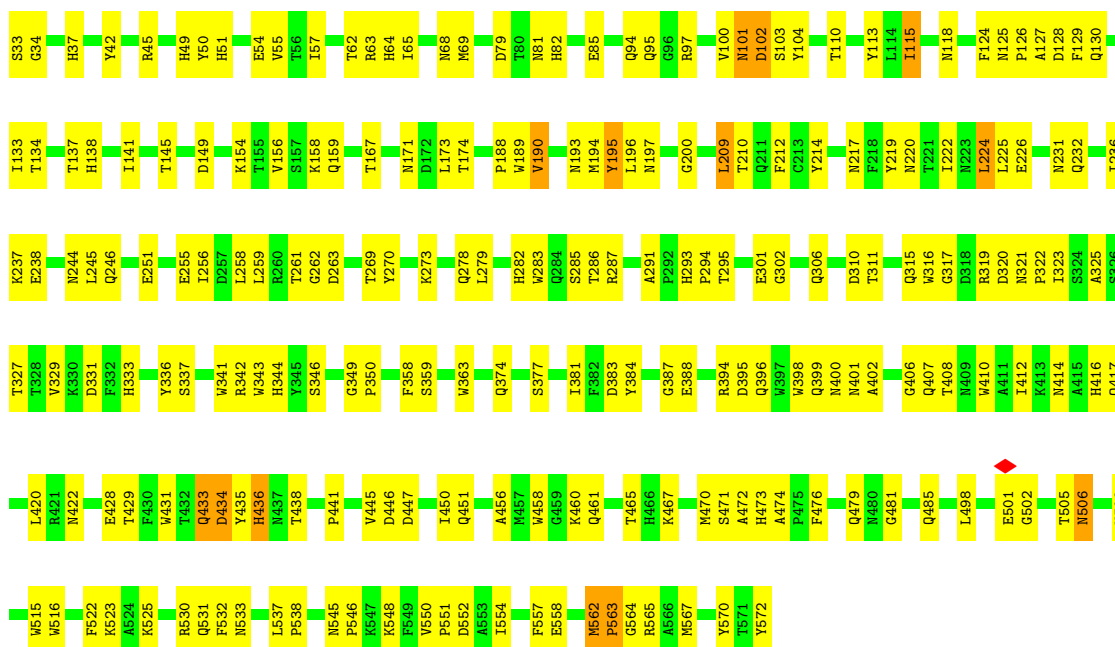


• Molecule 1: VP2



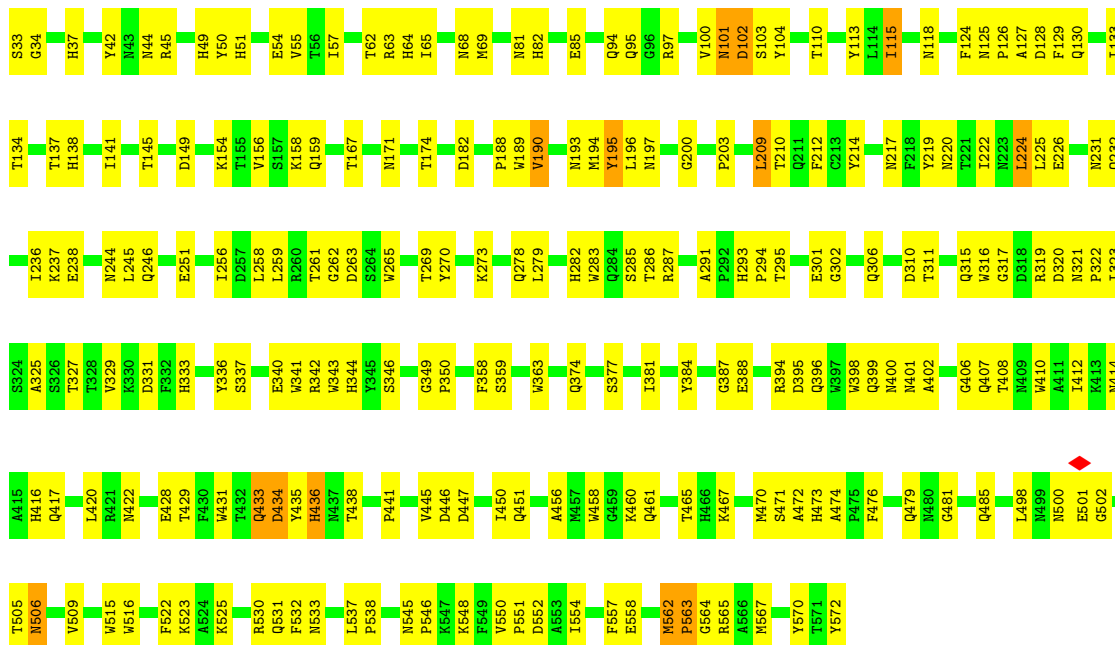
• Molecule 1: VP2





• Molecule 1: VP2

Chain y: 59% 39%



• Molecule 1: VP2

Chain z: 59% 38%





K237	E238	N244	L245	Q246	I256	D257	L258	L259	R260	T261	G262	D263	T269	Y270	K273	Q278	L279	H282	W283	Q284	S285	T286	R287	A291	P292	H293	P294	T295	E301	G302	Q306	D310	T311	Q315	W316	G317	D318	R319	D320	N321	P322	I323	S324	A325	S326	T327	T328	V329
K330	D331	F332	H333	Y336	S337	E340	W341	R342	W343	H344	Y345	S346	G349	P350	N353	P354	F358	S359	W363	Q374	S377	I381	F382	D383	Y384	G387	E388	R394	D395	Q396	W397	W398	Q399	N400	N401	A402	G406	Q407	T408	N409	W410	N414	A415	H416	Q417			
L420	R421	N422	E428	T429	F430	W431	T432	Q433	D434	Y435	H436	Y437	T438	P441	V445	D446	D447	I450	Q451	A456	R457	W458	G459	K460	Q461	T465	H466	K467	M470	S471	A472	H473	A474	P475	F476	Q479	N480	G481	Q485	L488	N489	N500	E501	G502	T505	N506	V509	
W515	W516	F522	K523	A524	K525	R530	Q531	F532	N533	L537	P538	N545	P546	K547	K548	F549	V550	P551	D552	A553	I554	F557	E558	M562	P563	G564	R565	A566	M567	Y570	T571	Y572																

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5234	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.310	Depositor
Minimum map value	-8.385	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	380.53998, 380.53998, 380.53998	wwPDB
Map dimensions	359, 359, 359	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.40	0/4500	0.62	7/6155 (0.1%)
1	1	0.40	0/4500	0.62	7/6155 (0.1%)
1	2	0.40	0/4500	0.62	7/6155 (0.1%)
1	3	0.40	0/4500	0.62	7/6155 (0.1%)
1	4	0.40	0/4500	0.62	7/6155 (0.1%)
1	5	0.40	0/4500	0.62	7/6155 (0.1%)
1	6	0.40	0/4500	0.62	7/6155 (0.1%)
1	7	0.40	0/4500	0.62	7/6155 (0.1%)
1	A	0.40	0/4500	0.62	7/6155 (0.1%)
1	B	0.40	0/4500	0.62	7/6155 (0.1%)
1	C	0.40	0/4500	0.62	7/6155 (0.1%)
1	D	0.40	0/4500	0.62	7/6155 (0.1%)
1	E	0.40	0/4500	0.62	7/6155 (0.1%)
1	F	0.40	0/4500	0.62	7/6155 (0.1%)
1	G	0.40	0/4500	0.62	7/6155 (0.1%)
1	H	0.40	0/4500	0.62	7/6155 (0.1%)
1	I	0.40	0/4500	0.62	7/6155 (0.1%)
1	J	0.40	0/4500	0.62	7/6155 (0.1%)
1	K	0.40	0/4500	0.62	7/6155 (0.1%)
1	L	0.40	0/4500	0.62	7/6155 (0.1%)
1	M	0.40	0/4500	0.62	7/6155 (0.1%)
1	N	0.40	0/4500	0.62	7/6155 (0.1%)
1	O	0.40	0/4500	0.62	7/6155 (0.1%)
1	P	0.40	0/4500	0.62	7/6155 (0.1%)
1	Q	0.40	0/4500	0.62	7/6155 (0.1%)
1	R	0.40	0/4500	0.62	7/6155 (0.1%)
1	S	0.40	0/4500	0.62	7/6155 (0.1%)
1	T	0.40	0/4500	0.62	7/6155 (0.1%)
1	U	0.40	0/4500	0.62	7/6155 (0.1%)
1	V	0.40	0/4500	0.62	7/6155 (0.1%)
1	W	0.40	0/4500	0.62	7/6155 (0.1%)
1	X	0.40	0/4500	0.62	7/6155 (0.1%)
1	Y	0.40	0/4500	0.62	7/6155 (0.1%)
1	Z	0.40	0/4500	0.62	7/6155 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.40	0/4500	0.62	7/6155 (0.1%)
1	b	0.40	0/4500	0.62	7/6155 (0.1%)
1	c	0.40	0/4500	0.62	7/6155 (0.1%)
1	d	0.40	0/4500	0.62	7/6155 (0.1%)
1	e	0.40	0/4500	0.62	7/6155 (0.1%)
1	f	0.40	0/4500	0.62	7/6155 (0.1%)
1	g	0.40	0/4500	0.62	7/6155 (0.1%)
1	h	0.40	0/4500	0.62	7/6155 (0.1%)
1	i	0.40	0/4500	0.62	7/6155 (0.1%)
1	j	0.40	0/4500	0.62	7/6155 (0.1%)
1	k	0.40	0/4500	0.62	7/6155 (0.1%)
1	l	0.40	0/4500	0.62	7/6155 (0.1%)
1	m	0.40	0/4500	0.62	7/6155 (0.1%)
1	n	0.40	0/4500	0.62	7/6155 (0.1%)
1	o	0.40	0/4500	0.62	7/6155 (0.1%)
1	p	0.40	0/4500	0.62	7/6155 (0.1%)
1	q	0.40	0/4500	0.62	7/6155 (0.1%)
1	r	0.40	0/4500	0.62	7/6155 (0.1%)
1	s	0.40	0/4500	0.62	7/6155 (0.1%)
1	t	0.40	0/4500	0.62	7/6155 (0.1%)
1	u	0.40	0/4500	0.62	7/6155 (0.1%)
1	v	0.40	0/4500	0.62	7/6155 (0.1%)
1	w	0.40	0/4500	0.62	7/6155 (0.1%)
1	x	0.40	0/4500	0.62	7/6155 (0.1%)
1	y	0.40	0/4500	0.62	7/6155 (0.1%)
1	z	0.40	0/4500	0.62	7/6155 (0.1%)
All	All	0.40	0/270000	0.62	420/369300 (0.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
1	Q	0	3
1	R	0	3
1	S	0	3
1	T	0	3
1	U	0	3
1	V	0	3
1	W	0	3
1	X	0	3
1	Y	0	3
1	Z	0	3
1	a	0	3
1	b	0	3
1	c	0	3
1	d	0	3
1	e	0	3
1	f	0	3
1	g	0	3
1	h	0	3
1	i	0	3
1	j	0	3
1	k	0	3
1	l	0	3
1	m	0	3
1	n	0	3
1	o	0	3
1	p	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	3
1	r	0	3
1	s	0	3
1	t	0	3
1	u	0	3
1	v	0	3
1	w	0	3
1	x	0	3
1	y	0	3
1	z	0	3
All	All	0	180

There are no bond length outliers.

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	433	GLN	N-CA-C	11.87	124.22	111.28
1	D	433	GLN	N-CA-C	11.87	124.22	111.28
1	X	433	GLN	N-CA-C	11.87	124.22	111.28
1	C	433	GLN	N-CA-C	11.85	124.20	111.28
1	Q	433	GLN	N-CA-C	11.85	124.20	111.28

There are no chirality outliers.

5 of 180 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	TYR	Peptide
1	A	434	ASP	Peptide
1	A	563	PRO	Peptide
1	B	195	TYR	Peptide
1	B	434	ASP	Peptide

## 5.2 Too-close contacts [i](#)

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4353	0	4043	214	0
1	1	4353	0	4043	214	0
1	2	4353	0	4043	217	0
1	3	4353	0	4043	214	0
1	4	4353	0	4043	216	0
1	5	4353	0	4043	215	0
1	6	4353	0	4043	212	0
1	7	4353	0	4043	213	0
1	A	4353	0	4043	210	0
1	B	4353	0	4043	218	0
1	C	4353	0	4043	212	0
1	D	4353	0	4043	215	0
1	E	4353	0	4043	210	0
1	F	4353	0	4043	218	0
1	G	4353	0	4043	211	0
1	H	4353	0	4043	213	0
1	I	4353	0	4043	214	0
1	J	4353	0	4043	215	0
1	K	4353	0	4043	219	0
1	L	4353	0	4043	213	0
1	M	4353	0	4043	214	0
1	N	4353	0	4043	216	0
1	O	4353	0	4043	215	0
1	P	4353	0	4043	215	0
1	Q	4353	0	4043	214	0
1	R	4353	0	4043	213	0
1	S	4353	0	4043	217	0
1	T	4353	0	4043	214	0
1	U	4353	0	4043	213	0
1	V	4353	0	4043	211	0
1	W	4353	0	4043	213	0
1	X	4353	0	4043	215	0
1	Y	4353	0	4043	214	0
1	Z	4353	0	4043	214	0
1	a	4353	0	4043	211	0
1	b	4353	0	4043	217	0
1	c	4353	0	4043	212	0
1	d	4353	0	4043	219	0
1	e	4353	0	4043	213	0
1	f	4353	0	4043	211	0
1	g	4353	0	4043	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	4353	0	4043	211	0
1	i	4353	0	4043	210	0
1	j	4353	0	4043	214	0
1	k	4353	0	4043	218	0
1	l	4353	0	4043	209	0
1	m	4353	0	4043	214	0
1	n	4353	0	4043	214	0
1	o	4353	0	4043	213	0
1	p	4353	0	4043	211	0
1	q	4353	0	4043	214	0
1	r	4353	0	4043	211	0
1	s	4353	0	4043	213	0
1	t	4353	0	4043	215	0
1	u	4353	0	4043	213	0
1	v	4353	0	4043	214	0
1	w	4353	0	4043	214	0
1	x	4353	0	4043	214	0
1	y	4353	0	4043	215	0
1	z	4353	0	4043	212	0
All	All	261180	0	242580	10552	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 21.

The worst 5 of 10552 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:S:501:GLU:HB2	1:S:502:GLY:HA3	1.32	1.12
1:2:501:GLU:HB2	1:2:502:GLY:HA3	1.32	1.12
1:P:501:GLU:HB2	1:P:502:GLY:HA3	1.32	1.12
1:V:501:GLU:HB2	1:V:502:GLY:HA3	1.32	1.12
1:X:501:GLU:HB2	1:X:502:GLY:HA3	1.32	1.12

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	0	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	1	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	2	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	3	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	4	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	5	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	6	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	7	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	A	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	B	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	C	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	D	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	E	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	F	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	G	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	H	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	I	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	J	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	K	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	L	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	M	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	N	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	O	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	P	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	Q	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	S	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	T	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	U	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	V	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	W	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	X	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	Y	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	Z	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	a	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	b	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	c	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	d	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	e	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	f	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	g	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	h	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	i	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	j	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	k	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	l	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	m	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	n	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	o	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	p	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	q	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	r	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	s	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	t	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	u	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	v	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	x	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	y	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
1	z	538/540 (100%)	516 (96%)	21 (4%)	1 (0%)	44	71
All	All	32280/32400 (100%)	30960 (96%)	1260 (4%)	60 (0%)	45	71

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	VAL
1	B	190	VAL
1	C	190	VAL
1	D	190	VAL
1	E	190	VAL

### 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	0	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	1	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	2	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	3	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	4	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	5	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	6	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	7	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	A	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	B	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	C	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	D	468/468 (100%)	463 (99%)	5 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	F	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	G	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	H	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	I	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	J	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	K	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	L	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	M	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	N	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	O	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	P	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	Q	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	R	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	S	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	T	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	U	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	V	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	W	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	X	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	Y	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	Z	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	a	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	b	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	c	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	d	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	e	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	f	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	g	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	h	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	i	468/468 (100%)	463 (99%)	5 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	k	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	l	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	m	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	n	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	o	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	p	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	q	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	r	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	s	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	t	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	u	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	v	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	w	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	x	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	y	468/468 (100%)	463 (99%)	5 (1%)	70	81
1	z	468/468 (100%)	463 (99%)	5 (1%)	70	81
All	All	28080/28080 (100%)	27780 (99%)	300 (1%)	69	81

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	o	115	ILE
1	z	115	ILE
1	p	224	LEU
1	u	65	ILE
1	T	209	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 948 such sidechains are listed below:

Mol	Chain	Res	Type
1	3	37	HIS
1	y	64	HIS
1	d	293	HIS
1	x	293	HIS

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Mol	Chain	Res	Type
1	7	451	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no 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.

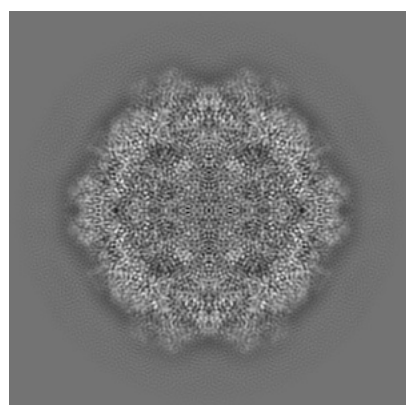
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7302. These allow visual inspection of the internal detail of the map and identification of artifacts.

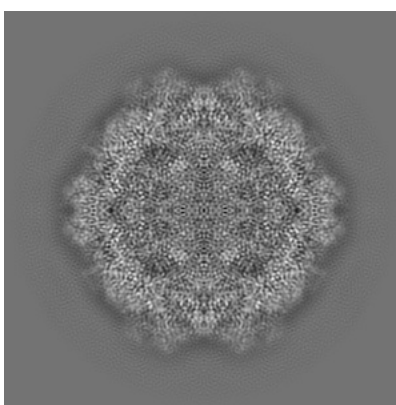
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

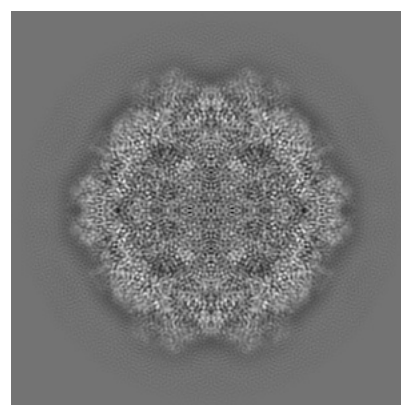
#### 6.1.1 Primary map



X



Y

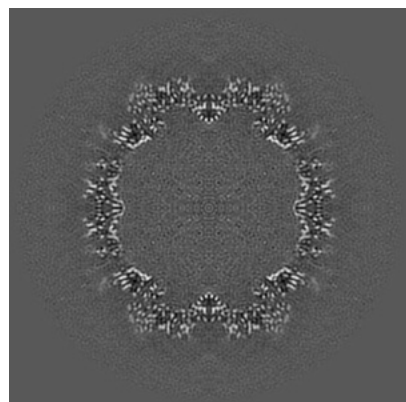


Z

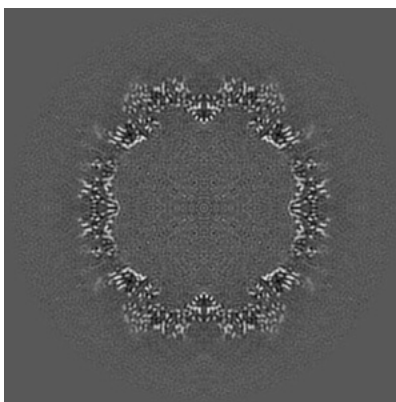
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

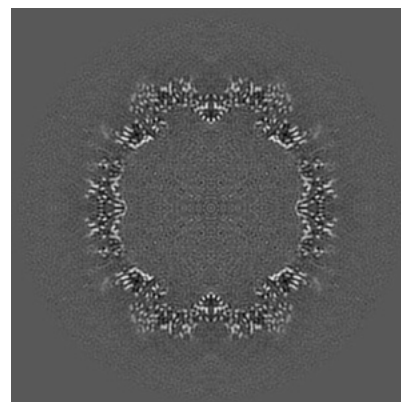
#### 6.2.1 Primary map



X Index: 179



Y Index: 179

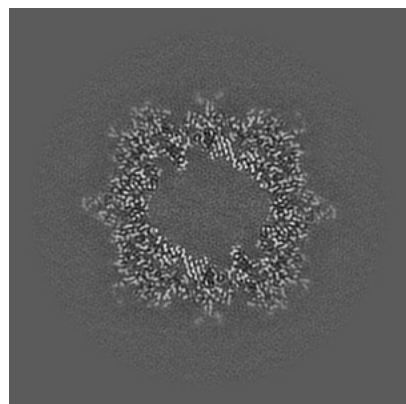


Z Index: 179

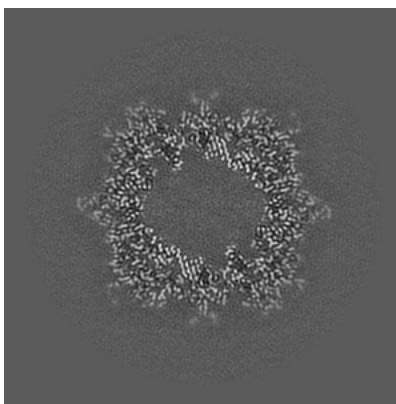
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

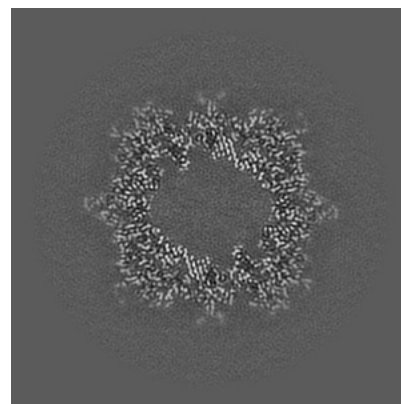
### 6.3.1 Primary map



X Index: 113



Y Index: 113

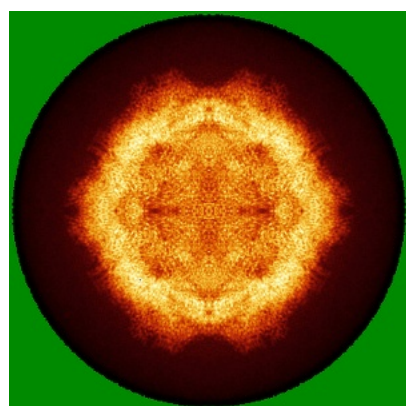


Z Index: 113

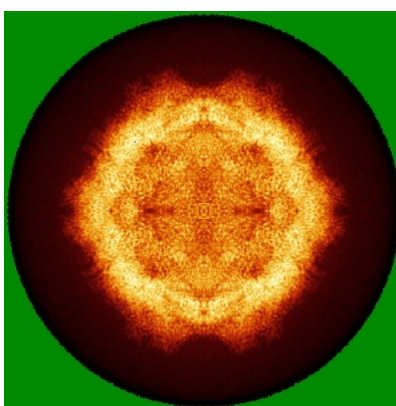
The images above show the largest variance slices of the map in three orthogonal directions.

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

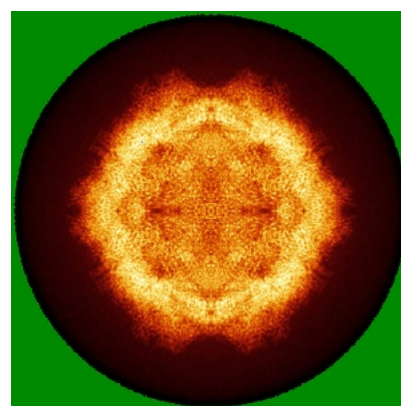
### 6.4.1 Primary map



X



Y

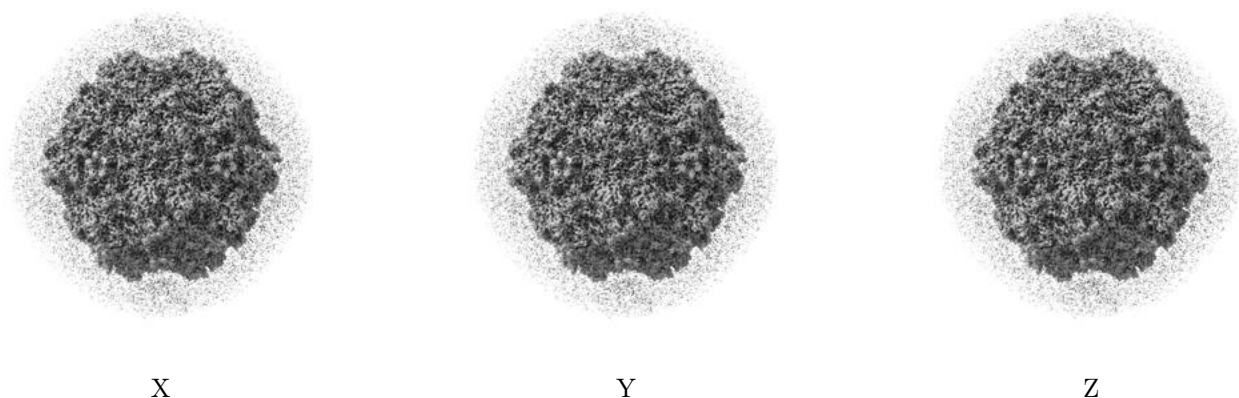


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

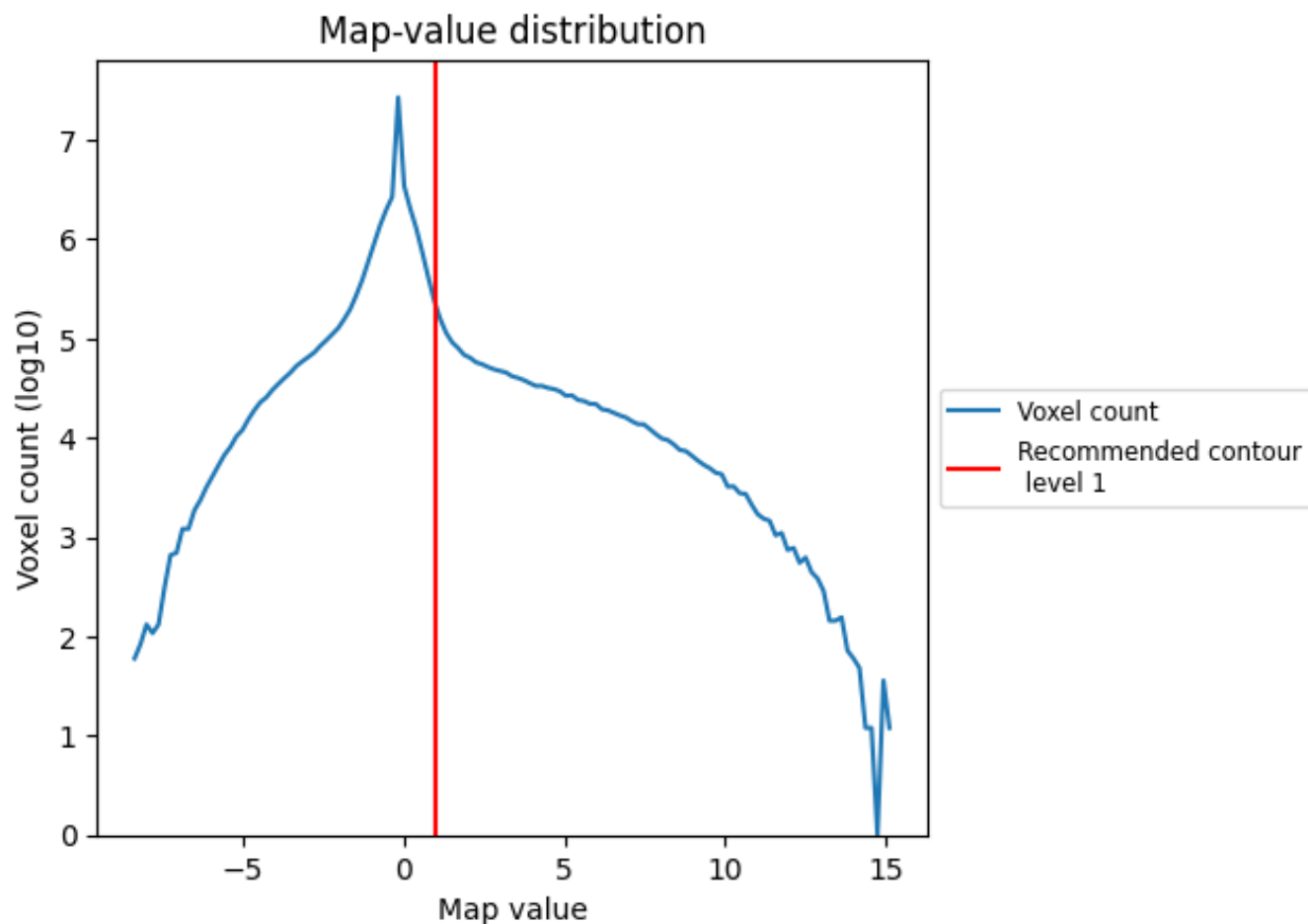
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

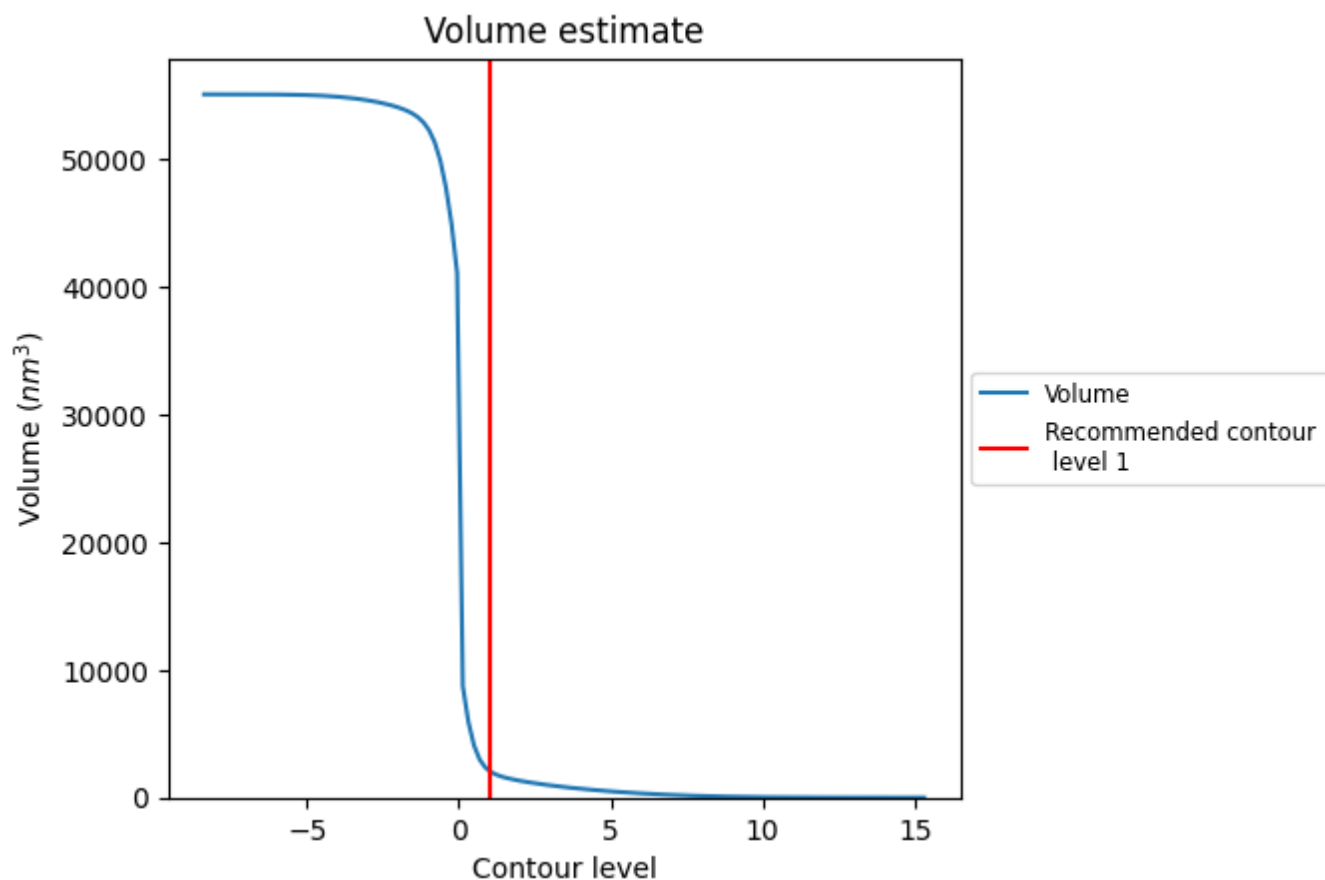
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

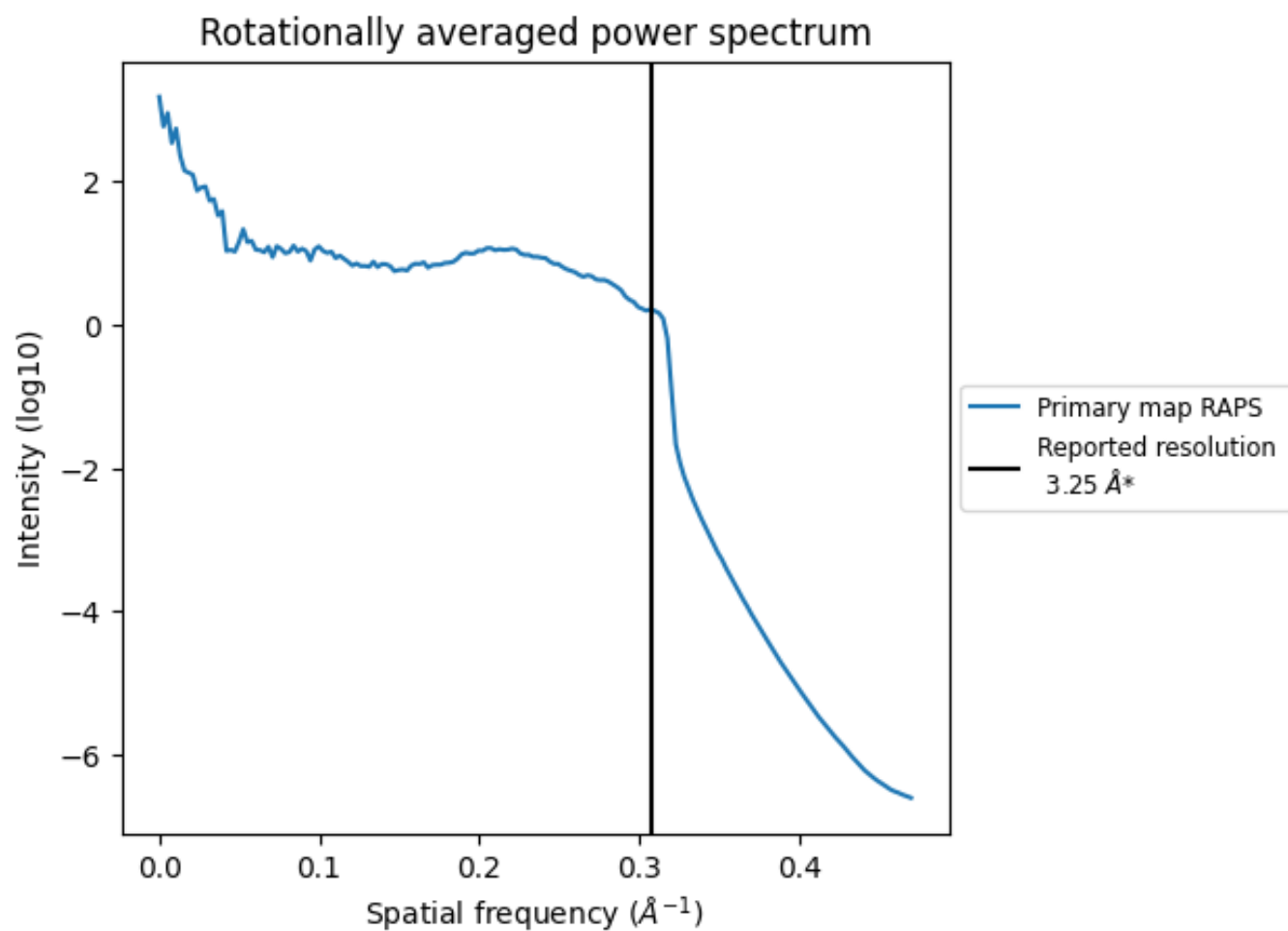


The volume at the recommended contour level is 2109 nm<sup>3</sup>; this corresponds to an approximate mass of 1905 kDa.

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 0.308 Å<sup>-1</sup>

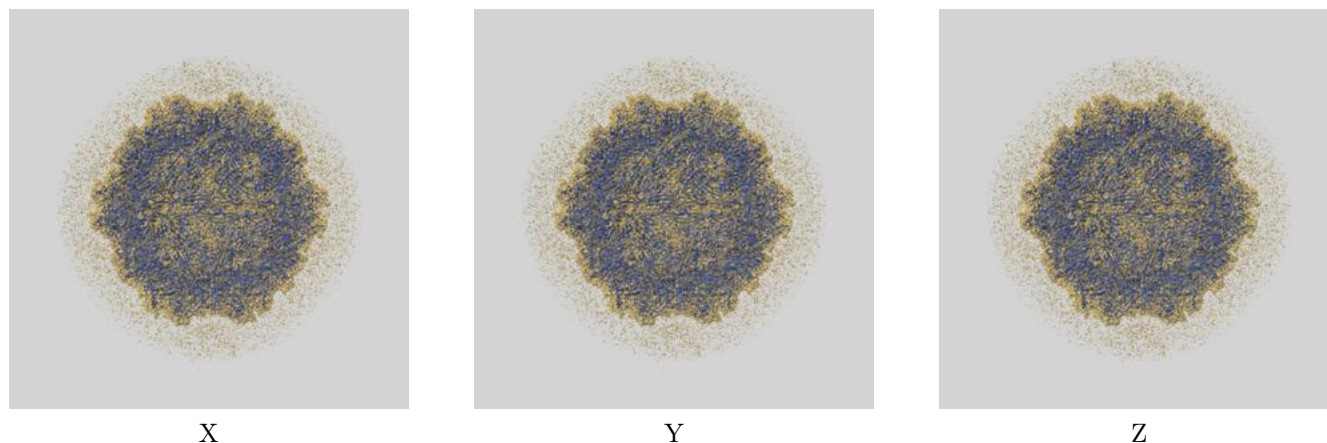
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

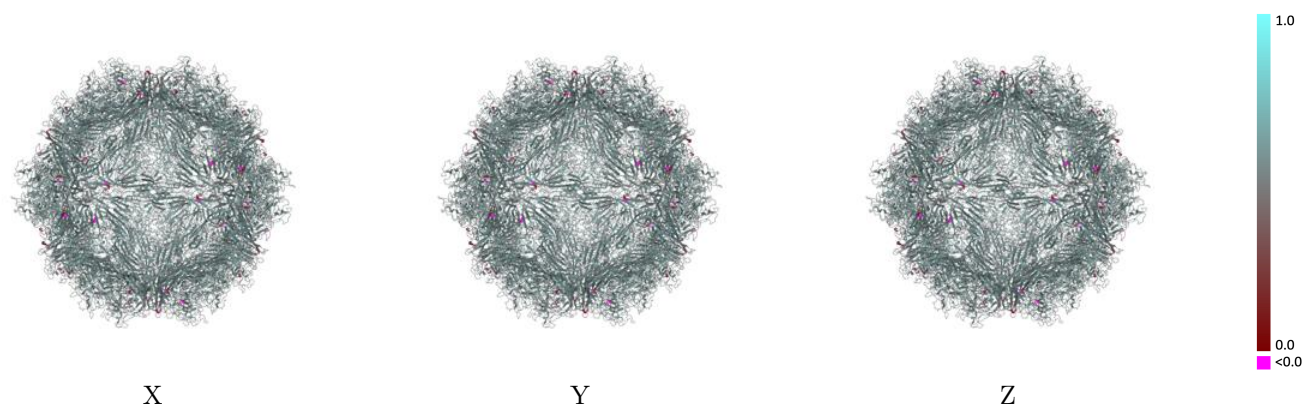
This section contains information regarding the fit between EMDB map EMD-7302 and PDB model 6BX1. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

### 9.1 Map-model overlay [i](#)



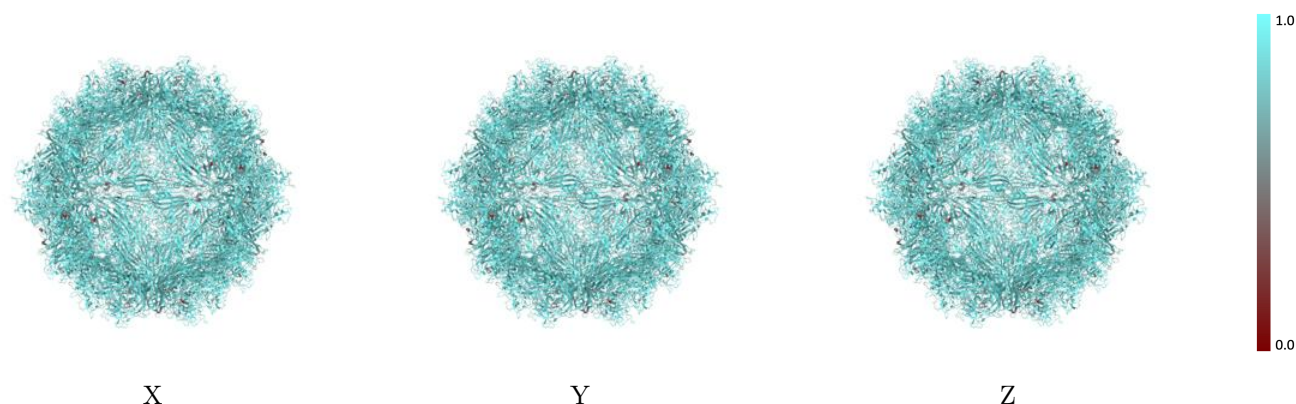
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



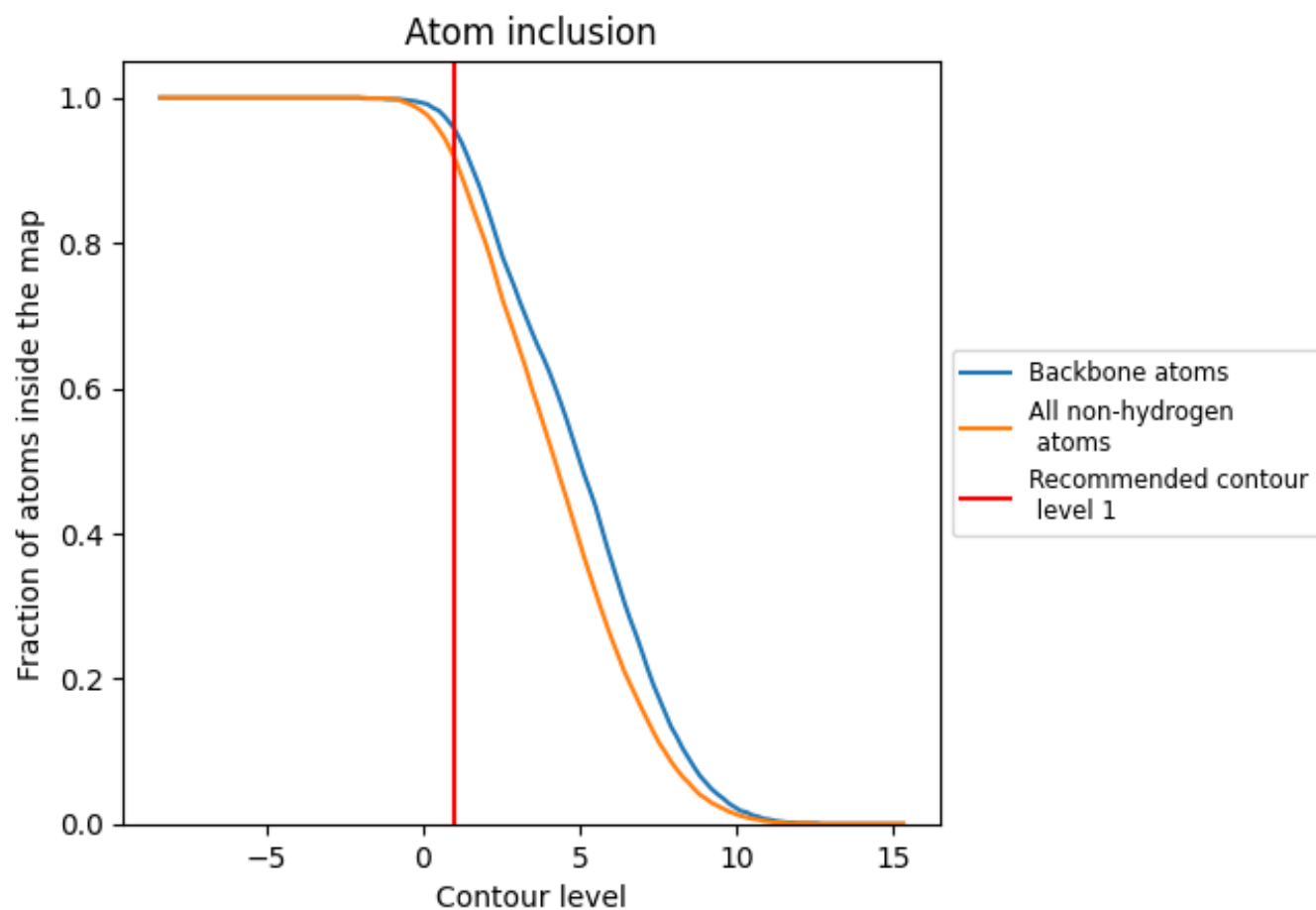
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.5500
0	 0.9180	 0.5510
1	 0.9190	 0.5510
2	 0.9180	 0.5510
3	 0.9190	 0.5500
4	 0.9140	 0.5500
5	 0.9180	 0.5500
6	 0.9140	 0.5510
7	 0.9180	 0.5500
A	 0.9140	 0.5500
B	 0.9160	 0.5500
C	 0.9190	 0.5510
D	 0.9170	 0.5520
E	 0.9180	 0.5510
F	 0.9180	 0.5510
G	 0.9170	 0.5500
H	 0.9190	 0.5490
I	 0.9160	 0.5480
J	 0.9140	 0.5500
K	 0.9180	 0.5510
L	 0.9170	 0.5490
M	 0.9190	 0.5510
N	 0.9160	 0.5510
O	 0.9160	 0.5500
P	 0.9140	 0.5520
Q	 0.9180	 0.5510
R	 0.9140	 0.5510
S	 0.9180	 0.5510
T	 0.9190	 0.5500
U	 0.9150	 0.5510
V	 0.9150	 0.5510
W	 0.9190	 0.5490
X	 0.9180	 0.5510
Y	 0.9190	 0.5500
Z	 0.9170	 0.5510



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Chain	Atom inclusion	Q-score
a	 0.9180	 0.5510
b	 0.9180	 0.5500
c	 0.9170	 0.5500
d	 0.9160	 0.5480
e	 0.9140	 0.5500
f	 0.9190	 0.5500
g	 0.9140	 0.5510
h	 0.9170	 0.5500
i	 0.9150	 0.5510
j	 0.9140	 0.5510
k	 0.9180	 0.5500
l	 0.9180	 0.5500
m	 0.9180	 0.5510
n	 0.9190	 0.5500
o	 0.9190	 0.5500
p	 0.9190	 0.5500
q	 0.9160	 0.5500
r	 0.9140	 0.5490
s	 0.9170	 0.5490
t	 0.9140	 0.5530
u	 0.9170	 0.5510
v	 0.9160	 0.5500
w	 0.9140	 0.5510
x	 0.9160	 0.5500
y	 0.9180	 0.5510
z	 0.9150	 0.5520