



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 06:50 PM EST

PDB ID : 3K1Q  
EMDB ID : EMD-1653  
Title : Backbone model of an aquareovirus virion by cryo-electron microscopy and bioinformatics  
Authors : Cheng, L.P.; Zhu, J.; Hiu, W.H.; Zhang, X.K.; Honig, B.; Fang, Q.; Zhou, Z.H.  
Deposited on : 2009-09-28  
Resolution : 4.50 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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

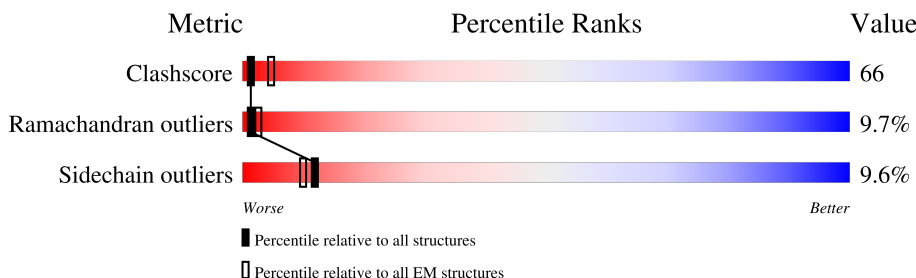
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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	158937	4297
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  $\geq 3$ , 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	A	1299	84% 35% 39% 17% 8%
2	B	1027	77% 37% 36% 20% 6%
3	C	1196	76% 39% 37% 17% 8%
4	D	412	81% 31% 38% 20% 11%
4	E	412	71% 33% 39% 20% 8%
5	F	276	94% 23% 34% 30% 13%
5	G	276	95% 24% 35% 29% 13%
5	H	276	95% 25% 32% 30% 14%

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Mol	Chain	Length	Quality of chain
5	L	276	<div>95%</div> <div>23% 35% 28% 14%</div>
5	M	276	<div>94%</div> <div>24% 33% 29% 13%</div>
5	N	276	<div>100%</div> <div>23% 35% 28% 13%</div>
5	R	276	<div>96%</div> <div>22% 34% 30% 14%</div>
5	S	276	<div>93%</div> <div>25% 32% 29% 14%</div>
5	T	276	<div>91%</div> <div>22% 35% 30% 13%</div>
5	Y	276	<div>100%</div> <div>25% 32% 29% 13%</div>
6	I	639	<div>89%</div> <div>27% 38% 24% 10%</div>
6	J	639	<div>85%</div> <div>27% 40% 23% 10%</div>
6	K	639	<div>86%</div> <div>28% 38% 23% 10%</div>
6	O	639	<div>89%</div> <div>27% 41% 23% 10%</div>
6	P	639	<div>90%</div> <div>28% 37% 24% 11%</div>
6	Q	639	<div>89%</div> <div>28% 38% 24% 10%</div>
6	U	639	<div>88%</div> <div>27% 38% 24% 10%</div>
6	V	639	<div>88%</div> <div>27% 38% 25% 10%</div>
6	W	639	<div>86%</div> <div>27% 39% 24% 10%</div>
6	X	639	<div>90%</div> <div>34% 39% 21% 6%</div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 101798 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1299	Total	C	N	O	S	0	0
			9989	6395	1700	1866	28		

- Molecule 2 is a protein called VP3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1027	Total	C	N	O	S	0	0
			7935	5067	1359	1462	47		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	455	GLU	GLN	CONFLICT	UNP Q9E3V8

- Molecule 3 is a protein called VP3B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1196	Total	C	N	O	S	0	0
			9154	5805	1575	1722	52		

- Molecule 4 is a protein called Core protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	412	Total	C	N	O	S	0	0
			3145	2013	545	571	16		
4	E	412	Total	C	N	O	S	0	0
			3145	2013	545	571	16		

- Molecule 5 is a protein called Outer capsid VP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	276	Total	C	N	O	S	0	0
			2085	1288	378	402	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	H	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	L	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	M	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	N	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	R	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	S	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	T	276	Total 2085	C 1288	N 378	O 402	S 17	0	0
5	Y	276	Total 2085	C 1288	N 378	O 402	S 17	0	0

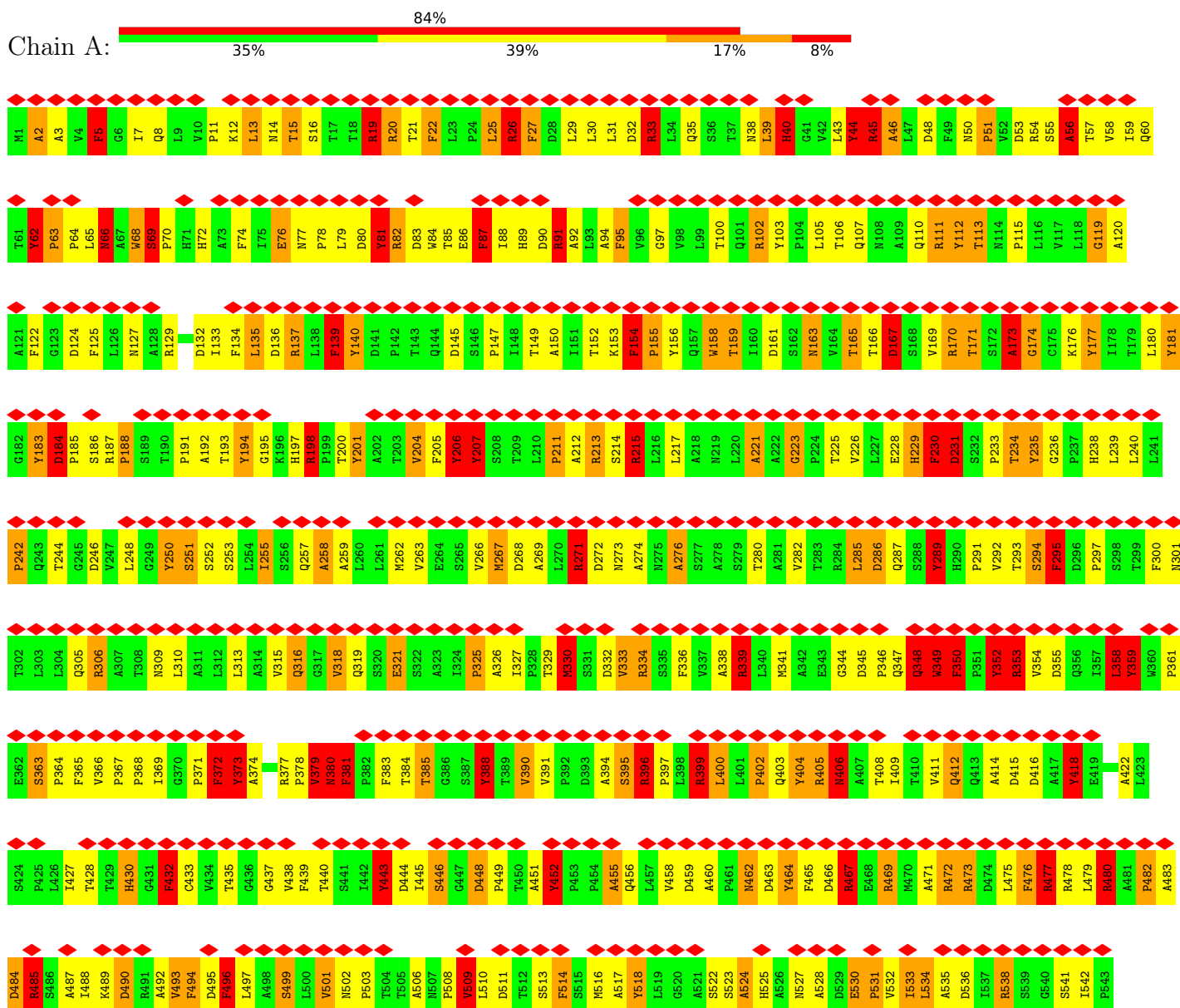
- Molecule 6 is a protein called Outer capsid VP5.

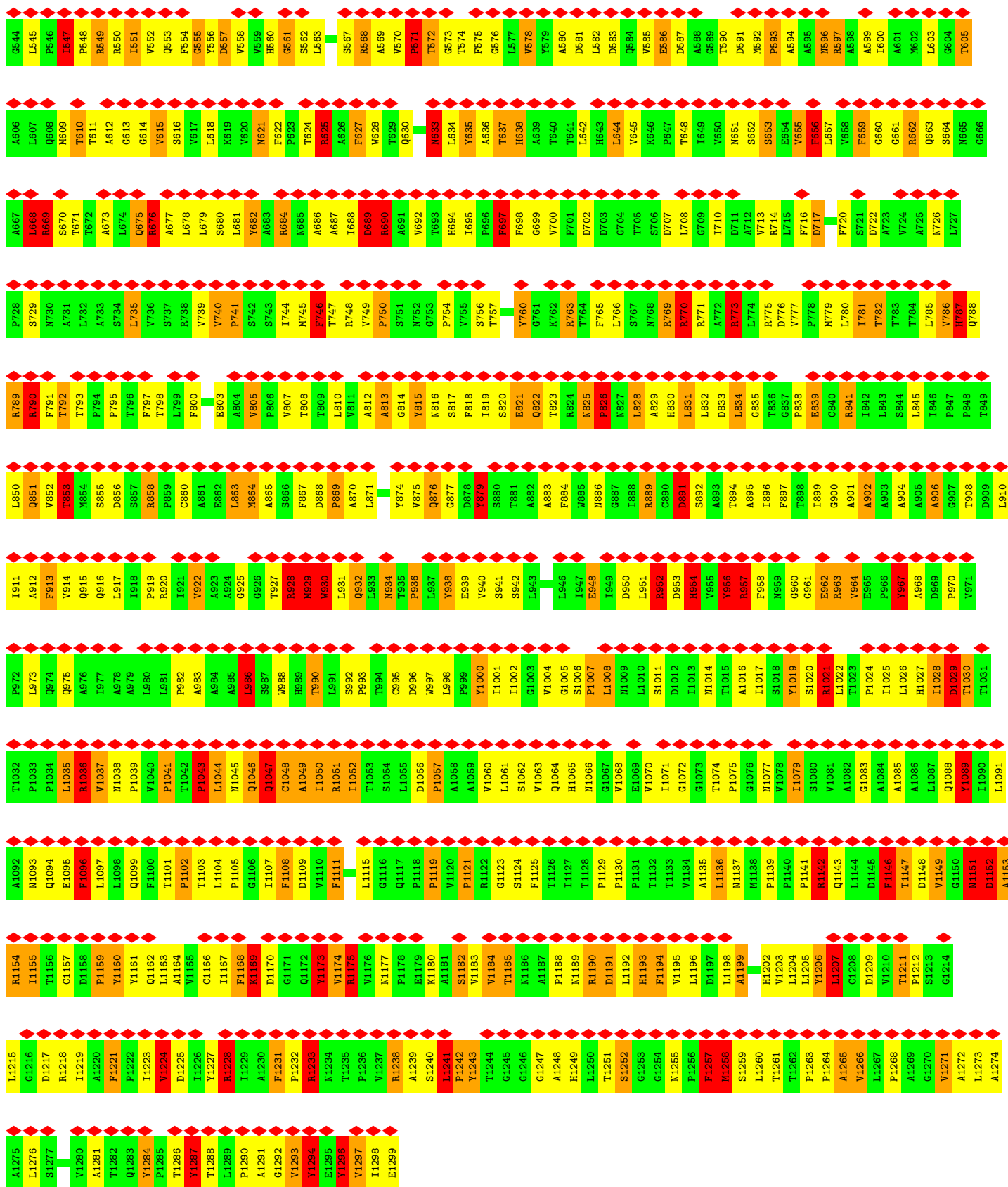
Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	J	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	K	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	O	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	P	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	Q	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	U	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	V	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	W	639	Total 4758	C 3012	N 801	O 927	S 18	0	0
6	X	639	Total 4758	C 3012	N 801	O 927	S 18	0	0

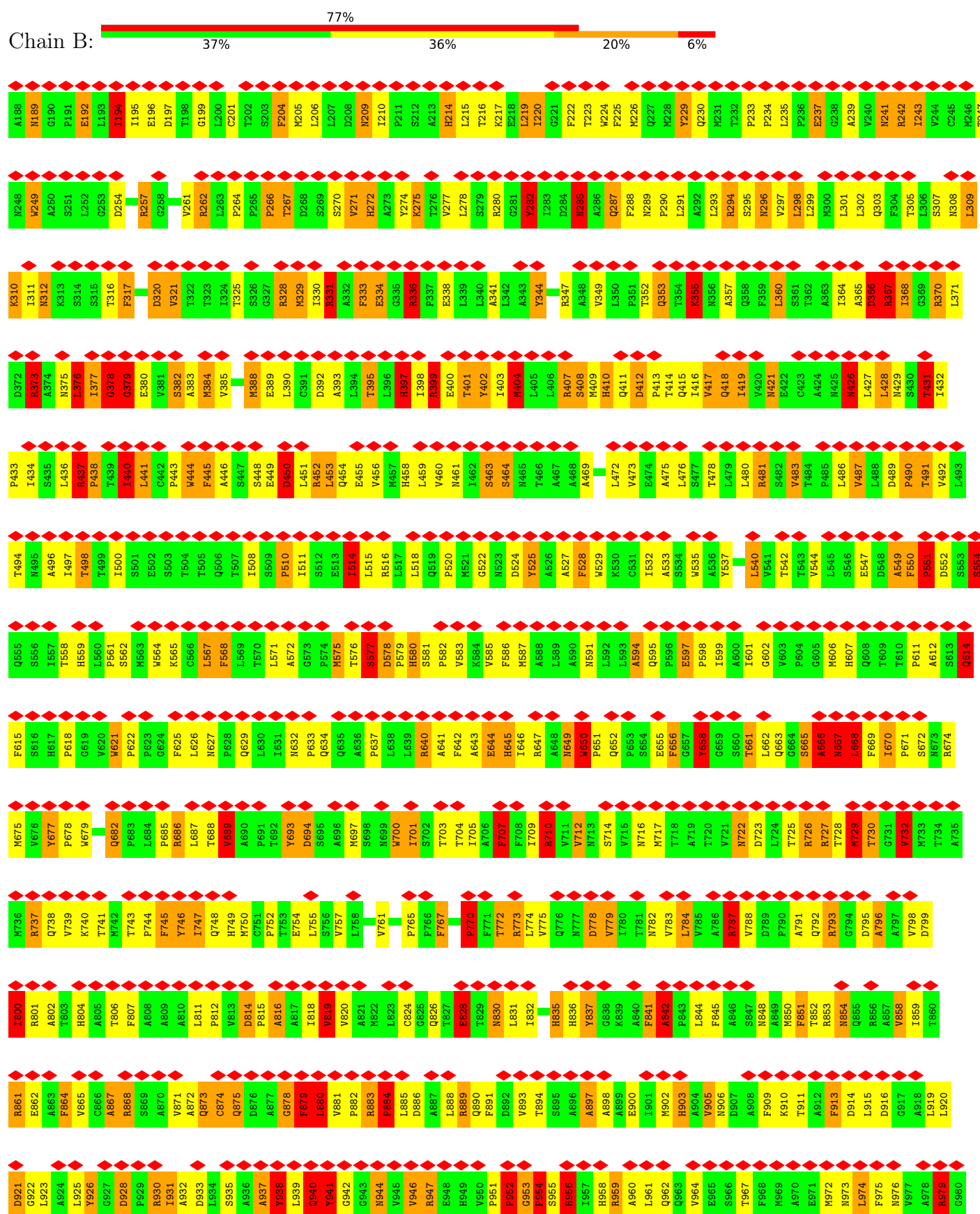
### 3 Residue-property plots

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.

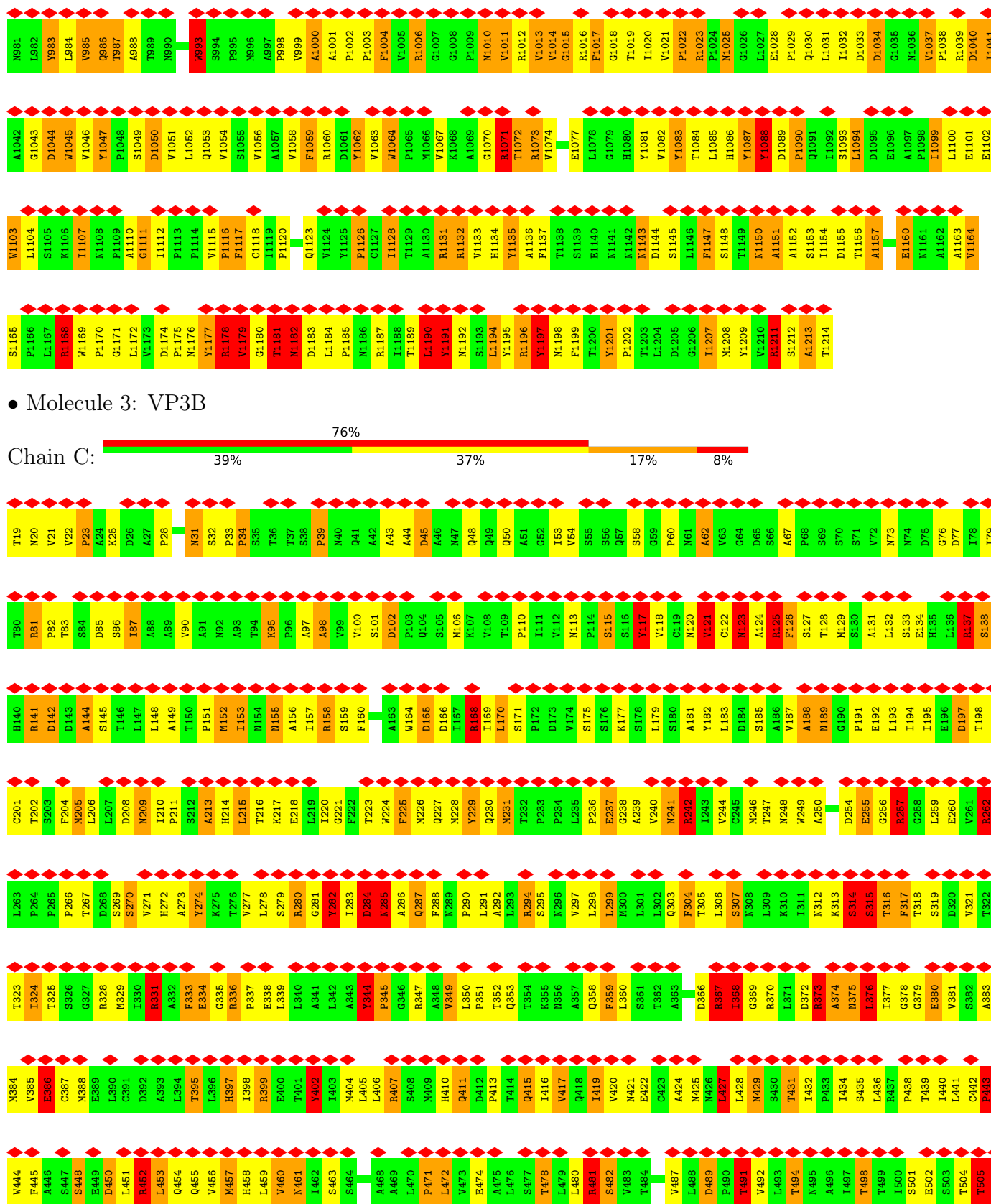
#### • Molecule 1: VP1



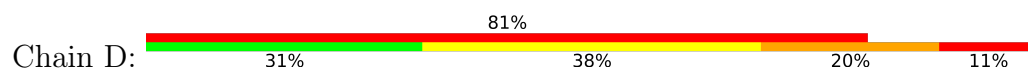




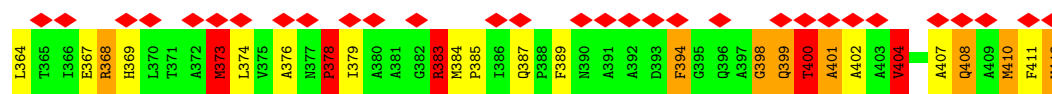




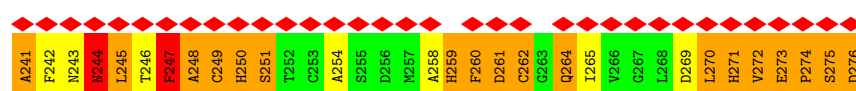
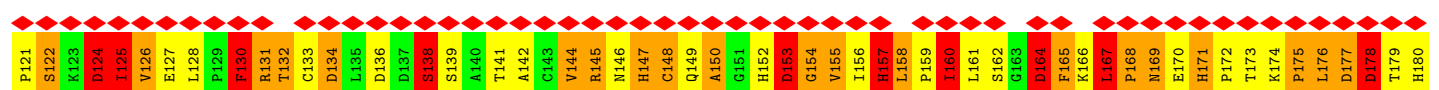
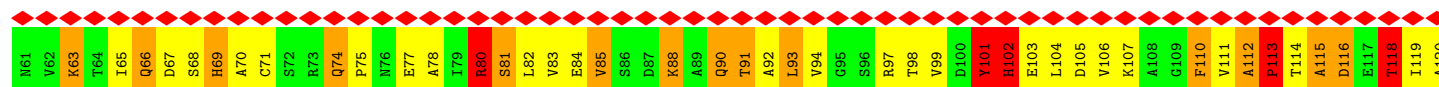
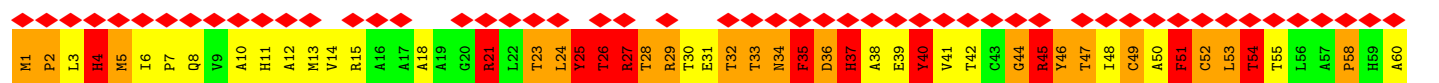
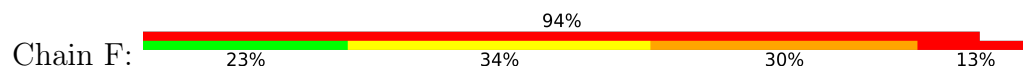
- Molecule 4: Core protein VP6



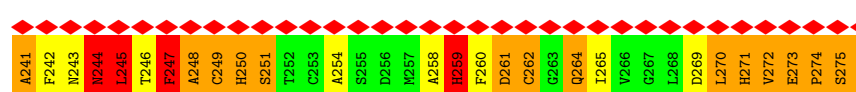
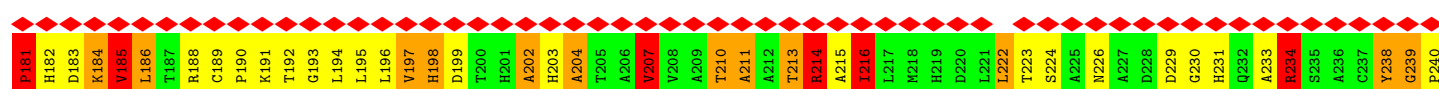
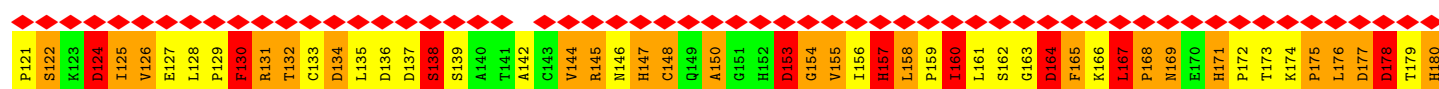
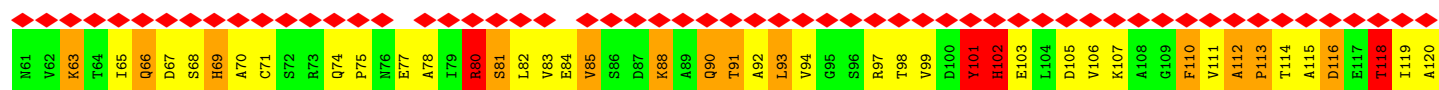
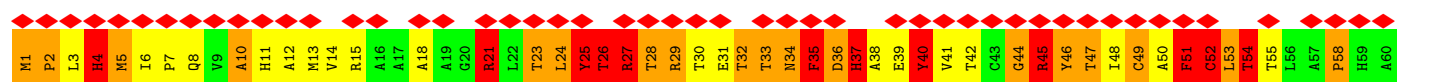
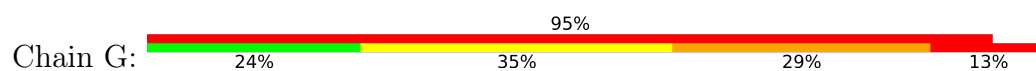




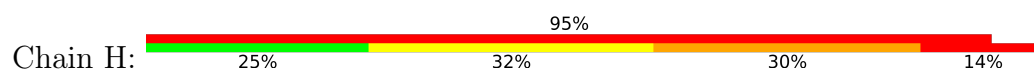
## • Molecule 5: Outer capsid VP7

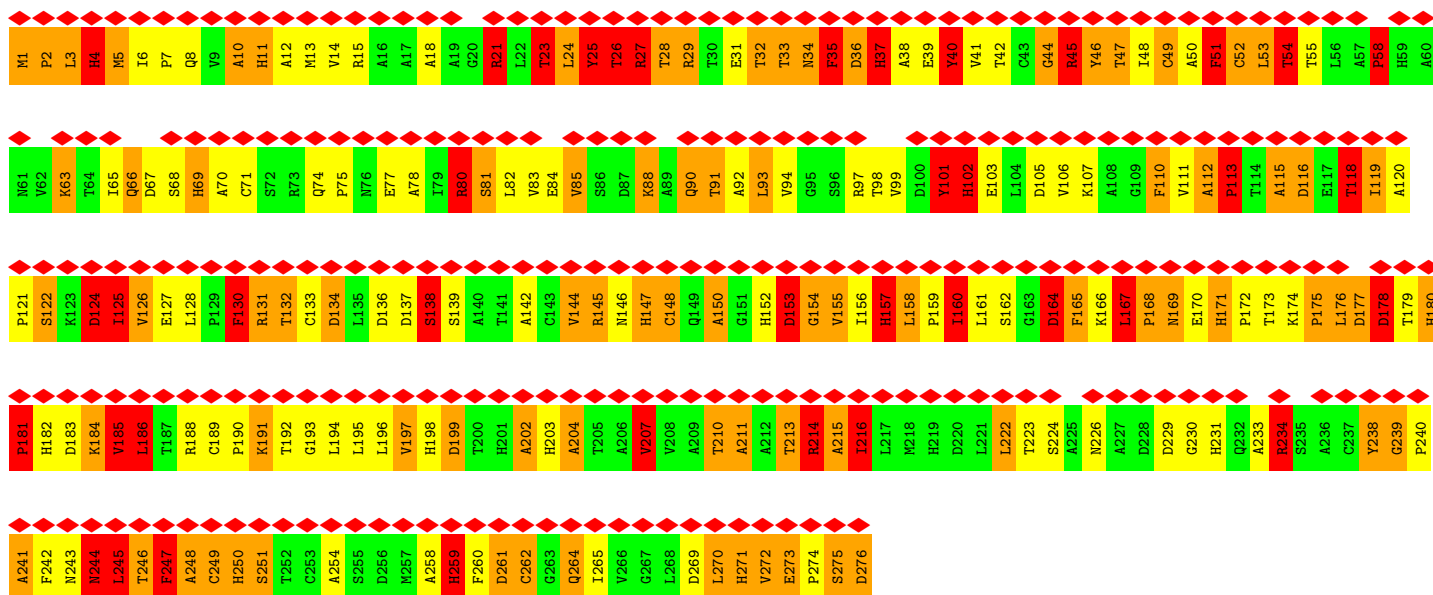


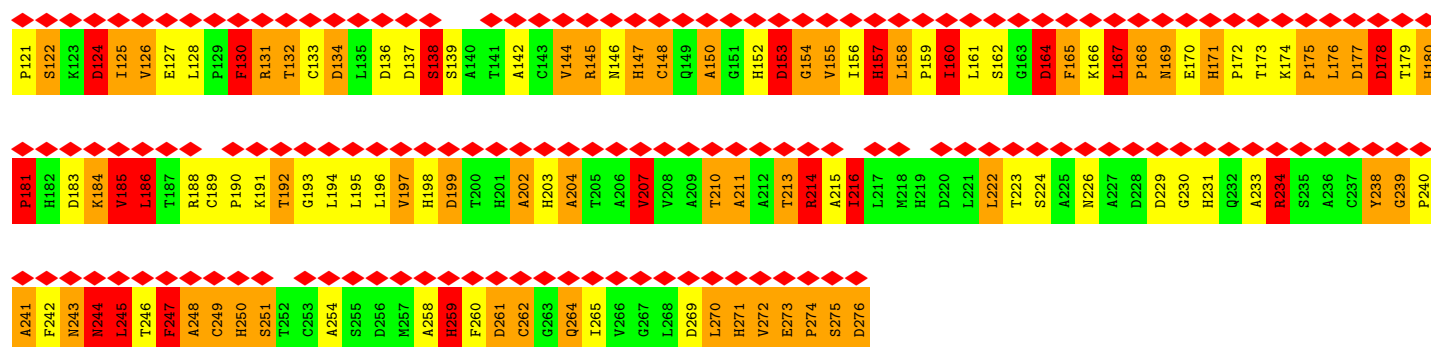
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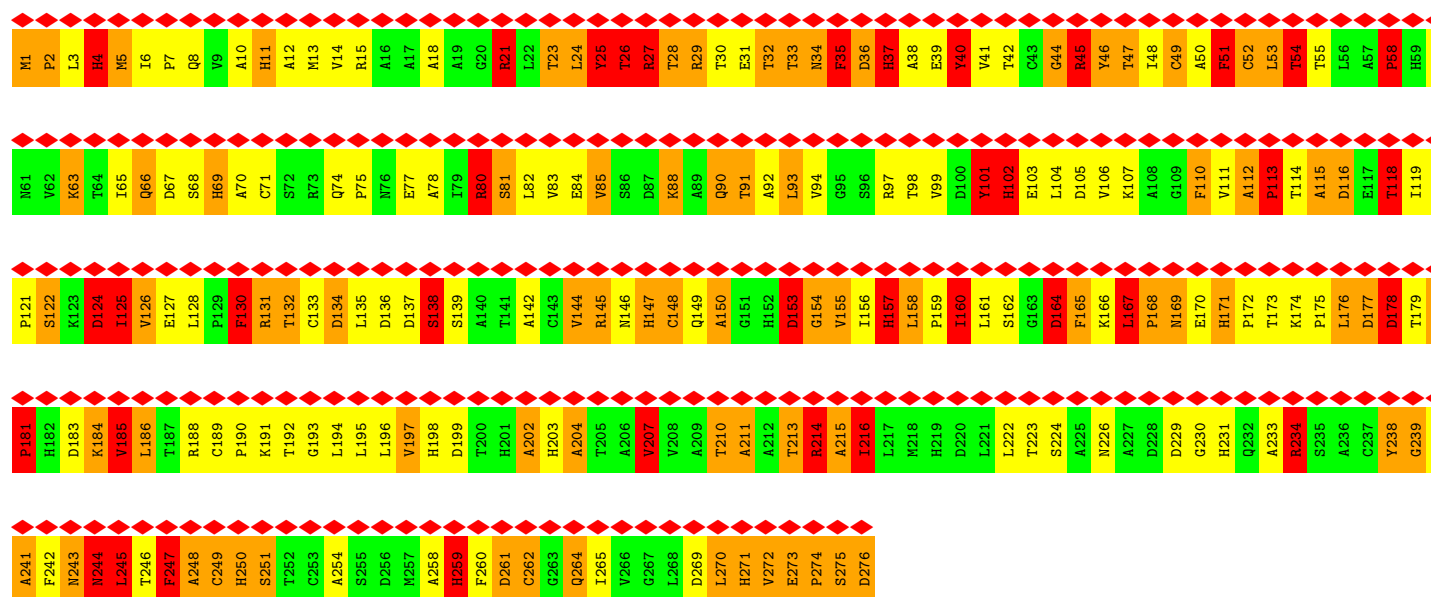
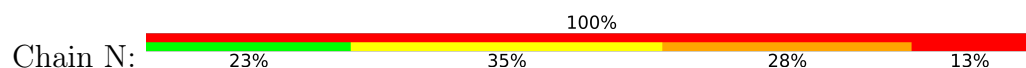
## • Molecule 5: Outer capsid VP7



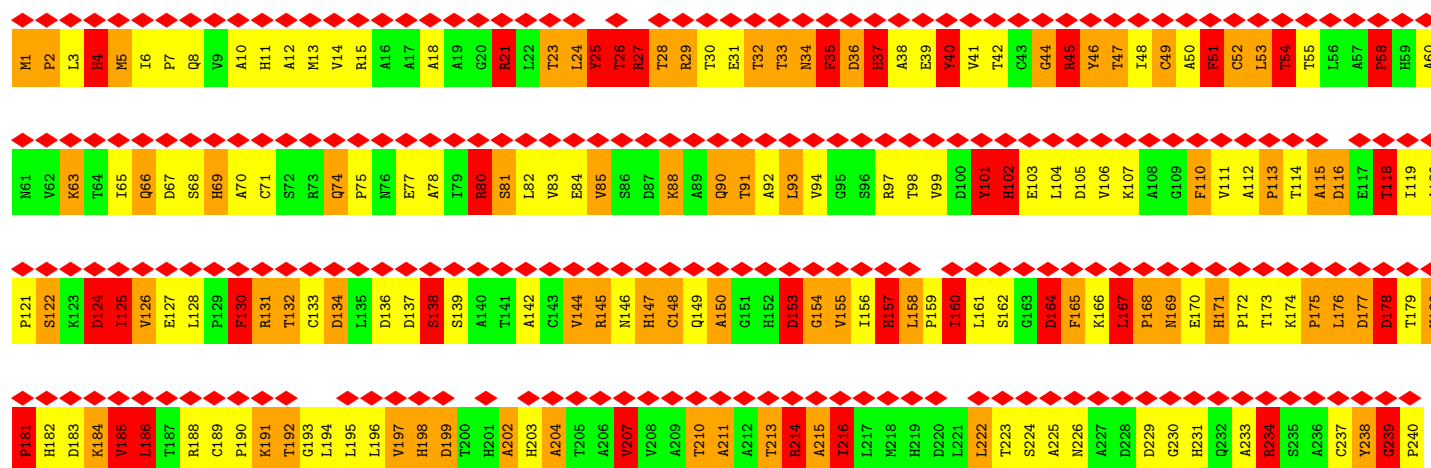
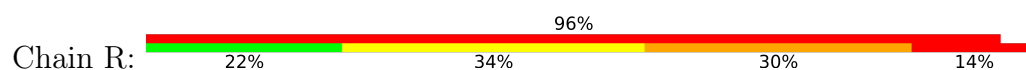


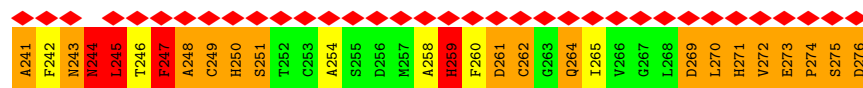


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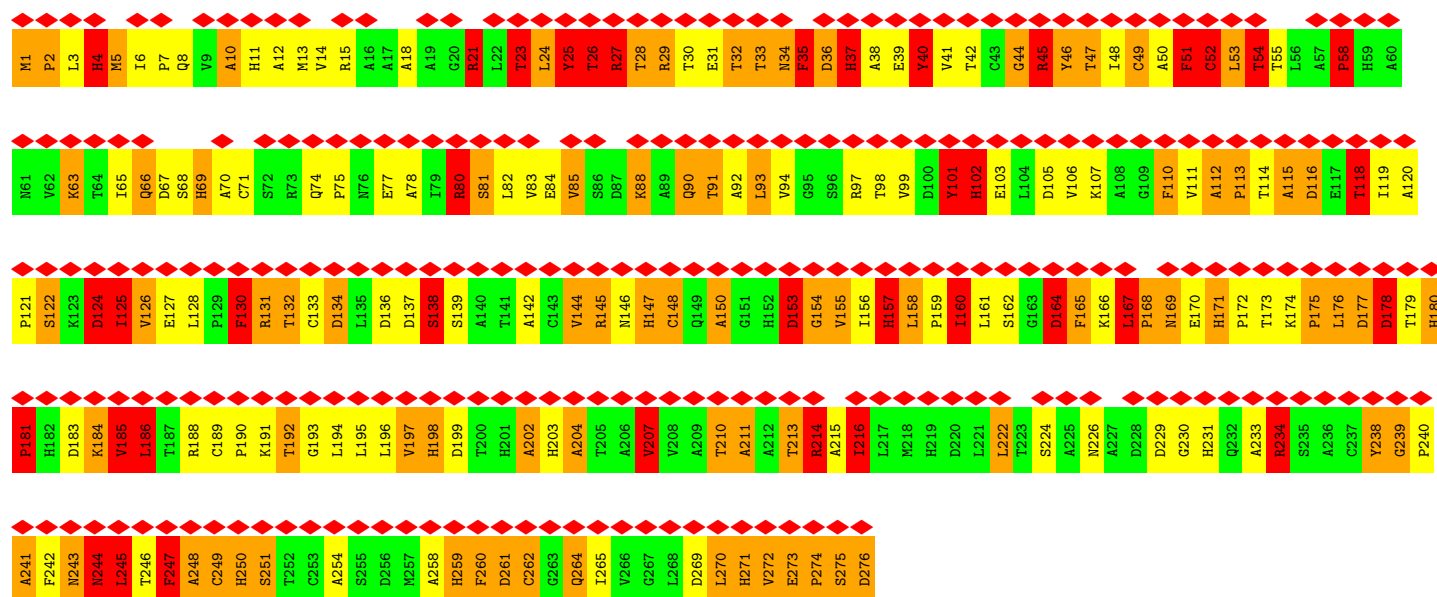
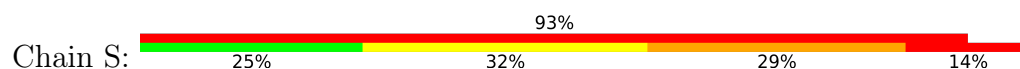


• Molecule 5: Outer capsid VP7

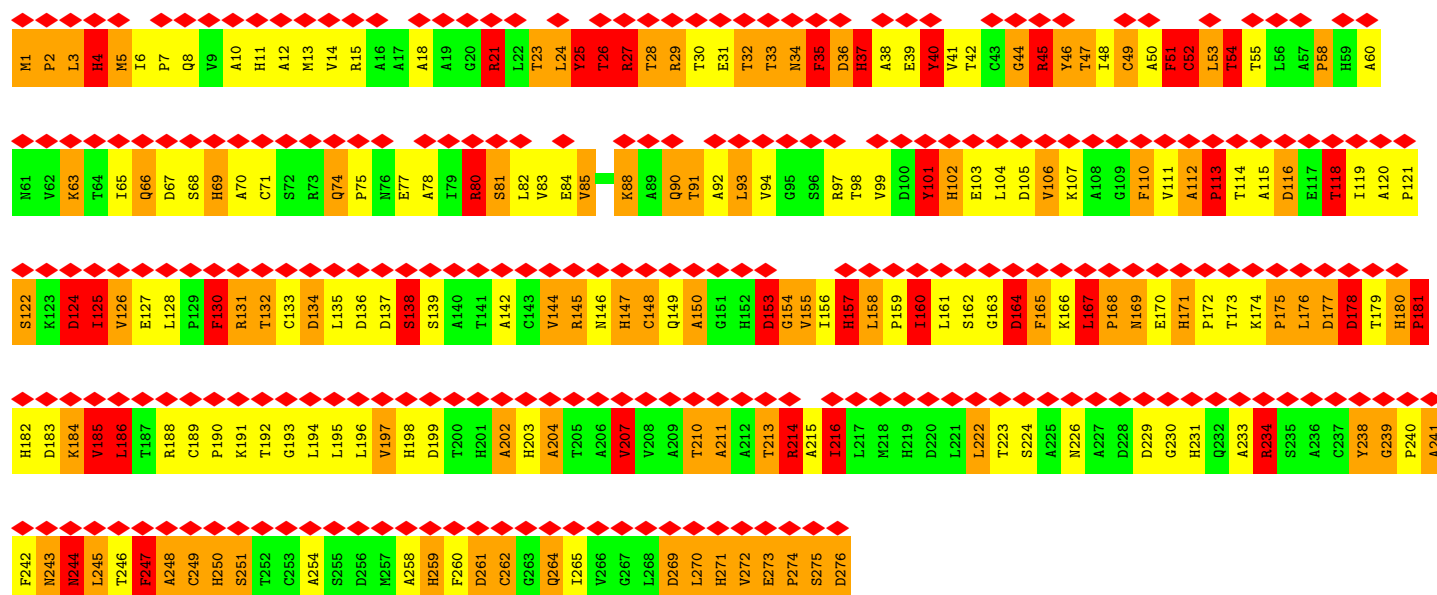
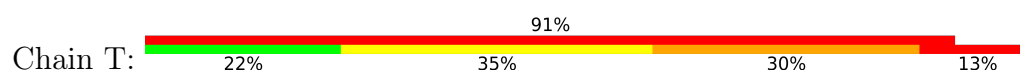




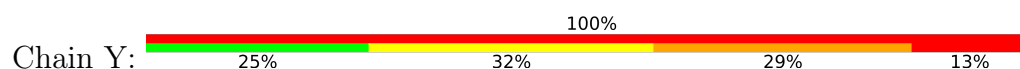
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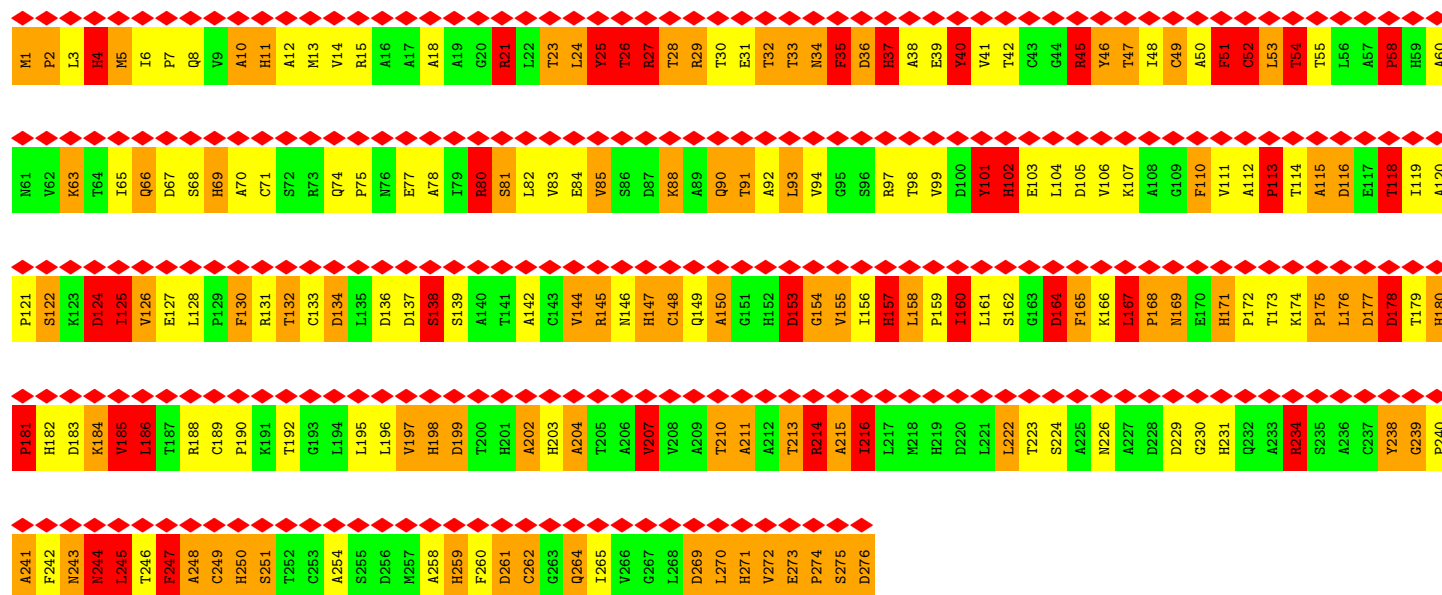


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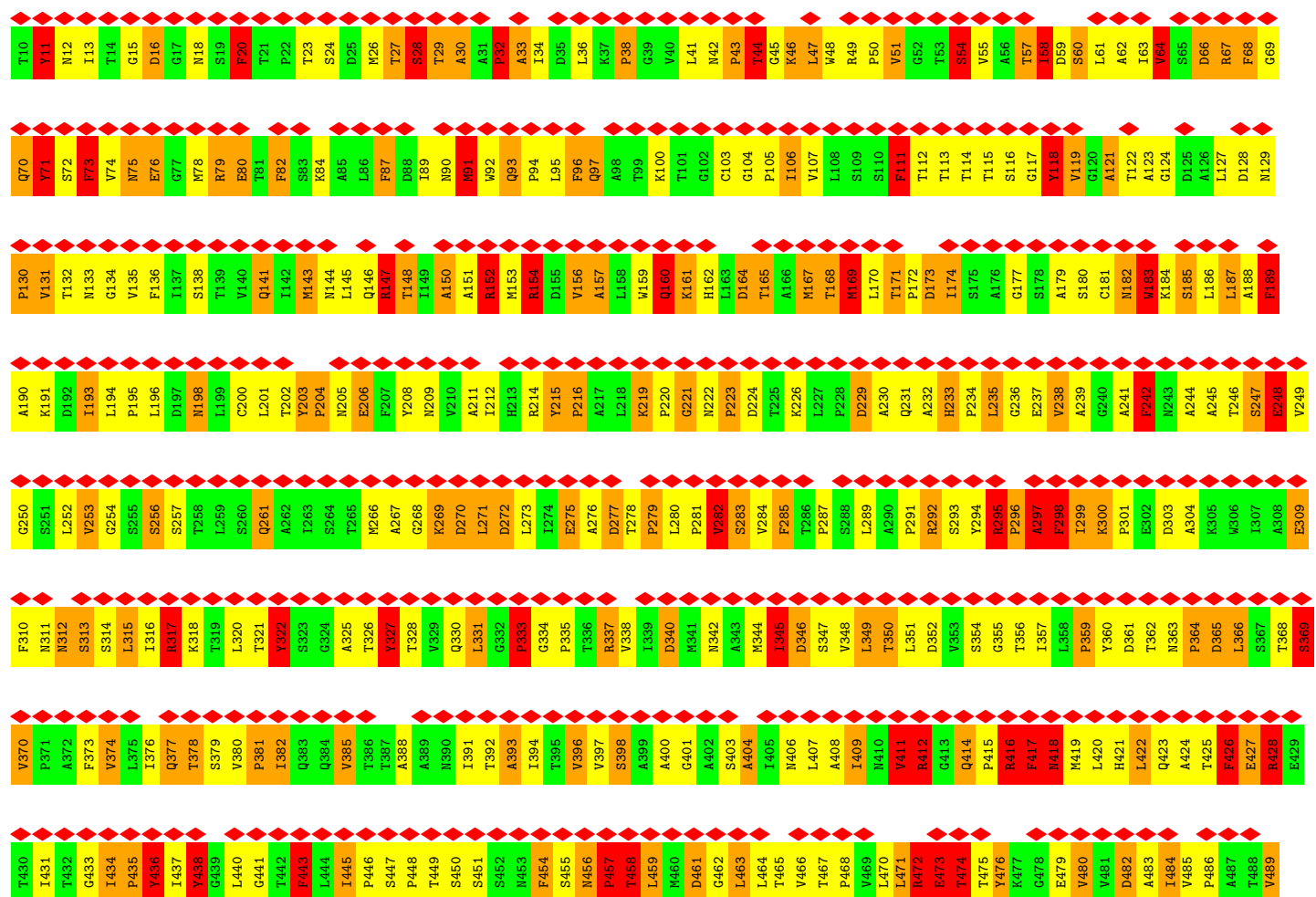
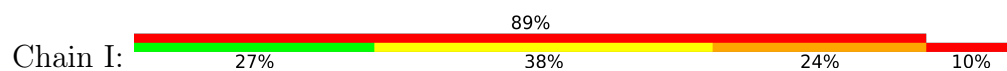


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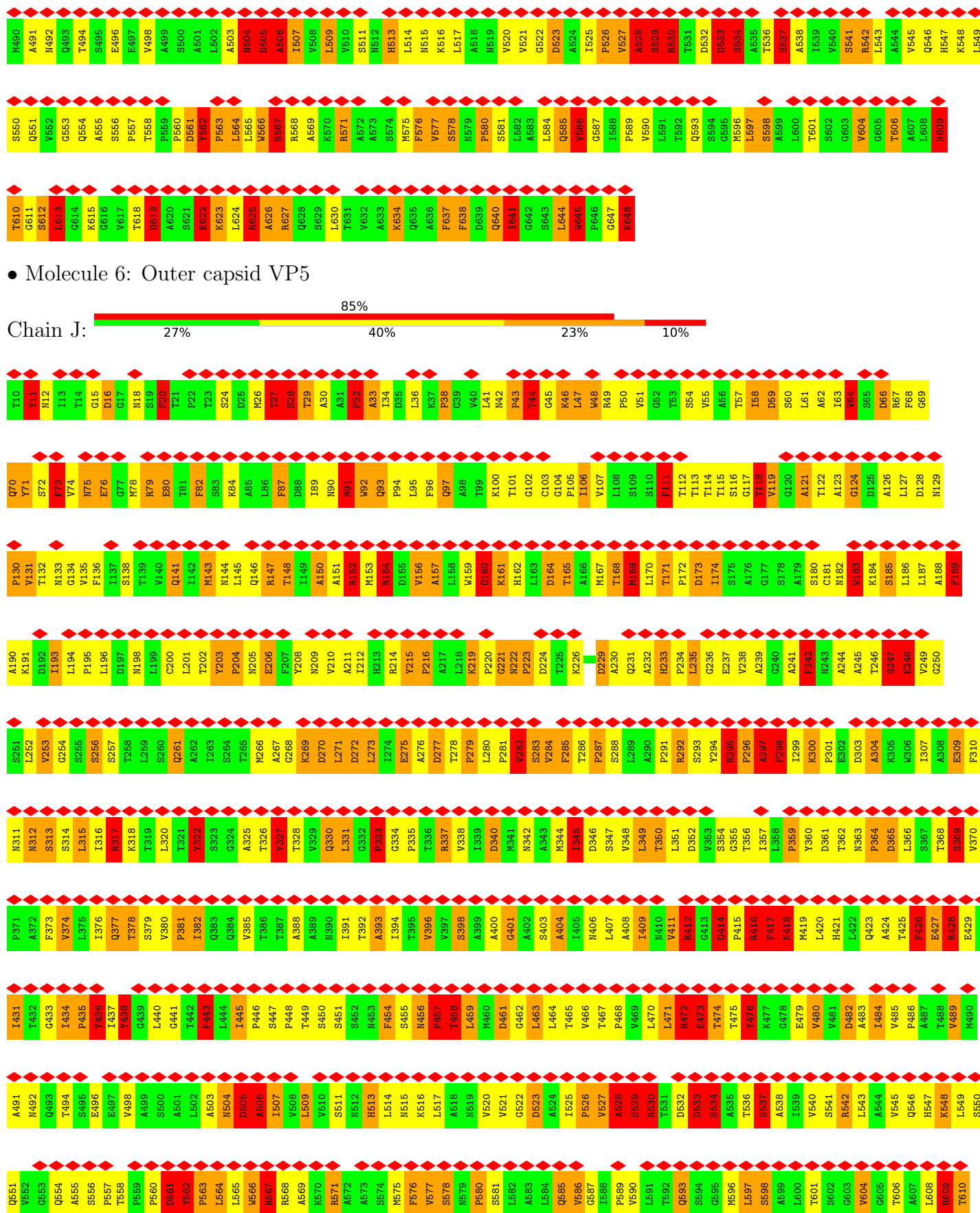


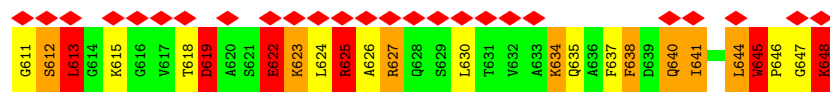


• Molecule 6: Outer capsid VP5

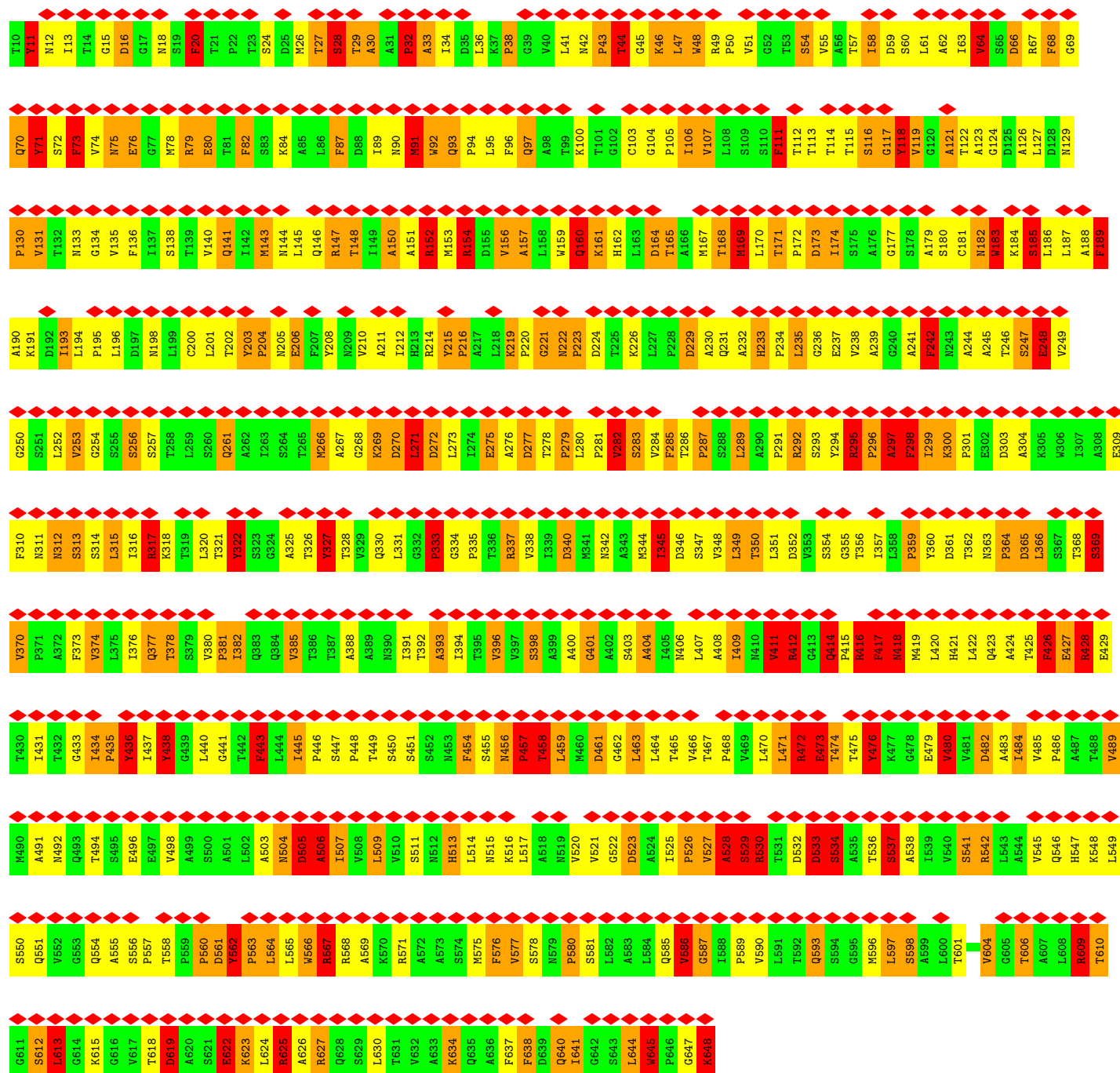
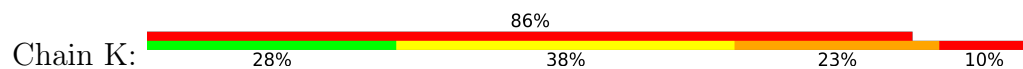




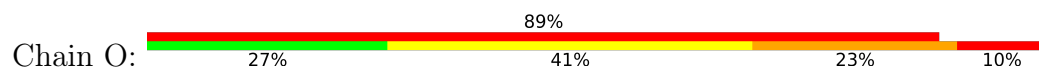


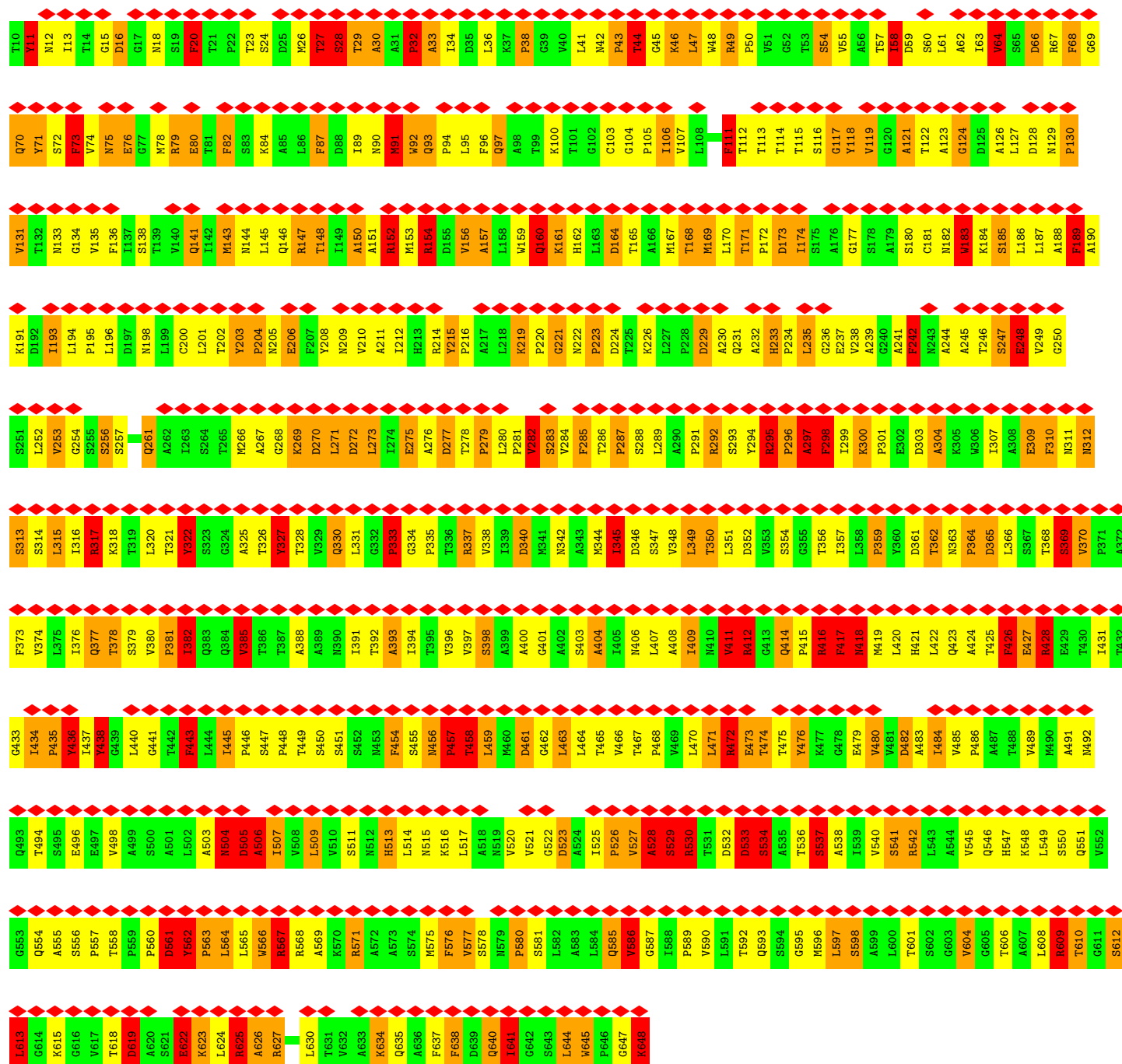


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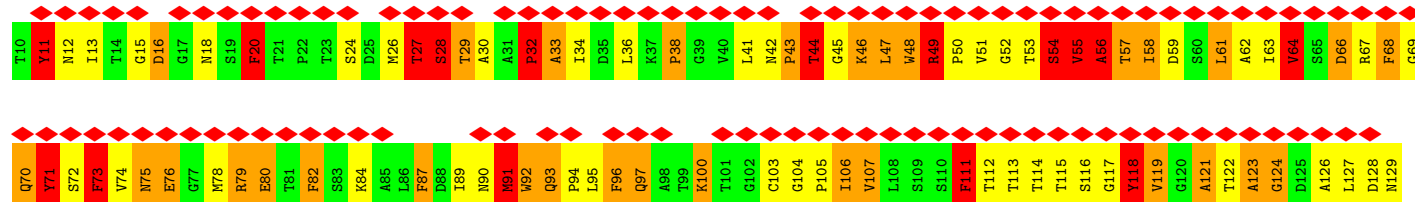
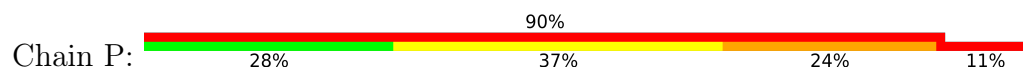


• Molecule 6: Outer capsid VP5

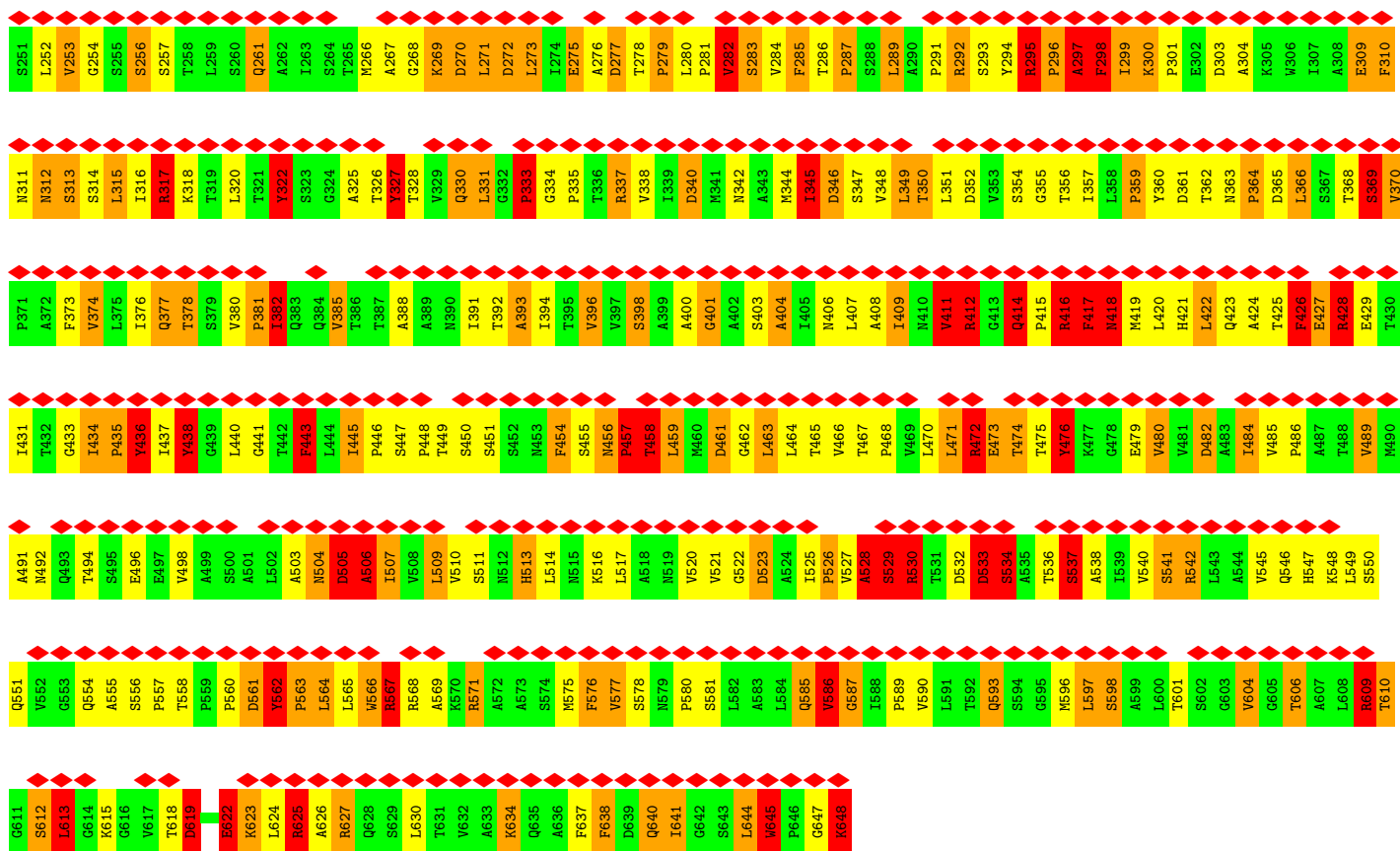




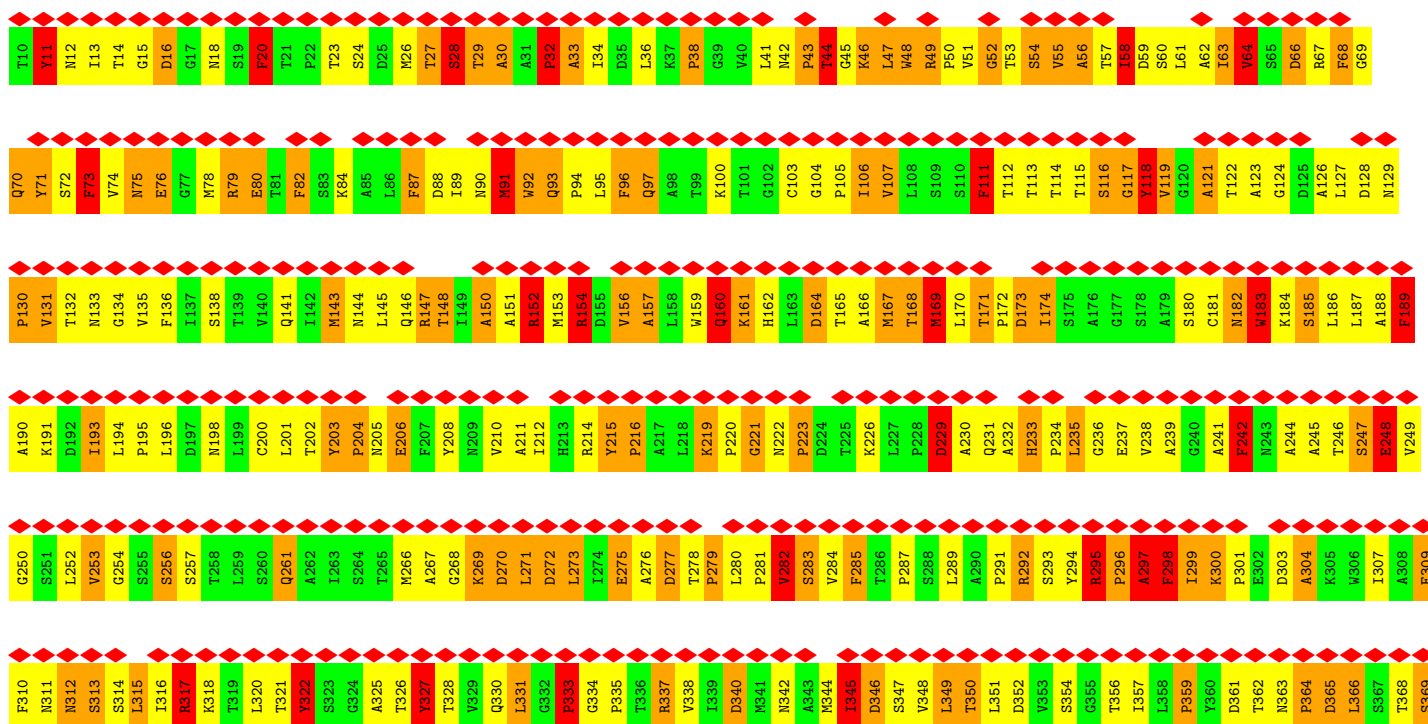
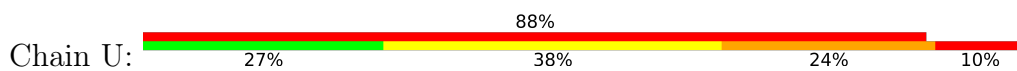
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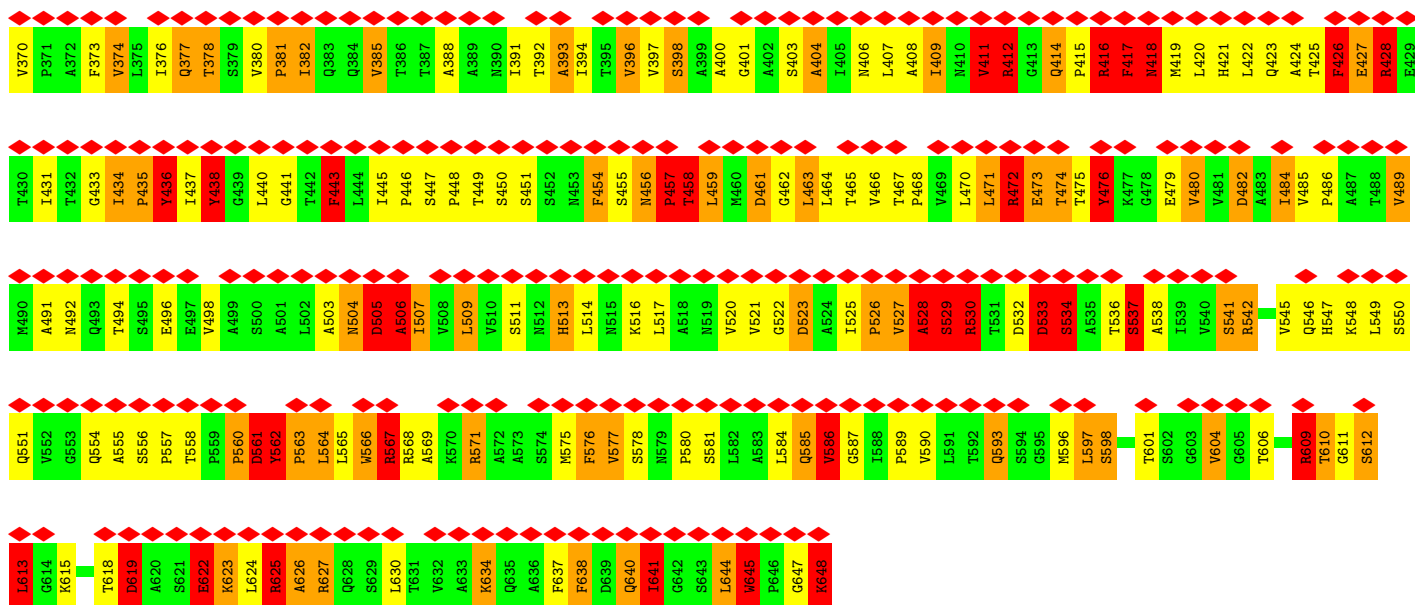




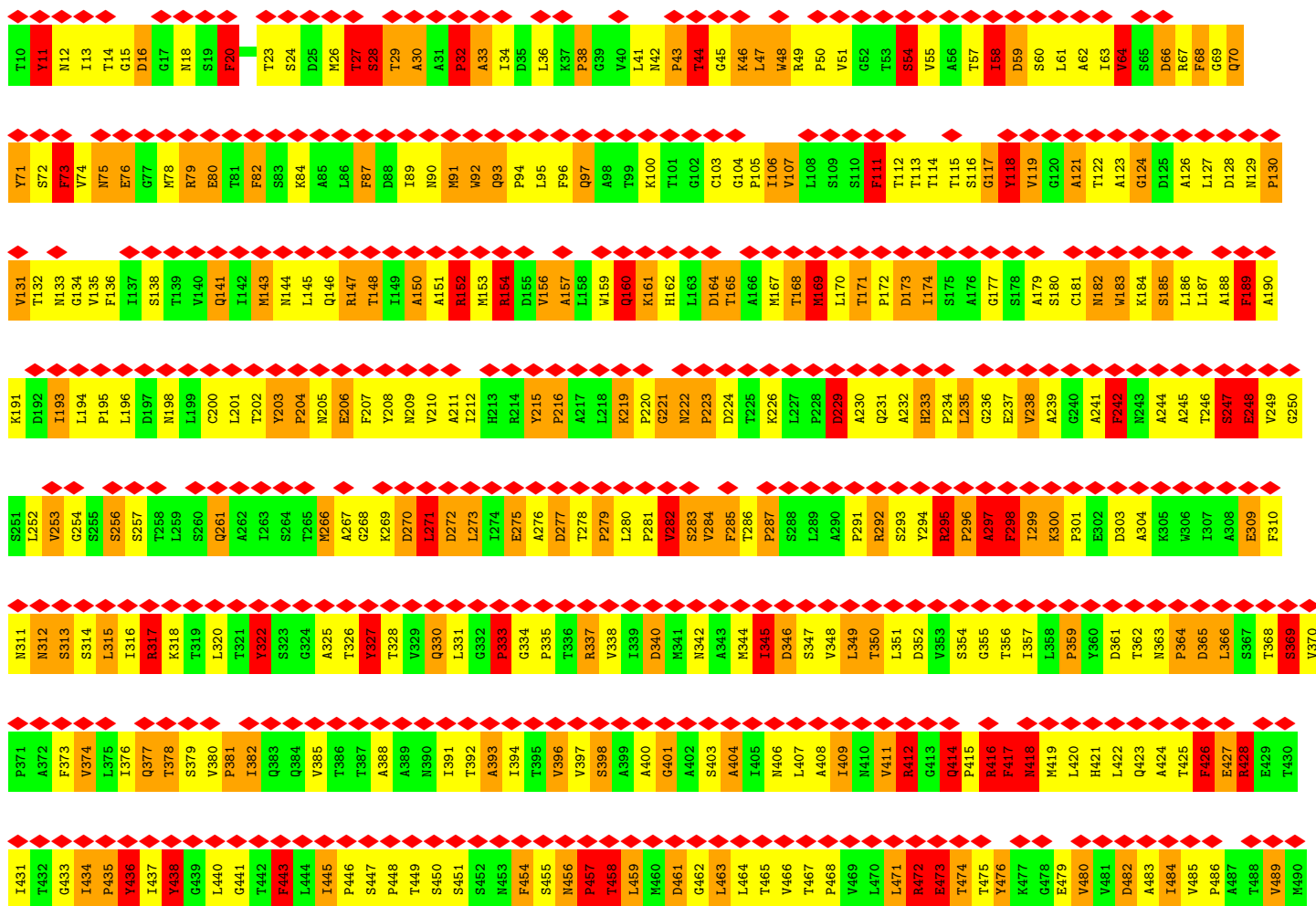
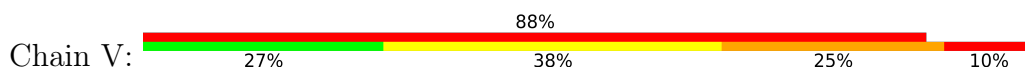


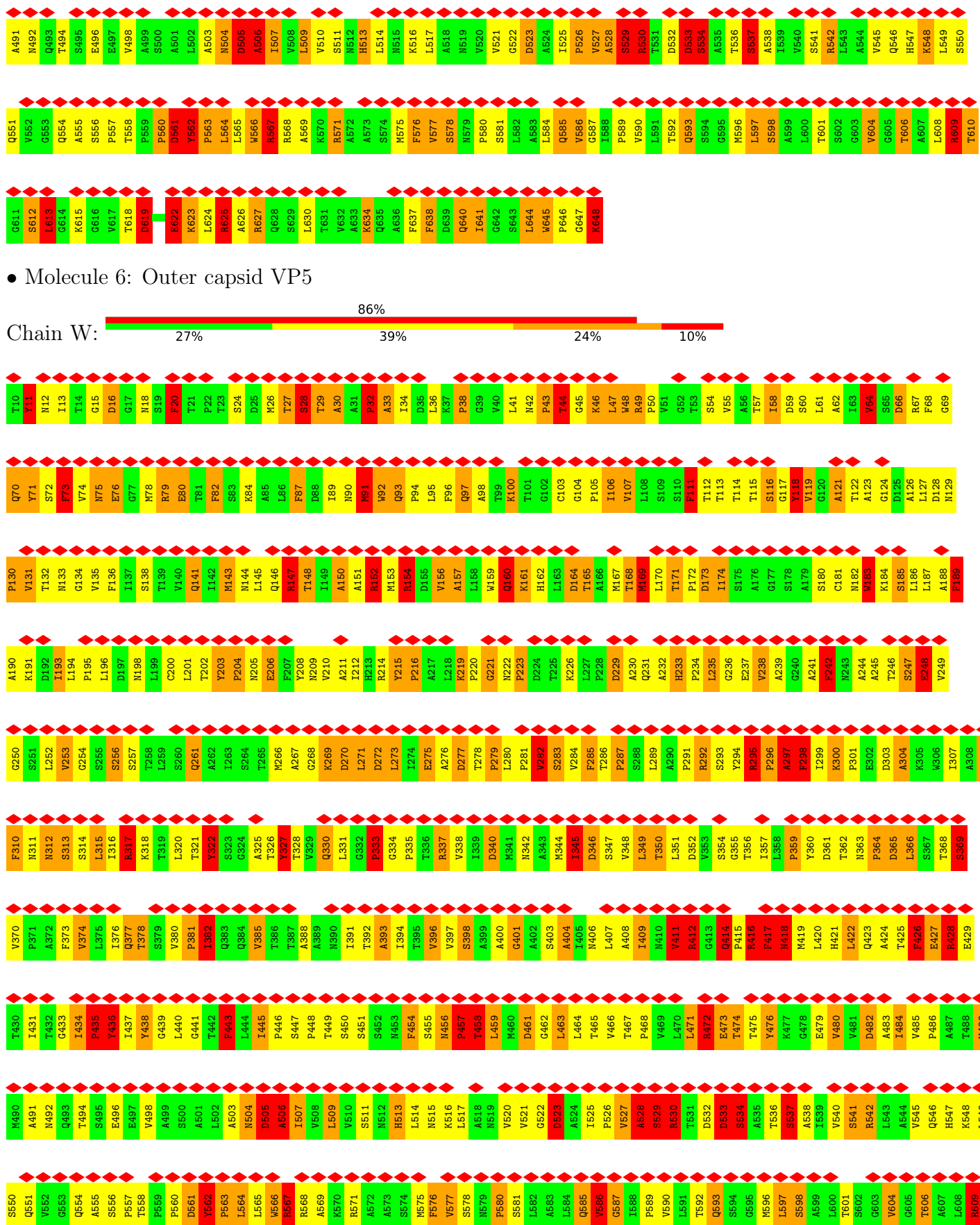
• Molecule 6: Outer capsid VP5





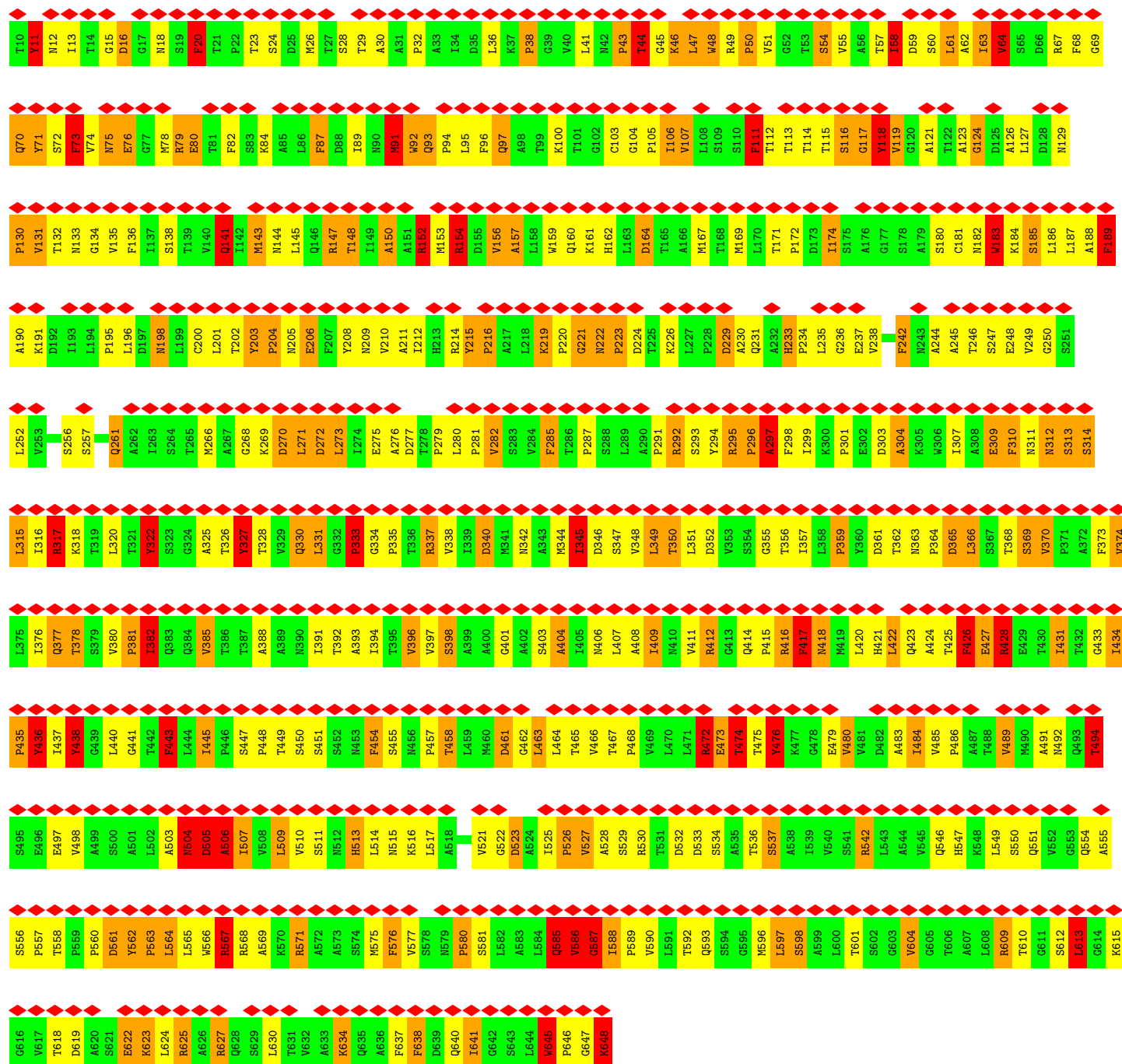
● Molecule 6: Outer capsid VP5







## • Molecule 6: Outer capsid VP5





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	15000	Depositor
Resolution determination method	Not provided	
CTF correction method	Fully corrected. See Zhou et al., 1999, J. Virol. 73, 3210-3218	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	154380	Depositor
Image detector	GENERIC CCD	Depositor
Maximum map value	6.460	Depositor
Minimum map value	-8.591	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.721	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	901.645, 901.645, 450.822	wwPDB
Map dimensions	929, 929, 465	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	0.9716, 0.9716, 0.9716	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	A	0.56	0/10259	2.41	538/14091 (3.8%)
2	B	0.55	0/8142	2.55	420/11160 (3.8%)
3	C	0.55	0/9383	2.56	471/12866 (3.7%)
4	D	0.55	0/3240	2.54	172/4453 (3.9%)
4	E	0.56	0/3240	2.44	181/4453 (4.1%)
5	F	0.50	0/2132	2.40	115/2912 (3.9%)
5	G	0.50	0/2132	2.41	113/2912 (3.9%)
5	H	0.50	0/2132	2.40	116/2912 (4.0%)
5	L	0.50	0/2132	2.40	116/2912 (4.0%)
5	M	0.51	0/2132	2.39	114/2912 (3.9%)
5	N	0.51	0/2132	2.39	111/2912 (3.8%)
5	R	0.51	0/2132	2.41	121/2912 (4.2%)
5	S	0.51	0/2132	2.40	116/2912 (4.0%)
5	T	0.51	0/2132	2.40	116/2912 (4.0%)
5	Y	0.50	0/2132	2.43	114/2912 (3.9%)
6	I	0.53	0/4856	3.09	312/6646 (4.7%)
6	J	0.53	0/4856	3.03	308/6646 (4.6%)
6	K	0.52	0/4856	3.02	312/6646 (4.7%)
6	O	0.53	0/4856	3.03	302/6646 (4.5%)
6	P	0.70	3/4856 (0.1%)	3.26	317/6646 (4.8%)
6	Q	0.53	0/4856	3.12	316/6646 (4.8%)
6	U	0.53	0/4856	3.04	312/6646 (4.7%)
6	V	0.53	0/4856	3.03	315/6646 (4.7%)
6	W	0.52	0/4856	3.08	313/6646 (4.7%)
6	X	0.53	0/4856	2.38	226/6646 (3.4%)
All	All	0.54	3/104144 (0.0%)	2.74	5967/142603 (4.2%)

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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
-----	-------	---------------------	---------------------

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	285
2	B	0	206
3	C	1	274
4	D	0	87
4	E	0	98
5	F	0	68
5	G	0	67
5	H	0	68
5	L	0	66
5	M	0	69
5	N	0	67
5	R	0	68
5	S	0	67
5	T	0	67
5	Y	0	68
6	I	0	155
6	J	0	142
6	K	0	149
6	O	0	145
6	P	0	147
6	Q	0	146
6	U	0	145
6	V	0	141
6	W	0	146
6	X	0	135
All	All	1	3076

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	56	ALA	CA-CB	25.04	2.05	1.52
6	P	56	ALA	N-CA	-14.68	1.17	1.46
6	P	56	ALA	CA-C	-11.44	1.23	1.52

The worst 5 of 5967 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	248	GLU	OE1-CD-OE2	-80.62	26.56	123.30
6	Q	248	GLU	OE1-CD-OE2	-80.09	27.19	123.30
6	K	248	GLU	OE1-CD-OE2	-77.76	29.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	248	GLU	OE1-CD-OE2	-76.08	32.01	123.30
6	U	248	GLU	OE1-CD-OE2	-75.94	32.18	123.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	315	SER	CA

5 of 3076 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	PRO	Mainchain
1	A	13	LEU	Mainchain
1	A	19	ARG	Sidechain
1	A	20	ARG	Sidechain
1	A	5	PHE	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9989	0	9916	381	0
2	B	7935	0	7904	765	0
3	C	9154	0	9092	604	0
4	D	3145	0	3071	587	0
4	E	3145	0	3071	274	0
5	F	2085	0	2019	225	0
5	G	2085	0	2019	232	0
5	H	2085	0	2019	238	0
5	L	2085	0	2019	221	0
5	M	2085	0	2019	226	0
5	N	2085	0	2019	241	0
5	R	2085	0	2019	221	0
5	S	2085	0	2019	235	0
5	T	2085	0	2019	244	0
5	Y	2085	0	2019	168	0
6	I	4758	0	4791	1941	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	4758	0	4792	1863	0
6	K	4758	0	4793	1854	0
6	O	4758	0	4792	1888	0
6	P	4758	0	4791	2017	0
6	Q	4758	0	4792	1844	0
6	U	4758	0	4792	2037	0
6	V	4758	0	4793	1877	0
6	W	4758	0	4790	1906	0
6	X	4758	0	4797	224	0
All	All	101798	0	101167	13378	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 66.

The worst 5 of 13378 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)
5:N:4:HIS:CG	6:O:586:VAL:HG22	1.19	1.72
6:U:66:ASP:HB2	6:V:232:ALA:CB	1.22	1.68
6:V:193:ILE:HG22	6:W:562:TYR:CE1	1.24	1.68
6:U:193:ILE:HG22	6:V:562:TYR:CE1	1.27	1.67
6:U:459:LEU:CB	6:V:414:GLN:HE22	1.05	1.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1297/1299 (100%)	974 (75%)	214 (16%)	109 (8%)	<a href="#">1</a> <a href="#">13</a>
2	B	1025/1027 (100%)	842 (82%)	136 (13%)	47 (5%)	<a href="#">2</a> <a href="#">24</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	1194/1196 (100%)	904 (76%)	201 (17%)	89 (8%)	1	15
4	D	410/412 (100%)	317 (77%)	54 (13%)	39 (10%)	0	11
4	E	410/412 (100%)	307 (75%)	75 (18%)	28 (7%)	1	17
5	F	274/276 (99%)	167 (61%)	66 (24%)	41 (15%)	0	4
5	G	274/276 (99%)	170 (62%)	61 (22%)	43 (16%)	0	4
5	H	274/276 (99%)	170 (62%)	62 (23%)	42 (15%)	0	4
5	L	274/276 (99%)	168 (61%)	62 (23%)	44 (16%)	0	3
5	M	274/276 (99%)	170 (62%)	62 (23%)	42 (15%)	0	4
5	N	274/276 (99%)	170 (62%)	62 (23%)	42 (15%)	0	4
5	R	274/276 (99%)	170 (62%)	61 (22%)	43 (16%)	0	4
5	S	274/276 (99%)	170 (62%)	61 (22%)	43 (16%)	0	4
5	T	274/276 (99%)	169 (62%)	62 (23%)	43 (16%)	0	4
5	Y	274/276 (99%)	169 (62%)	62 (23%)	43 (16%)	0	4
6	I	637/639 (100%)	477 (75%)	105 (16%)	55 (9%)	1	13
6	J	637/639 (100%)	476 (75%)	106 (17%)	55 (9%)	1	13
6	K	637/639 (100%)	479 (75%)	102 (16%)	56 (9%)	1	12
6	O	637/639 (100%)	478 (75%)	102 (16%)	57 (9%)	1	12
6	P	637/639 (100%)	476 (75%)	103 (16%)	58 (9%)	1	12
6	Q	637/639 (100%)	481 (76%)	102 (16%)	54 (8%)	1	13
6	U	637/639 (100%)	477 (75%)	105 (16%)	55 (9%)	1	13
6	V	637/639 (100%)	479 (75%)	100 (16%)	58 (9%)	1	12
6	W	637/639 (100%)	482 (76%)	99 (16%)	56 (9%)	1	12
6	X	637/639 (100%)	482 (76%)	99 (16%)	56 (9%)	1	12
All	All	13446/13496 (100%)	9824 (73%)	2324 (17%)	1298 (10%)	1	11

5 of 1298 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	40	HIS
1	A	69	SER
1	A	76	GLU
1	A	153	LYS

### 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	A	1092/1092 (100%)	987 (90%)	105 (10%)	8	29
2	B	875/875 (100%)	788 (90%)	87 (10%)	8	28
3	C	1017/1017 (100%)	926 (91%)	91 (9%)	9	33
4	D	326/326 (100%)	283 (87%)	43 (13%)	4	20
4	E	326/326 (100%)	286 (88%)	40 (12%)	4	22
5	F	228/228 (100%)	199 (87%)	29 (13%)	4	21
5	G	228/228 (100%)	200 (88%)	28 (12%)	4	22
5	H	228/228 (100%)	199 (87%)	29 (13%)	4	21
5	L	228/228 (100%)	200 (88%)	28 (12%)	4	22
5	M	228/228 (100%)	200 (88%)	28 (12%)	4	22
5	N	228/228 (100%)	200 (88%)	28 (12%)	4	22
5	R	228/228 (100%)	199 (87%)	29 (13%)	4	21
5	S	228/228 (100%)	200 (88%)	28 (12%)	4	22
5	T	228/228 (100%)	199 (87%)	29 (13%)	4	21
5	Y	228/228 (100%)	200 (88%)	28 (12%)	4	22
6	I	528/528 (100%)	483 (92%)	45 (8%)	10	36
6	J	528/528 (100%)	486 (92%)	42 (8%)	12	38
6	K	528/528 (100%)	486 (92%)	42 (8%)	12	38
6	O	528/528 (100%)	485 (92%)	43 (8%)	11	37
6	P	528/528 (100%)	488 (92%)	40 (8%)	13	40
6	Q	528/528 (100%)	485 (92%)	43 (8%)	11	37
6	U	528/528 (100%)	485 (92%)	43 (8%)	11	37
6	V	528/528 (100%)	487 (92%)	41 (8%)	12	38
6	W	528/528 (100%)	485 (92%)	43 (8%)	11	37
6	X	528/528 (100%)	484 (92%)	44 (8%)	11	36
All	All	11196/11196 (100%)	10120 (90%)	1076 (10%)	12	29

5 of 1076 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	V	143	MET
6	V	558	THR
6	V	133	ASN
6	X	575	MET
5	F	210	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 252 such sidechains are listed below:

Mol	Chain	Res	Type
6	K	233	HIS
6	V	593	GLN
5	N	231	HIS
6	V	456	ASN
6	X	146	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

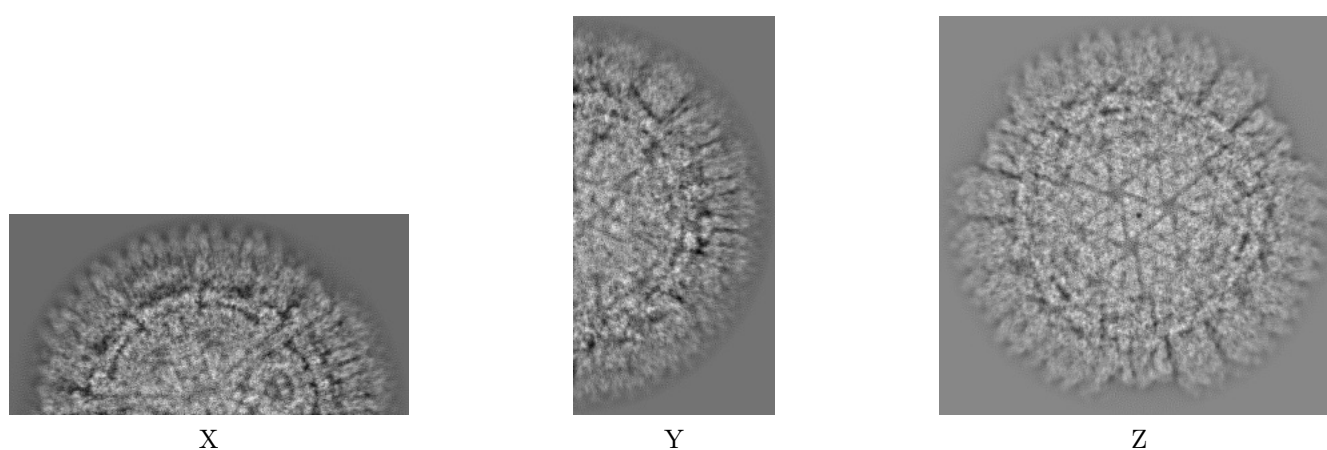
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1653. 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](#)

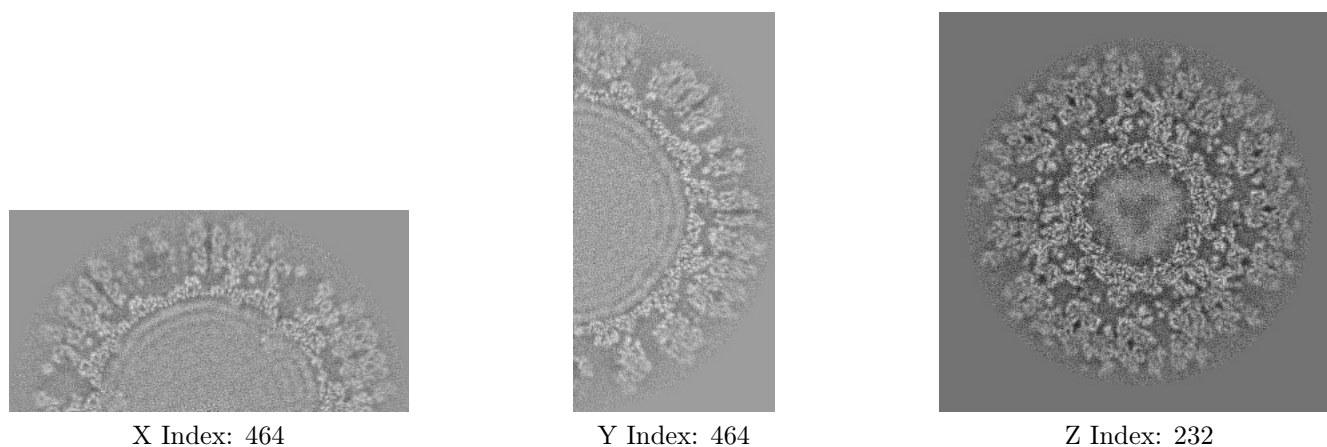
#### 6.1.1 Primary map



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

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

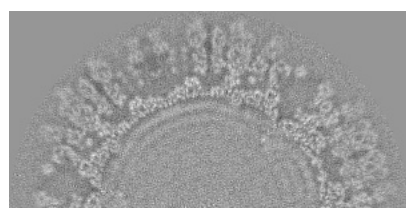
#### 6.2.1 Primary map



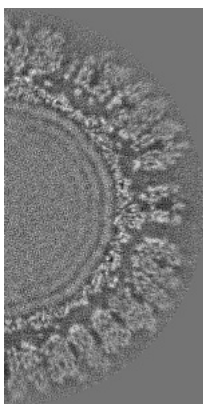
The images above show central slices of the map in three orthogonal directions.

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

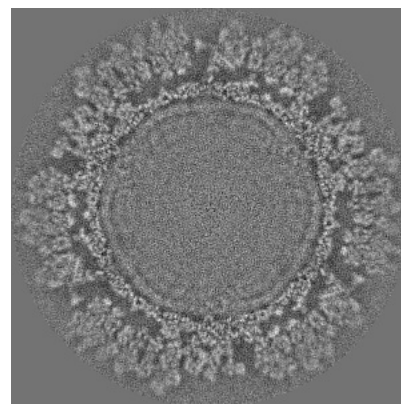
### 6.3.1 Primary map



X Index: 464



Y Index: 501

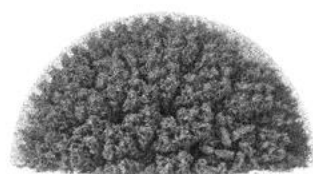


Z Index: 18

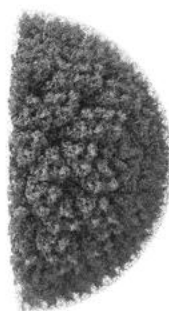
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

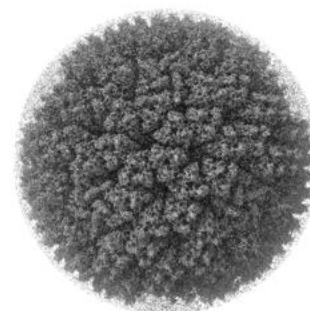
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

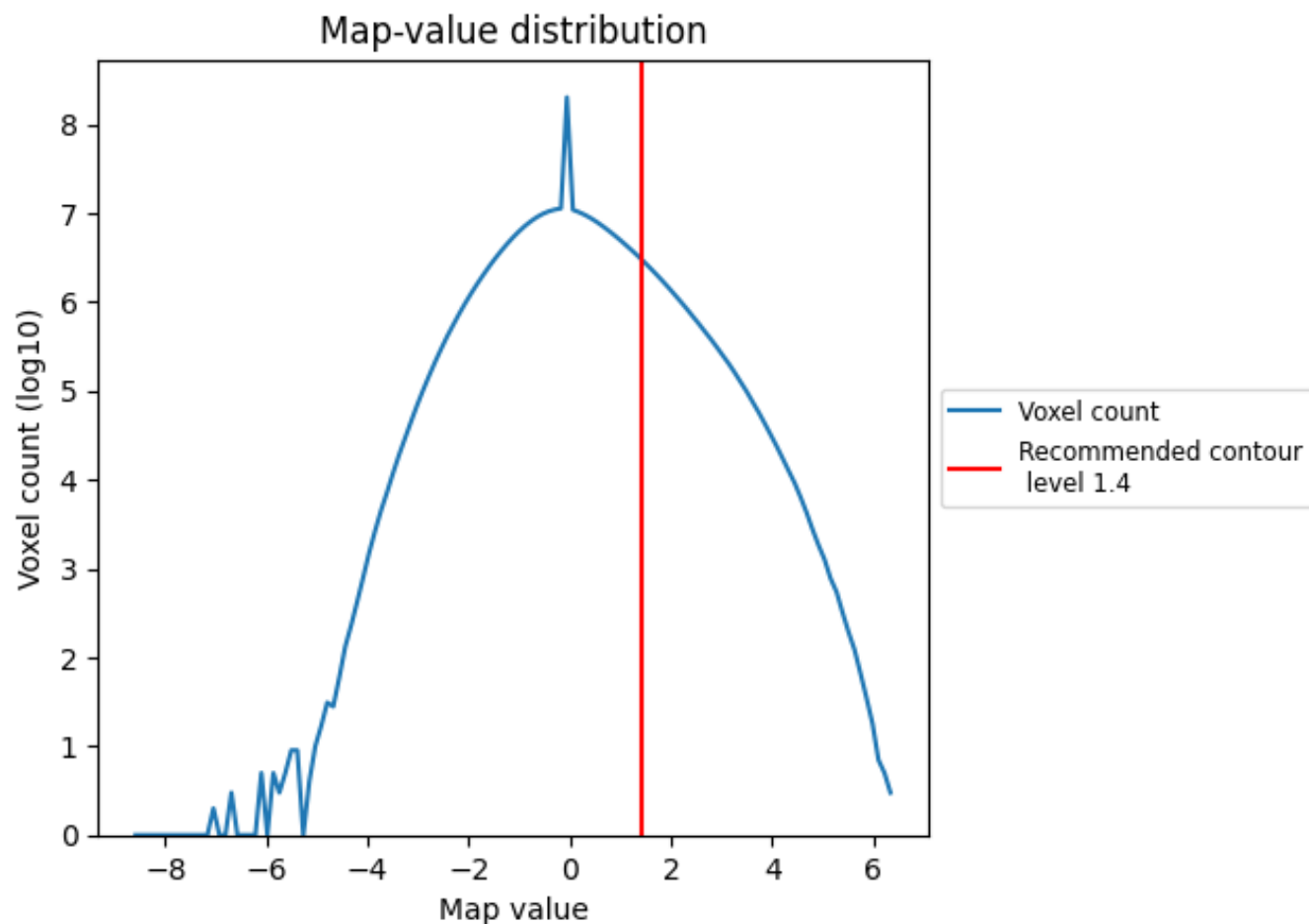
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

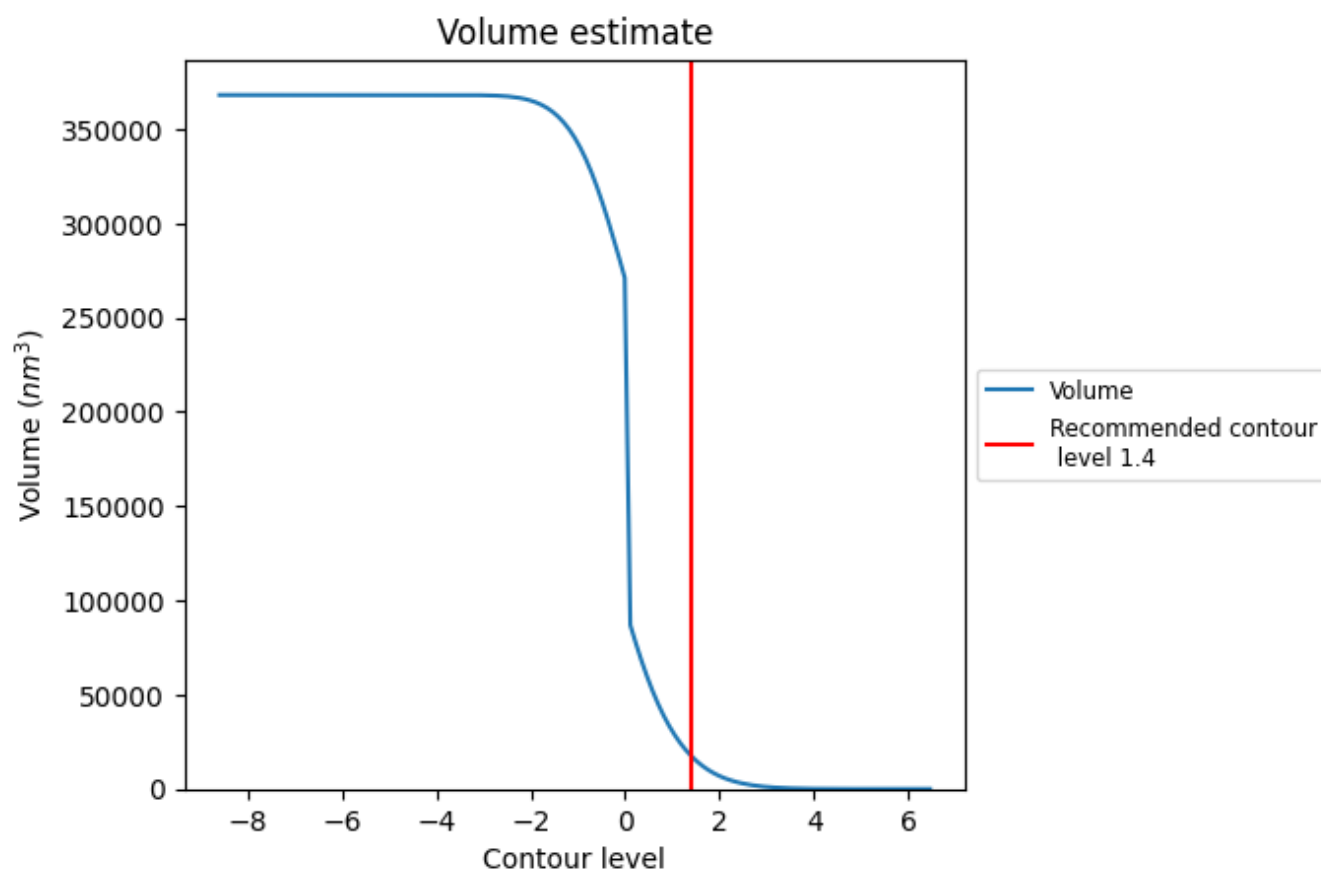
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 17524 nm<sup>3</sup>; this corresponds to an approximate mass of 15830 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 8 Fourier-Shell correlation

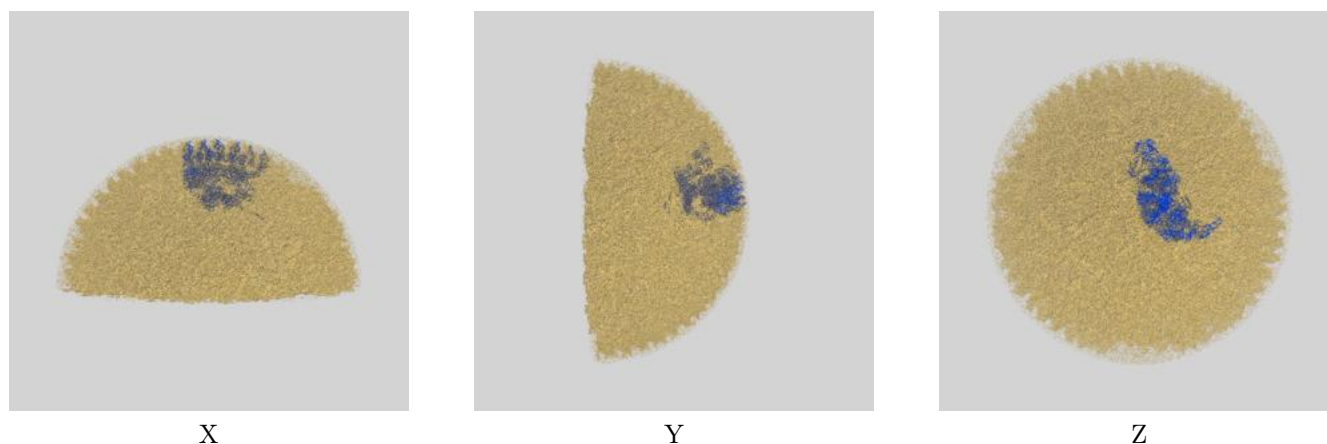
This section was not generated. No FSC curve or half-maps provided.

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

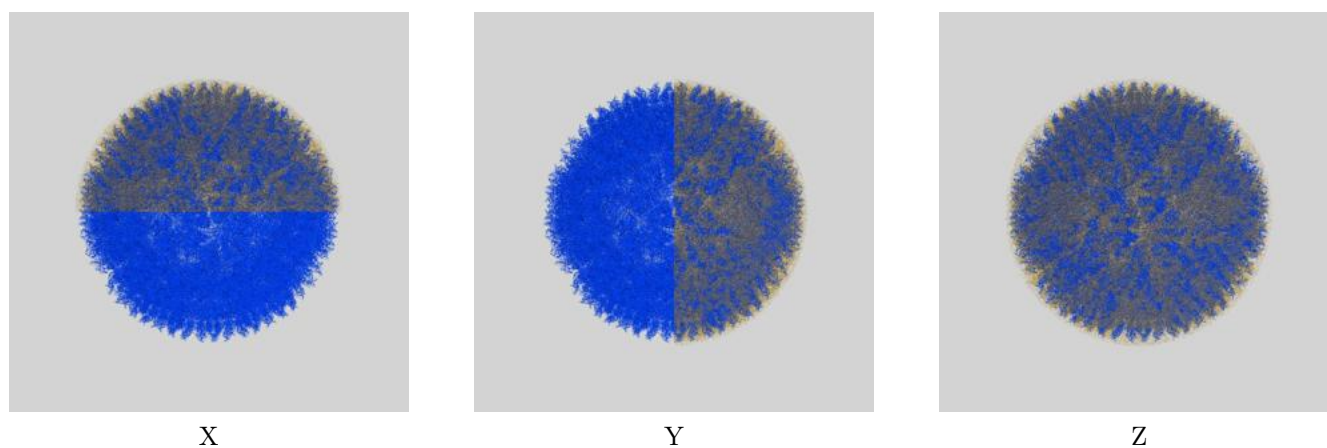
This section contains information regarding the fit between EMDB map EMD-1653 and PDB model 3K1Q. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

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



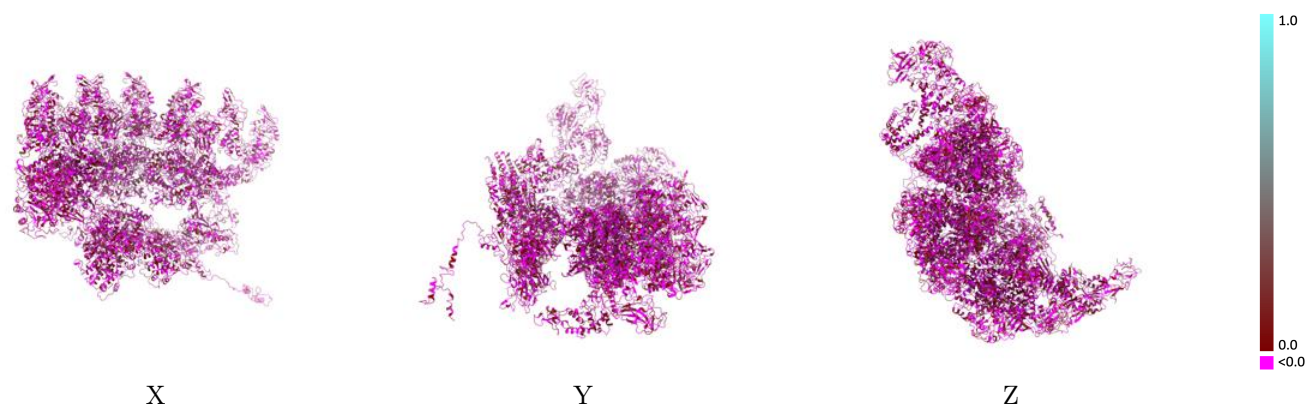
#### 9.1.2 Map-model assembly overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.4 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.

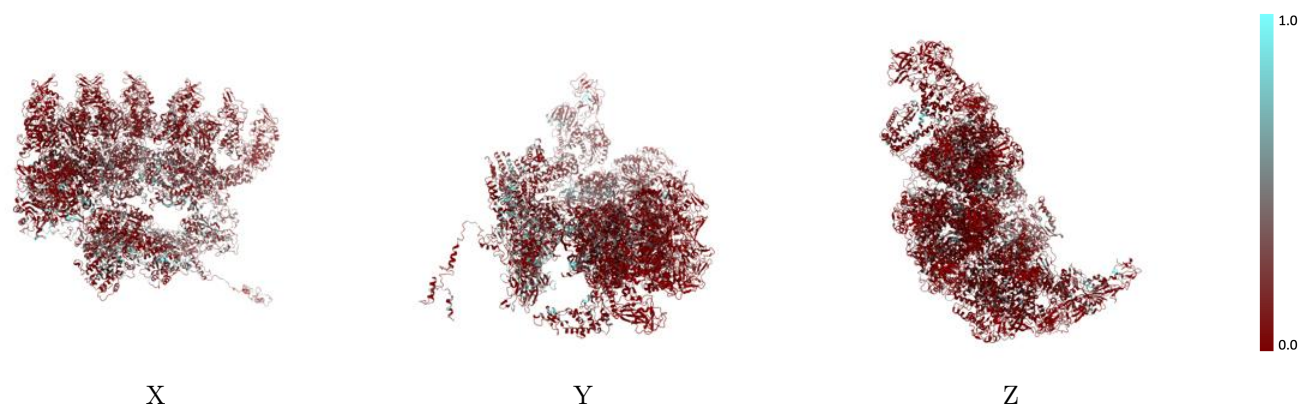


## 9.2 Q-score mapped to coordinate model [i](#)



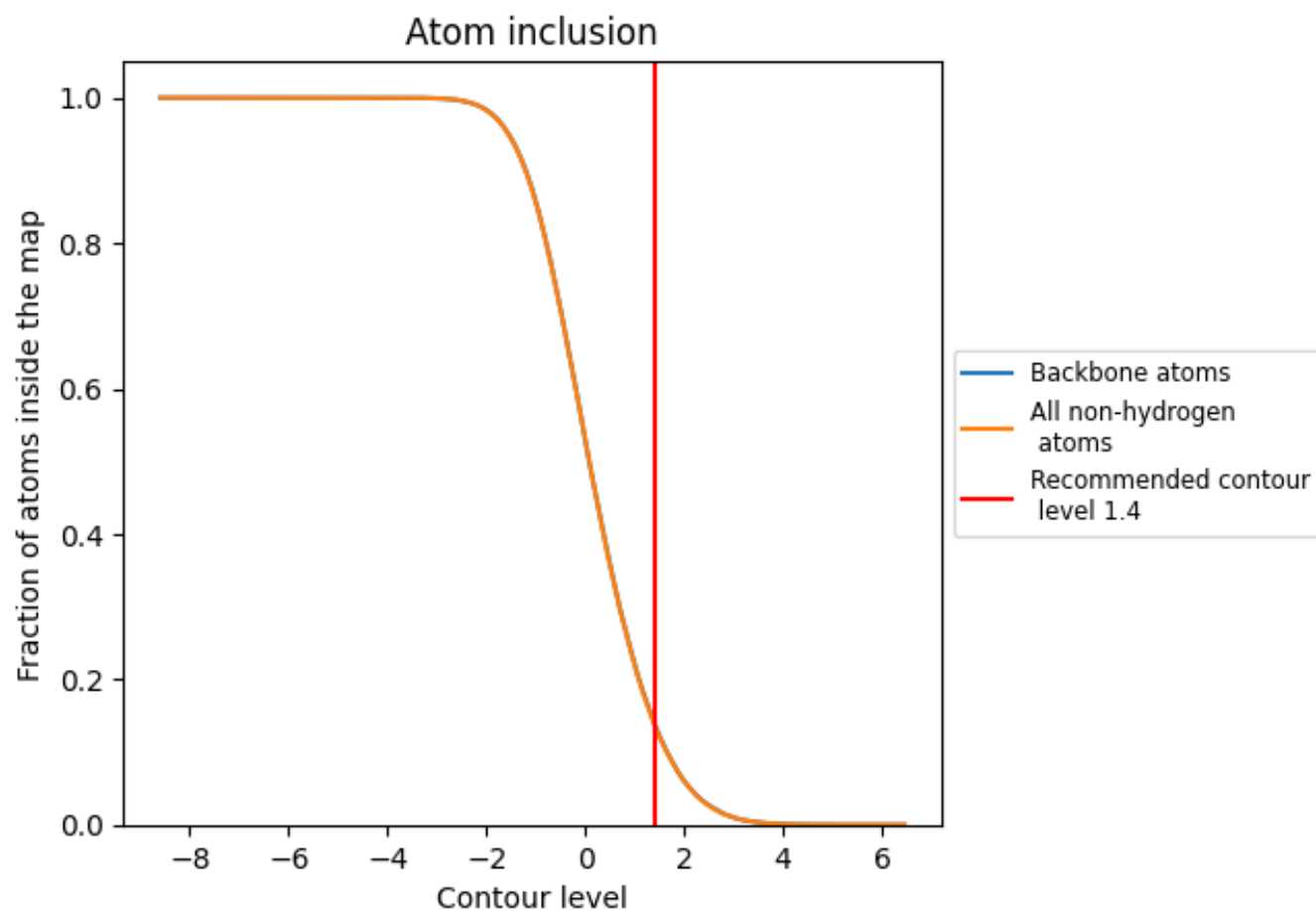
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.4).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 14% of all backbone atoms, 14% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1374	 -0.0000
A	 0.1556	 0.0070
B	 0.2247	 0.0040
C	 0.2280	 0.0010
D	 0.1744	 -0.0070
E	 0.2600	 0.0160
F	 0.0818	 0.0040
G	 0.0686	 0.0000
H	 0.0706	 0.0180
I	 0.1228	 -0.0100
J	 0.1505	 -0.0010
K	 0.1499	 0.0060
L	 0.0589	 0.0070
M	 0.0638	 -0.0050
N	 0.0019	 0.0050
O	 0.1102	 0.0000
P	 0.1072	 0.0080
Q	 0.1166	 -0.0080
R	 0.0755	 -0.0150
S	 0.0818	 0.0050
T	 0.0925	 0.0000
U	 0.1256	 -0.0060
V	 0.1258	 -0.0130
W	 0.1475	 -0.0100
X	 0.0970	 -0.0090
Y	 0.0044	 -0.0050

