



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 03:35 AM JST

PDB ID : 5ZVS  
EMDB ID : EMD-6968  
Title : Structure of RNA polymerase complex and genome within a dsRNA virus provides insights into the mechanisms of transcription and assembly  
Authors : Liu, H.; Fang, Q.; Cheng, L.  
Deposited on : 2018-05-12  
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.dev113  
MolProbity : 4.02b-467  
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) : 2.39

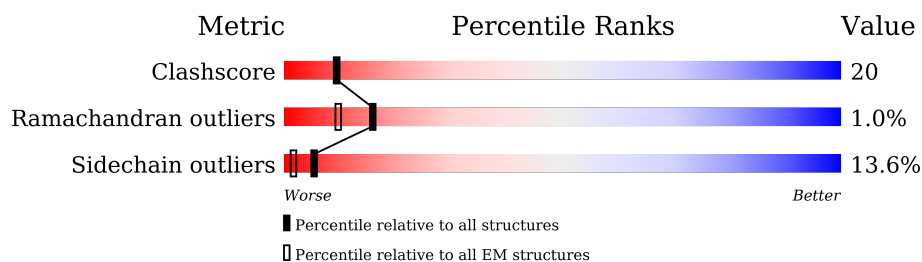
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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




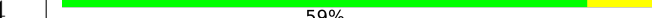


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1214	 60% 23% 5% 13%
1	B	1214	 66% 26% • 5%
1	C	1214	 61% 22% • 13%
1	D	1214	 66% 25% • 5%
1	E	1214	 58% 22% 5% 15%
1	F	1214	 65% 26% • 5%
1	G	1214	 60% 22% 5% 13%
1	H	1214	 68% 23% • 5%

*Continued on next page...*

Mol	Chain	Length	Quality of chain
1	I	1214	
1	J	1214	
2	2	1274	
3	4	728	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 99250 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 VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1060	Total	C	N	O	S	0	0
			8190	5232	1400	1510	48		
1	B	1154	Total	C	N	O	S	0	0
			8839	5608	1525	1656	50		
1	D	1154	Total	C	N	O	S	0	0
			8838	5608	1525	1655	50		
1	C	1060	Total	C	N	O	S	0	0
			8190	5232	1400	1510	48		
1	E	1032	Total	C	N	O	S	0	0
			7973	5095	1363	1468	47		
1	F	1154	Total	C	N	O	S	0	0
			8839	5608	1525	1656	50		
1	G	1062	Total	C	N	O	S	0	0
			8205	5244	1402	1511	48		
1	H	1155	Total	C	N	O	S	0	0
			8847	5612	1527	1658	50		
1	I	1059	Total	C	N	O	S	0	0
			8184	5229	1399	1508	48		
1	J	1154	Total	C	N	O	S	0	0
			8839	5608	1525	1656	50		

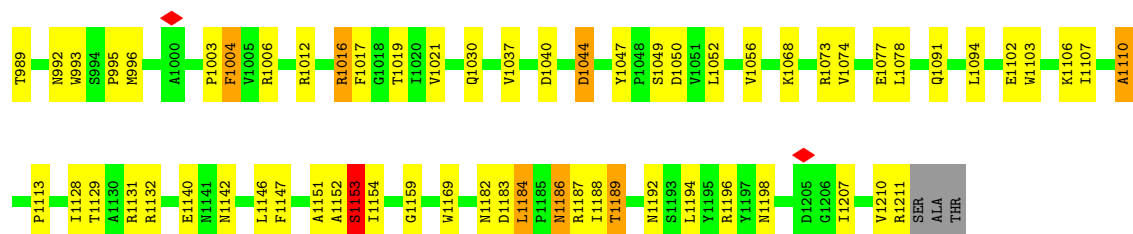
- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1245	Total	C	N	O	S	0	0
			9771	6257	1693	1777	44		

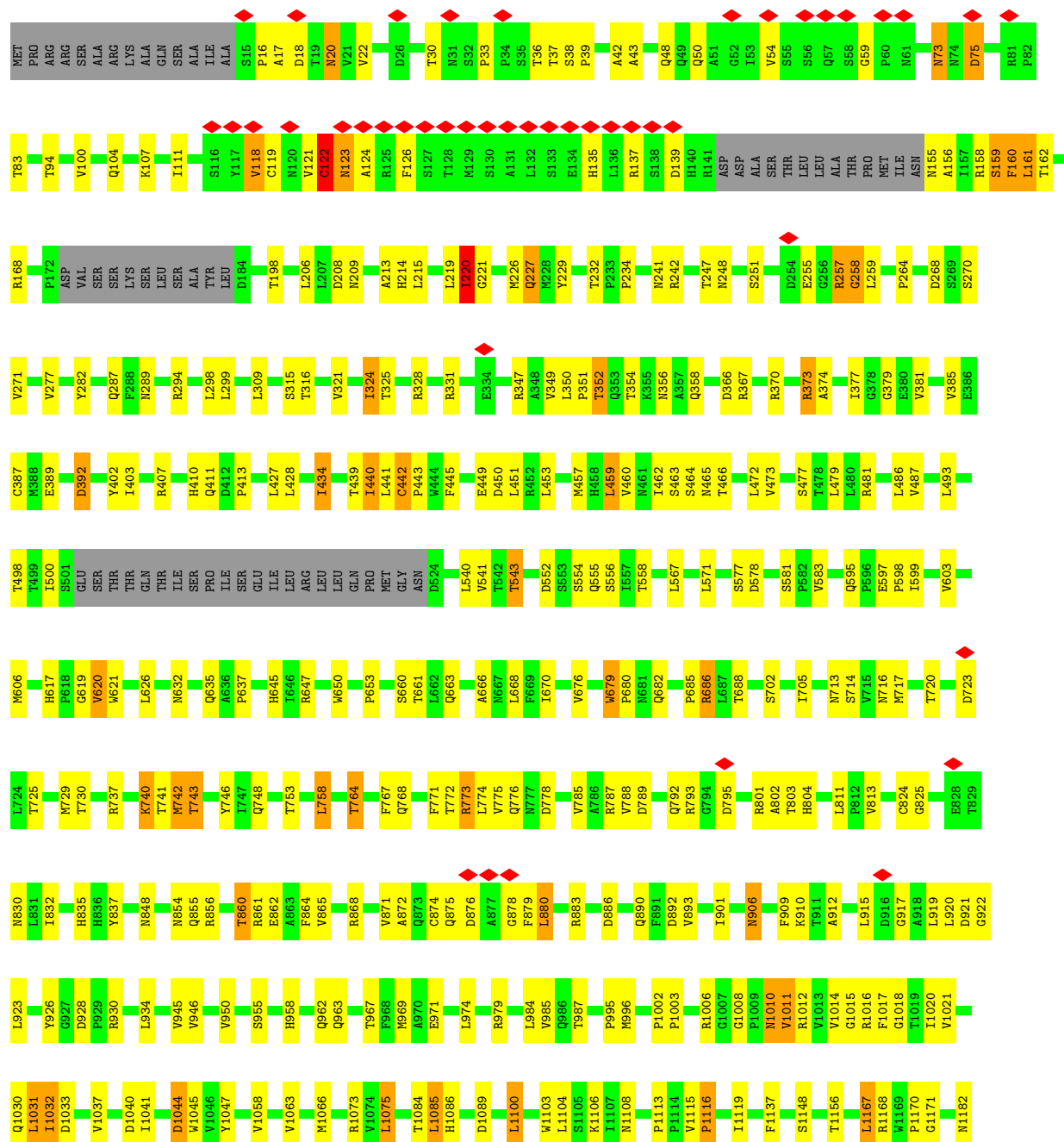
- Molecule 3 is a protein called Putative core protein NTPase/VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	583	Total	C	N	O	S	0	0
			4535	2916	788	817	14		





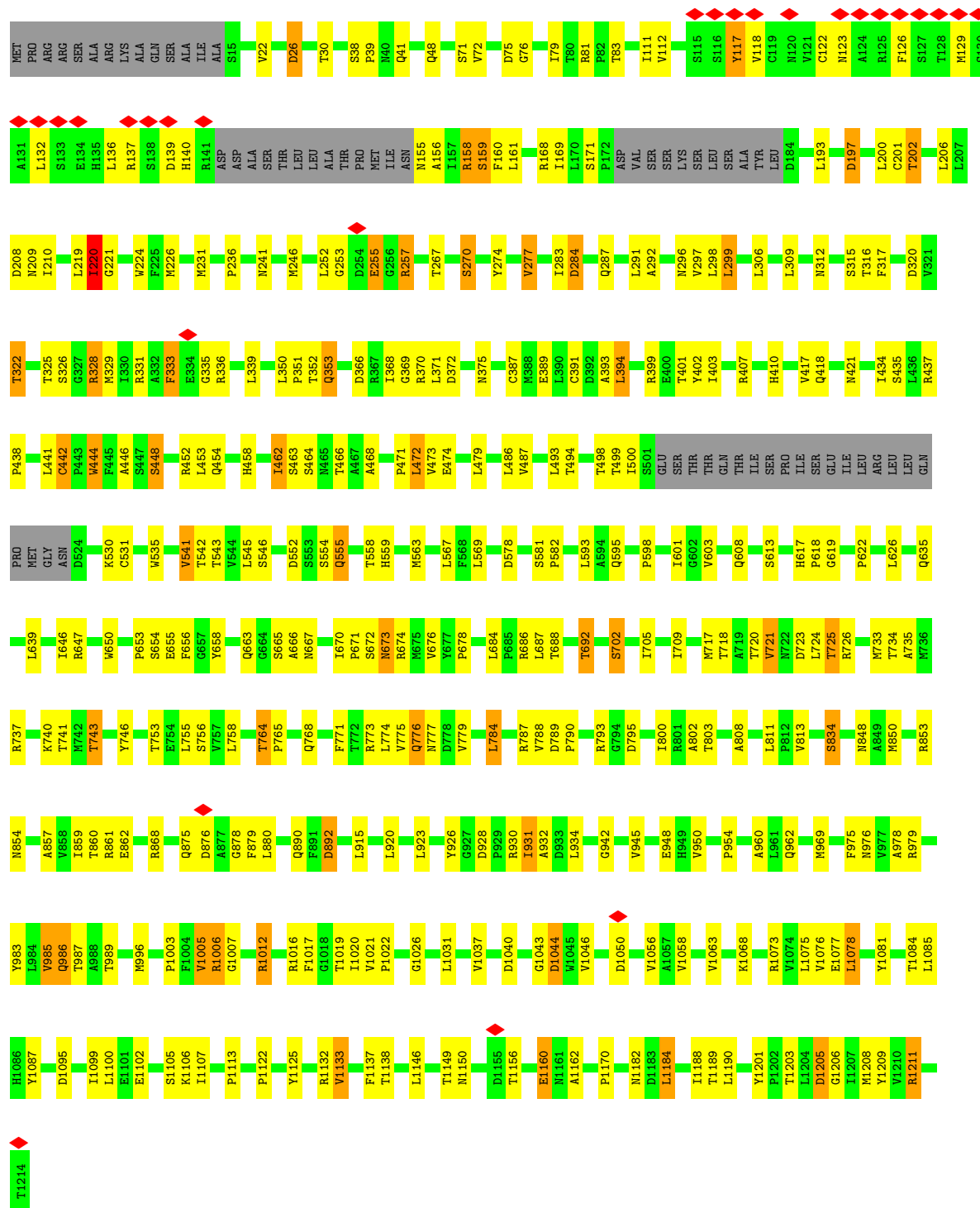
• Molecule 1: VP3





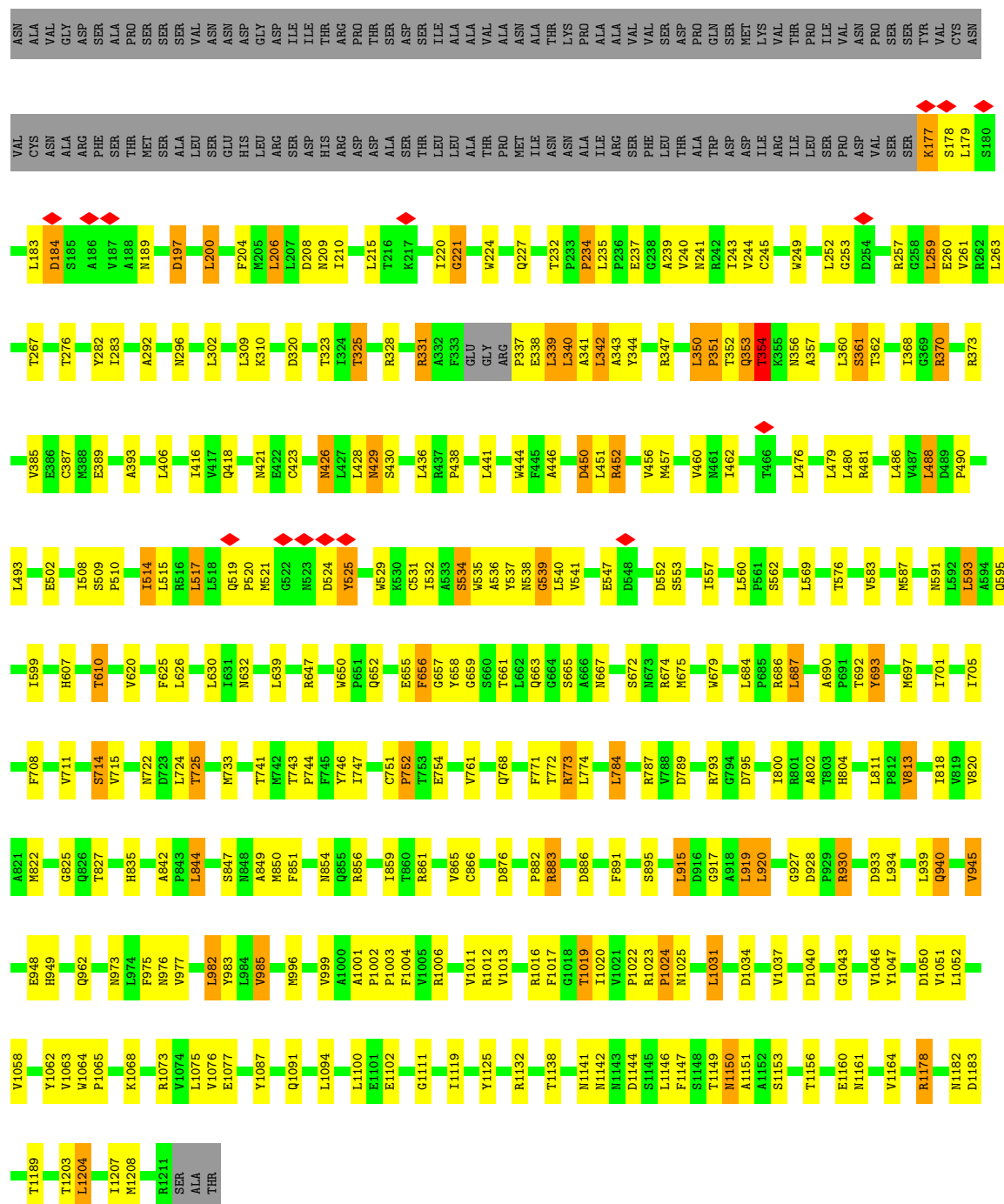
• Molecule 1: VP3

Chain D: 66% 25% 5%



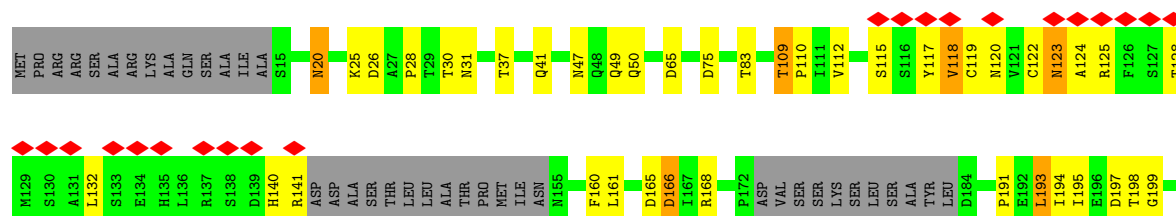






### • Molecule 1: VP3

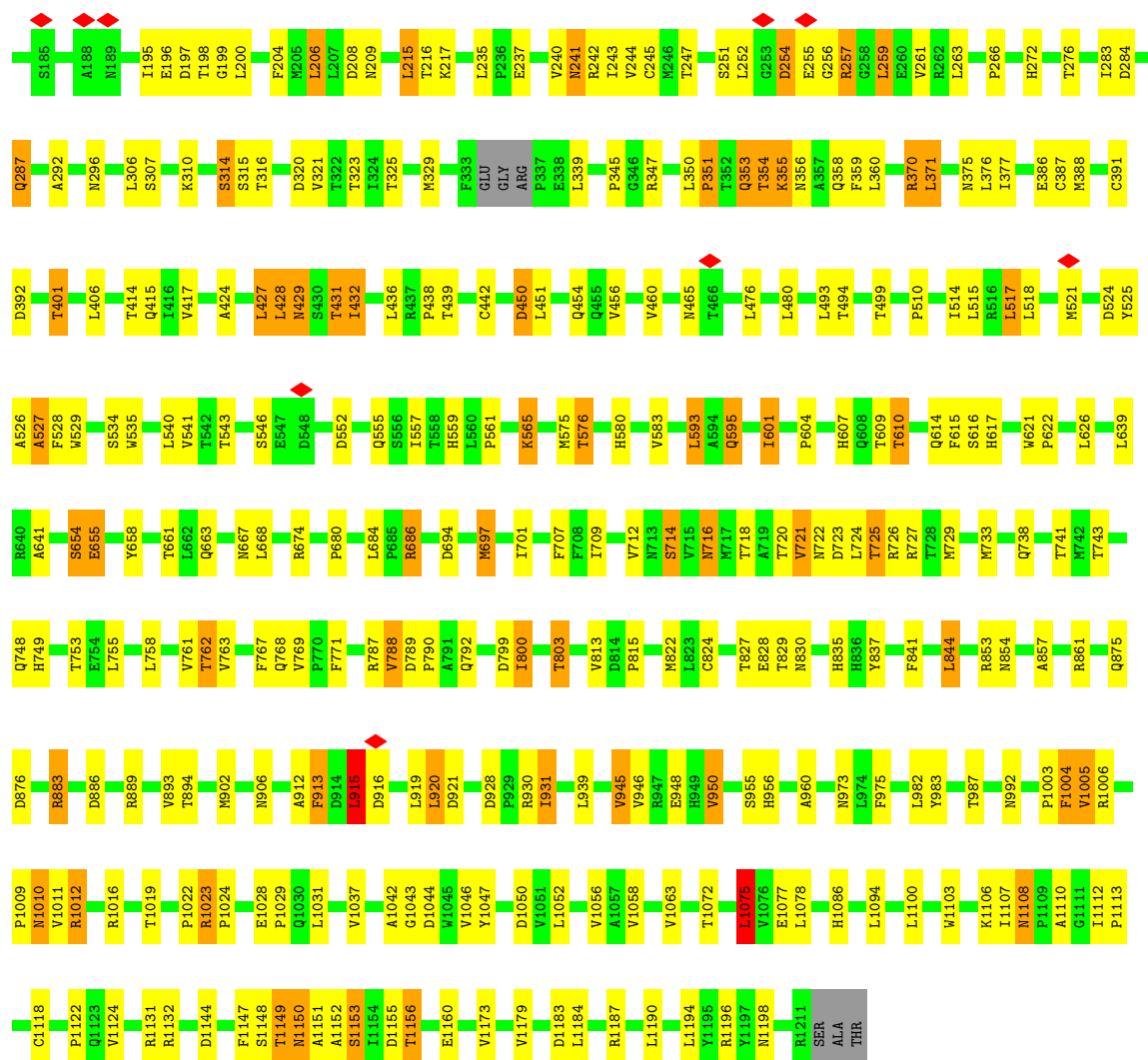
Chain F: 65% 26% 5%





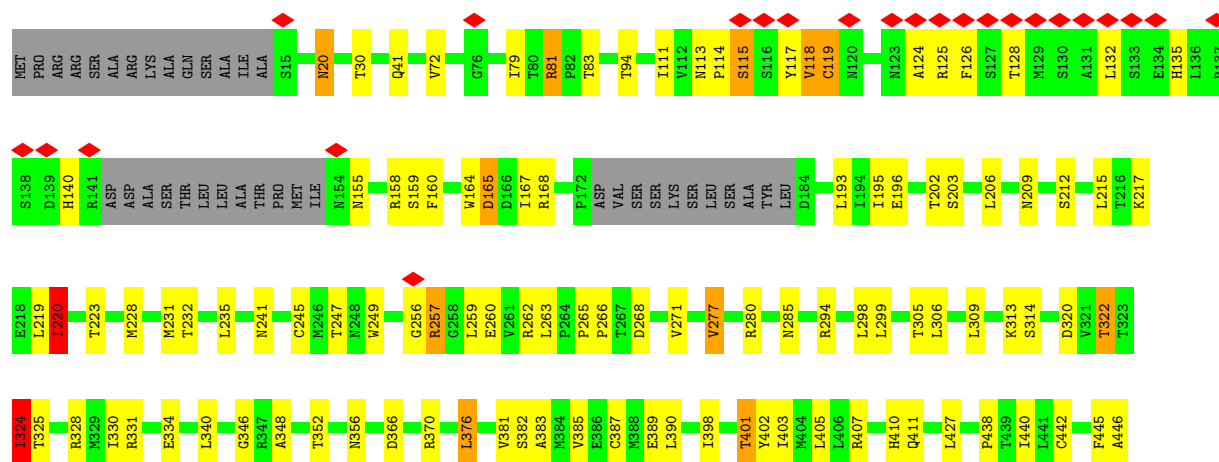
Frequency	Percentage
Daily	60%
Weekly	22%
Monthly	5%
Never	13%

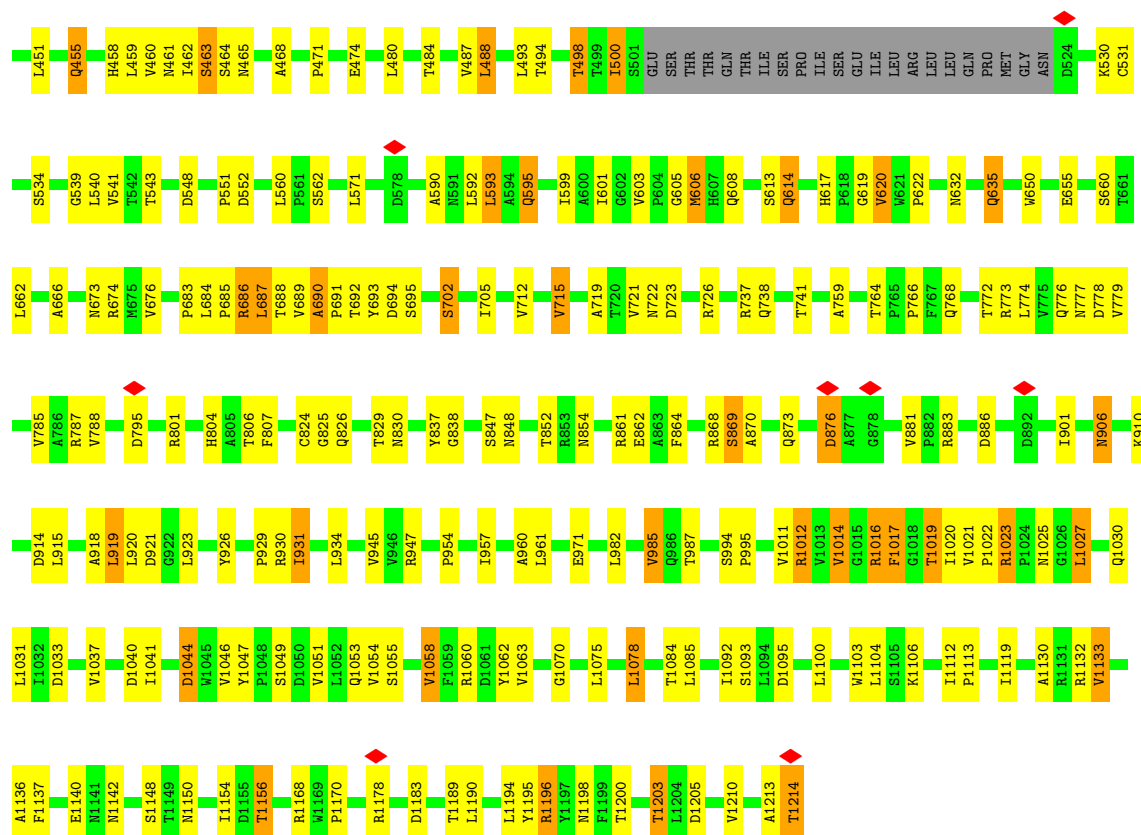




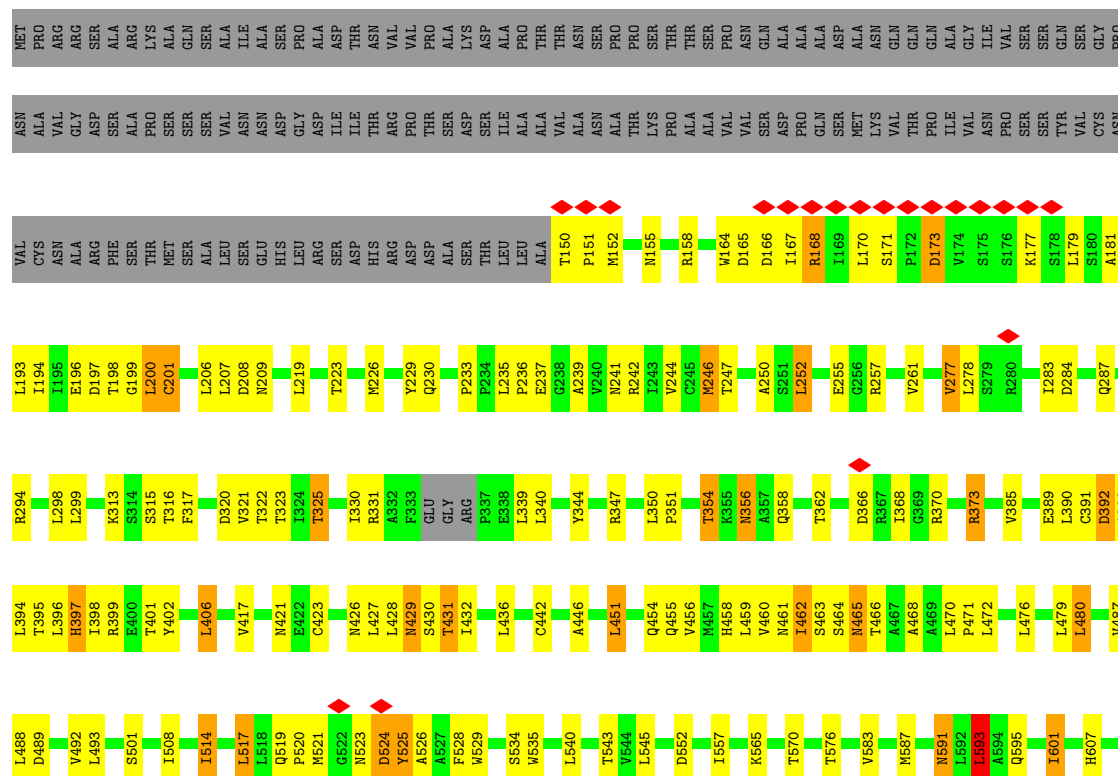
• Molecule 1: VP3

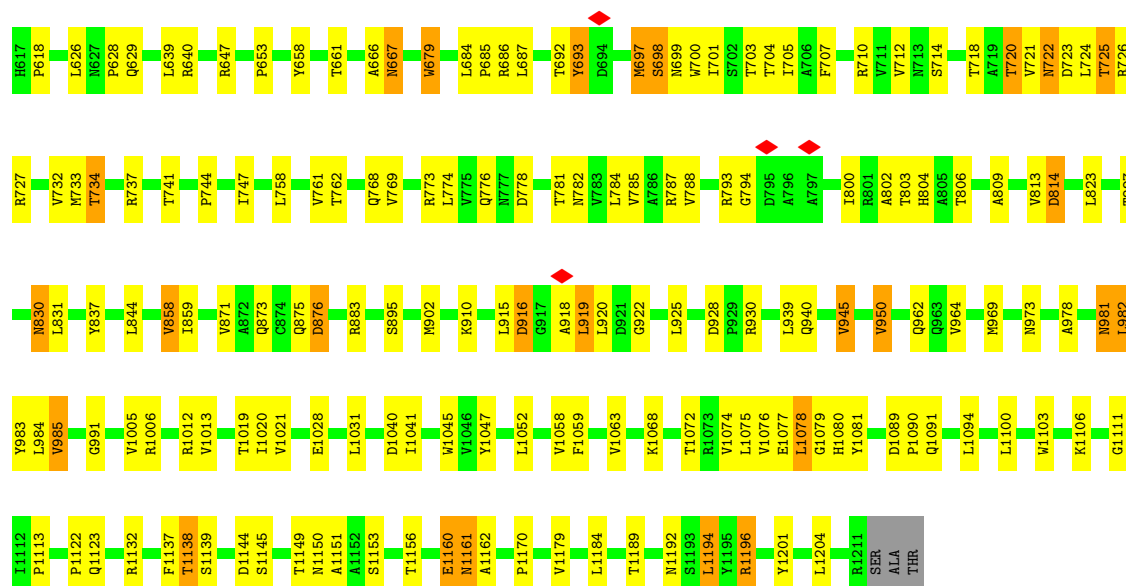
Chain H: 68% 23% 5%





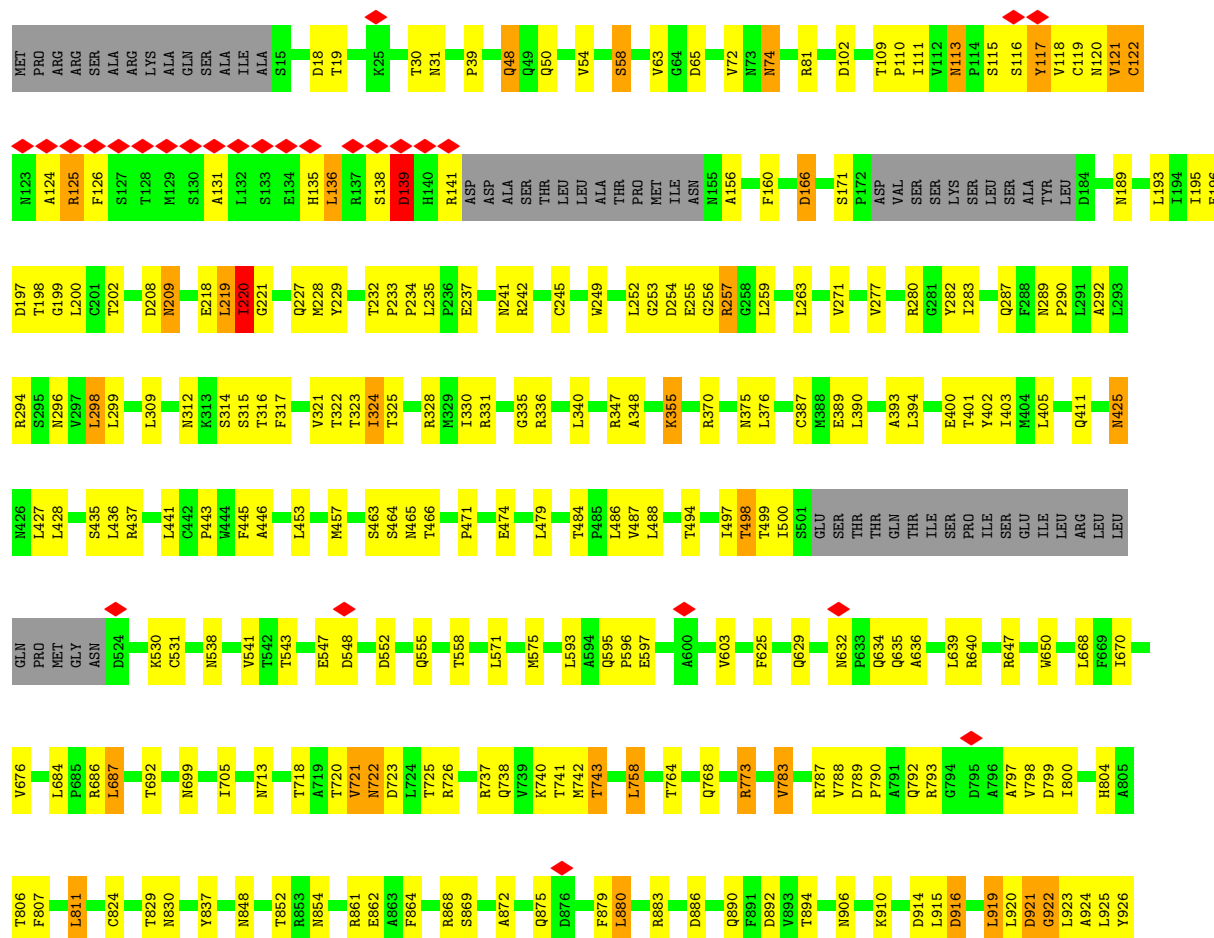
### • Molecule 1: VP3

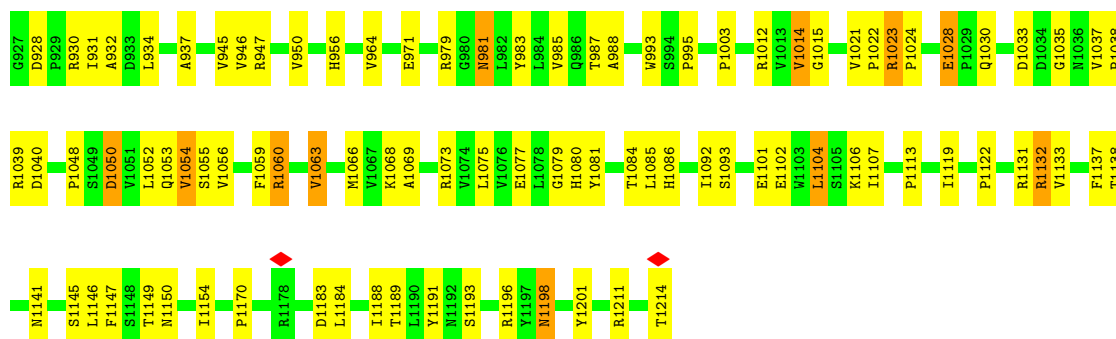




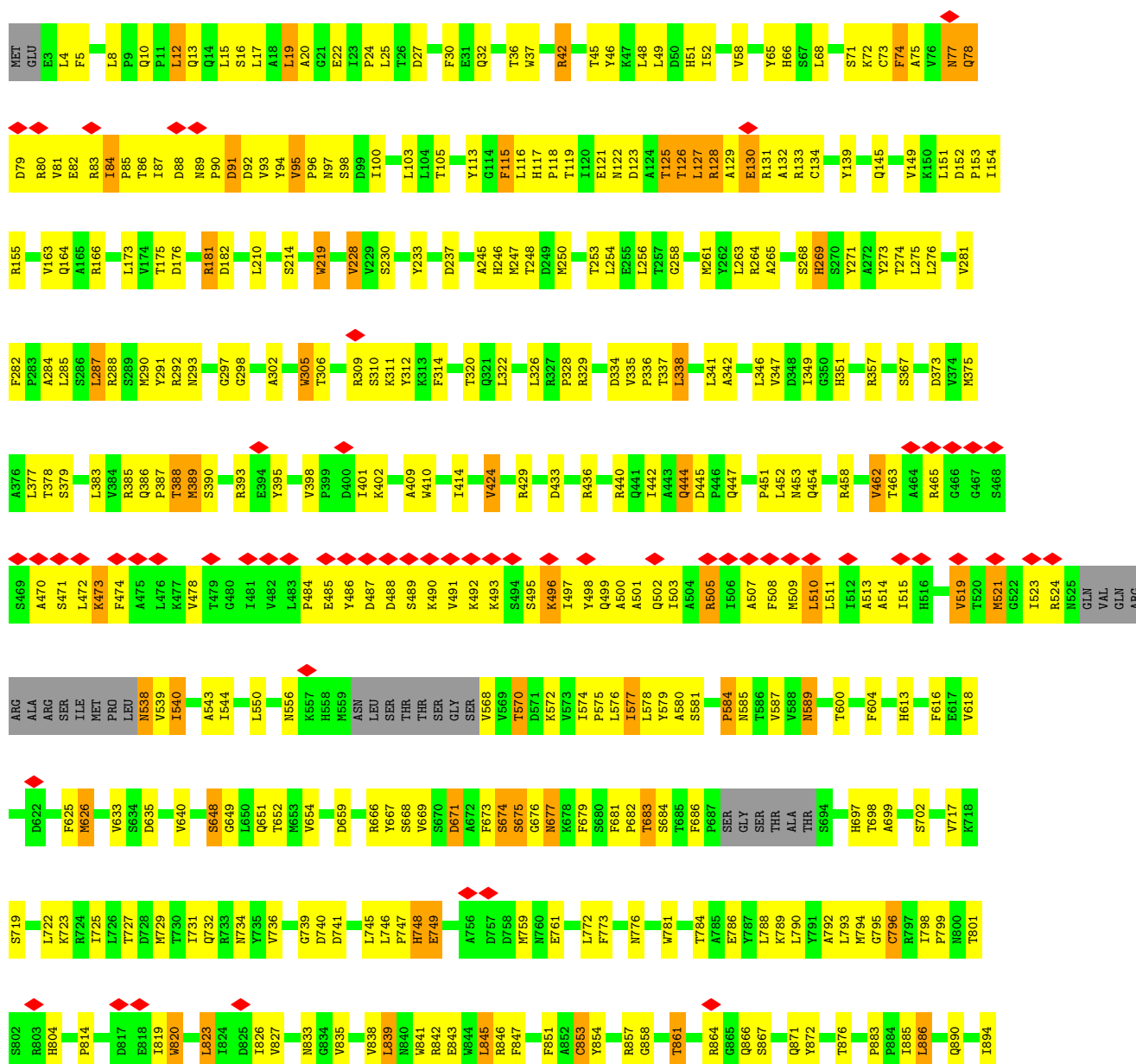
### • Molecule 1: VP3

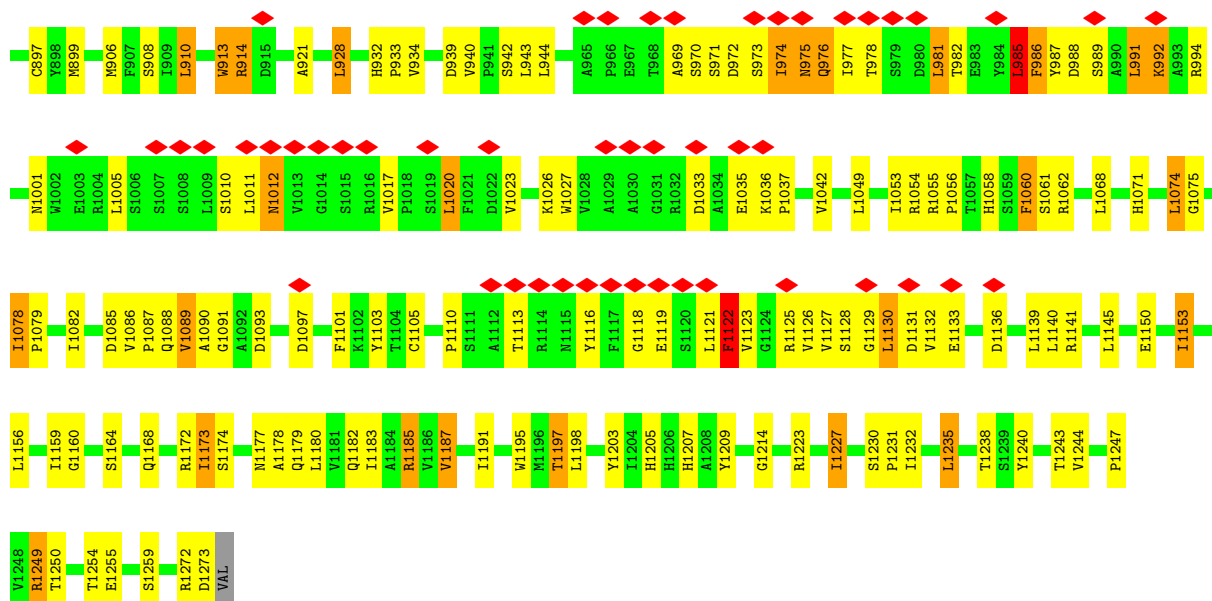
Chain J: 67% 25% 5%



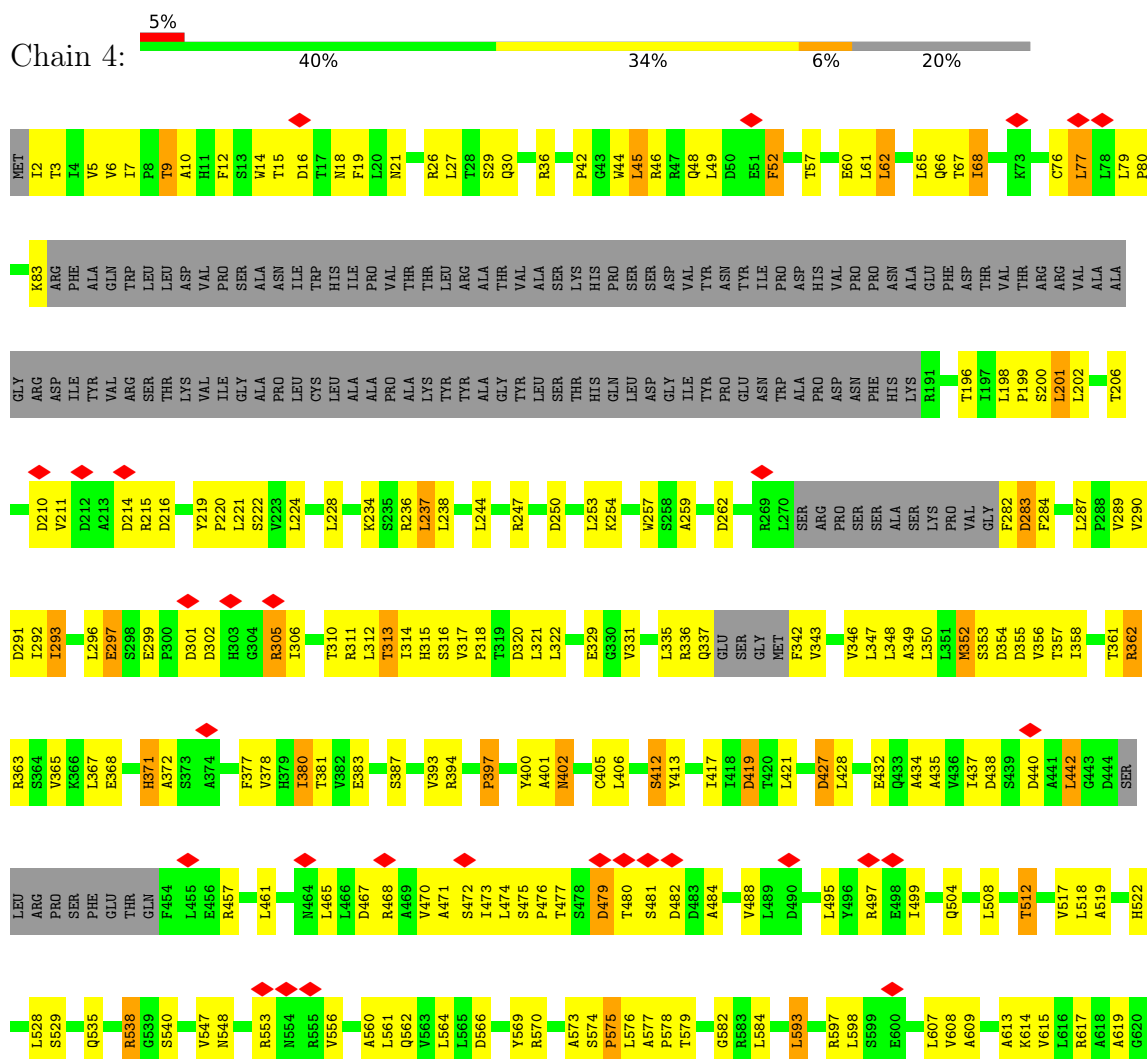


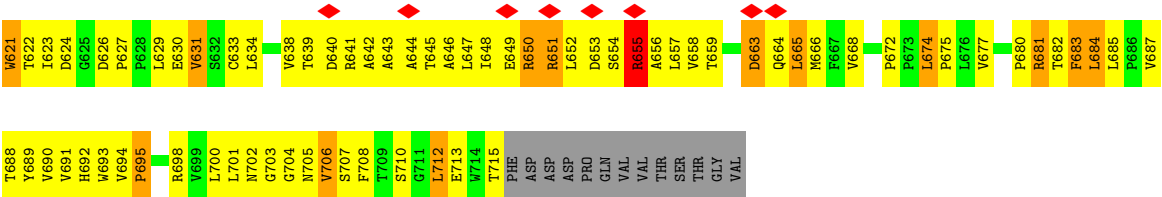
• Molecule 2: VP2





• Molecule 3: Putative core protein NTPase/VP5







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	54.858	Depositor
Minimum map value	-26.854	Depositor
Average map value	0.739	Depositor
Map value standard deviation	4.089	Depositor
Recommended contour level	8	Depositor
Map size (Å)	838.8, 838.8, 838.8	wwPDB
Map dimensions	900, 900, 900	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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	0.43	0/8402	0.59	8/11515 (0.1%)
1	B	0.41	0/9062	0.56	7/12422 (0.1%)
1	C	0.43	0/8402	0.56	3/11515 (0.0%)
1	D	0.42	0/9061	0.56	5/12422 (0.0%)
1	E	0.42	0/8180	0.57	4/11210 (0.0%)
1	F	0.42	0/9062	0.59	4/12422 (0.0%)
1	G	0.42	0/8417	0.57	4/11535 (0.0%)
1	H	0.44	0/9070	0.59	4/12433 (0.0%)
1	I	0.45	0/8396	0.58	4/11506 (0.0%)
1	J	0.44	0/9062	0.58	3/12422 (0.0%)
2	2	0.44	0/10051	0.62	6/13731 (0.0%)
3	4	0.39	0/4637	0.66	2/6343 (0.0%)
All	All	0.43	0/101802	0.58	54/139476 (0.0%)

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	A	0	1
1	H	0	1
3	4	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	559	HIS	N-CA-C	-9.16	86.28	111.00
2	2	749	GLU	N-CA-C	-8.56	87.88	111.00
1	H	593	LEU	CA-CB-CG	8.15	134.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	655	ARG	N-CA-C	-7.86	89.78	111.00
1	H	119	CYS	N-CA-C	-7.73	90.12	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	655	ARG	Mainchain,Sidechain
1	A	426	ASN	Mainchain
1	H	1023	ARG	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	8190	0	8167	336	0
1	B	8839	0	8761	307	0
1	C	8190	0	8168	280	0
1	D	8838	0	8762	310	0
1	E	7973	0	7952	276	0
1	F	8839	0	8762	326	0
1	G	8205	0	8189	296	0
1	H	8847	0	8768	276	0
1	I	8184	0	8163	322	0
1	J	8839	0	8762	288	0
2	2	9771	0	9677	679	0
3	4	4535	0	4670	431	0
All	All	99250	0	98801	3916	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 20.

The worst 5 of 3916 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)
2:2:827:VAL:HG22	2:2:851:PHE:CE2	1.09	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:558:THR:HB	1:F:720:THR:CG2	1.12	1.59
1:B:457:MET:CE	1:B:920:LEU:HG	1.06	1.53
2:2:84:ILE:CG2	2:2:93:VAL:HG23	1.39	1.52
2:2:827:VAL:CG2	2:2:851:PHE:HE2	1.15	1.52

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	1056/1214 (87%)	948 (90%)	98 (9%)	10 (1%)	14	45
1	B	1146/1214 (94%)	1018 (89%)	117 (10%)	11 (1%)	13	44
1	C	1056/1214 (87%)	947 (90%)	102 (10%)	7 (1%)	19	52
1	D	1146/1214 (94%)	1031 (90%)	108 (9%)	7 (1%)	22	55
1	E	1028/1214 (85%)	916 (89%)	100 (10%)	12 (1%)	11	40
1	F	1146/1214 (94%)	1040 (91%)	92 (8%)	14 (1%)	11	40
1	G	1058/1214 (87%)	959 (91%)	91 (9%)	8 (1%)	16	49
1	H	1147/1214 (94%)	1023 (89%)	112 (10%)	12 (1%)	13	44
1	I	1055/1214 (87%)	961 (91%)	87 (8%)	7 (1%)	19	52
1	J	1146/1214 (94%)	1029 (90%)	103 (9%)	14 (1%)	11	40
2	2	1237/1274 (97%)	1116 (90%)	106 (9%)	15 (1%)	11	40
3	4	573/728 (79%)	506 (88%)	62 (11%)	5 (1%)	14	45
All	All	12794/14142 (90%)	11494 (90%)	1178 (9%)	122 (1%)	16	44

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	THR

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Mol	Chain	Res	Type
1	A	520	PRO
1	A	1153	SER
1	B	220	ILE
1	B	324	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	A	905/1030 (88%)	785 (87%)	120 (13%)	3	18
1	B	978/1030 (95%)	851 (87%)	127 (13%)	3	18
1	C	905/1030 (88%)	792 (88%)	113 (12%)	3	19
1	D	978/1030 (95%)	849 (87%)	129 (13%)	3	18
1	E	880/1030 (85%)	767 (87%)	113 (13%)	3	18
1	F	978/1030 (95%)	850 (87%)	128 (13%)	3	18
1	G	906/1030 (88%)	768 (85%)	138 (15%)	2	14
1	H	979/1030 (95%)	862 (88%)	117 (12%)	4	19
1	I	904/1030 (88%)	777 (86%)	127 (14%)	3	17
1	J	978/1030 (95%)	862 (88%)	116 (12%)	4	20
2	2	1066/1091 (98%)	900 (84%)	166 (16%)	2	14
3	4	502/626 (80%)	409 (82%)	93 (18%)	1	8
All	All	10959/12017 (91%)	9472 (86%)	1487 (14%)	5	17

5 of 1487 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	673	ASN
1	J	376	LEU
1	H	985	VAL
1	H	662	LEU
1	I	525	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 258 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	293	ASN
2	2	697	HIS
1	E	673	ASN
1	E	649	ASN
2	2	866	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.

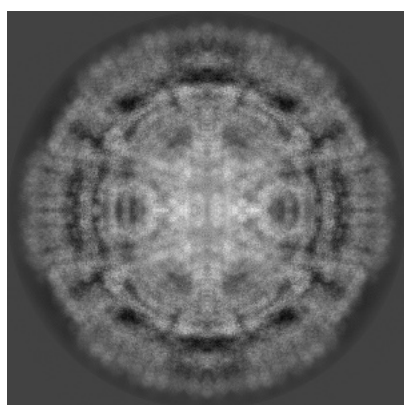
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6968. These allow visual inspection of the internal detail of the map and identification of artifacts.

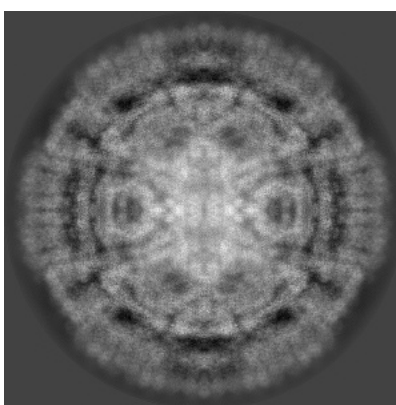
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

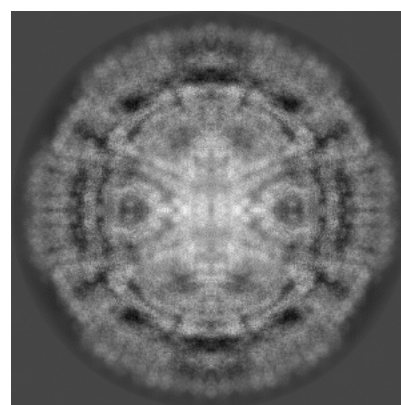
#### 6.1.1 Primary map



X



Y

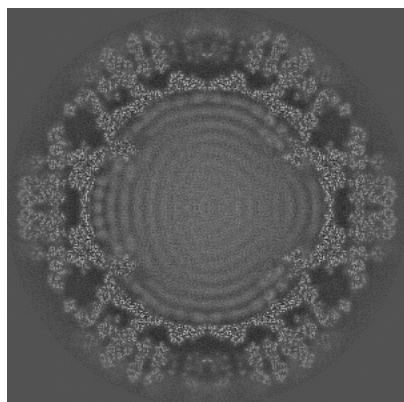


Z

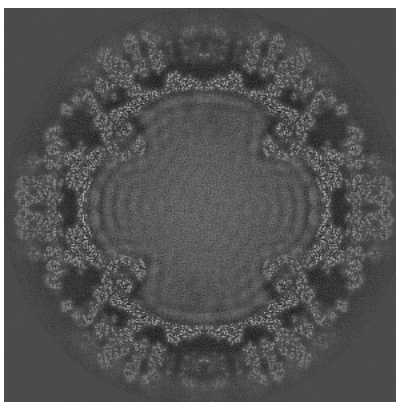
The images above show the map projected in three orthogonal directions.

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

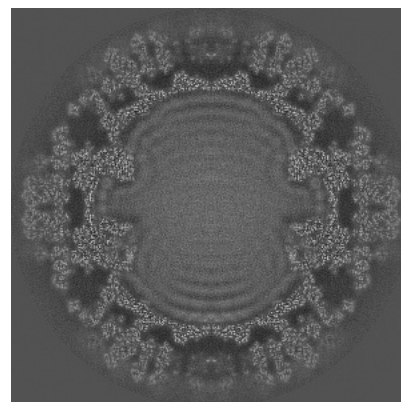
#### 6.2.1 Primary map



X Index: 450



Y Index: 450



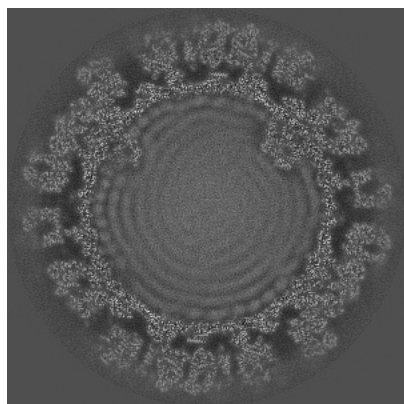
Z Index: 450



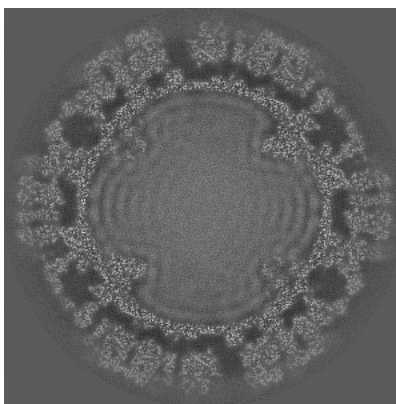
The images above show central slices of the map in three orthogonal directions.

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

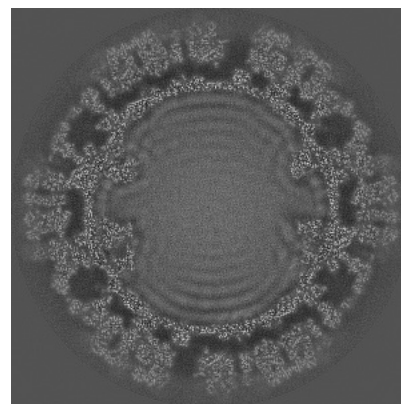
### 6.3.1 Primary map



X Index: 494



Y Index: 460

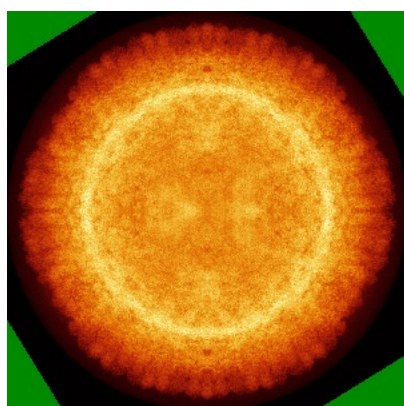


Z Index: 440

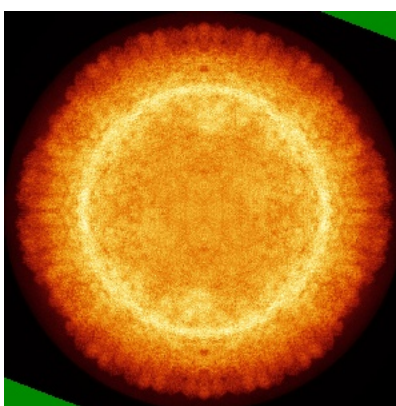
The images above show the largest variance slices of the map in three orthogonal directions.

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

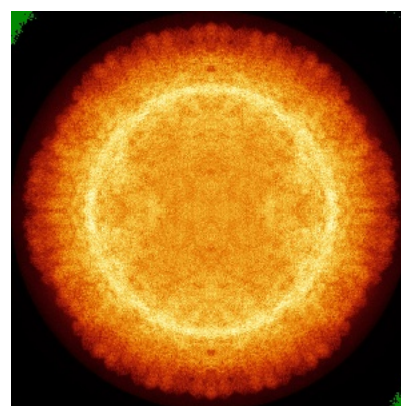
### 6.4.1 Primary map



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](#)

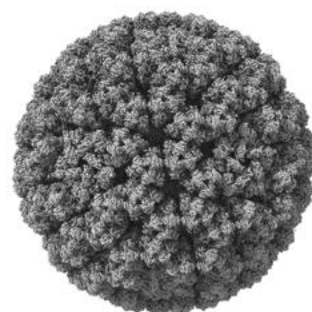
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

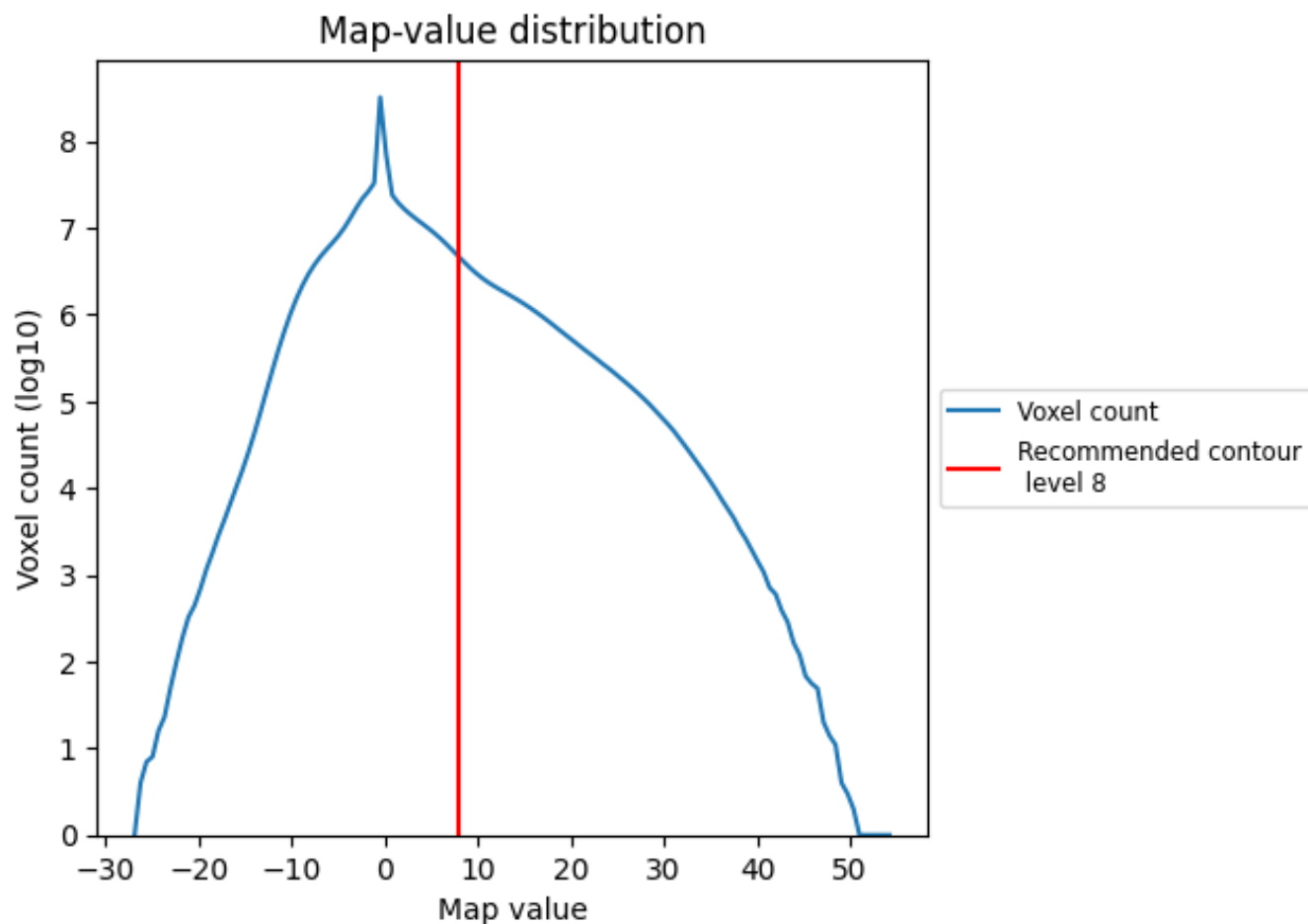
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

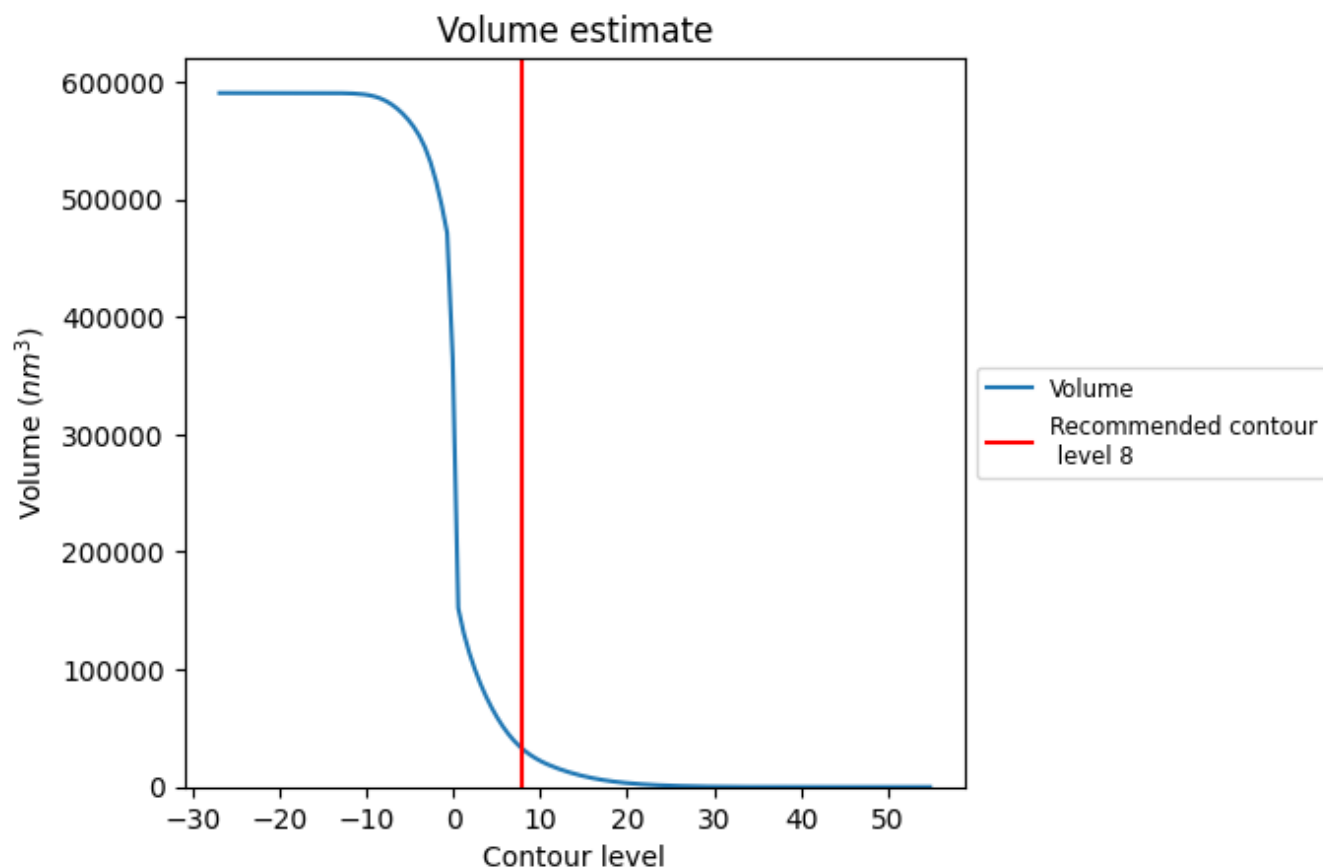
This section contains the results of statistical analysis of the map.

### 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.

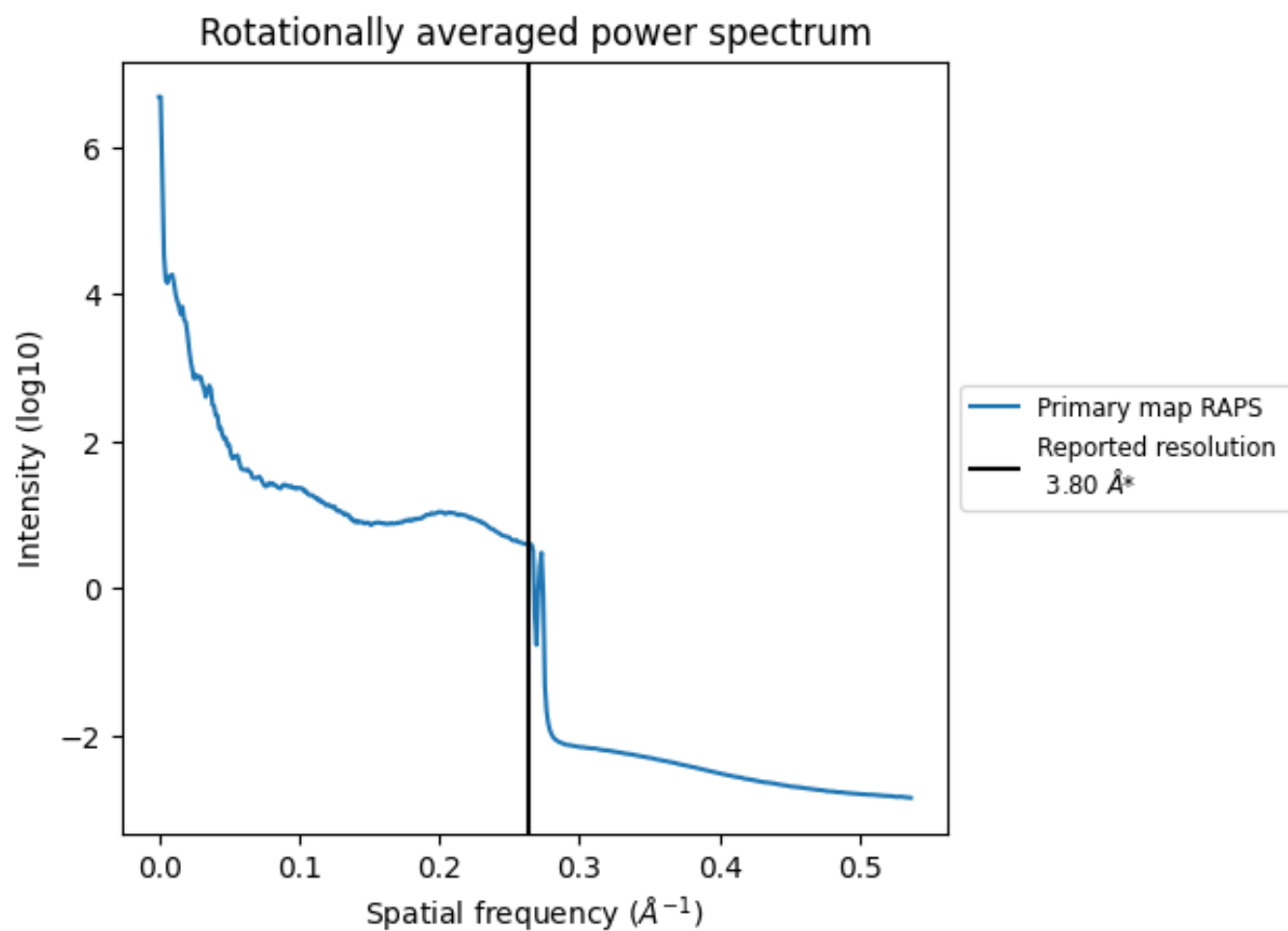
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 32351  $\text{nm}^3$ ; this corresponds to an approximate mass of 29223 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 0.263 Å<sup>-1</sup>

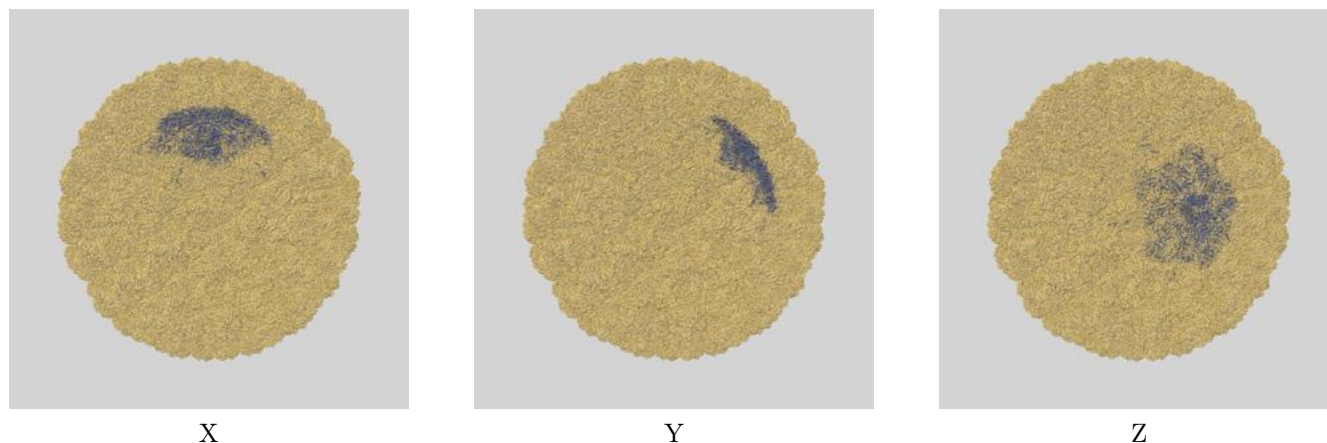
## 8 Fourier-Shell correlation

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

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

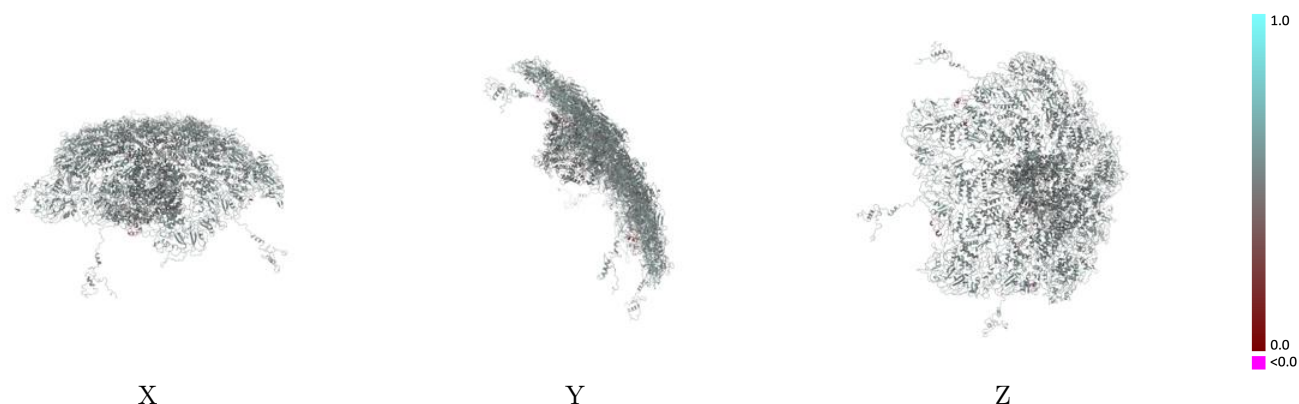
This section contains information regarding the fit between EMDB map EMD-6968 and PDB model 5ZVS. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



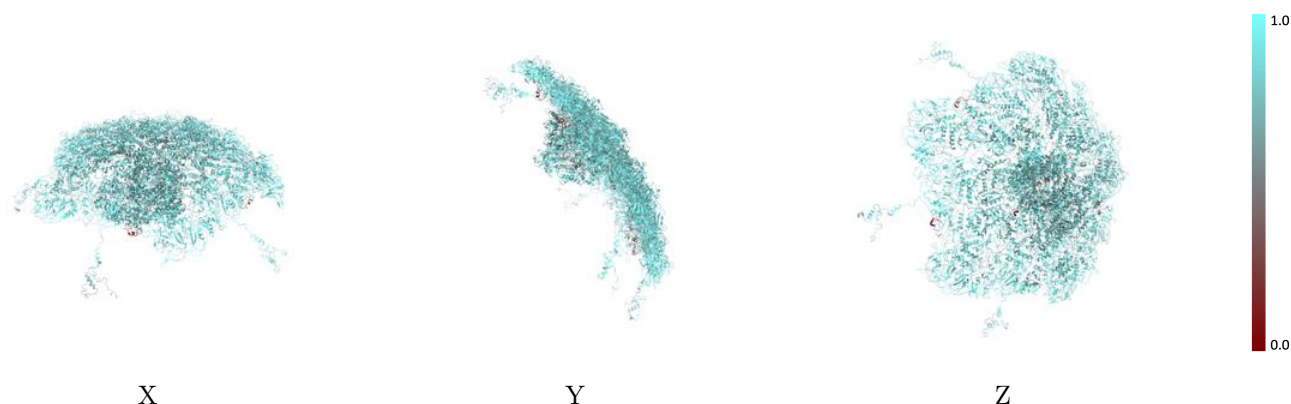
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



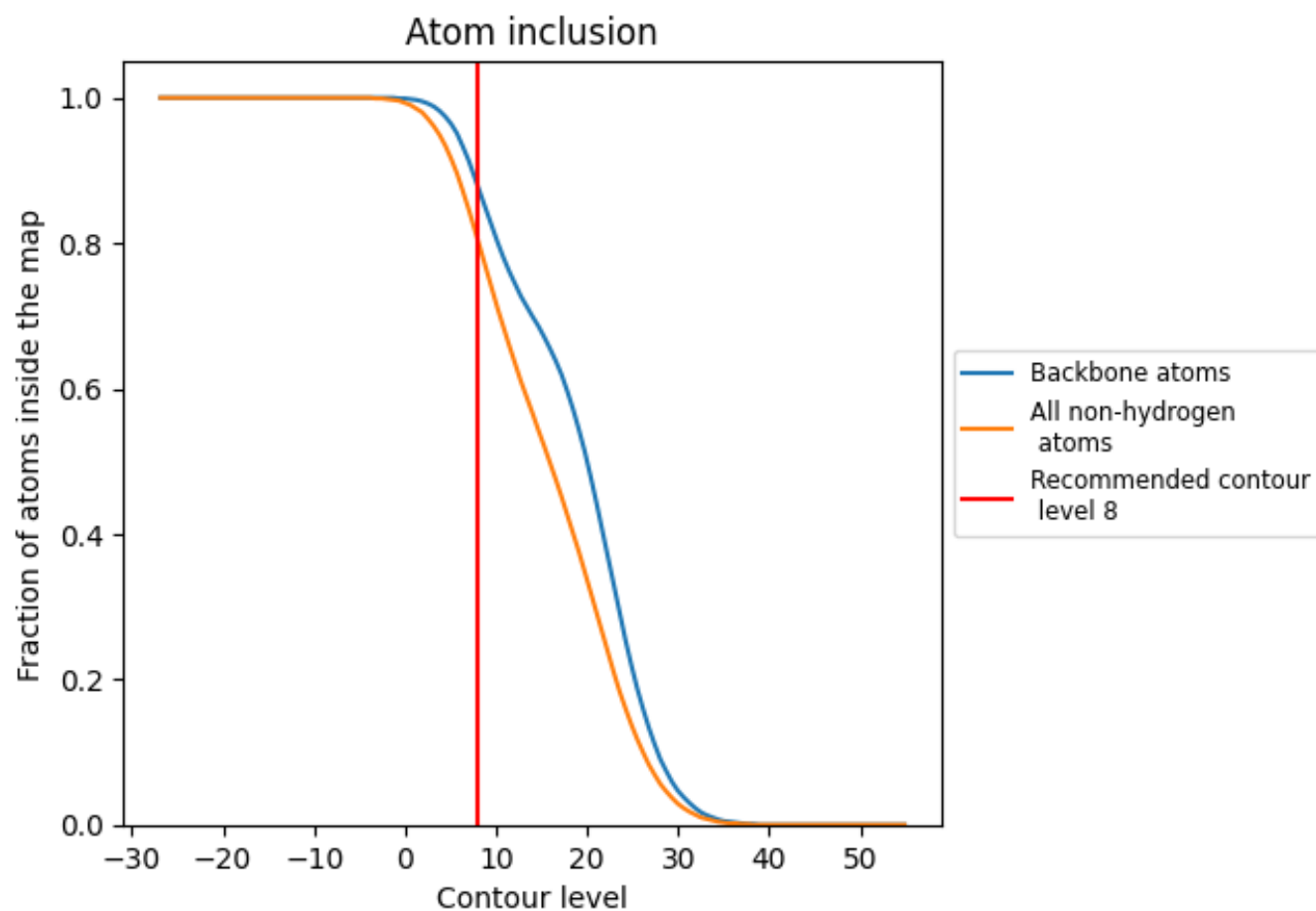
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8040	<div><div></div></div> 0.5110
2	<div><div></div></div> 0.7500	<div><div></div></div> 0.4900
4	<div><div></div></div> 0.7490	<div><div></div></div> 0.4910
A	<div><div></div></div> 0.8080	<div><div></div></div> 0.5170
B	<div><div></div></div> 0.7940	<div><div></div></div> 0.5120
C	<div><div></div></div> 0.8160	<div><div></div></div> 0.5180
D	<div><div></div></div> 0.8160	<div><div></div></div> 0.5140
E	<div><div></div></div> 0.8250	<div><div></div></div> 0.5160
F	<div><div></div></div> 0.8170	<div><div></div></div> 0.5130
G	<div><div></div></div> 0.8180	<div><div></div></div> 0.5140
H	<div><div></div></div> 0.8120	<div><div></div></div> 0.5150
I	<div><div></div></div> 0.8110	<div><div></div></div> 0.5150
J	<div><div></div></div> 0.8090	<div><div></div></div> 0.5150

1.0

0.0

<0.0