



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:49 PM BST

PDB ID : 3GZU  
EMDB ID: : EMD-1571  
Title : VP7 recoated rotavirus DLP  
Authors : Chen, J.Z.; Settembre, E.C.; Harrison, S.C.; Grigorieff, N.  
Deposited on : 2009-04-07  
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

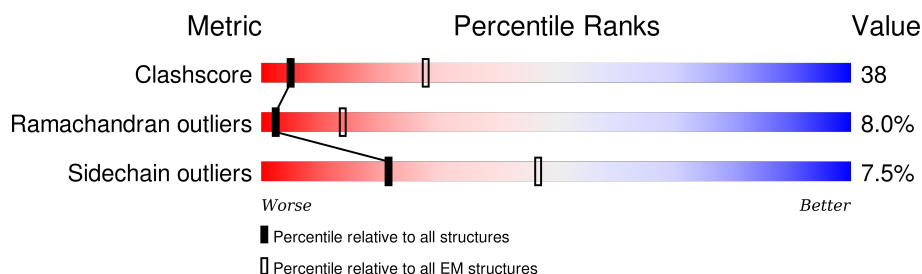
# 1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	800	19% 56% 20% . .
1	B	800	20% 57% 22% .
2	C	397	61% 32% 6% .
2	D	397	59% 34% 7% .
2	E	397	60% 33% 6% .
2	F	397	61% 32% 6% .
2	G	397	60% 33% 7% .
2	H	397	59% 34% 7% .
2	I	397	60% 33% 6% .

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Mol	Chain	Length	Quality of chain
2	J	397	<div><div></div><div>60%</div><div>32%</div><div>7%</div><div></div></div>
2	K	397	<div><div></div><div>61%</div><div>32%</div><div>7%</div><div></div></div>
2	L	397	<div><div></div><div>60%</div><div>33%</div><div>6%</div><div></div></div>
2	M	397	<div><div></div><div>59%</div><div>34%</div><div>7%</div><div></div></div>
2	N	397	<div><div></div><div>60%</div><div>33%</div><div>7%</div><div></div></div>
2	O	397	<div><div></div><div>61%</div><div>31%</div><div>7%</div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 53996 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	781	Total	C	N	O	S	1	0
			6383	4054	1099	1194	36		
1	B	800	Total	C	N	O	S	0	0
			6541	4157	1124	1224	36		

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	D	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	E	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	F	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	G	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	H	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	I	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	J	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	K	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	L	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	M	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	N	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		
2	O	397	Total	C	N	O	S	0	0
			3159	2002	546	596	15		

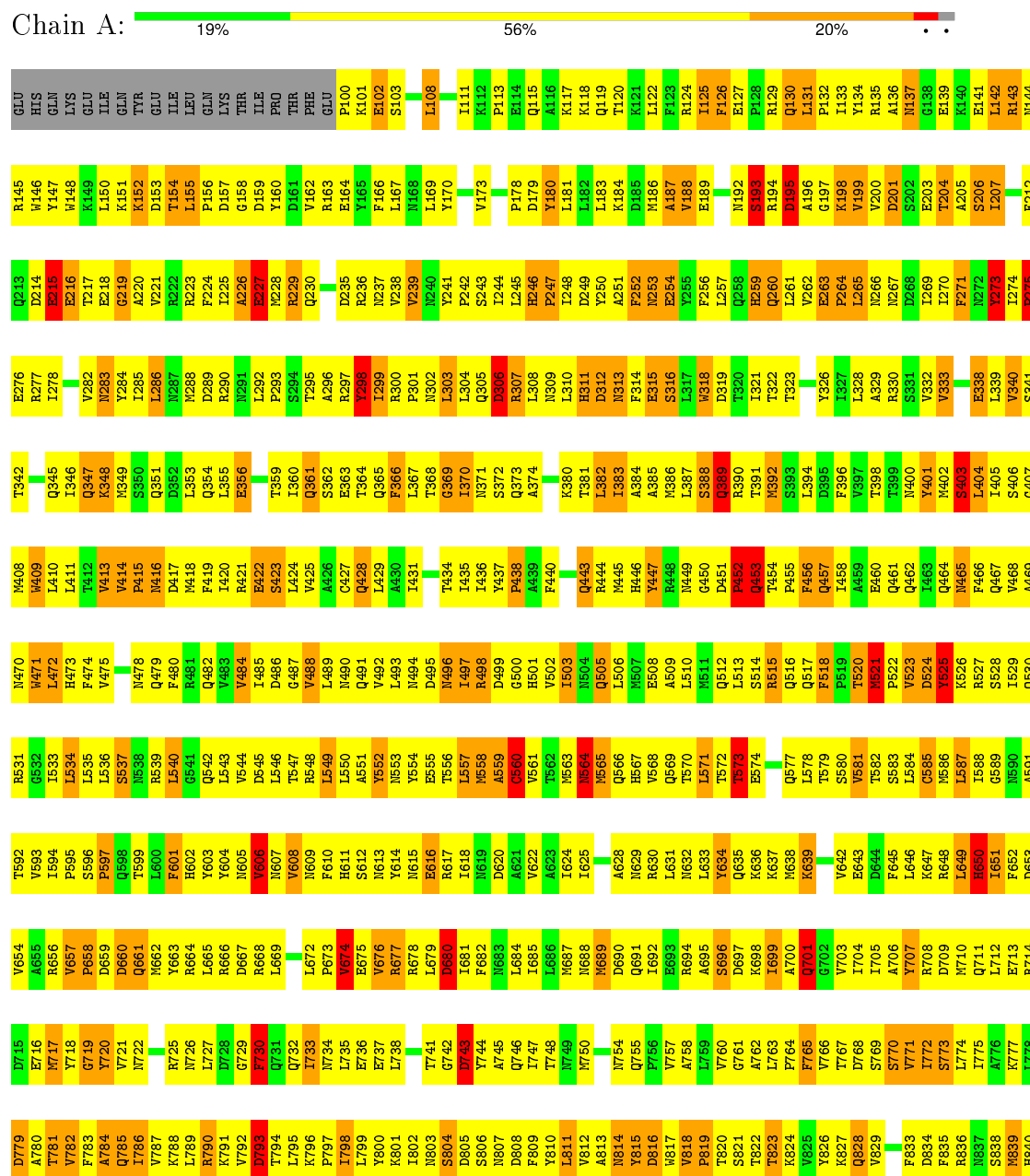
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total 1	Zn 1	0
3	J	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	N	1	Total 1	Zn 1	0
3	O	1	Total 1	Zn 1	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

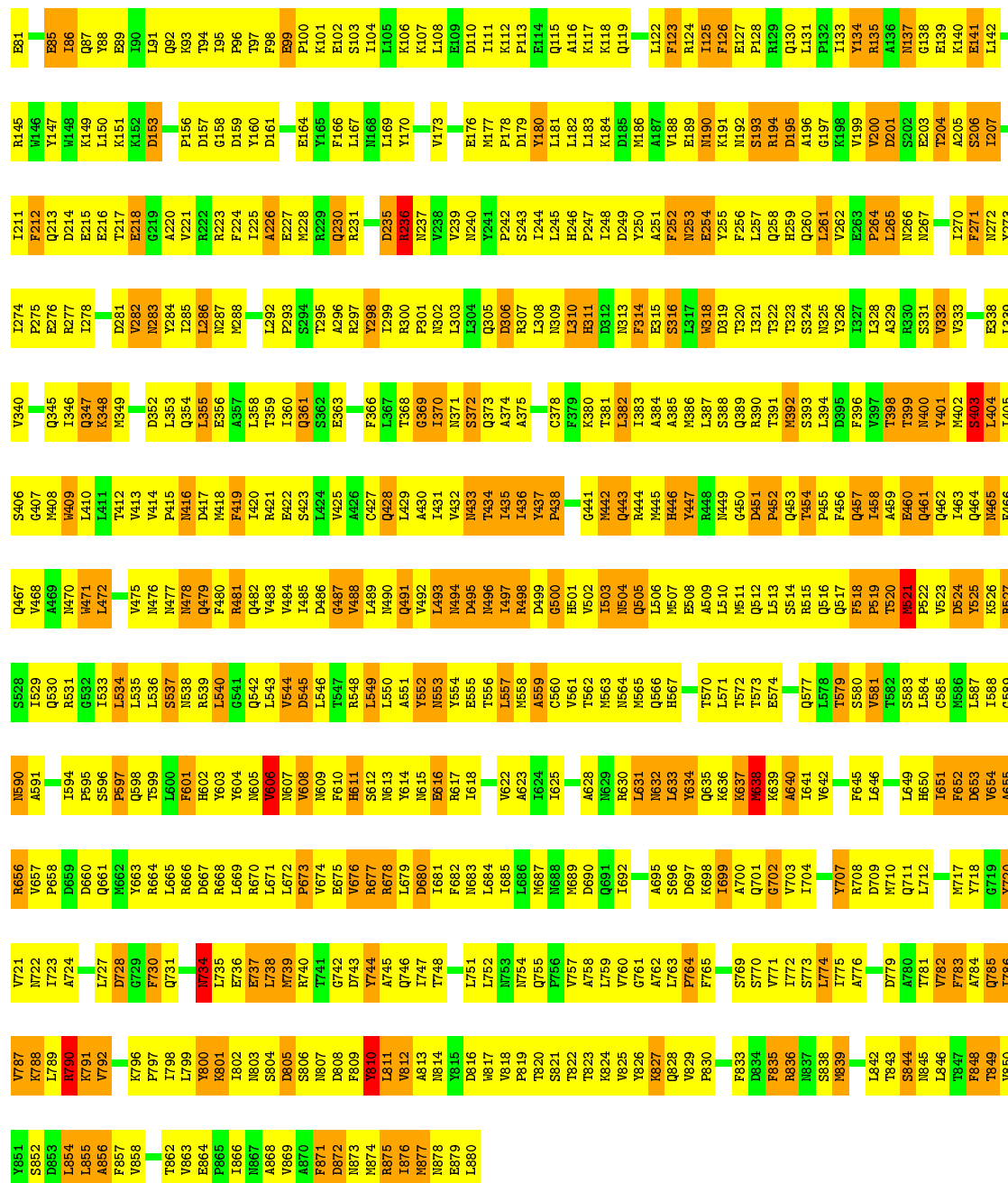
#### • Molecule 1: Inner capsid protein VP2





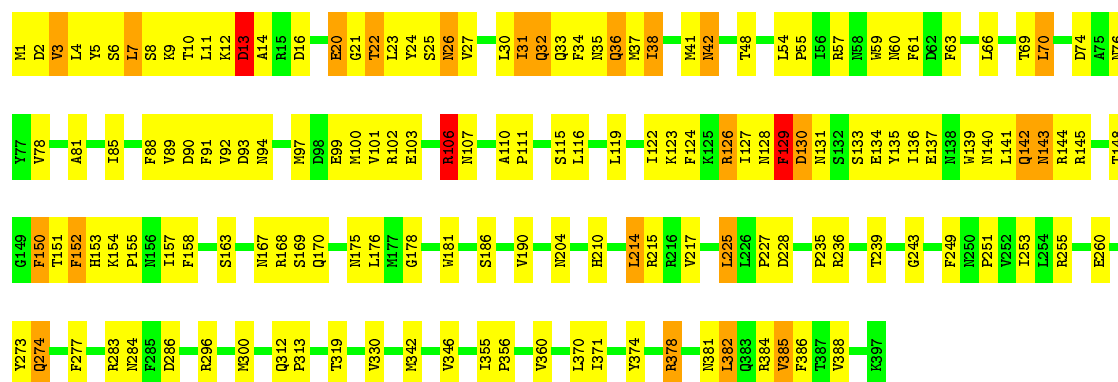
● Molecule 1: Inner capsid protein VP2

Chain B: 20% 57% 22%



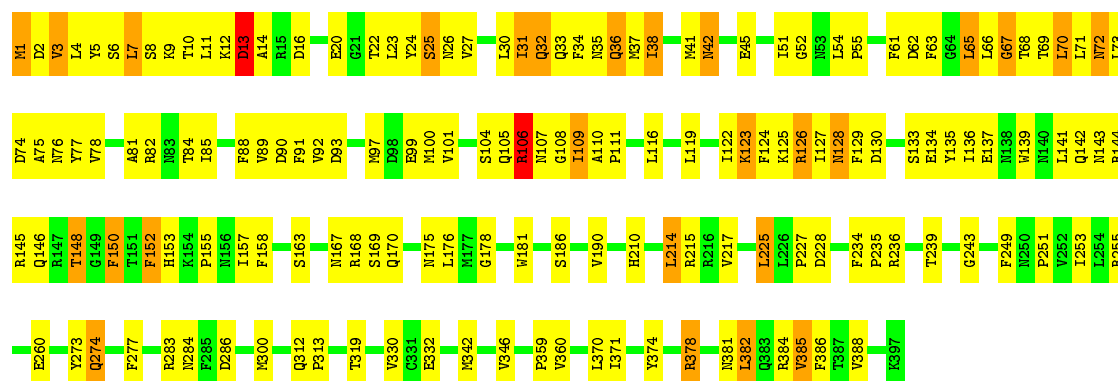
● Molecule 2: Intermediate capsid protein VP6

Chain C: 61% 32% 6%



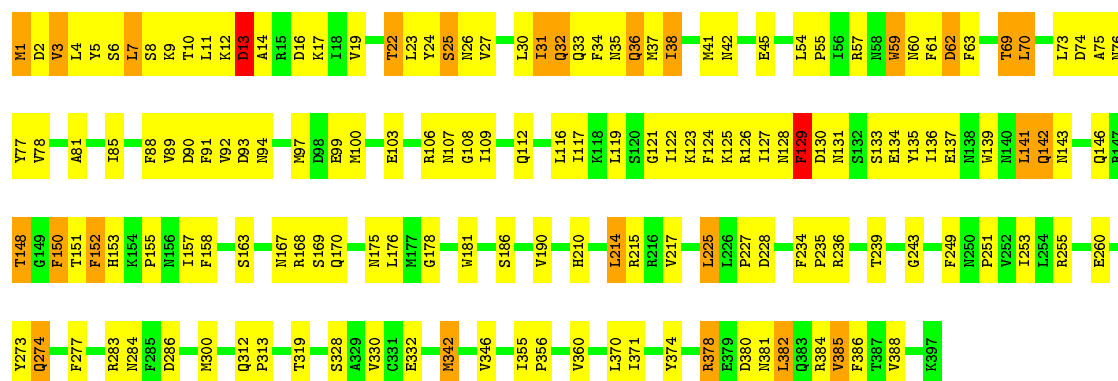
• Molecule 2: Intermediate capsid protein VP6

Chain D: 59% 34% 7% .



• Molecule 2: Intermediate capsid protein VP6

Chain E: 60% 33% 6% .

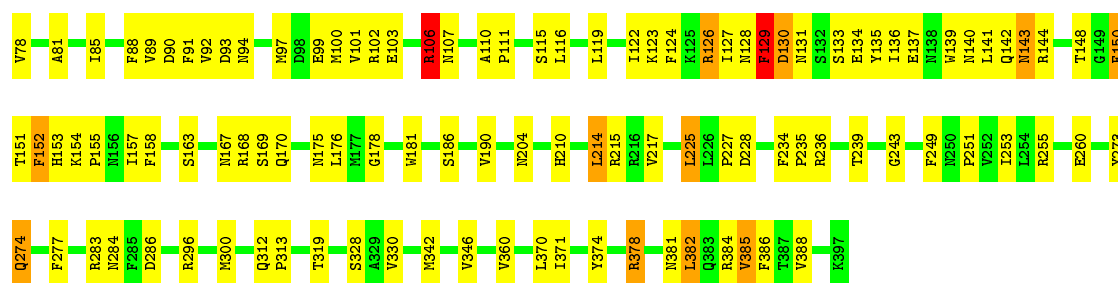


• Molecule 2: Intermediate capsid protein VP6

Chain F: 61% 32% 6% .

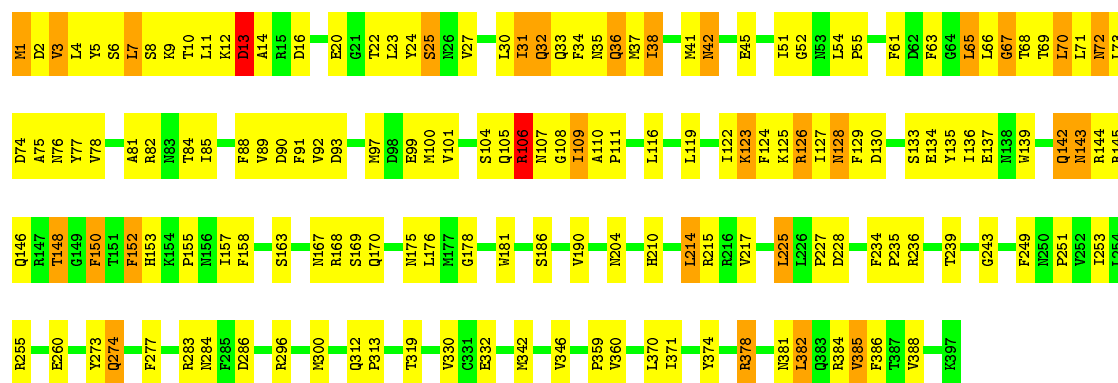






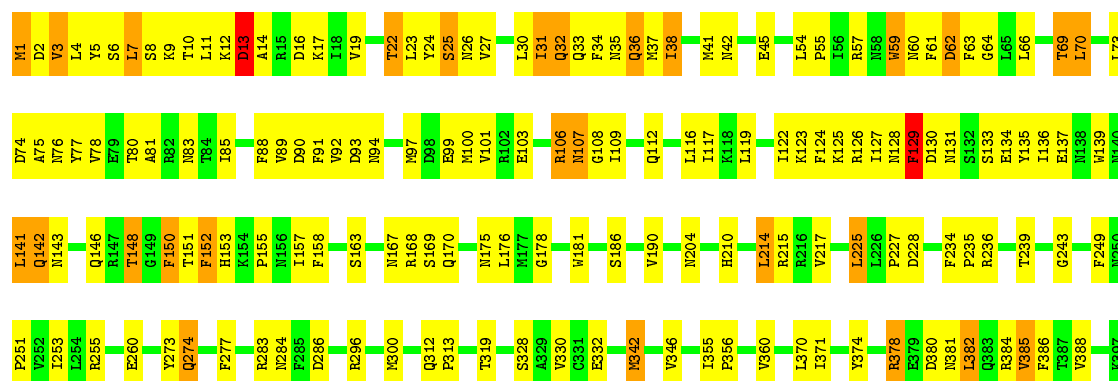
- Molecule 2: Intermediate capsid protein VP6

Chain G: 60% 33% 7% .



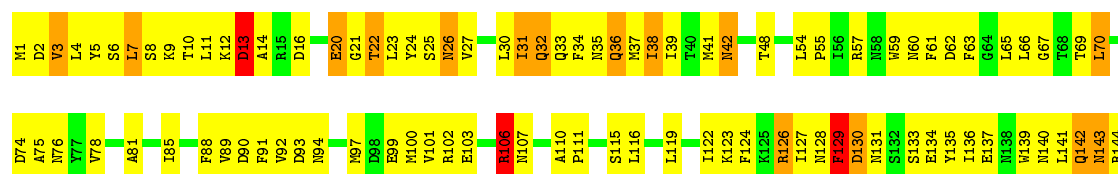
- Molecule 2: Intermediate capsid protein VP6

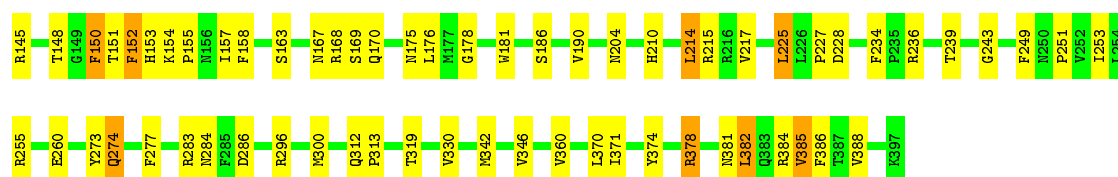
Chain H: 59% 34% 7% .



- Molecule 2: Intermediate capsid protein VP6

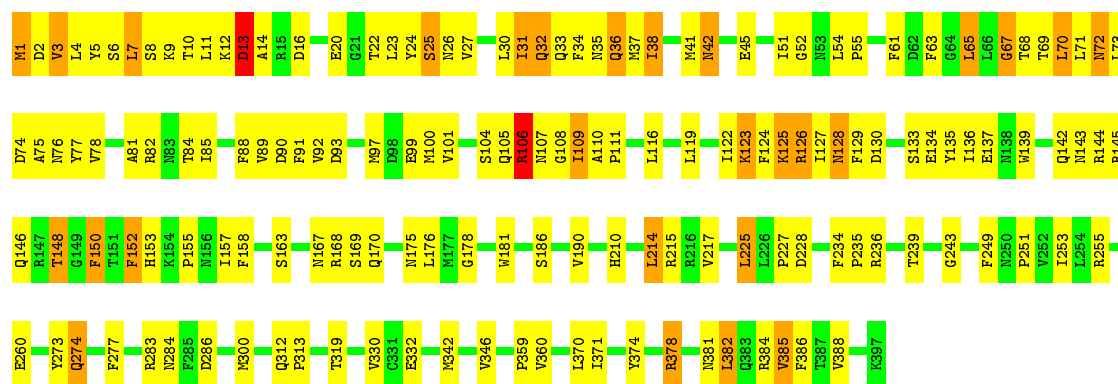
Chain I: 60% 33% 6% .





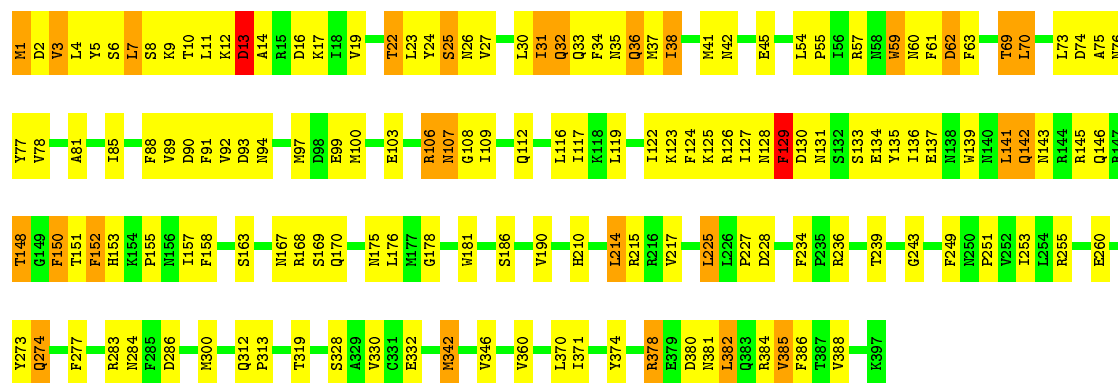
• Molecule 2: Intermediate capsid protein VP6

Chain J: 60% 32% 7%



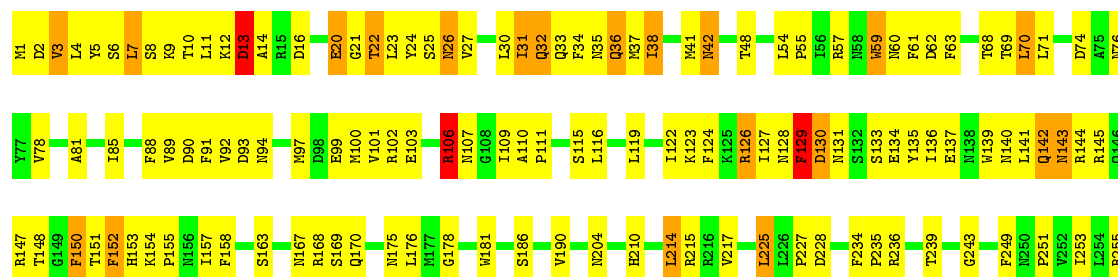
• Molecule 2: Intermediate capsid protein VP6

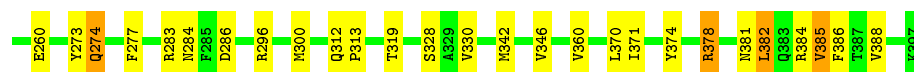
Chain K: 61% 32% 7%



• Molecule 2: Intermediate capsid protein VP6

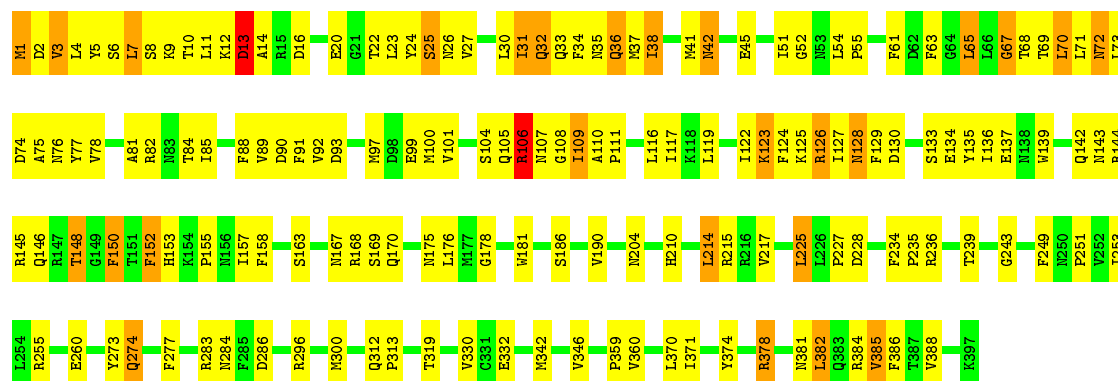
Chain L: 60% 33% 6%





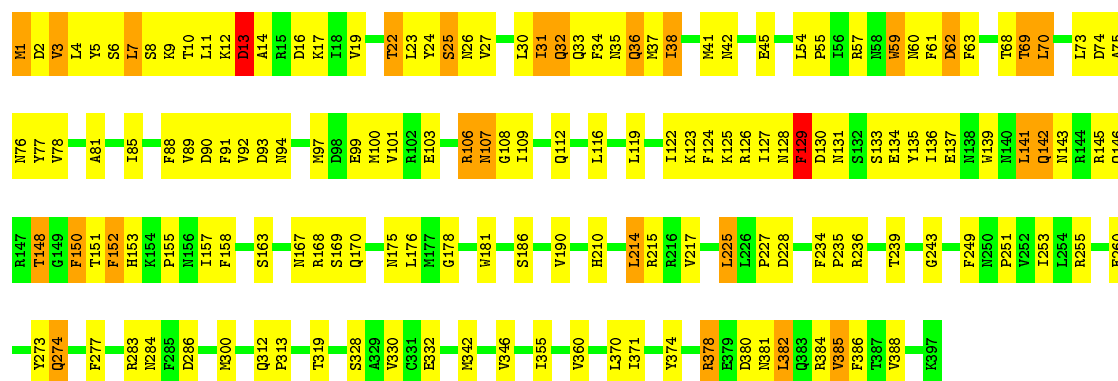
• Molecule 2: Intermediate capsid protein VP6

Chain M: 59% 34% 7%



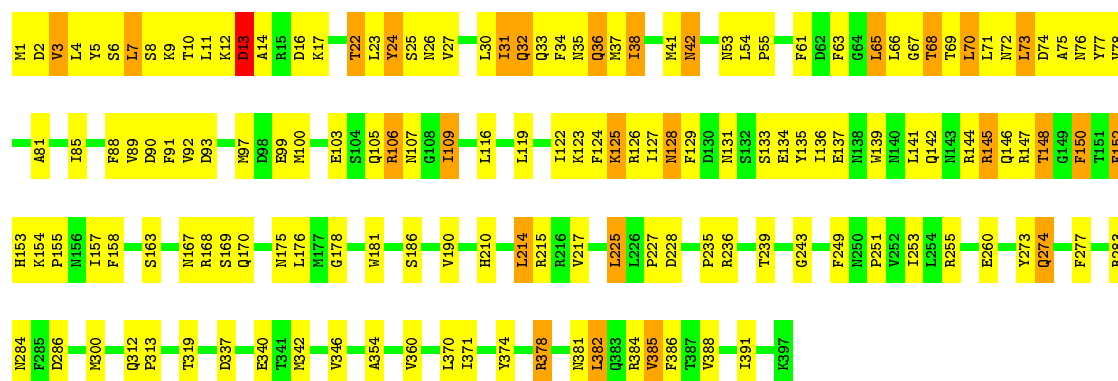
• Molecule 2: Intermediate capsid protein VP6

Chain N: 60% 33% 7%



• Molecule 2: Intermediate capsid protein VP6

Chain O: 61% 31% 7%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	individual particle CTF	Depositor
Microscope	TF30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2500	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	film	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.52	0/6500	0.85	10/8819 (0.1%)
1	B	0.59	2/6662 (0.0%)	0.84	10/9038 (0.1%)
2	C	0.50	0/3229	0.76	5/4394 (0.1%)
2	D	0.50	0/3229	0.76	5/4394 (0.1%)
2	E	0.50	0/3229	0.76	5/4394 (0.1%)
2	F	0.50	0/3229	0.76	5/4394 (0.1%)
2	G	0.50	0/3229	0.76	5/4394 (0.1%)
2	H	0.50	0/3229	0.76	5/4394 (0.1%)
2	I	0.50	0/3229	0.76	5/4394 (0.1%)
2	J	0.50	0/3229	0.76	5/4394 (0.1%)
2	K	0.50	0/3229	0.76	5/4394 (0.1%)
2	L	0.50	0/3229	0.76	5/4394 (0.1%)
2	M	0.50	0/3229	0.76	5/4394 (0.1%)
2	N	0.50	0/3229	0.76	5/4394 (0.1%)
2	O	0.51	0/3229	0.77	5/4394 (0.1%)
All	All	0.51	2/55139 (0.0%)	0.78	85/74979 (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	A	0	3
1	B	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	848	PHE	C-N	-17.55	0.93	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	ALA	C-N	-10.49	1.09	1.34

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD1	-11.13	114.32	121.00
1	A	273	TYR	CB-CG-CD2	10.46	127.28	121.00
1	A	674	VAL	O-C-N	-9.91	106.84	122.70
1	B	273	TYR	CB-CG-CD1	9.20	126.52	121.00
1	B	273	TYR	CB-CG-CD2	-9.16	115.50	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263[A]	GLU	Mainchain
1	A	273	TYR	Sidechain
1	A	674	VAL	Mainchain
1	B	810	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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	6383	0	6398	1021	0
1	B	6541	0	6551	1252	0
2	C	3159	0	3102	144	0
2	D	3159	0	3102	153	0
2	E	3159	0	3102	142	0
2	F	3159	0	3100	141	0
2	G	3159	0	3102	184	0
2	H	3159	0	3101	198	0
2	I	3159	0	3100	215	0
2	J	3159	0	3102	189	0
2	K	3159	0	3101	158	0
2	L	3159	0	3099	178	0
2	M	3159	0	3102	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	3159	0	3101	177	0
2	O	3159	0	3102	135	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
All	All	53996	0	53265	4052	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 38.

The worst 5 of 4052 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:B:498:ARG:HH12	2:J:25:SER:CB	1.22	1.46
1:B:498:ARG:NH1	2:J:25:SER:HB3	1.24	1.46
2:K:145:ARG:CD	2:L:143:ASN:HA	1.45	1.44
1:B:630:ARG:HD3	2:L:71:LEU:CB	1.07	1.44
1:A:473:HIS:CD2	2:G:70:LEU:CD1	2.01	1.44

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	780/800 (98%)	433 (56%)	201 (26%)	146 (19%)	<b>0</b> <b>3</b>
1	B	798/800 (100%)	460 (58%)	210 (26%)	128 (16%)	<b>0</b> <b>5</b>
2	C	395/397 (100%)	326 (82%)	49 (12%)	20 (5%)	<b>2</b> <b>31</b>
2	D	395/397 (100%)	330 (84%)	43 (11%)	22 (6%)	<b>2</b> <b>29</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	395/397 (100%)	331 (84%)	45 (11%)	19 (5%)	3	32
2	F	395/397 (100%)	326 (82%)	49 (12%)	20 (5%)	2	31
2	G	395/397 (100%)	329 (83%)	45 (11%)	21 (5%)	2	30
2	H	395/397 (100%)	331 (84%)	45 (11%)	19 (5%)	3	32
2	I	395/397 (100%)	326 (82%)	49 (12%)	20 (5%)	2	31
2	J	395/397 (100%)	329 (83%)	45 (11%)	21 (5%)	2	30
2	K	395/397 (100%)	331 (84%)	45 (11%)	19 (5%)	3	32
2	L	395/397 (100%)	326 (82%)	49 (12%)	20 (5%)	2	31
2	M	395/397 (100%)	330 (84%)	44 (11%)	21 (5%)	2	30
2	N	395/397 (100%)	331 (84%)	45 (11%)	19 (5%)	3	32
2	O	395/397 (100%)	320 (81%)	52 (13%)	23 (6%)	2	28
All	All	6713/6761 (99%)	5159 (77%)	1016 (15%)	538 (8%)	2	19

5 of 538 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	A	131	LEU
1	A	154	THR
1	A	187	ALA
1	A	198	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	716/734 (98%)	628 (88%)	88 (12%)	6	34
1	B	734/734 (100%)	645 (88%)	89 (12%)	6	34
2	C	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	D	350/350 (100%)	328 (94%)	22 (6%)	22	63
2	E	350/350 (100%)	329 (94%)	21 (6%)	24	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	G	350/350 (100%)	328 (94%)	22 (6%)	22	63
2	H	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	I	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	J	350/350 (100%)	328 (94%)	22 (6%)	22	63
2	K	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	L	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	M	350/350 (100%)	328 (94%)	22 (6%)	22	63
2	N	350/350 (100%)	329 (94%)	21 (6%)	24	65
2	O	350/350 (100%)	331 (95%)	19 (5%)	27	68
All	All	6000/6018 (100%)	5548 (92%)	452 (8%)	21	57

5 of 452 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	129	PHE
2	F	225	LEU
2	N	107	ASN
2	D	214	LEU
2	E	152	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 196 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	53	ASN
2	G	131	ASN
2	N	142	GLN
2	E	131	ASN
2	F	32	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.