wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:41 PM BST

PDB ID	:	3IYK
EMDB ID:	:	EMD-5147
Title	:	Bluetongue virus structure reveals a sialic acid binding domain, amphipathic helices and a central coiled coil in the outer capsid proteins
Authors	:	Zhang, X.; Boyce, M.; Bhattacharya, B.; Zhang, X.; Schein, S.; Roy, P.; Zhou, Z.H.
Deposited on	:	2010-01-25
Resolution	:	7.00 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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

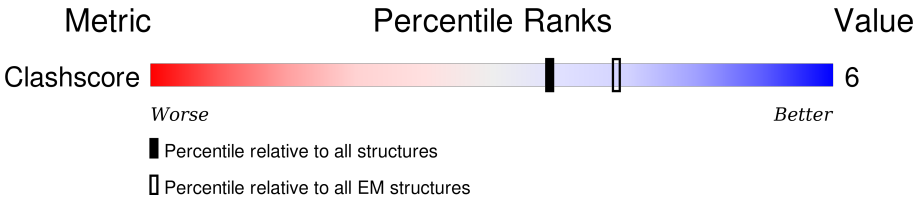
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.00 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

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	526	58% 42%
1	B	526	58% 42%
1	C	526	58% 42%
1	D	526	58% 42%
1	E	526	58% 42%
1	F	526	58% 42%
2	G	600	23% • 77%
2	I	600	23% • 77%
2	K	600	23% • 77%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2331 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.

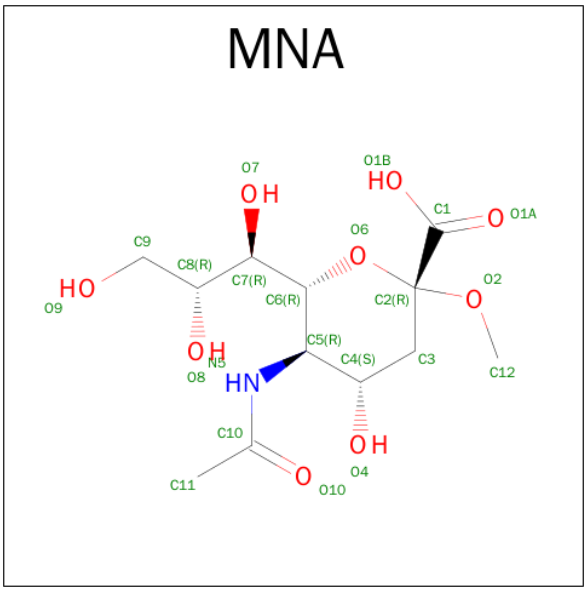
- Molecule 1 is a protein called VP5.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	307	Total C 307 307	0	307
1	B	307	Total C 307 307	0	307
1	C	307	Total C 307 307	0	307
1	D	307	Total C 307 307	0	307
1	E	307	Total C 307 307	0	307
1	F	307	Total C 307 307	0	307

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	G	141	Total C 141 141	0	141
2	I	141	Total C 141 141	0	141
2	K	141	Total C 141 141	0	141

- Molecule 3 is 2-O-METHYL-5-N-ACETYL-ALPHA-D- NEURAMINIC ACID (three-letter code: MNA) (formula: $C_{12}H_{21}NO_9$).



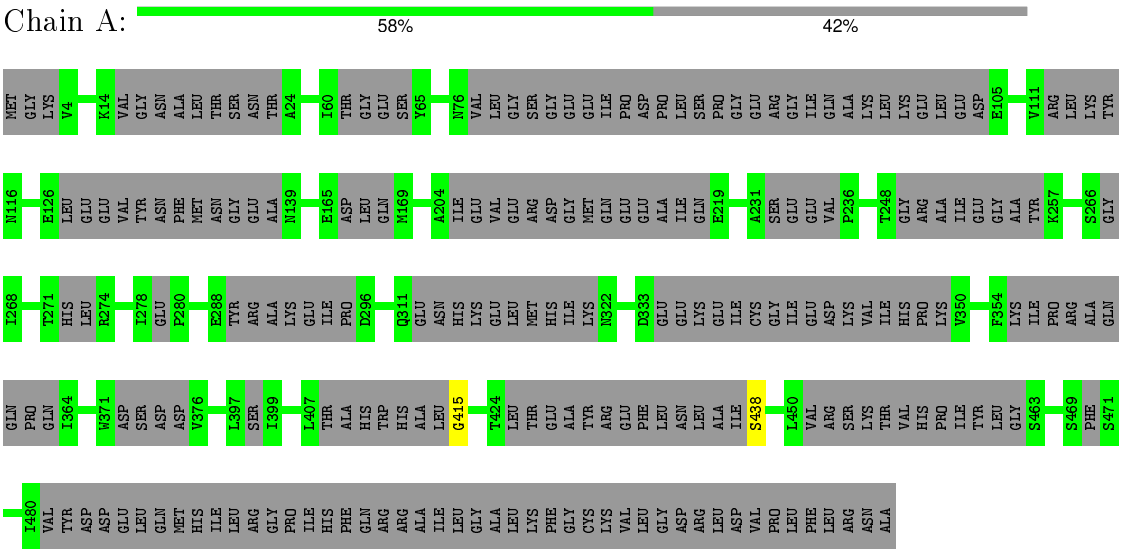
Mol	Chain	Residues	Atoms				AltConf
3	G	1	Total	C	N	O	1
			22	12	1	9	
3	I	1	Total	C	N	O	1
			22	12	1	9	
3	K	1	Total	C	N	O	1
			22	12	1	9	

3 Residue-property plots (i)

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.

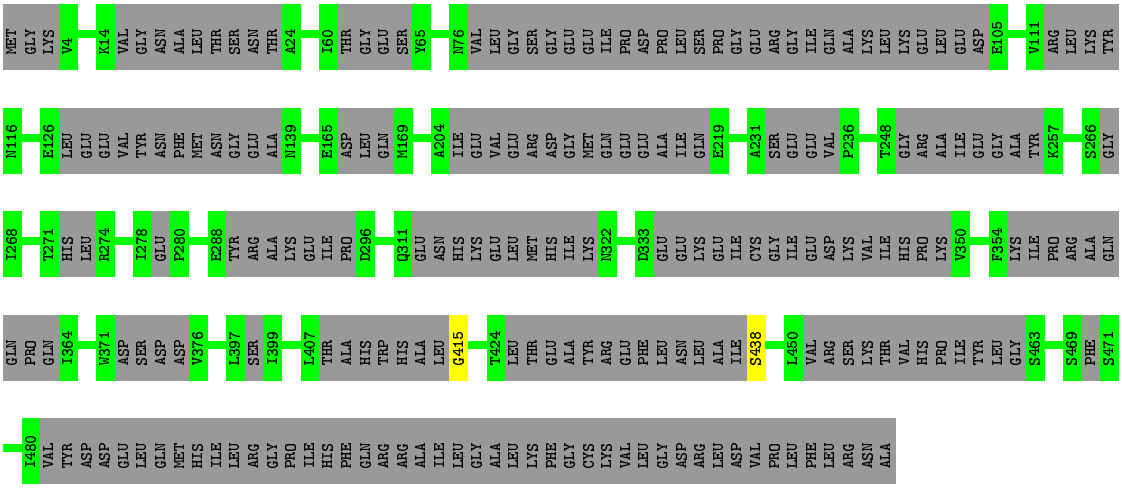
- Molecule 1: VP5

Chain A:



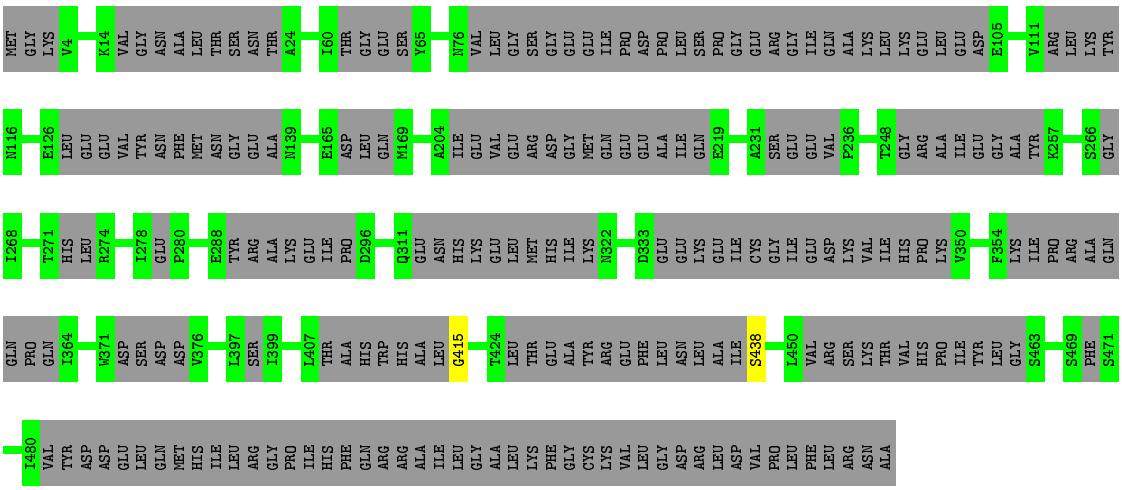
- Molecule 1: VP5

Chain B:



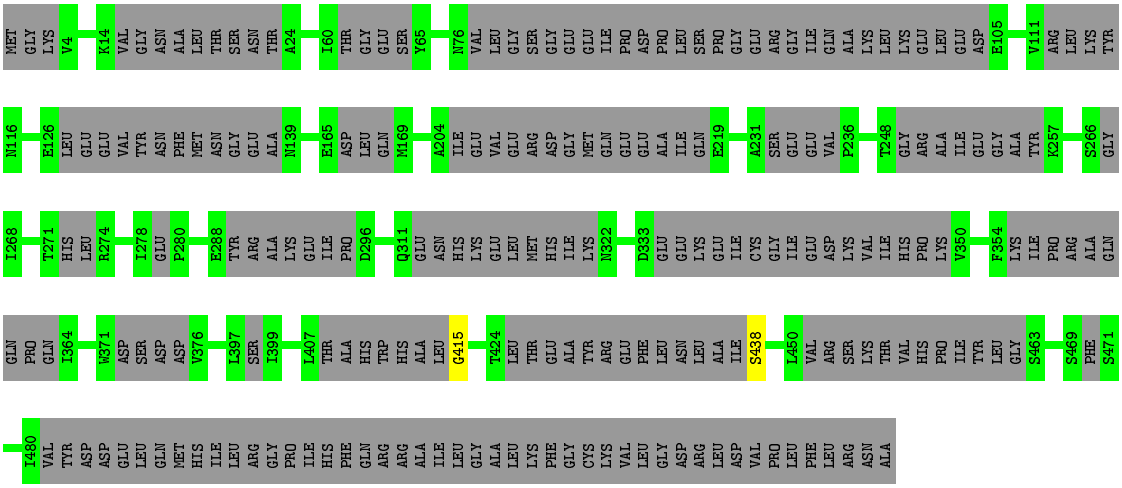
- Molecule 1: VP5

Chain C:



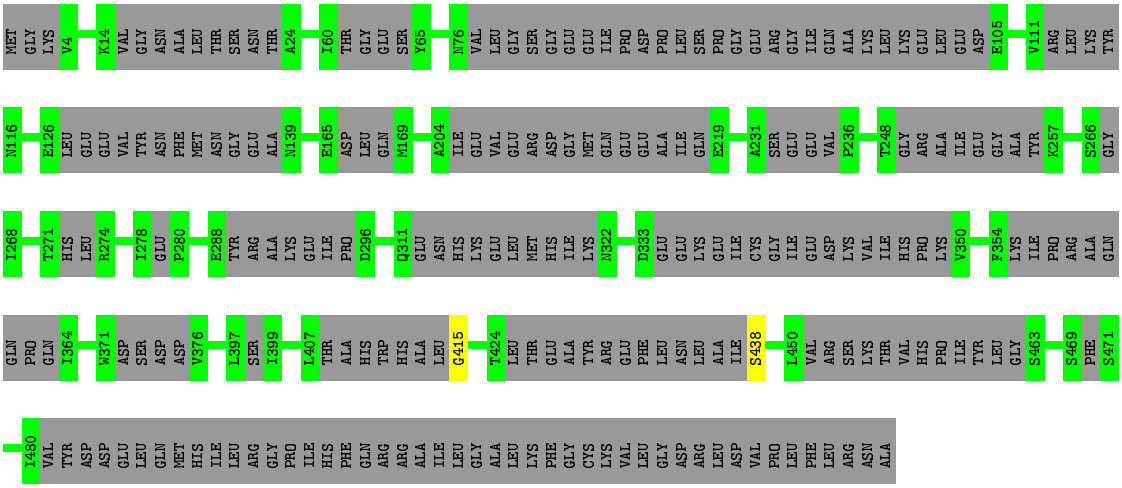
- Molecule 1: VP5

Chain D:



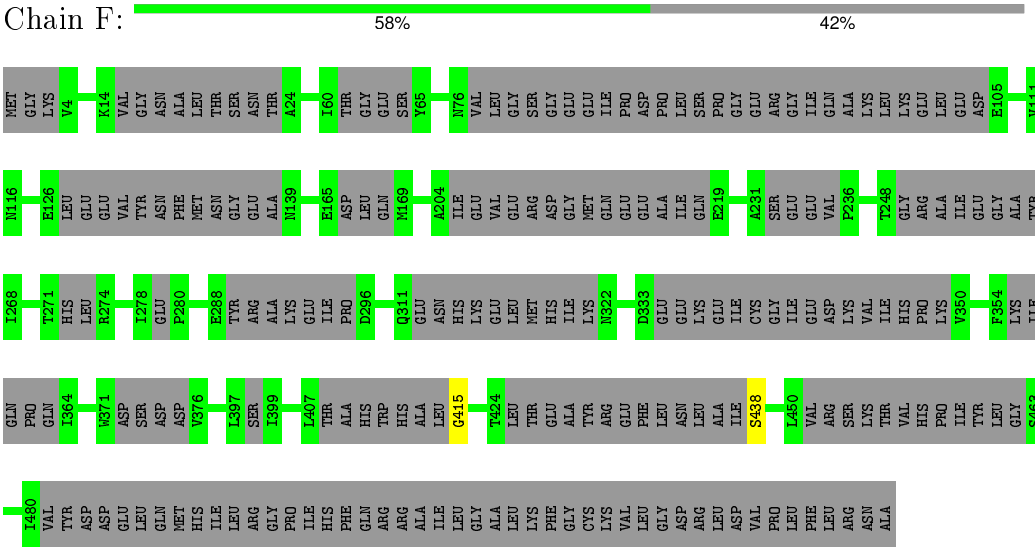
- Molecule 1: VP5

Chain E:



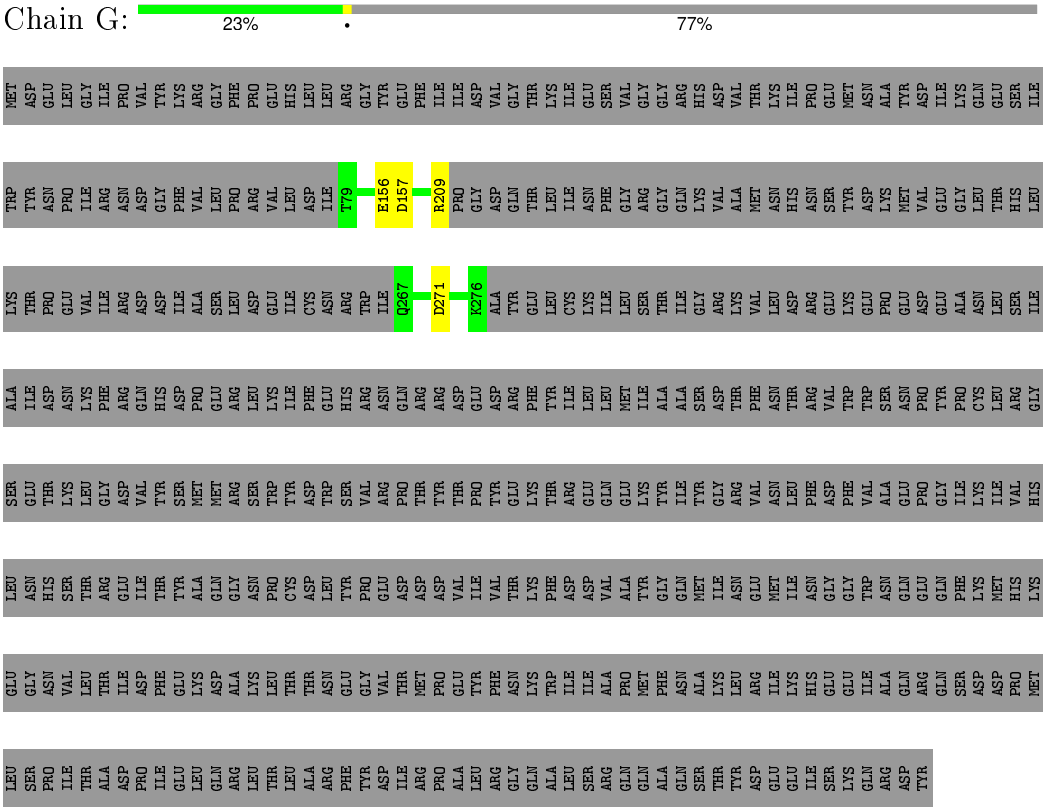
- Molecule 1: VP5

Chain F:



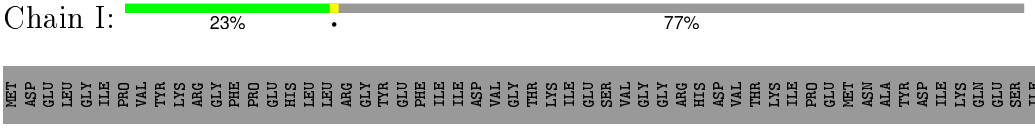
- Molecule 2: VP2

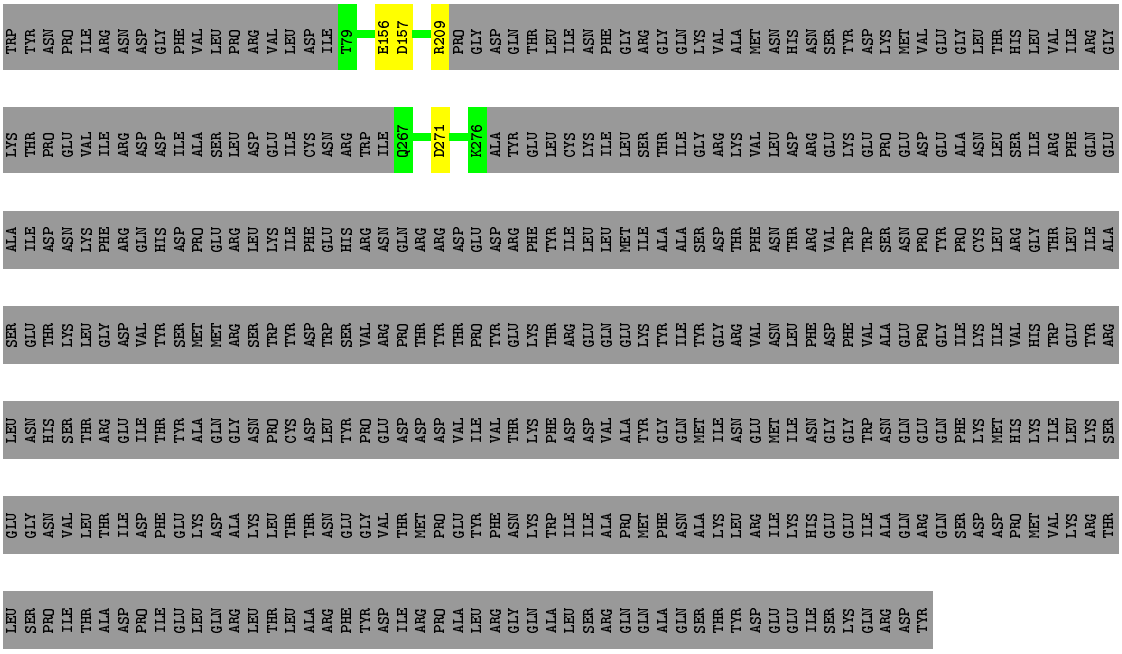
Chain G:



- Molecule 2: VP2

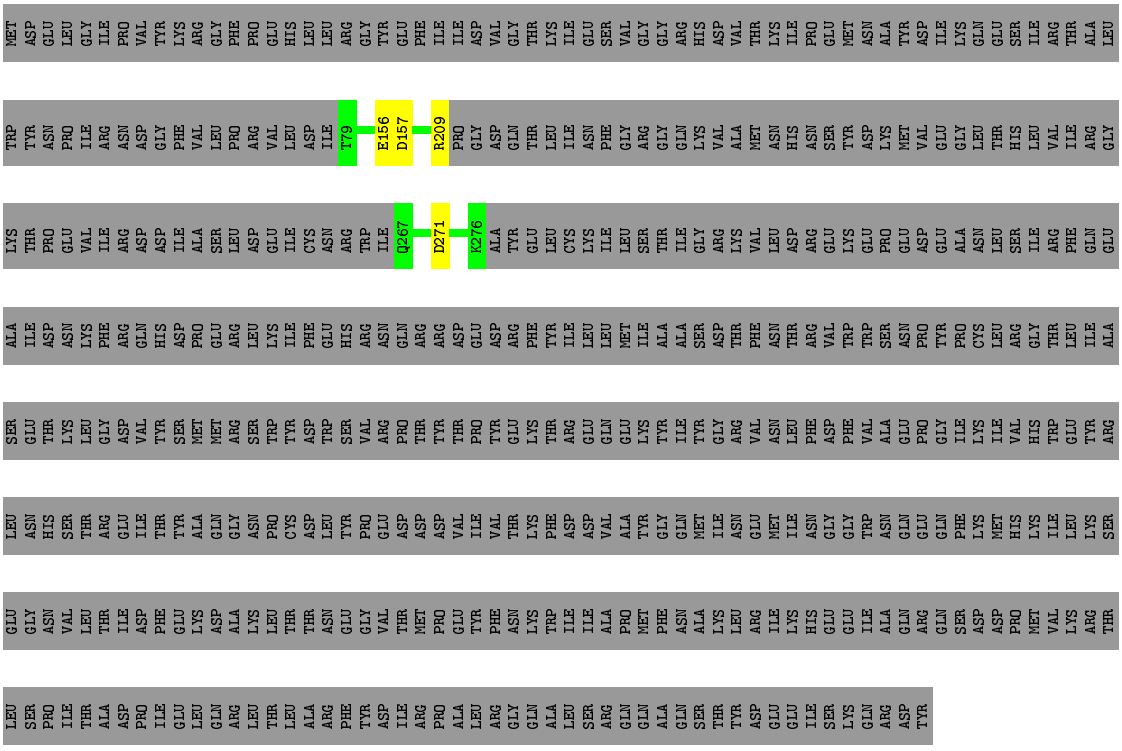
Chain I:





- Molecule 2: VP2

Chain K:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	3400	Depositor
Resolution determination method	FSC 0.143 cut-off	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	80000	Depositor
Image detector	CCD	Depositor

5 Model quality

5.1 Standard geometry

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	307	0	0	1	0
1	B	307	0	0	1	0
1	C	307	0	0	1	0
1	D	307	0	0	1	0
1	E	307	0	0	1	0
1	F	307	0	0	1	0
2	G	141	0	0	3	0
2	I	141	0	0	3	0
2	K	141	0	0	3	0
3	G	22	0	20	0	0
3	I	22	0	20	0	0
3	K	22	0	20	0	0
All	All	2331	0	60	12	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 6.

The worst 5 of 12 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:E:415:GLY:CA	1:E:438:SER:CA	2.38	1.02
1:C:415:GLY:CA	1:C:438:SER:CA	2.38	1.02
1:D:415:GLY:CA	1:D:438:SER:CA	2.38	1.02
1:B:415:GLY:CA	1:B:438:SER:CA	2.38	1.01
1:A:415:GLY:CA	1:A:438:SER:CA	2.38	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MNA	G	1000[A]	-	19,22,22	1.17	2 (10%)	17,32,32	0.80	1 (5%)
3	MNA	I	1000[B]	-	19,22,22	1.19	2 (10%)	17,32,32	0.80	1 (5%)
3	MNA	K	1000[C]	-	19,22,22	1.20	2 (10%)	17,32,32	0.81	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MNA	G	1000[A]	-	-	0/17/41/41	0/1/1/1
3	MNA	I	1000[B]	-	-	0/17/41/41	0/1/1/1
3	MNA	K	1000[C]	-	-	0/17/41/41	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1000[B]	MNA	C4-C5	2.13	1.55	1.53
3	G	1000[A]	MNA	C4-C5	2.13	1.55	1.53
3	K	1000[C]	MNA	C4-C5	2.18	1.55	1.53
3	G	1000[A]	MNA	C3-C2	3.67	1.55	1.52
3	K	1000[C]	MNA	C3-C2	3.72	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1000[B]	MNA	C12-O2-C2	2.06	117.33	115.29
3	G	1000[A]	MNA	C12-O2-C2	2.09	117.36	115.29
3	K	1000[C]	MNA	C12-O2-C2	2.11	117.39	115.29

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.