

# Full wwPDB X-ray Structure Validation Report (i)

#### Dec 4, 2023 - 07:04 pm GMT

PDB ID : 1WCE

Title : Crystal structure of the T13 IBDV viral particle reveals a missing link in

icosahedral viruses evolution

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Deposited on : 2004-11-12

Resolution : 7.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$ 

EDS: 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

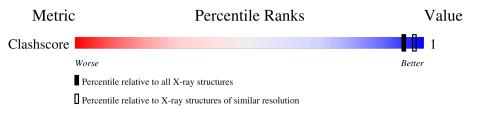
Validation Pipeline (wwPDB-VP) : 2.36

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

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	Similar resolution	
Medic	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$	
Clashscore	141614	1069 (10.00-3.90)	

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain	
1	A	441	96%	
1	В	441	97%	
1	С	441	98%	·
1	D	441	96%	·
1	Е	441	97%	·
1	F	441	98%	
1	G	441	96%	·
1	Н	441	96%	
1	I	441	95%	5%
1	J	441	96%	
1	K	441	94%	6%

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Mol	Chain	Length	Quality of chain
1	L	441	97%
1	M	441	96%



### 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5533 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 MAJOR STRUCTURAL PROTEIN VP2.

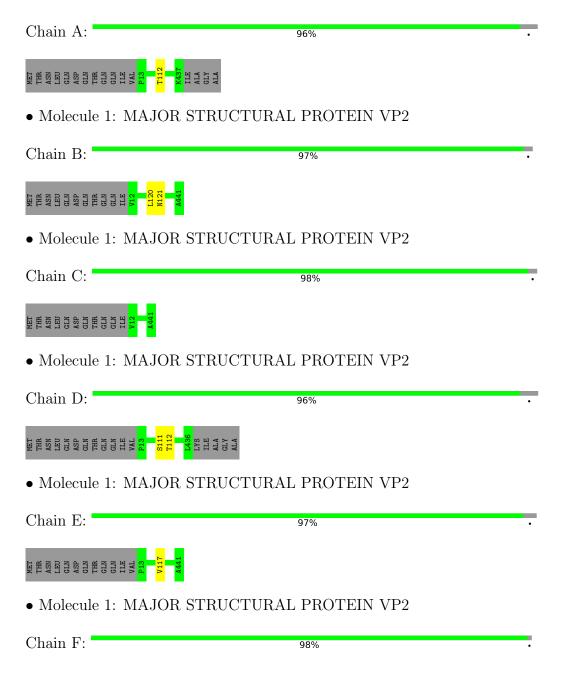
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	425	Total C 425 425	0	0	425
1	В	430	Total C 430 430	0	0	430
1	С	430	Total C 430 430	0	0	430
1	D	424	Total C 424 424	0	0	424
1	Е	429	Total C 429 429	0	0	429
1	F	436	Total C 436 436	0	0	436
1	G	426	Total C 426 426	0	0	426
1	Н	423	Total C 423 423	0	0	423
1	I	417	Total C 417 417	0	0	417
1	J	423	Total C 423 423	0	0	423
1	K	416	Total C 416 416	0	0	416
1	L	429	Total C 429 429	0	0	429
1	M	425	Total C 425 425	0	0	425



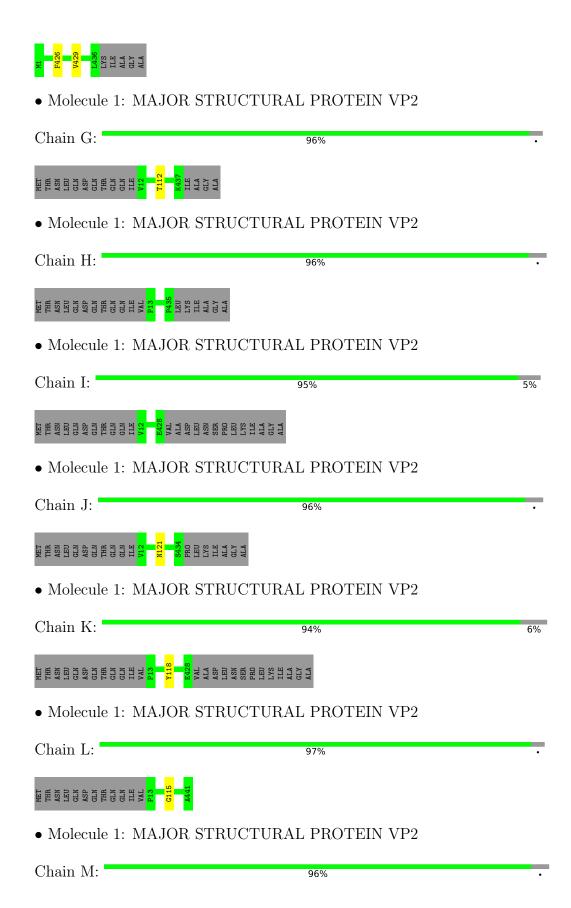
## 3 Residue-property plots (i)

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. 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.

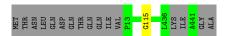
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2













## 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	854.01Å 692.23Å 792.41Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	50.00 - 7.00	Depositor	
resolution (A)	49.86 - 6.97	EDS	
% Data completeness	75.1 (50.00-7.00)	Depositor	
(in resolution range)	74.7 (49.86-6.97)	EDS	
$R_{merge}$	0.14	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.90  (at  6.68Å)	Xtriage	
Refinement program	CNS 1.1	Depositor	
$R, R_{free}$	(Not available) , (Not available)	Depositor	
it, it <sub>free</sub>	0.371, (Not available)	DCC	
$R_{free}$ test set	No test flags present.	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	190.2	Xtriage	
Anisotropy	0.155	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	1.78, 49.1	EDS	
L-test for twinning <sup>2</sup>	$< L >=0.45, < L^2>=0.27$	Xtriage	
Estimated twinning fraction	0.327 for -h,-k,l	Xtriage	
$F_o, F_c$ correlation	0.67	EDS	
Total number of atoms	5533	wwPDB-VP	
Average B, all atoms $(\mathring{A}^2)$	52.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

#### 5.1 Standard geometry (i)

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

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 (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	425	0	0	2	0
1	В	430	0	0	2	0
1	С	430	0	0	0	0
1	D	424	0	0	1	0
1	Ε	429	0	0	1	0
1	F	436	0	0	1	0
1	G	426	0	0	1	0
1	Н	423	0	0	0	0
1	I	417	0	0	0	0
1	J	423	0	0	1	0
1	K	416	0	0	1	0
1	L	429	0	0	1	0
1	M	425	0	0	1	0
All	All	5533	0	0	7	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 1.

All (7) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:D:111:SER:CA	1:D:112:THR:CA	1.85	1.51
1:E:117:VAL:CA	1:M:115:GLY:CA	2.26	1.13
1:A:112:THR:CA	1:B:121:ASN:CA	2.64	0.76
1:K:118:TYR:CA	1:L:115:GLY:CA	2.82	0.58
1:A:112:THR:CA	1:B:120:LEU:CA	2.96	0.43
1:F:426:PHE:CA	1:F:429:VAL:CA	3.00	0.40
1:G:112:THR:CA	1:J:121:ASN:CA	2.99	0.40

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

#### 5.3.2 Protein sidechains (i)

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

#### 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 (i)

There are no chain breaks in this entry.



### 6 Fit of model and data (i)

#### 6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

