



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 09:17 am GMT

PDB ID : 1WCE
Title : Crystal structure of the T13 IBDV viral particle reveals a missing link in icosahedral viruses evolution
Authors : Coulibaly, F.; Chevalier, C.; Gutsche, I.; Pous, J.; Bressanelli, S.; Navaza, J.; Delmas, B.; Rey, F.A.
Deposited on : 2004-11-12
Resolution : 7.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

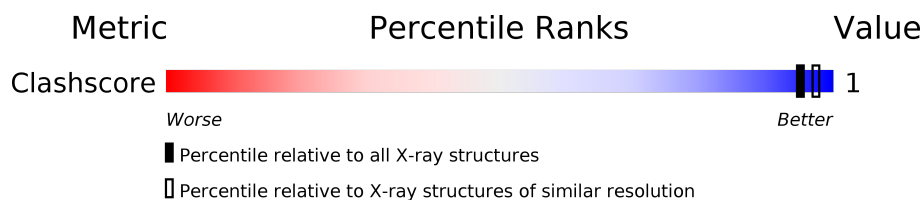
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

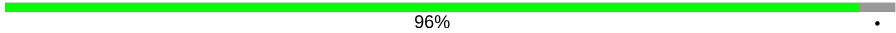
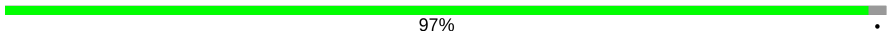

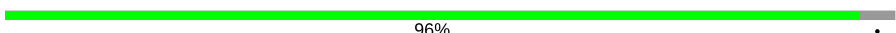

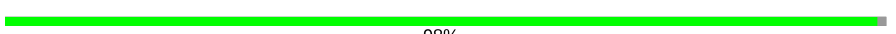
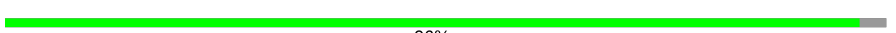




The reported resolution of this entry is 7.00 Å.

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.



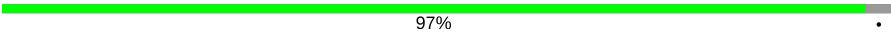
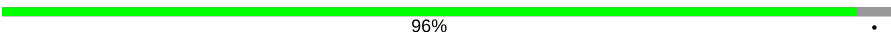
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	1146 (10.00-3.80)

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 on the lower 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	441	 96% .
1	B	441	 97% .
1	C	441	 98% .
1	D	441	 96% .
1	E	441	 97% .
1	F	441	 98% .
1	G	441	 96% .
1	H	441	 96% .
1	I	441	 95% 5%
1	J	441	 96% .
1	K	441	 94% 6%

Continued on next page...

Continued from previous page...

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

2 Entry composition

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.

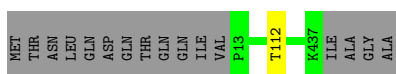
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	425	Total C 425 425	0	0	425
1	B	430	Total C 430 430	0	0	430
1	C	430	Total C 430 430	0	0	430
1	D	424	Total C 424 424	0	0	424
1	E	429	Total C 429 429	0	0	429
1	F	436	Total C 436 436	0	0	436
1	G	426	Total C 426 426	0	0	426
1	H	423	Total C 423 423	0	0	423
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 and DNA 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.

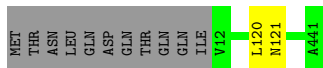
- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain A:  96%



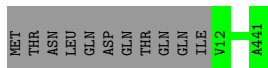
- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain B:  97%



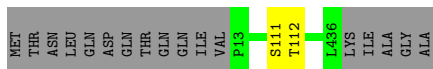
- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain C:  98%



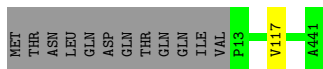
- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain D:  96%



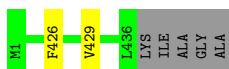
- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain E:  97%

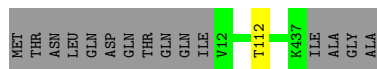


- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

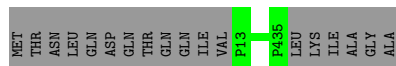
Chain F:  98%



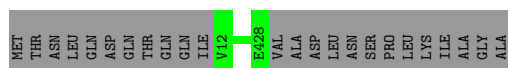
● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain G:  96% .

● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain H:  96% .

● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain I:  95% 5% .

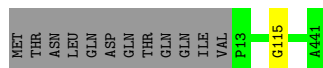
● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain J:  96% .

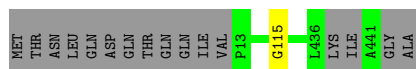
● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain K:  94% 6% .

● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain L:  97% .

● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain M:  96% .

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	854.01Å 692.23Å 792.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 7.00 49.86 – 6.97	Depositor EDS
% Data completeness (in resolution range)	75.1 (50.00-7.00) 74.7 (49.86-6.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 6.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	(Not available) , (Not available) 0.371 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	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 ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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 (Å 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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	B	430	0	0	2	0
1	C	430	0	0	0	0
1	D	424	0	0	1	0
1	E	429	0	0	1	0
1	F	436	0	0	1	0
1	G	426	0	0	1	0
1	H	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.

The worst 5 of 7 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: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

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 carbohydrates 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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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