



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:06 PM 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

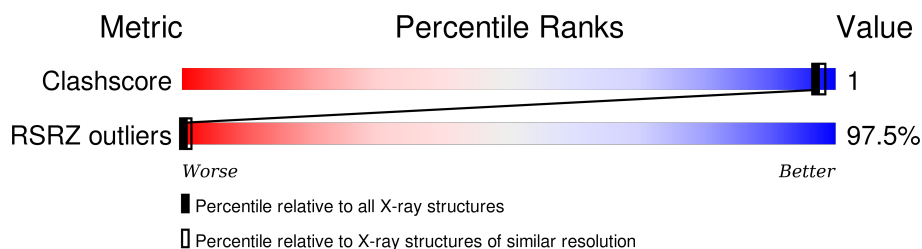
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

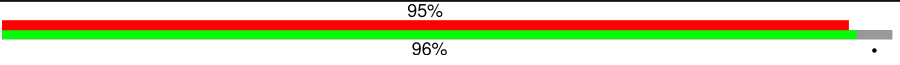
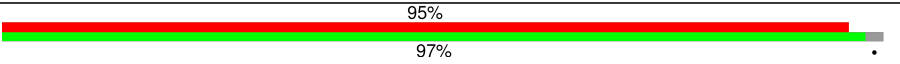
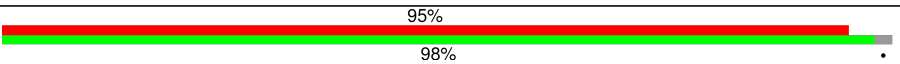
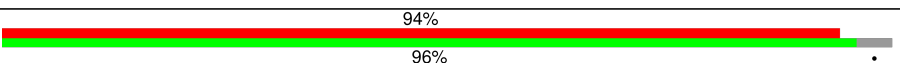
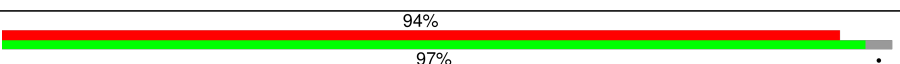
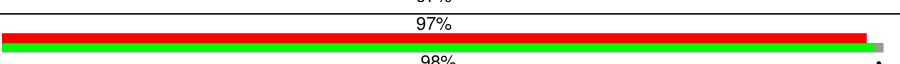
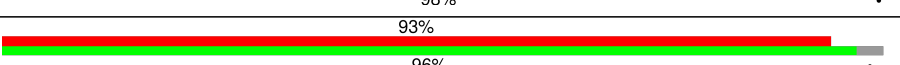
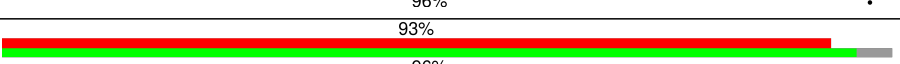
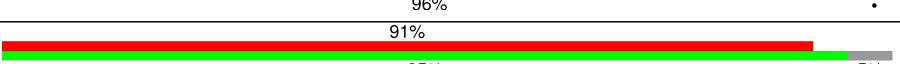
The reported resolution of this entry is 7.00 Å.

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	102246	1063 (10.00-3.70)
RSRZ outliers	91569	1013 (9.50-3.66)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	441	
1	B	441	
1	C	441	
1	D	441	
1	E	441	
1	F	441	
1	G	441	
1	H	441	
1	I	441	

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Mol	Chain	Length	Quality of chain
1	J	441	<div><div></div><div>95%</div><div></div><div></div><div>96%</div><div></div><div>.</div></div>
1	K	441	<div><div></div><div>93%</div><div></div><div></div><div>94%</div><div></div><div>6%</div></div>
1	L	441	<div><div></div><div>95%</div><div></div><div></div><div>97%</div><div></div><div>.</div></div>
1	M	441	<div><div></div><div>94%</div><div></div><div></div><div>96%</div><div></div><div>.</div></div>

## 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.

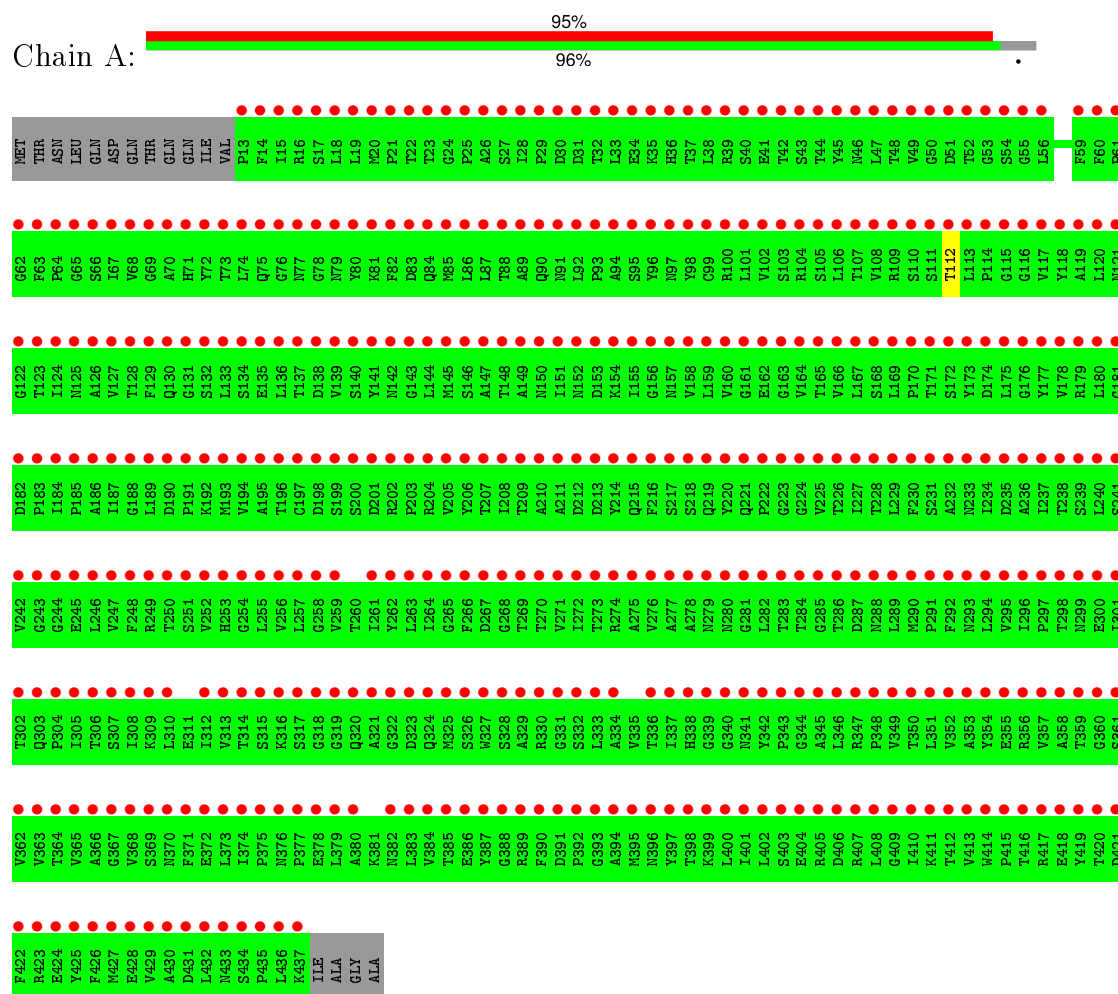
- Molecule 1 is a protein called MAJOR STRUCTURAL PROTEIN VP2.

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

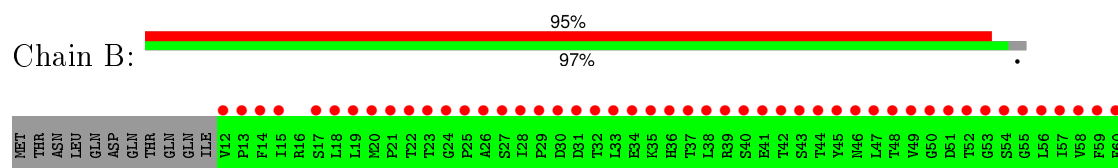
### 3 Residue-property plots

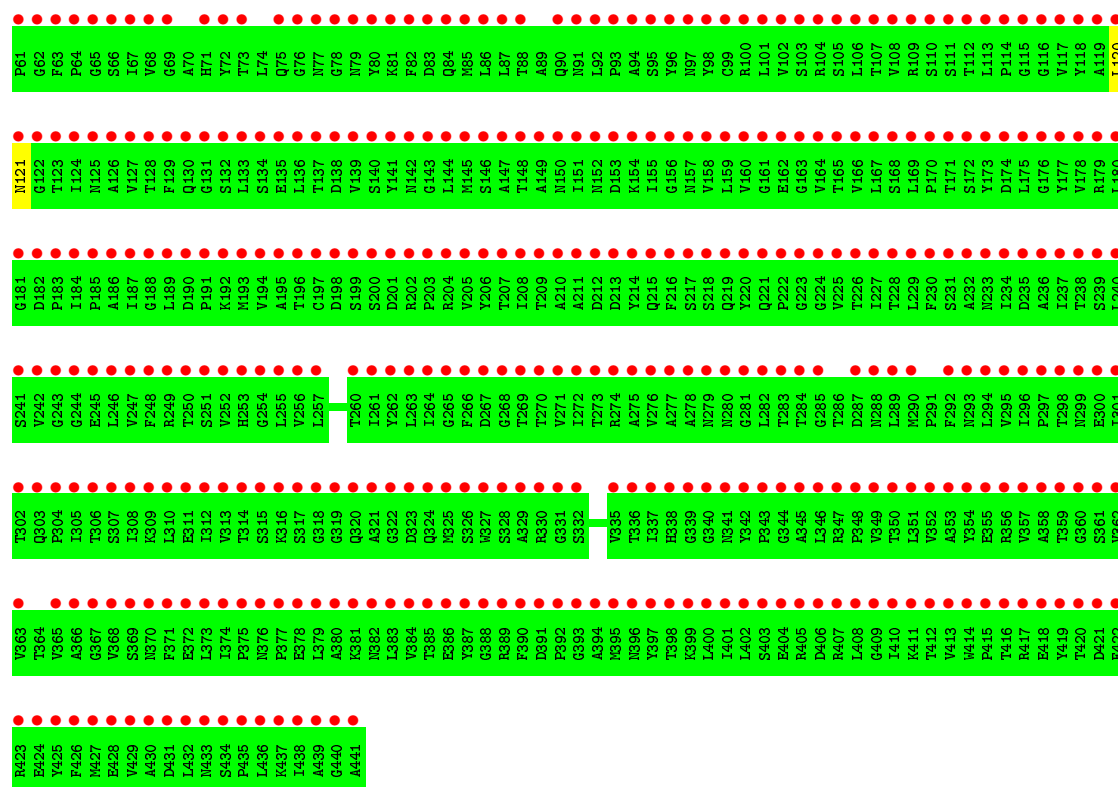
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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

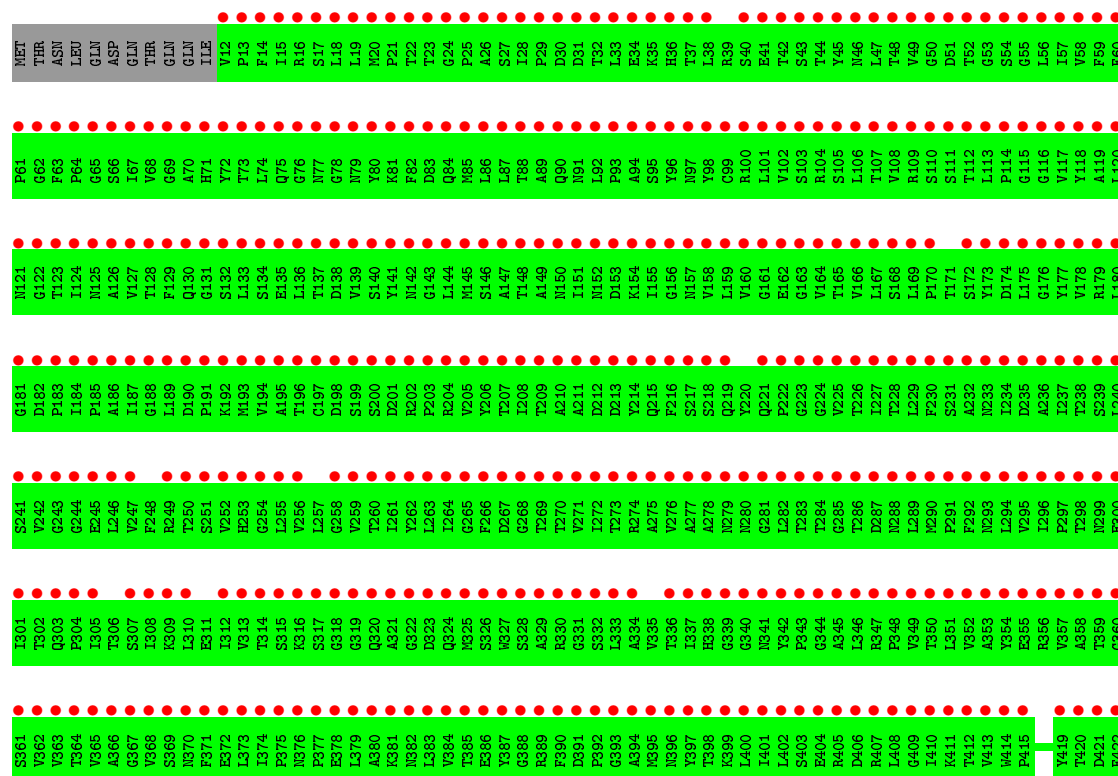


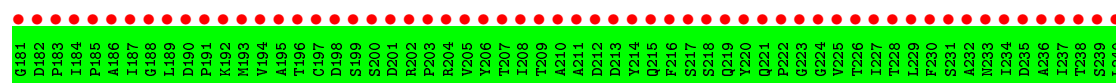
#### • Molecule 1: MAJOR STRUCTURAL PROTEIN VP2





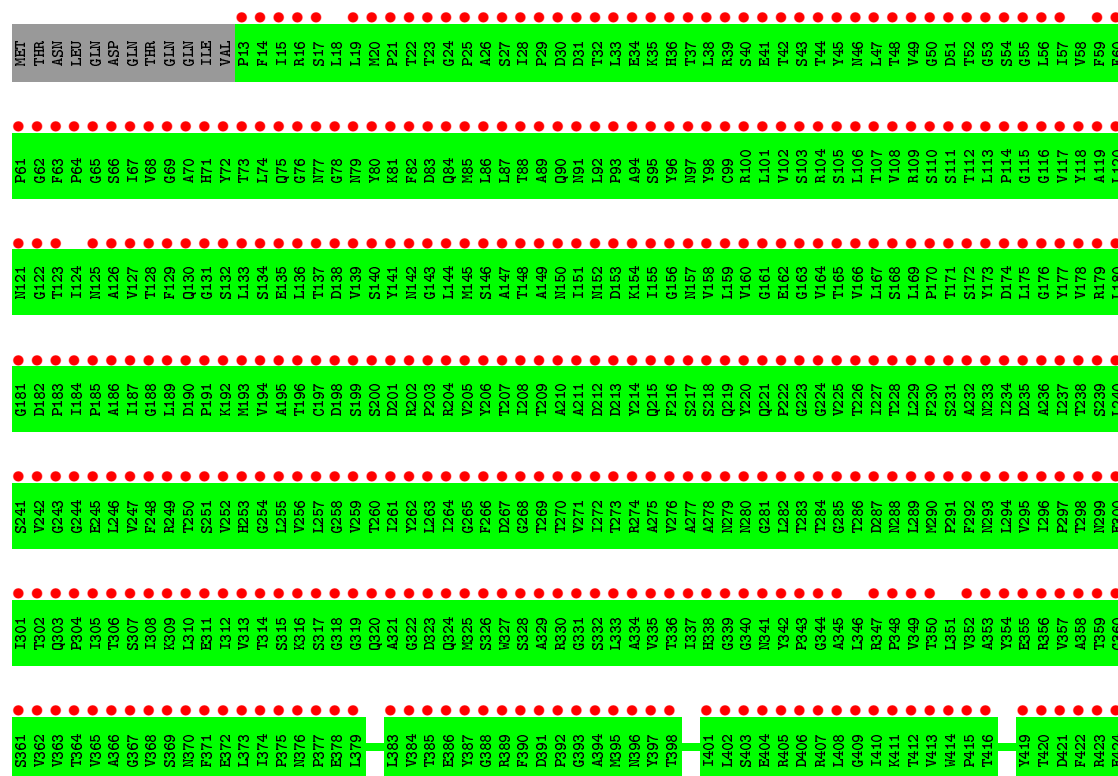
• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

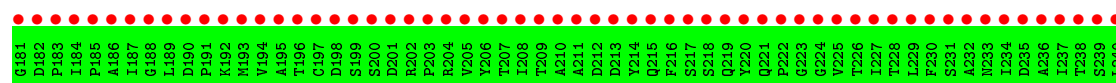












D421	F422	E423	E424	Y425	F426	M427	E428	V429	A430	D431	I432	L433	N434	P435	P436	P437	P438	P439	P440	P441	P442	P443	P444	P445	P446	P447	P448	P449	P450	P451	P452	P453	P454	P455	P456	P457	P458	P459	P460	P461	P462	P463	P464	P465	P466	P467	P468	P469	P470
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• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

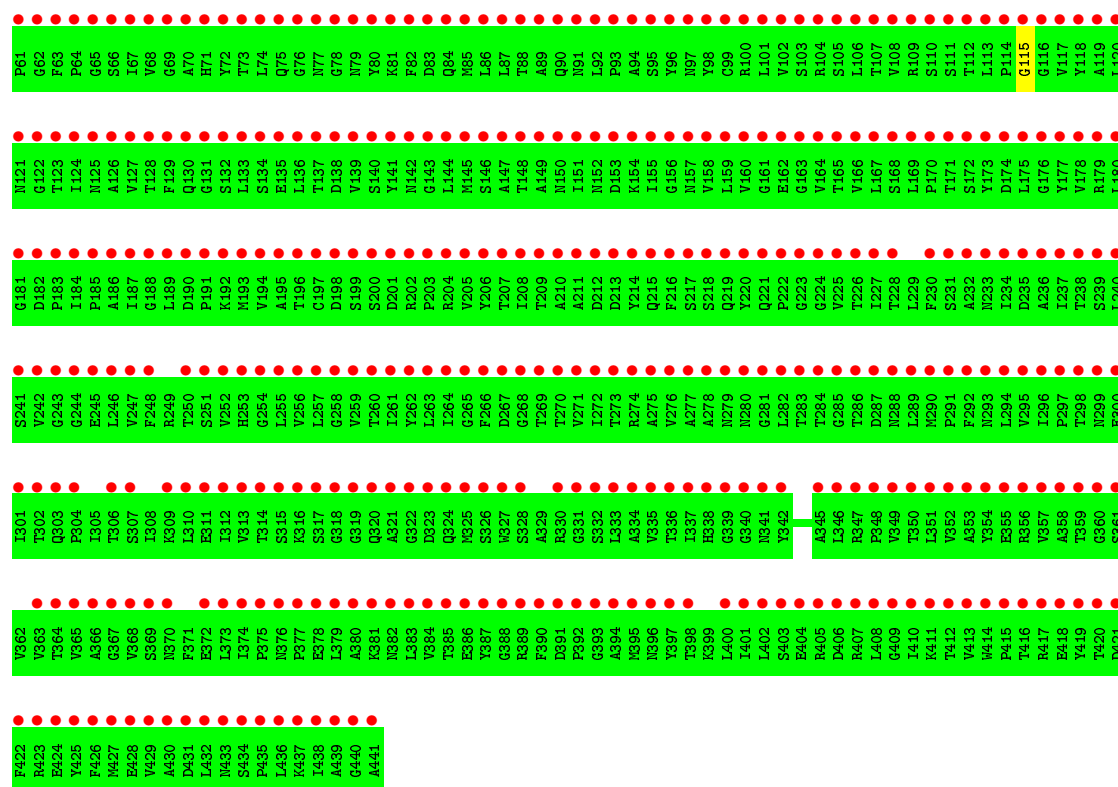


D421	S361	I301	S241	G181	N121	P61	MET
F422	V362	T302	V242	D182	G122	G62	THR
R423	V363	Q303	G243	P183	T122	F63	ASN
E424	T364	P304	G244	I184	I124	P64	LEU
Y425	V365	I305	E245	P185	N125	G65	GLN
F426	A366	T306	L246	A186	A126	S66	ASP
M427	G367	S307	V247	L187	T127	L67	GLN
E428	V368	I308	F248	G188	T128	V68	THR
VAL	S369	K309	R249	L189	F129	G69	GLN
ALA	N370	L310	T250	D190	Q130	A70	GLN
ASP	F371	E311	S251	P191	G131	H71	ILE
LEU	E372	I312	V252	K192	S132	V72	VAL
ASN	L373	V313	H253	M193	L133	T73	P13
SER	I374	T314	G254	V194	E135	L74	F14
PRO	P375	S315	L255	A195	E335	Q75	I15
LYS	N376	K316	V256	T196	L136	G76	R16
LEU	P377	S317	L257	C197	T137	N77	S17
ILE	E378	G318	G258	D198	D138	G78	L18
GLY	L379	G319	V259	S199	V139	N79	L19
GLY	A380	Q320	T260	S200	S140	Y80	N20
ALA	K381	A321	D261	D201	I141	K81	P21
	N382	G322	Y262	R202	N142	F82	T22
	L383	D323	L263	P203	G143	D83	T23
	S384	Q324	I264	R204	L144	Q84	G24
	T385	M325	G265	V205	M145	M85	P25
	E386	S326	F266	Y206	S146	L86	A26
	V387	N327	D267	T207	A147	L87	S27
	G388	S328	G268	L208	T148	T88	I28
	R389	A329	T269	T209	A149	A89	P29
	F390	N330	T270	A210	N150	Q90	S30
	D391	G331	V271	A211	I151	N91	D31
	P392	S332	I272	D212	N152	L92	T32
	G393	L333	T273	D213	D153	P93	L33
	A394	A334	R274	Y214	K154	A94	E34
	N395	V335	A275	Q215	I155	S95	K35
	N396	T336	V276	F216	G156	Y96	H36
	V397	I337	A277	S217	N157	N97	T37
	T398	H338	A278	S218	V158	Y98	L38
	K399	G339	N279	Q219	L159	C99	R39
	L400	N340	N280	Y220	V160	R100	S40
	L401	G341	G281	Q221	G161	L101	E41
	L402	Y342	L282	P222	E162	V102	T42
	S403	P343	T283	G223	G163	S103	S43
	E404	E404	G284	G224	V164	R104	T44
	R405	A345	G285	V225	T165	S105	V45
	D406	L346	T286	T226	V166	L106	M46
	R407	R347	N287	I227	L167	T107	L47
	L408	P348	N288	T228	S168	V108	T48
	G409	V349	L289	L229	L169	R109	V49
	L410	T350	N290	F230	P170	S110	G50
	K411	L351	P291	S231	T171	S111	D51
	T412	V352	F292	A232	S172	T112	T52
	V413	G353	N293	N233	G173	L113	G53
	W414	T354	L294	L234	D174	P114	S54
	F415	E355	V295	D235	L175	G115	G55
	T416	R356	L296	A236	G176	G116	L56
	R417	V357	T297	I237	Y177	V117	I57
	E418	A358	T298	T238	V178	Y118	V58
	V419	T359	N299	S239	R179	A119	F59
	T420	G360	E300	L240	L180	L120	P60

• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2



MET	THR	ASN	LEU	GLN	ASP	GLN	THR	GLN	GLN	GLN	ILE	VAL	P13	F14	I15	R16	S17	L18	L19	N20	P21	T22	T23	G24	P25	A26	S27	L28	R29	S40	E41	T42	S43	T44	Y45	M46	T47	T48	V49	G50	D51	T52	G53	S54	G55	L56	I57	V58	F59	P60
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E424	•
Y425	•
F426	•
M427	•
E428	•
V429	•
A430	•
D431	•
L432	•
M433	•
S434	•
P435	•
L436	•
LYS	
ILE	•
A441	
GLY	
ALA	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 74.8 (49.86-6.97)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 6.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.411 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	190.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 27.2	EDS
Estimated twinning fraction	0.327 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 1089556 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.65	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	425/441 (96%)	7.27	419 (98%) 0 0	20, 47, 95, 99	0
1	B	430/441 (97%)	6.81	419 (97%) 0 1	20, 47, 95, 99	0
1	C	430/441 (97%)	6.88	419 (97%) 0 1	20, 47, 95, 99	0
1	D	424/441 (96%)	6.85	414 (97%) 0 1	20, 47, 95, 99	0
1	E	429/441 (97%)	6.77	416 (96%) 0 1	20, 47, 95, 99	0
1	F	436/441 (98%)	7.11	427 (97%) 0 1	20, 46, 95, 99	0
1	G	426/441 (96%)	6.86	409 (96%) 0 1	20, 47, 95, 99	0
1	H	423/441 (95%)	6.76	411 (97%) 0 1	20, 47, 95, 99	0
1	I	417/441 (94%)	7.04	402 (96%) 0 1	20, 47, 96, 99	0
1	J	423/441 (95%)	7.20	417 (98%) 0 0	20, 47, 95, 99	0
1	K	416/441 (94%)	6.70	408 (98%) 0 1	20, 47, 96, 99	0
1	L	429/441 (97%)	7.03	419 (97%) 0 1	20, 47, 95, 99	0
1	M	425/441 (96%)	6.97	414 (97%) 0 1	20, 47, 95, 99	0
All	All	5533/5733 (96%)	6.94	5394 (97%) 0 1	20, 47, 96, 99	0

The worst 5 of 5394 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	150	ASN	25.7
1	C	209	THR	25.7
1	A	64	PRO	23.9
1	F	83	ASP	23.4
1	D	391	ASP	23.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.