



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:56 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

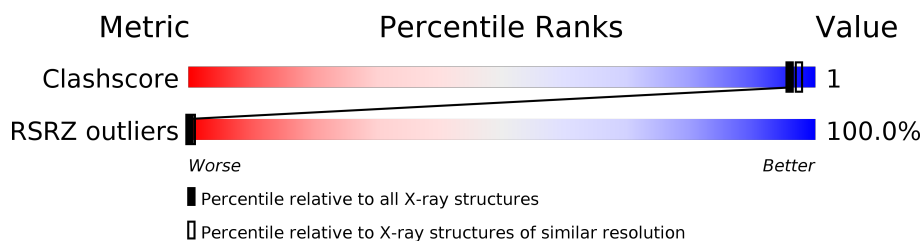
1 Overall quality at a glance

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	112137	1035 (10.00-3.80)
RSRZ outliers	101464	1003 (10.00-3.72)

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 $\leq 5\%$. 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	<div> <div>96%</div> <div> <div></div> <div>96%</div> <div>96%</div> <div>96%</div> <div>96%</div> </div> </div>
1	B	441	<div> <div>98%</div> <div> <div></div> <div>97%</div> <div>97%</div> <div>97%</div> <div>97%</div> </div> </div>
1	C	441	<div> <div>98%</div> <div> <div></div> <div>98%</div> <div>98%</div> <div>98%</div> <div>98%</div> </div> </div>
1	D	441	<div> <div>96%</div> <div> <div></div> <div>96%</div> <div>96%</div> <div>96%</div> <div>96%</div> </div> </div>
1	E	441	<div> <div>97%</div> <div> <div></div> <div>97%</div> <div>97%</div> <div>97%</div> <div>97%</div> </div> </div>
1	F	441	<div> <div>99%</div> <div> <div></div> <div>98%</div> <div>98%</div> <div>98%</div> <div>98%</div> </div> </div>
1	G	441	<div> <div>97%</div> <div> <div></div> <div>96%</div> <div>96%</div> <div>96%</div> <div>96%</div> </div> </div>
1	H	441	<div> <div>96%</div> <div> <div></div> <div>96%</div> <div>96%</div> <div>96%</div> <div>96%</div> </div> </div>
1	I	441	<div> <div>95%</div> <div> <div></div> <div>95%</div> <div>95%</div> <div>95%</div> <div>95%</div> </div> </div>

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

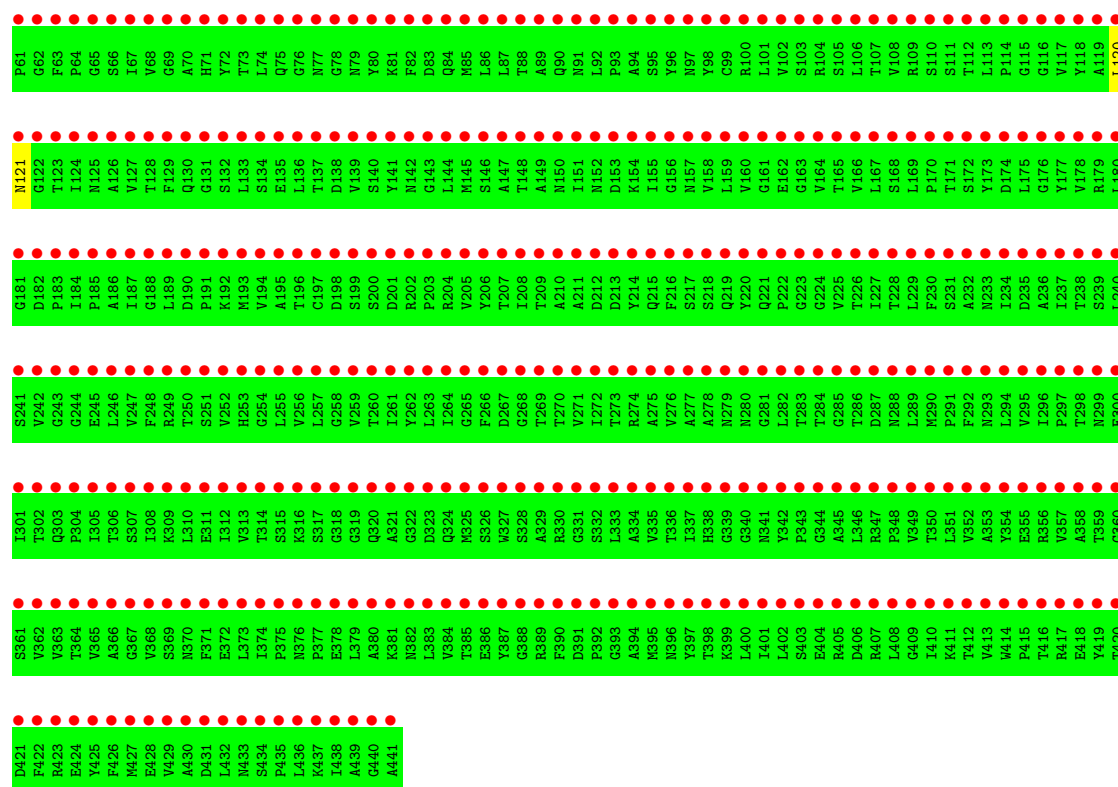
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	425	Total C 425 425	0	0	425
1	B	430	Total C 430 430	0	0	430
1	C	430	Total C 430 430	0	0	430
1	D	424	Total C 424 424	0	0	424
1	E	429	Total C 429 429	0	0	429
1	F	436	Total C 436 436	0	0	436
1	G	426	Total C 426 426	0	0	426
1	H	423	Total C 423 423	0	0	423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

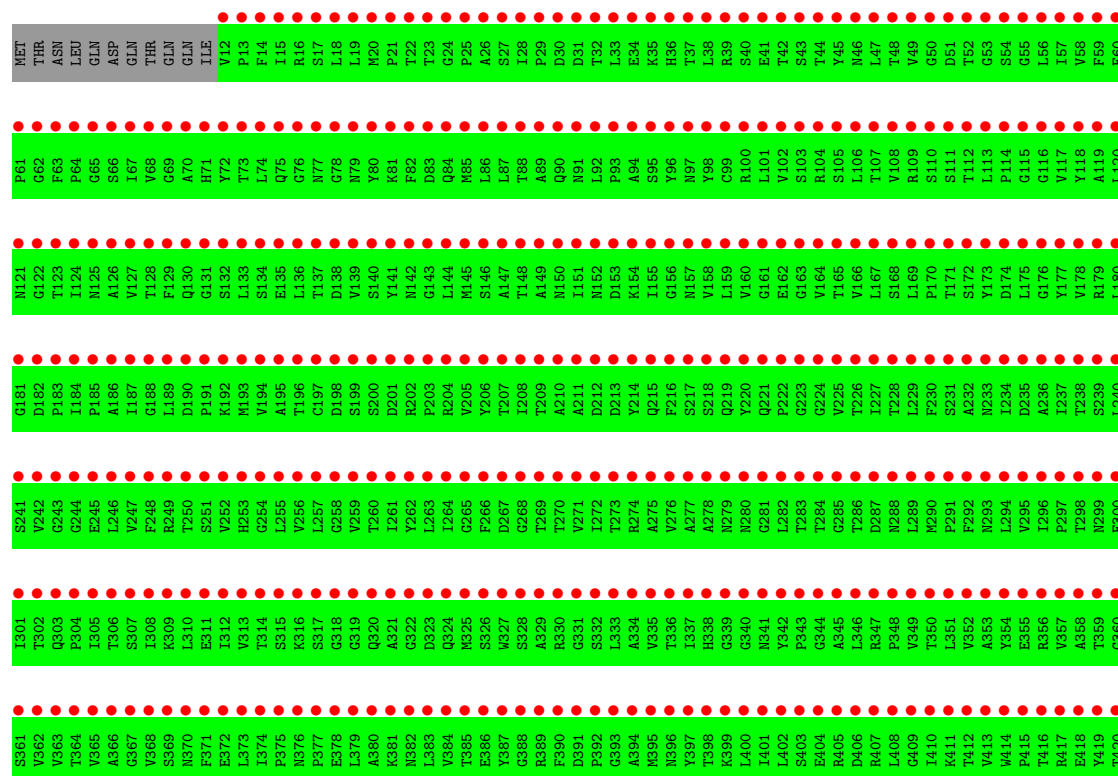
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



D421
 F422
 R423
 E424
 Y425
 F426
 M427
 E428
 V429
 A430
 D431
 L432
 N433
 S434
 P435
 L436
 K437
 I438
 A439
 G440
 A441

● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain D: 

MET THR ASN LEU GLN THR GLN ILE VAL P13 P14 P15 P16 P17 P18 P19 P20 P21 P22 P23 P24 P25 P26 P27 P28 P29 P30 P31 P32 P33 P34 P35 P36 P37 P38 P39 P40 P41 P42 P43 P44 P45 P46 P47 P48 P49 P50 P51 P52 P53 P54 P55 P56 P57 P58 P59 P60
 P61 P62 P63 P64 P65 P66 P67 P68 P69 P70 P71 P72 P73 P74 P75 P76 P77 P78 P79 P80 P81 P82 P83 P84 P85 P86 P87 P88 P89 P90 P91 P92 P93 P94 P95 P96 P97 P98 P99 C00 C01 C02 C03 C04 C05 C06 C07 C08 C09 C10 C11 C12 C13 C14 C15 C16 C17 C18 C19 C20 C21 C22 C23 C24 C25 C26 C27 C28 C29 C30 C31 C32 C33 C34 C35 C36 C37 C38 C39 C40 C41 C42 C43 C44 C45 C46 C47 C48 C49 C50 C51 C52 C53 C54 C55 C56 C57 C58 C59 C60
 M121 G122 G123 G124 G125 G126 G127 G128 G129 G130 G131 G132 G133 G134 G135 G136 G137 G138 G139 G140 G141 G142 G143 G144 G145 G146 G147 G148 G149 G150 G151 G152 G153 G154 G155 G156 G157 G158 G159 G160 G161 G162 G163 G164 G165 G166 G167 G168 G169 G170 G171 G172 G173 G174 G175 G176 G177 G178 G179 G180
 G181 D182 P183 I184 A185 A186 A187 G188 L189 L190 P191 P192 K193 K194 V195 V196 V197 V198 V199 S200 S201 S202 S203 S204 S205 S206 S207 S208 S209 S210 S211 S212 S213 S214 S215 S216 S217 S218 S219 S220 S221 S222 S223 S224 S225 S226 S227 S228 S229 S230 S231 S232 S233 S234 S235 S236 S237 S238 S239 S240
 S241 V242 G243 G244 G245 G246 G247 G248 G249 G250 G251 G252 G253 G254 G255 G256 G257 G258 G259 G260 G261 G262 G263 G264 G265 G266 G267 G268 G269 G270 G271 G272 G273 G274 G275 G276 G277 G278 G279 G280 G281 G282 G283 G284 G285 G286 G287 G288 G289 G290 G291 G292 G293 G294 G295 G296 G297 G298 G299 E300
 L301 T302 Q303 P304 L305 T306 T307 L308 L309 K309 K310 L311 E311 E312 L313 L314 T314 S315 S316 K316 P317 P318 G318 G319 G320 Q321 A321 G322 D323 L323 Q324 M325 M326 M327 M328 M329 M330 R330 R331 G331 S332 S333 L333 A334 A335 M336 M337 M338 M339 M340 M341 M342 M343 M344 M345 M346 M347 M348 M349 M350 M351 M352 M353 M354 M355 M356 M357 M358 M359 M360 M361 M362 M363 M364 M365 M366 M367 M368 M369 M370 M371 M372 M373 M374 M375 M376 M377 M378 M379 M380 M381 M382 M383 M384 M385 M386 M387 M388 M389 M390 M391 M392 M393 M394 M395 M396 M397 M398 M399 M400 M401 M402 M403 M404 M405 M406 M407 M408 M409 M410 M411 M412 M413 M414 M415 M416 M417 M418 M419 M420
 D421 F422 R423 E424 Y425 F426 M427 E428 V429 A430 D431 L432 L433 S434 P435 L436 LYS ILE ALA GLY ALA

● Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

Chain E: 

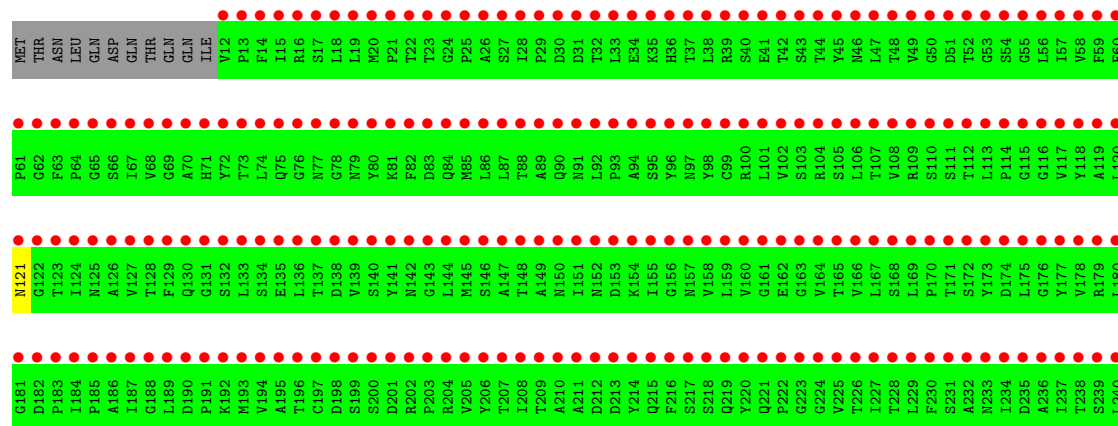
MET THR ASN GLN ASP GLN THR GLN ILE VAL P13 P14 P15 P16 P17 P18 P19 P20 P21 P22 P23 P24 P25 P26 P27 P28 P29 P30 P31 P32 P33 P34 P35 P36 P37 P38 P39 P40 P41 P42 P43 P44 P45 P46 P47 P48 P49 P50 P51 P52 P53 P54 P55 P56 P57 P58 P59 P60
 P61 P62 P63 P64 P65 P66 P67 P68 P69 P70 P71 P72 P73 P74 P75 P76 P77 P78 P79 P80 P81 P82 P83 P84 P85 P86 P87 P88 P89 P90 P91 P92 P93 P94 P95 P96 P97 P98 P99 C00 C01 C02 C03 C04 C05 C06 C07 C08 C09 C10 C11 C12 C13 C14 C15 C16 C17 C18 C19 C20 C21 C22 C23 C24 C25 C26 C27 C28 C29 C30 C31 C32 C33 C34 C35 C36 C37 C38 C39 C40 C41 C42 C43 C44 C45 C46 C47 C48 C49 C50 C51 C52 C53 C54 C55 C56 C57 C58 C59 C60
 M121 G122 G123 G124 G125 G126 G127 G128 G129 G130 G131 G132 G133 G134 G135 G136 G137 G138 G139 G140 G141 G142 G143 G144 G145 G146 G147 G148 G149 G150 G151 G152 G153 G154 G155 G156 G157 G158 G159 G160 G161 G162 G163 G164 G165 G166 G167 G168 G169 G170 G171 G172 G173 G174 G175 G176 G177 G178 G179 G180
 G181 D182 P183 I184 A185 A186 A187 G188 L189 L190 P191 P192 K193 K194 V195 V196 V197 V198 V199 S200 S201 S202 S203 S204 S205 S206 S207 S208 S209 S210 S211 S212 S213 S214 S215 S216 S217 S218 S219 S220 S221 S222 S223 S224 S225 S226 S227 S228 S229 S230 S231 S232 S233 S234 S235 S236 S237 S238 S239 S240
 L432 L433 S434 P435 L436 LYS ILE ALA GLY ALA

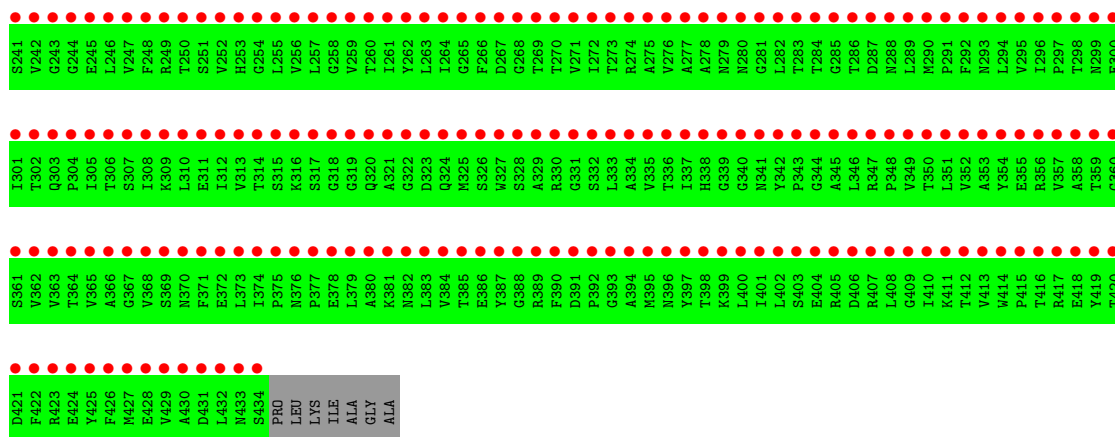
D421	S361	I301	S241	G181	N121	P61
F422	V362	Q302	V242	D182	G122	G62
R423	P363	T303	G243	P183	T123	F63
E424	T364	P304	G244	I184	I124	P64
Y425	V365	T305	F245	P185	N125	G65
F426	A366	T306	L246	A186	A126	S66
M427	G367	S307	V247	I187	V127	I67
E428	V368	L308	F248	G188	T128	V68
V429	S369	K309	R249	D189	F129	G69
A430	N370	L310	T250	L190	Q130	A70
D431	F371	E311	S251	P191	G131	H71
L432	E372	L312	V252	K192	S132	Y72
M433	L373	V313	H253	M193	L133	T73
S434	I374	T314	G254	V194	S134	L74
P435	P375	S315	L255	A195	E135	Q75
L436	N376	G316	V256	T196	L136	G76
K437	P377	S317	L257	C197	T137	N77
ILE	E378	G318	G258	D198	D138	G78
	L379	G319	V259	S199	V139	N79
	A380	Q320	T260	S200	S140	Y80
GLY	K381	A321	L261	D201	Y141	K81
ALA	N382	G322	V262	R202	N142	F82
	L383	D323	L263	P203	G143	D83
	V384	Q324	L264	R204	L144	Q84
	T385	K325	G265	K205	M145	M85
	E386	S326	F266	Y206	S146	L86
	T387	W327	D267	T207	A147	L87
	G388	S328	G268	L208	T148	T88
	R389	A329	T269	S209	A149	A89
	F390	R330	T270	A210	N150	Q90
	D391	G331	V271	D211	I151	N91
	P392	S332	L272	D212	N152	L92
	G393	L333	T273	D213	D153	P93
	A394	A334	R274	Y214	K154	A94
	N395	V335	A275	Q215	I155	S95
	N396	T336	V276	F216	G156	Y96
	Y397	T337	A277	S217	N157	N97
	T398	H338	R278	Q218	V158	Y98
	K399	G339	N279	S219	L159	C99
	L400	G340	G280	Y220	V160	R100
	L401	N341	G281	Q221	G161	L101
	L402	Y342	L282	P222	E162	V102
	S403	P343	T283	G223	G163	S103
	E404	G344	T284	G224	V164	R104
	R405	A345	G285	V225	T165	S105
	D406	L346	T286	T226	V166	L106
	R407	P347	D287	L227	L167	T107
	L408	R348	N288	T228	S168	V108
	G409	V349	L289	L229	L169	R109
	I410	T350	M290	F230	P170	S110
	K411	L351	P291	S231	T171	S111
	T412	V352	F292	A232	S172	T112
	V413	A353	N293	N233	Y173	L113
	W414	Y354	L294	T234	D174	P114
	P415	E355	V295	D235	L175	G115
	T416	R356	L296	A236	G176	V116
	R417	V357	P297	L237	Y177	V117
	E418	A358	T298	T238	V178	N118
	Y419	T359	N299	S239	R179	A119
	T420	G360	F298	L240	L180	L120

• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

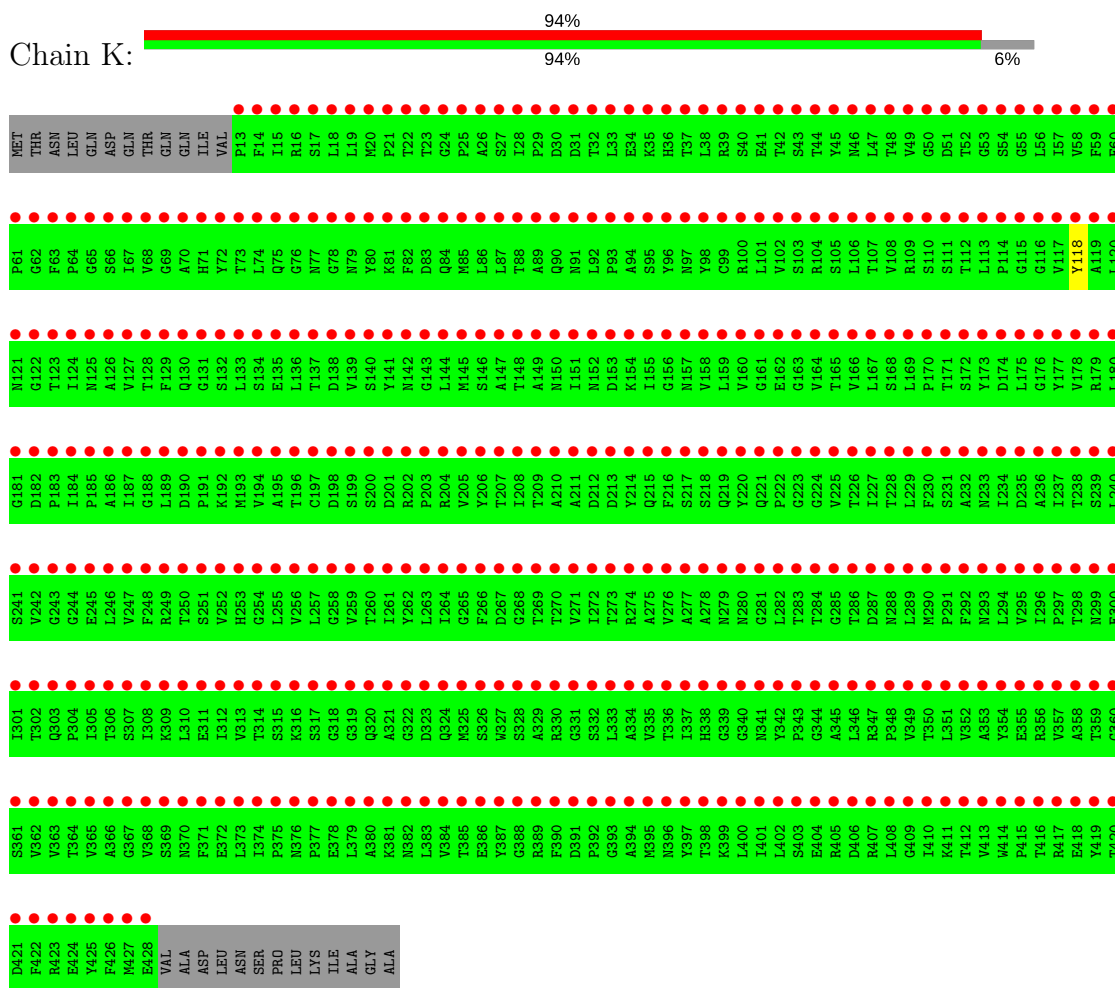


MET	THR	ASN	LEU	GLN	ASP	GLN	THR	GLN	GLN	ILE	VAL	P13	F14	I15	R16	S17	L18	L19	M20	P21	T22	T23	G24	P25	A26	S27	L28	P29	D30	G31	T32	L33	E34	K35	H36	T37	L38	R39	S40	E41	T42	S43	T44	Y45	N46	L47	T48	V49	G50	D51	T52	G53	S54	G55	L56	I57	V58	F59	F60	
P61	G62	F63	P64	G65	S66	I67	V68	G69	A70	H71	Y72	T73	L74	Q75	G76	N77	G78	N79	K80	K81	F82	D83	Q84	N85	L86	L87	T88	A89	Q90	N91	L92	P93	A94	S95	Y96	N97	Y98	C99	R100	L101	V102	S103	S104	S105	L106	T107	V108	R109	S110	S111	T112	L113	P114	G115	V116	V117	A118	N119	L120	
N121	G122	T123	I124	N125	A126	V127	T128	F129	Q130	G131	S132	L133	S134	E135	L136	T137	D138	V139	S140	Y141	D142	R202	G143	L144	M145	S146	T148	A149	N150	L151	D152	D153	K154	L155	G156	M157	L158	Q159	V160	G161	E162	G163	G164	T165	V166	L167	S168	L169	P170	T171	S172	Y173	D174	L175	G176	V177	V178	R179	L180	
G181	D182	P183	I184	P185	A186	I187	G188	L189	D190	P191	K192	L193	V194	A195	T196	C197	D198	S199	S200	D201	R202	P203	R204	V205	Y206	T207	T208	T209	A210	A211	D212	D213	Y214	L215	F216	S217	S218	Q219	Q220	Q221	P222	G223	G224	V225	T226	L227	T228	L229	F230	S231	S232	A233	T234	D235	L236	T237	T238	S239	L240	
S241	V242	G243	G244	E245	L246	V247	F248	R249	Q250	S251	V252	H253	G254	L255	V256	L257	G258	V259	T260	D261	R262	G263	L264	G265	F266	G267	T268	G269	A270	N271	L272	T273	R274	Y275	V276	A277	A278	N279	N280	G281	L282	T283	T284	G285	T286	D287	N288	L289	M290	F291	F292	N293	L294	V295	L296	P297	T298	N299	E300	
T301	T302	Q303	P304	T305	T306	S307	L308	K309	L310	E311	T312	V313	T314	S315	G316	P317	G318	G319	Q320	A321	G322	D323	Q324	K325	S326	W327	G328	S329	A329	R330	G331	S332	L333	A334	V335	T336	I337	H338	G339	G340	L341	N342	P343	G344	A345	D346	R347	P348	V349	T350	L351	V352	A353	V354	E355	R356	V357	A358	T359	G360
S361	V362	P363	E364	V365	A366	G367	V368	S369	N370	F371	E372	L373	I374	P375	N376	P377	E378	L379	A380	K381	G382	L383	V384	T385	E386	T387	G388	R389	F390	D391	P392	G393	A394	N395	N396	Y397	T398	K399	L400	L401	L402	S403	E404	R405	D406	R407	L408	G409	I410	K411	T412	V413	W414	P415	T416	R417	E418	Y419	T420	

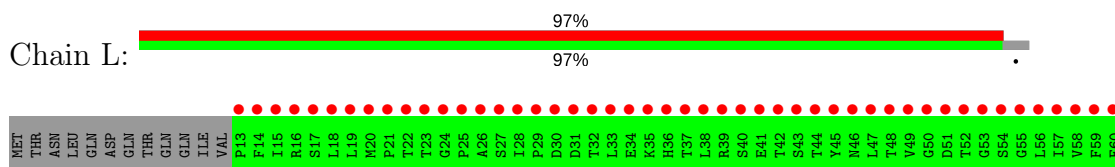


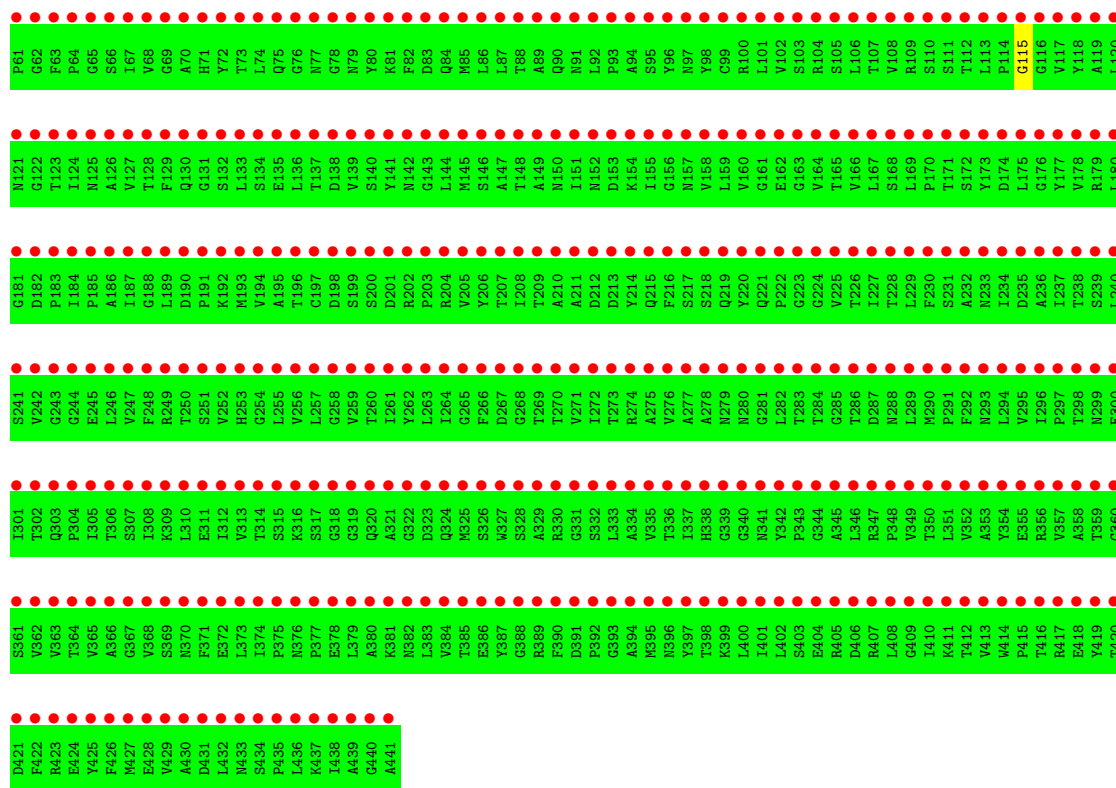


- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2

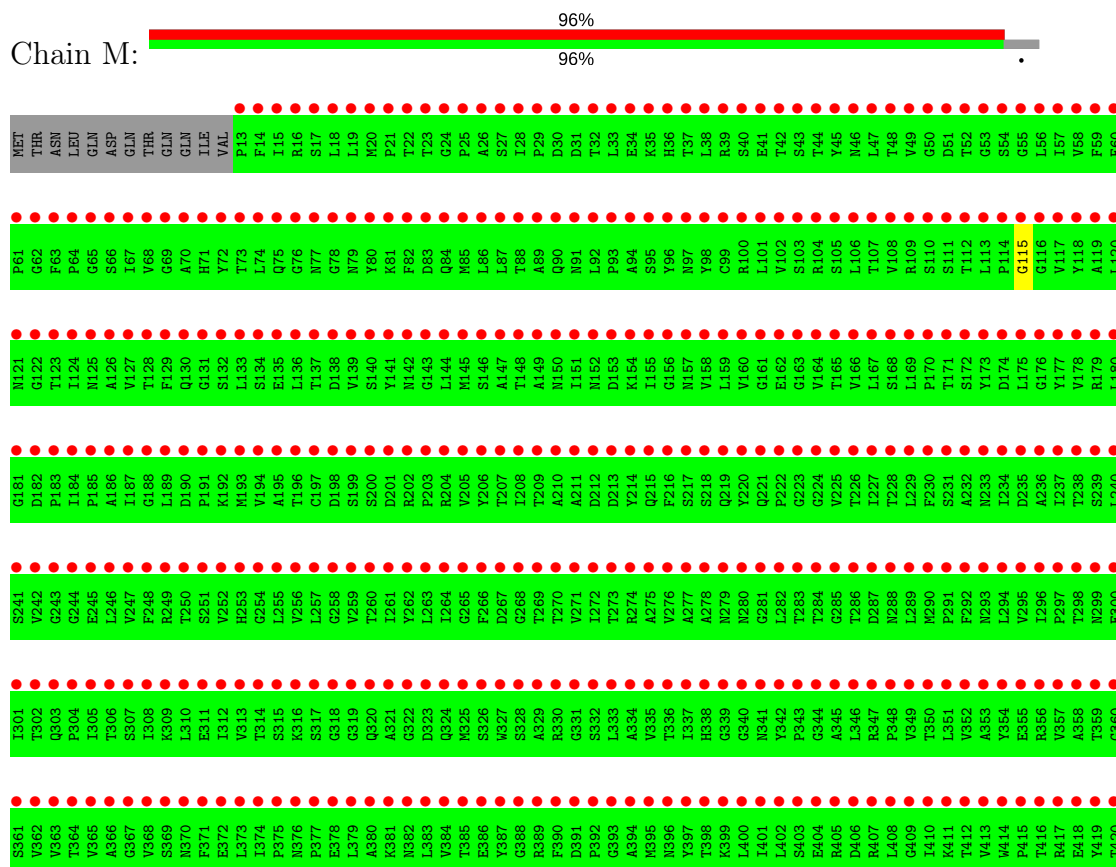


- Molecule 1: MAJOR STRUCTURAL PROTEIN VP2





• Molecule 1: MAJOR STRUCTURAL PROTEIN VP2



D421	
F422	
R423	
E424	
Y425	
F426	
M427	
E428	
V429	
A430	
D431	
L432	
N433	
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, 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) 0.411 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 [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, 95th 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 ²)	Q<0.9
1	A	425/441 (96%)	19.75	425 (100%) 0 0	20, 47, 95, 99	0
1	B	430/441 (97%)	18.85	430 (100%) 0 0	20, 47, 95, 99	0
1	C	430/441 (97%)	20.28	430 (100%) 0 0	20, 47, 95, 99	0
1	D	424/441 (96%)	19.43	424 (100%) 0 0	20, 47, 95, 99	0
1	E	429/441 (97%)	18.23	429 (100%) 0 0	20, 47, 95, 99	0
1	F	436/441 (98%)	18.20	435 (99%) 0 0	20, 46, 95, 99	0
1	G	426/441 (96%)	20.65	426 (100%) 0 0	20, 47, 95, 99	0
1	H	423/441 (95%)	19.29	423 (100%) 0 0	20, 47, 95, 99	0
1	I	417/441 (94%)	20.03	417 (100%) 0 0	20, 47, 96, 99	0
1	J	423/441 (95%)	19.81	423 (100%) 0 0	20, 47, 95, 99	0
1	K	416/441 (94%)	20.36	416 (100%) 0 0	20, 47, 96, 99	0
1	L	429/441 (97%)	20.66	429 (100%) 0 0	20, 47, 95, 99	0
1	M	425/441 (96%)	19.58	425 (100%) 0 0	20, 47, 95, 99	0
All	All	5533/5733 (96%)	19.62	5532 (99%) 0 0	20, 47, 96, 99	0

The worst 5 of 5532 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	291	PRO	73.6
1	D	331	GLY	72.6
1	G	203	PRO	72.4
1	H	418	GLU	71.9
1	G	341	ASN	70.8

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.