



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 06:12 AM EDT

PDB ID : 2DF7 / pdb_00002df7
Title : Crystal structure of infectious bursal disease virus VP2 subviral particle
Authors : Ko, T.P.; Lee, C.C.; Wang, M.Y.; Wang, A.H.
Deposited on : 2006-02-27
Resolution : 2.60 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

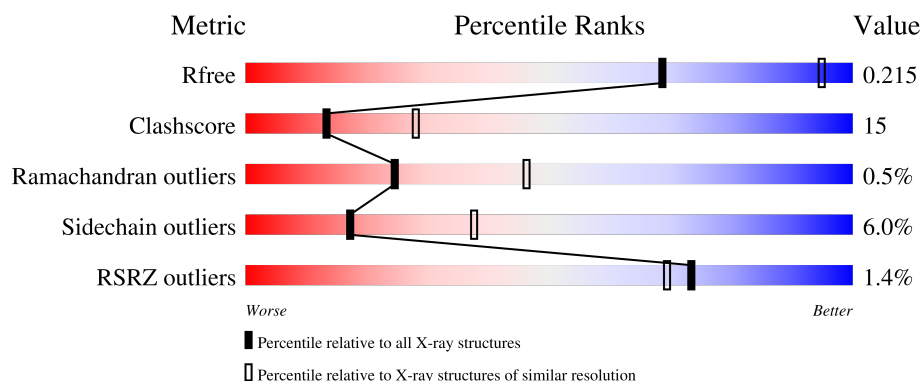
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	458	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>24%</div> <div>5%</div> <div>8%</div> </div> </div>
1	B	458	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	458	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	458	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>•</div> <div>10%</div> </div> </div>
1	E	458	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	458	
1	G	458	
1	H	458	
1	I	458	
1	J	458	
1	K	458	
1	L	458	
1	M	458	
1	N	458	
1	O	458	
1	P	458	
1	Q	458	
1	R	458	
1	S	458	
1	T	458	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 66956 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 structural polyprotein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3162	2006	520	626	10			
1	B	418	Total	C	N	O	S	0	0	0
			3149	1997	518	624	10			
1	C	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	D	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	E	415	Total	C	N	O	S	0	0	0
			3130	1985	515	620	10			
1	F	413	Total	C	N	O	S	0	0	0
			3113	1974	513	616	10			
1	G	412	Total	C	N	O	S	0	0	0
			3110	1971	512	617	10			
1	H	413	Total	C	N	O	S	0	0	0
			3117	1976	513	618	10			
1	I	413	Total	C	N	O	S	0	0	0
			3118	1977	513	618	10			
1	J	411	Total	C	N	O	S	0	0	0
			3102	1965	511	616	10			
1	K	417	Total	C	N	O	S	0	0	0
			3137	1988	517	622	10			
1	L	418	Total	C	N	O	S	0	0	0
			3150	1998	518	624	10			
1	M	412	Total	C	N	O	S	0	0	0
			3110	1971	512	617	10			
1	N	413	Total	C	N	O	S	0	0	0
			3109	1970	513	616	10			
1	O	412	Total	C	N	O	S	0	0	0
			3109	1970	512	617	10			
1	P	417	Total	C	N	O	S	0	0	0
			3138	1989	517	622	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	417	Total	C	N	O	S	0	0	0
			3138	1989	517	622	10			
1	R	411	Total	C	N	O	S	0	0	0
			3101	1966	511	614	10			
1	S	414	Total	C	N	O	S	0	0	0
			3116	1975	514	617	10			
1	T	418	Total	C	N	O	S	0	0	0
			3150	1998	518	624	10			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	GLU	ASP	engineered mutation	UNP Q6S9I7
A	330	SER	MET	engineered mutation	UNP Q6S9I7
A	331	GLY	TRP	engineered mutation	UNP Q6S9I7
A	453	HIS	-	expression tag	UNP Q6S9I7
A	454	HIS	-	expression tag	UNP Q6S9I7
A	455	HIS	-	expression tag	UNP Q6S9I7
A	456	HIS	-	expression tag	UNP Q6S9I7
A	457	HIS	-	expression tag	UNP Q6S9I7
A	458	HIS	-	expression tag	UNP Q6S9I7
B	135	GLU	ASP	engineered mutation	UNP Q6S9I7
B	330	SER	MET	engineered mutation	UNP Q6S9I7
B	331	GLY	TRP	engineered mutation	UNP Q6S9I7
B	453	HIS	-	expression tag	UNP Q6S9I7
B	454	HIS	-	expression tag	UNP Q6S9I7
B	455	HIS	-	expression tag	UNP Q6S9I7
B	456	HIS	-	expression tag	UNP Q6S9I7
B	457	HIS	-	expression tag	UNP Q6S9I7
B	458	HIS	-	expression tag	UNP Q6S9I7
C	135	GLU	ASP	engineered mutation	UNP Q6S9I7
C	330	SER	MET	engineered mutation	UNP Q6S9I7
C	331	GLY	TRP	engineered mutation	UNP Q6S9I7
C	453	HIS	-	expression tag	UNP Q6S9I7
C	454	HIS	-	expression tag	UNP Q6S9I7
C	455	HIS	-	expression tag	UNP Q6S9I7
C	456	HIS	-	expression tag	UNP Q6S9I7
C	457	HIS	-	expression tag	UNP Q6S9I7
C	458	HIS	-	expression tag	UNP Q6S9I7
D	135	GLU	ASP	engineered mutation	UNP Q6S9I7
D	330	SER	MET	engineered mutation	UNP Q6S9I7
D	331	GLY	TRP	engineered mutation	UNP Q6S9I7
D	453	HIS	-	expression tag	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	HIS	-	expression tag	UNP Q6S9I7
D	455	HIS	-	expression tag	UNP Q6S9I7
D	456	HIS	-	expression tag	UNP Q6S9I7
D	457	HIS	-	expression tag	UNP Q6S9I7
D	458	HIS	-	expression tag	UNP Q6S9I7
E	135	GLU	ASP	engineered mutation	UNP Q6S9I7
E	330	SER	MET	engineered mutation	UNP Q6S9I7
E	331	GLY	TRP	engineered mutation	UNP Q6S9I7
E	453	HIS	-	expression tag	UNP Q6S9I7
E	454	HIS	-	expression tag	UNP Q6S9I7
E	455	HIS	-	expression tag	UNP Q6S9I7
E	456	HIS	-	expression tag	UNP Q6S9I7
E	457	HIS	-	expression tag	UNP Q6S9I7
E	458	HIS	-	expression tag	UNP Q6S9I7
F	135	GLU	ASP	engineered mutation	UNP Q6S9I7
F	330	SER	MET	engineered mutation	UNP Q6S9I7
F	331	GLY	TRP	engineered mutation	UNP Q6S9I7
F	453	HIS	-	expression tag	UNP Q6S9I7
F	454	HIS	-	expression tag	UNP Q6S9I7
F	455	HIS	-	expression tag	UNP Q6S9I7
F	456	HIS	-	expression tag	UNP Q6S9I7
F	457	HIS	-	expression tag	UNP Q6S9I7
F	458	HIS	-	expression tag	UNP Q6S9I7
G	135	GLU	ASP	engineered mutation	UNP Q6S9I7
G	330	SER	MET	engineered mutation	UNP Q6S9I7
G	331	GLY	TRP	engineered mutation	UNP Q6S9I7
G	453	HIS	-	expression tag	UNP Q6S9I7
G	454	HIS	-	expression tag	UNP Q6S9I7
G	455	HIS	-	expression tag	UNP Q6S9I7
G	456	HIS	-	expression tag	UNP Q6S9I7
G	457	HIS	-	expression tag	UNP Q6S9I7
G	458	HIS	-	expression tag	UNP Q6S9I7
H	135	GLU	ASP	engineered mutation	UNP Q6S9I7
H	330	SER	MET	engineered mutation	UNP Q6S9I7
H	331	GLY	TRP	engineered mutation	UNP Q6S9I7
H	453	HIS	-	expression tag	UNP Q6S9I7
H	454	HIS	-	expression tag	UNP Q6S9I7
H	455	HIS	-	expression tag	UNP Q6S9I7
H	456	HIS	-	expression tag	UNP Q6S9I7
H	457	HIS	-	expression tag	UNP Q6S9I7
H	458	HIS	-	expression tag	UNP Q6S9I7
I	135	GLU	ASP	engineered mutation	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	330	SER	MET	engineered mutation	UNP Q6S9I7
I	331	GLY	TRP	engineered mutation	UNP Q6S9I7
I	453	HIS	-	expression tag	UNP Q6S9I7
I	454	HIS	-	expression tag	UNP Q6S9I7
I	455	HIS	-	expression tag	UNP Q6S9I7
I	456	HIS	-	expression tag	UNP Q6S9I7
I	457	HIS	-	expression tag	UNP Q6S9I7
I	458	HIS	-	expression tag	UNP Q6S9I7
J	135	GLU	ASP	engineered mutation	UNP Q6S9I7
J	330	SER	MET	engineered mutation	UNP Q6S9I7
J	331	GLY	TRP	engineered mutation	UNP Q6S9I7
J	453	HIS	-	expression tag	UNP Q6S9I7
J	454	HIS	-	expression tag	UNP Q6S9I7
J	455	HIS	-	expression tag	UNP Q6S9I7
J	456	HIS	-	expression tag	UNP Q6S9I7
J	457	HIS	-	expression tag	UNP Q6S9I7
J	458	HIS	-	expression tag	UNP Q6S9I7
K	135	GLU	ASP	engineered mutation	UNP Q6S9I7
K	330	SER	MET	engineered mutation	UNP Q6S9I7
K	331	GLY	TRP	engineered mutation	UNP Q6S9I7
K	453	HIS	-	expression tag	UNP Q6S9I7
K	454	HIS	-	expression tag	UNP Q6S9I7
K	455	HIS	-	expression tag	UNP Q6S9I7
K	456	HIS	-	expression tag	UNP Q6S9I7
K	457	HIS	-	expression tag	UNP Q6S9I7
K	458	HIS	-	expression tag	UNP Q6S9I7
L	135	GLU	ASP	engineered mutation	UNP Q6S9I7
L	330	SER	MET	engineered mutation	UNP Q6S9I7
L	331	GLY	TRP	engineered mutation	UNP Q6S9I7
L	453	HIS	-	expression tag	UNP Q6S9I7
L	454	HIS	-	expression tag	UNP Q6S9I7
L	455	HIS	-	expression tag	UNP Q6S9I7
L	456	HIS	-	expression tag	UNP Q6S9I7
L	457	HIS	-	expression tag	UNP Q6S9I7
L	458	HIS	-	expression tag	UNP Q6S9I7
M	135	GLU	ASP	engineered mutation	UNP Q6S9I7
M	330	SER	MET	engineered mutation	UNP Q6S9I7
M	331	GLY	TRP	engineered mutation	UNP Q6S9I7
M	453	HIS	-	expression tag	UNP Q6S9I7
M	454	HIS	-	expression tag	UNP Q6S9I7
M	455	HIS	-	expression tag	UNP Q6S9I7
M	456	HIS	-	expression tag	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	457	HIS	-	expression tag	UNP Q6S9I7
M	458	HIS	-	expression tag	UNP Q6S9I7
N	135	GLU	ASP	engineered mutation	UNP Q6S9I7
N	330	SER	MET	engineered mutation	UNP Q6S9I7
N	331	GLY	TRP	engineered mutation	UNP Q6S9I7
N	453	HIS	-	expression tag	UNP Q6S9I7
N	454	HIS	-	expression tag	UNP Q6S9I7
N	455	HIS	-	expression tag	UNP Q6S9I7
N	456	HIS	-	expression tag	UNP Q6S9I7
N	457	HIS	-	expression tag	UNP Q6S9I7
N	458	HIS	-	expression tag	UNP Q6S9I7
O	135	GLU	ASP	engineered mutation	UNP Q6S9I7
O	330	SER	MET	engineered mutation	UNP Q6S9I7
O	331	GLY	TRP	engineered mutation	UNP Q6S9I7
O	453	HIS	-	expression tag	UNP Q6S9I7
O	454	HIS	-	expression tag	UNP Q6S9I7
O	455	HIS	-	expression tag	UNP Q6S9I7
O	456	HIS	-	expression tag	UNP Q6S9I7
O	457	HIS	-	expression tag	UNP Q6S9I7
O	458	HIS	-	expression tag	UNP Q6S9I7
P	135	GLU	ASP	engineered mutation	UNP Q6S9I7
P	330	SER	MET	engineered mutation	UNP Q6S9I7
P	331	GLY	TRP	engineered mutation	UNP Q6S9I7
P	453	HIS	-	expression tag	UNP Q6S9I7
P	454	HIS	-	expression tag	UNP Q6S9I7
P	455	HIS	-	expression tag	UNP Q6S9I7
P	456	HIS	-	expression tag	UNP Q6S9I7
P	457	HIS	-	expression tag	UNP Q6S9I7
P	458	HIS	-	expression tag	UNP Q6S9I7
Q	135	GLU	ASP	engineered mutation	UNP Q6S9I7
Q	330	SER	MET	engineered mutation	UNP Q6S9I7
Q	331	GLY	TRP	engineered mutation	UNP Q6S9I7
Q	453	HIS	-	expression tag	UNP Q6S9I7
Q	454	HIS	-	expression tag	UNP Q6S9I7
Q	455	HIS	-	expression tag	UNP Q6S9I7
Q	456	HIS	-	expression tag	UNP Q6S9I7
Q	457	HIS	-	expression tag	UNP Q6S9I7
Q	458	HIS	-	expression tag	UNP Q6S9I7
R	135	GLU	ASP	engineered mutation	UNP Q6S9I7
R	330	SER	MET	engineered mutation	UNP Q6S9I7
R	331	GLY	TRP	engineered mutation	UNP Q6S9I7
R	453	HIS	-	expression tag	UNP Q6S9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	454	HIS	-	expression tag	UNP Q6S9I7
R	455	HIS	-	expression tag	UNP Q6S9I7
R	456	HIS	-	expression tag	UNP Q6S9I7
R	457	HIS	-	expression tag	UNP Q6S9I7
R	458	HIS	-	expression tag	UNP Q6S9I7
S	135	GLU	ASP	engineered mutation	UNP Q6S9I7
S	330	SER	MET	engineered mutation	UNP Q6S9I7
S	331	GLY	TRP	engineered mutation	UNP Q6S9I7
S	453	HIS	-	expression tag	UNP Q6S9I7
S	454	HIS	-	expression tag	UNP Q6S9I7
S	455	HIS	-	expression tag	UNP Q6S9I7
S	456	HIS	-	expression tag	UNP Q6S9I7
S	457	HIS	-	expression tag	UNP Q6S9I7
S	458	HIS	-	expression tag	UNP Q6S9I7
T	135	GLU	ASP	engineered mutation	UNP Q6S9I7
T	330	SER	MET	engineered mutation	UNP Q6S9I7
T	331	GLY	TRP	engineered mutation	UNP Q6S9I7
T	453	HIS	-	expression tag	UNP Q6S9I7
T	454	HIS	-	expression tag	UNP Q6S9I7
T	455	HIS	-	expression tag	UNP Q6S9I7
T	456	HIS	-	expression tag	UNP Q6S9I7
T	457	HIS	-	expression tag	UNP Q6S9I7
T	458	HIS	-	expression tag	UNP Q6S9I7

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	P	1	Total Cl 1 1	0	0
2	R	1	Total Cl 1 1	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	I	1	Total 1	Ca 1	0	0
3	P	1	Total 1	Ca 1	0	0
3	R	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	252	Total 252	O 252	0	0
4	B	250	Total 250	O 250	0	0
4	C	204	Total 204	O 204	0	0
4	D	245	Total 245	O 245	0	0
4	E	211	Total 211	O 211	0	0
4	F	235	Total 235	O 235	0	0
4	G	226	Total 226	O 226	0	0
4	H	195	Total 195	O 195	0	0
4	I	202	Total 202	O 202	0	0
4	J	213	Total 213	O 213	0	0
4	K	226	Total 226	O 226	0	0

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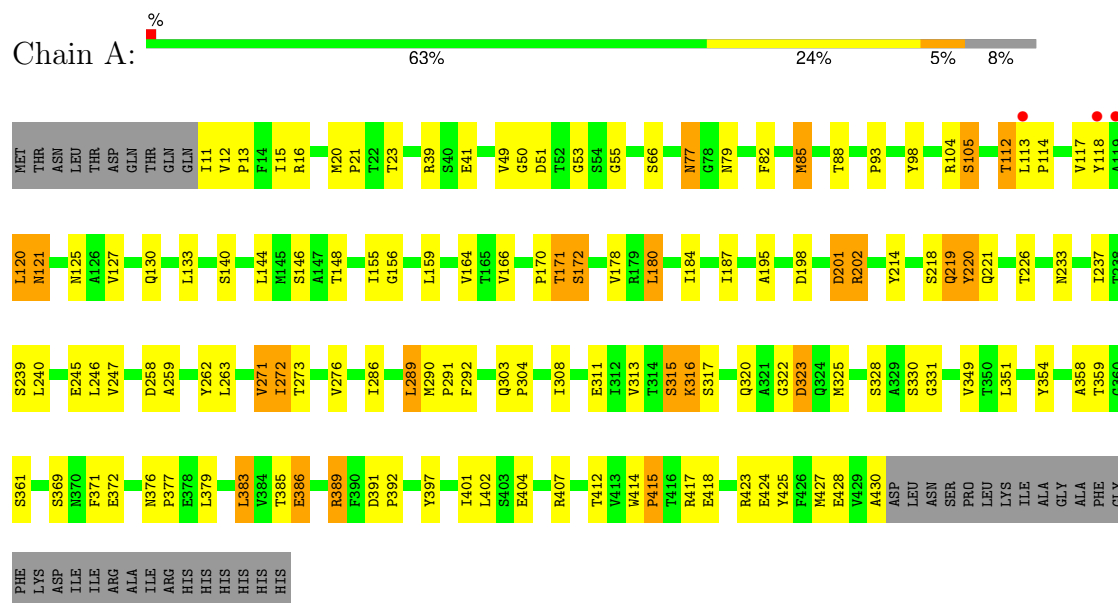
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	234	Total 234	O 234	0	0
4	M	235	Total 235	O 235	0	0
4	N	195	Total 195	O 195	0	0
4	O	216	Total 216	O 216	0	0
4	P	183	Total 183	O 183	0	0
4	Q	201	Total 201	O 201	0	0
4	R	226	Total 226	O 226	0	0
4	S	226	Total 226	O 226	0	0
4	T	270	Total 270	O 270	0	0

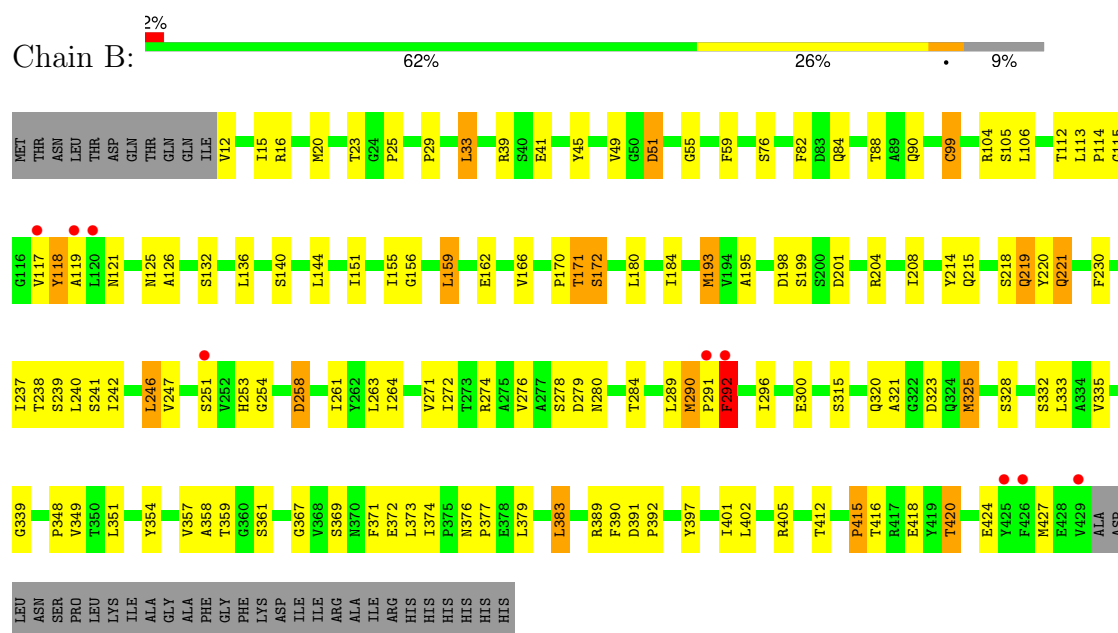
3 Residue-property plots

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 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 ($RSRZ > 2$). 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: structural polypeptide VP2



• Molecule 1: structural polypeptide VP2



Chain C:

2%

64%

23%

10%

0.00 0.05 0.10 0.15 0.20 0.25

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238

LYS ASP ILE ILE ARG ALA ILE ARG HIS HIS HIS HIS HIS HIS HIS HIS VAL ASP LEU SER PRO LEU LYS ILE ALA GLY ALA PHE GLY THR

L246 H249 T250 L285 A296 L297 A298 D259 T260 I261 I262 L263 I264 V271 I272 I273 R274 D279 D287 T296 E300 I305 T306 S307 L310 V313 T314 S317 A321 M325 S326 W327 A328 A329 S330 G331 G339 P348 V349 T350 L351 E355 R356 V357

MET THR ASN LEU THR ASP GLN GLN T11 V12 P13 I14 M20 P25 I155 P29 E34 K35 S40 E41 T44 V49 S54 G55 L56 S66 I67 T88 S95 C99 R100 R104 S105 L106 R109 T112 L113 P114 GLY VAL TYR THR

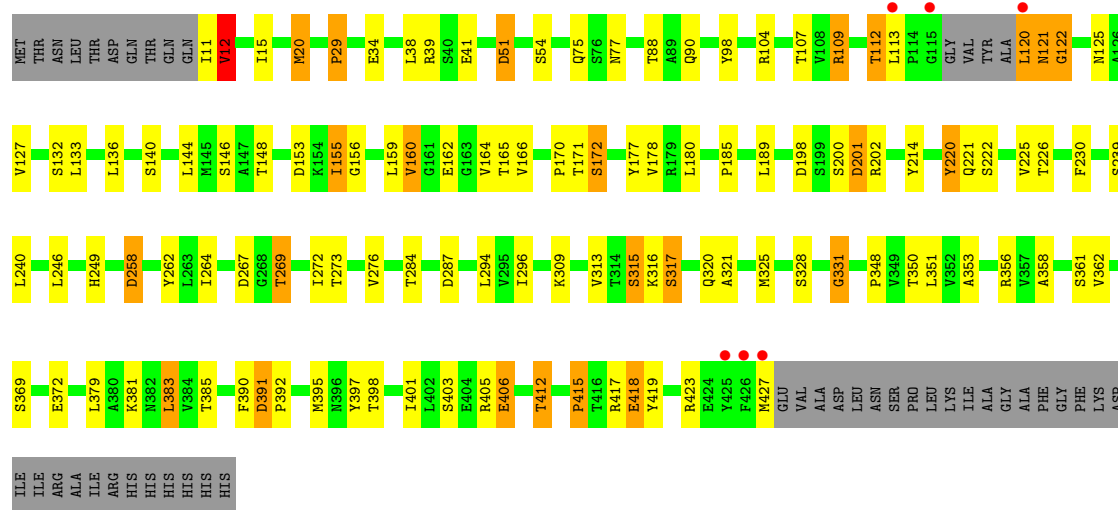
L120 M121 G122 F129 Q130 L133 L136 S140 L144 M145 S146 D153 K154 I155 G156 L159 V160 G161 E162 G163 V164 P170 I171 S172 Y177 L189 D190 K192 M193 D198 D201 A211 Y214 Q219 Y220 Q221 S222 G223 F230 I237 T238

[illegible]

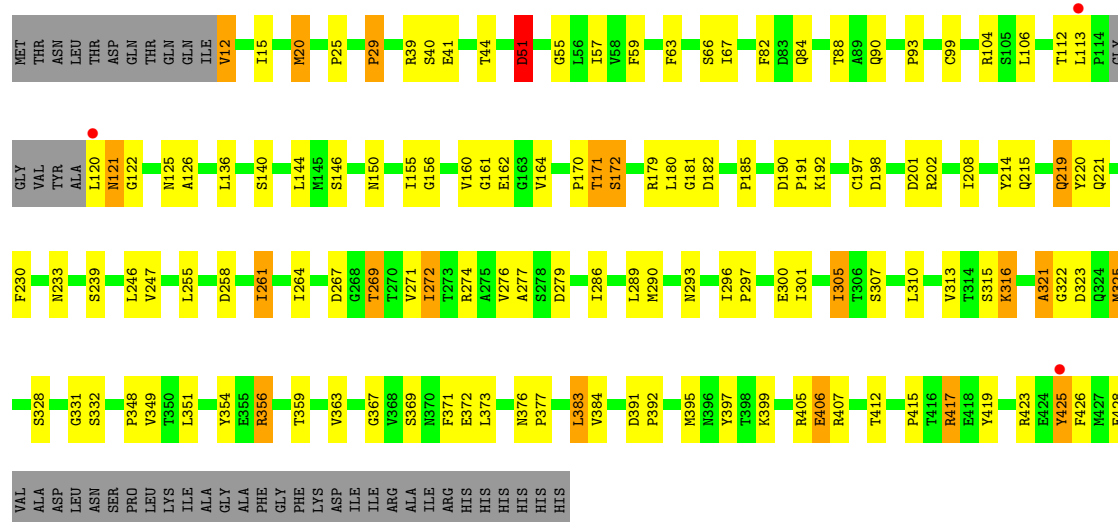
Chain E:

Amino Acid	Percentage
MET	3%
THR	
ASN	
LEU	
THR	
ASP	
GLN	
THR	
GLN	
I11	
I15	
M20	
P25	
L33	
E34	
K35	
S40	
E41	
L47	
D51	
G55	
V58	
S66	
H71	
S76	
F82	
D83	
Q84	
T88	
P93	
C99	
R100	
R104	
V108	
S111	
T112	
L113	
P114	
G115	
VAL	
TYR	
ALA	
L120	
M121	
G122	
M125	
A126	
Q130	
G131	
S132	
L136	
V139	
S140	
Y141	
L144	
I155	
G156	
L159	
V160	
G161	
E162	
G163	
V164	
L169	
P170	
T171	
S172	
Y177	
L180	
G181	
P185	
M193	
C197	
D198	
S199	
D200	
R201	
R202	
I208	
A211	
Y214	
Q215	
G216	

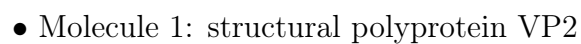
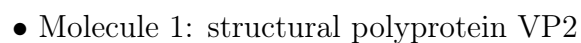
- Molecule 1: structural polyprotein VP2

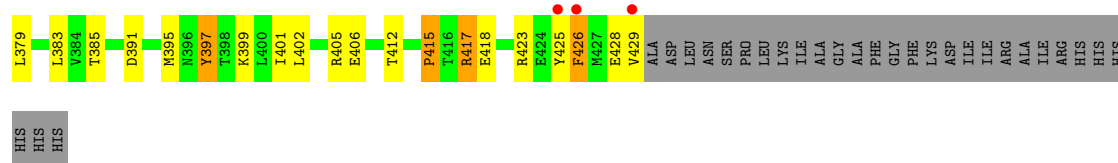


- Molecule 1: structural polyprotein VP2

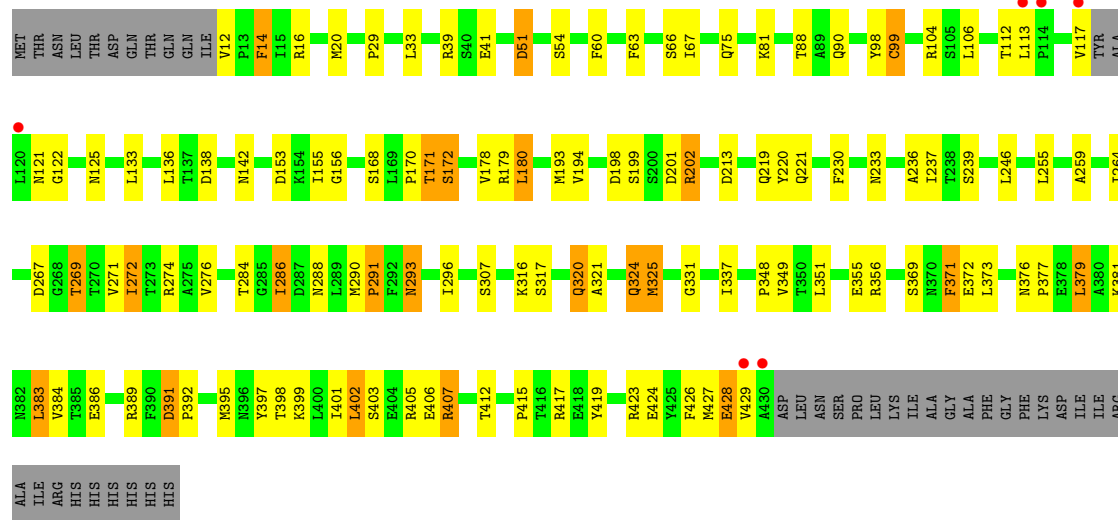


- Molecule 1: structural polyprotein VP2

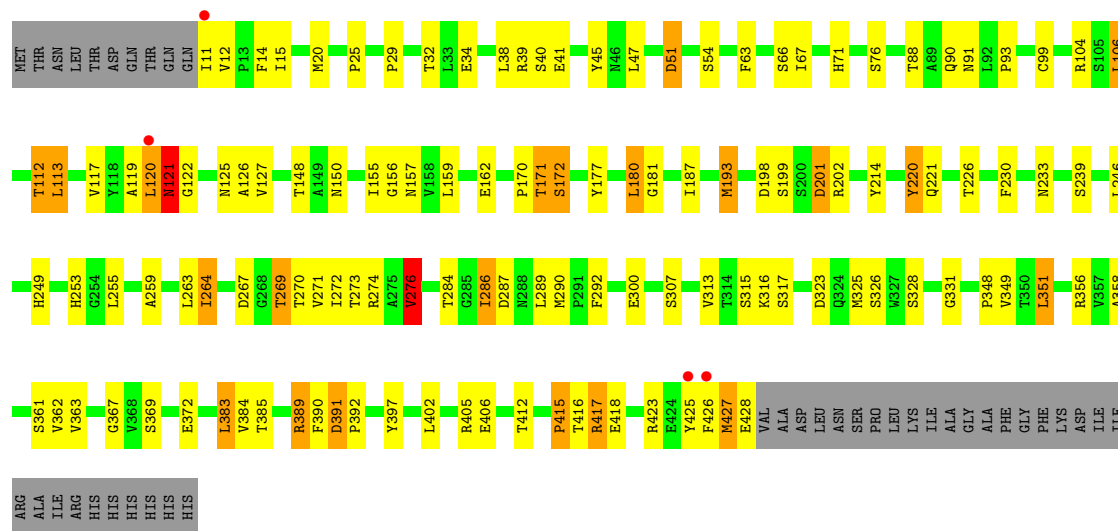




• Molecule 1: structural polypeptide VP2

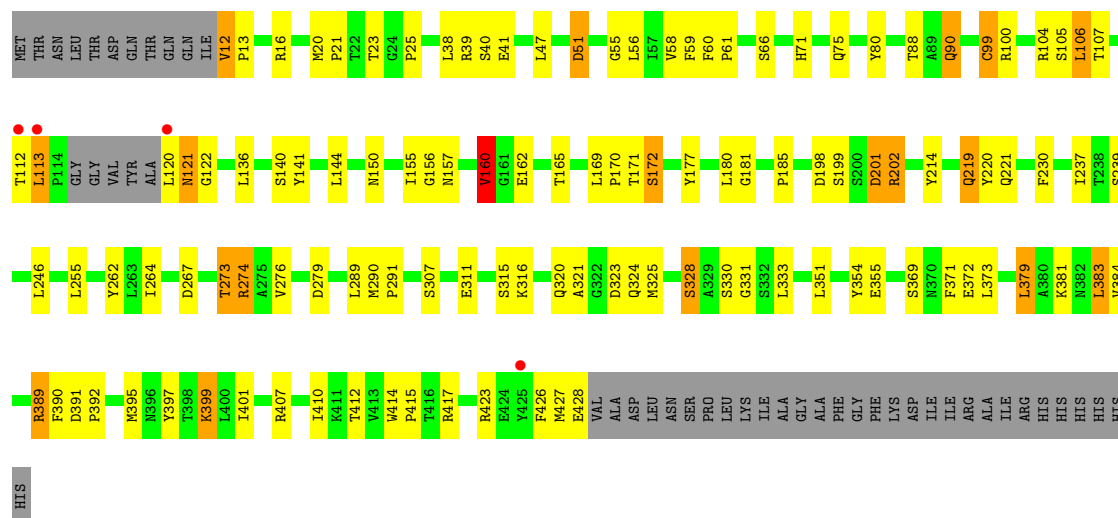


• Molecule 1: structural polypeptide VP2



• Molecule 1: structural polypeptide VP2

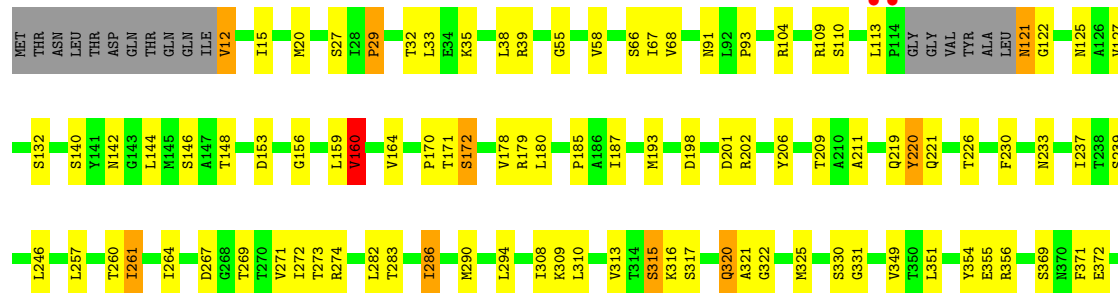


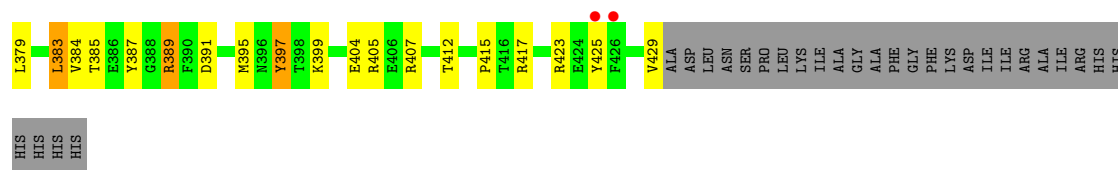


• Molecule 1: structural polypeptide VP2

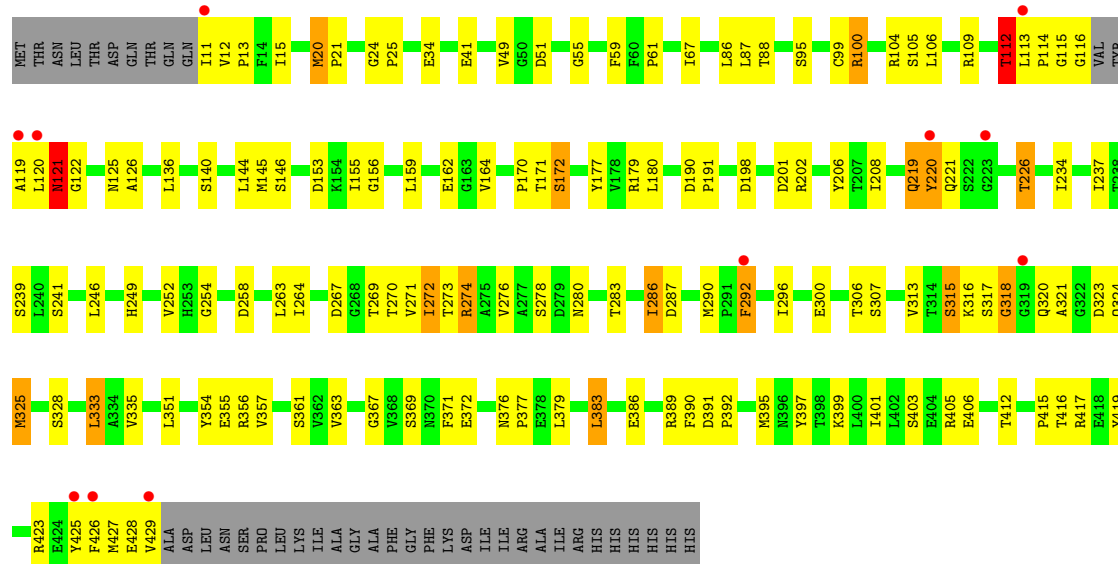


• Molecule 1: structural polypeptide VP2

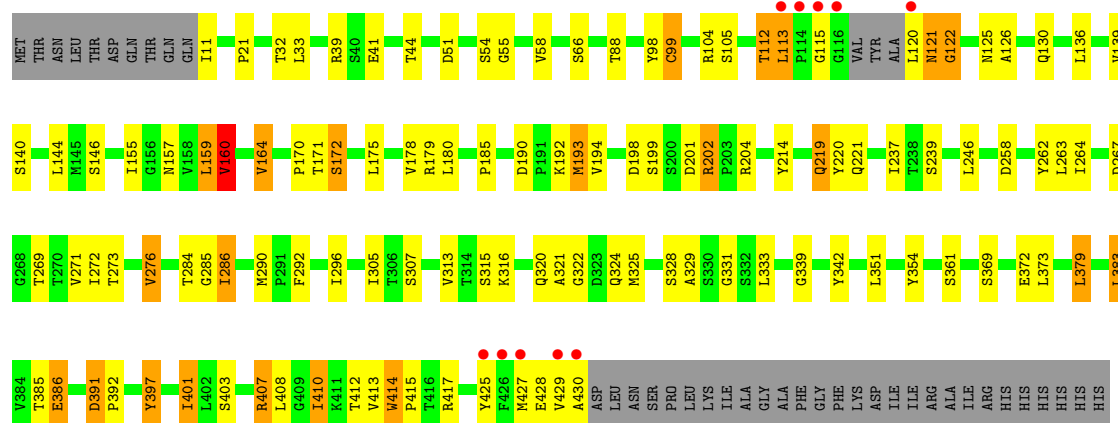




• Molecule 1: structural polypeptide VP2

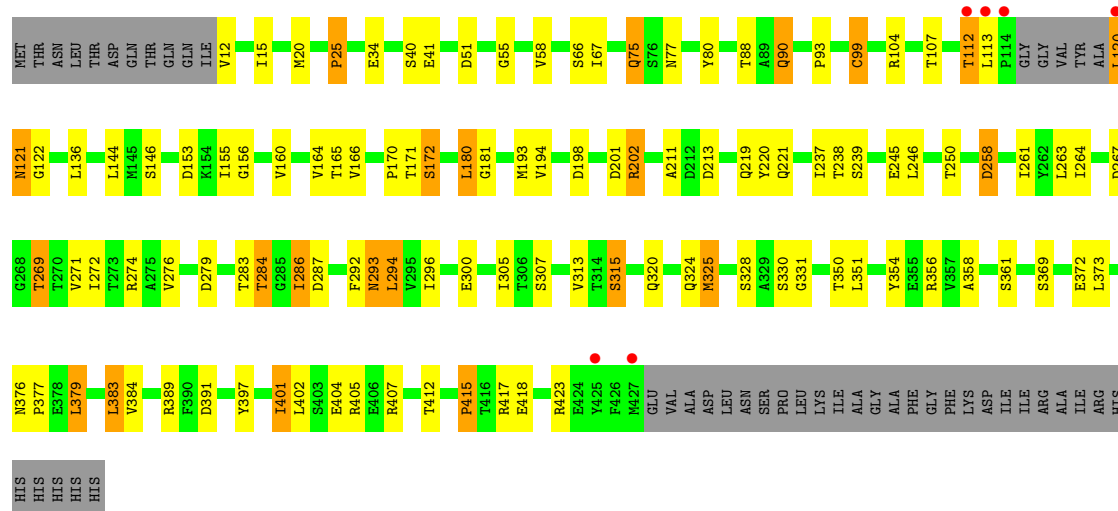


• Molecule 1: structural polypeptide VP2



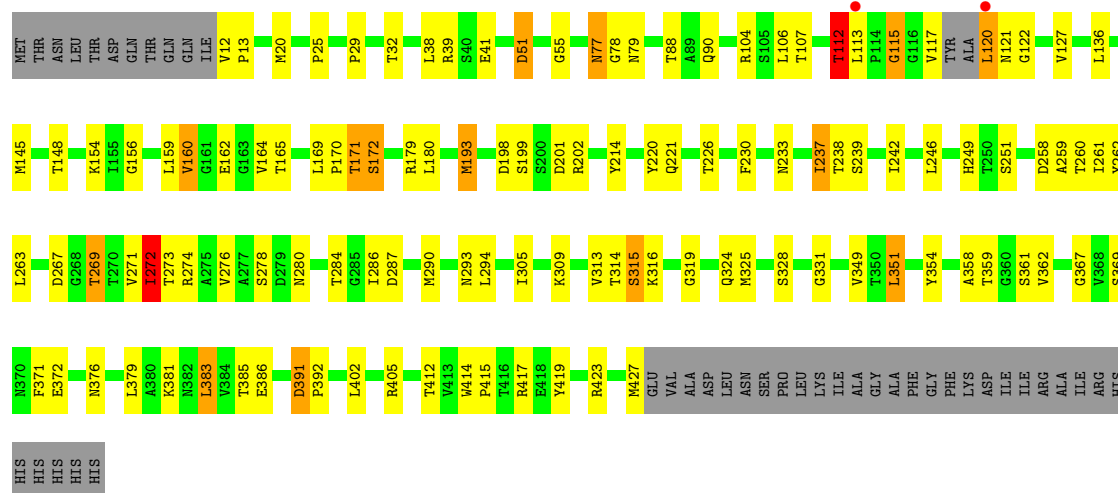
• Molecule 1: structural polypeptide VP2





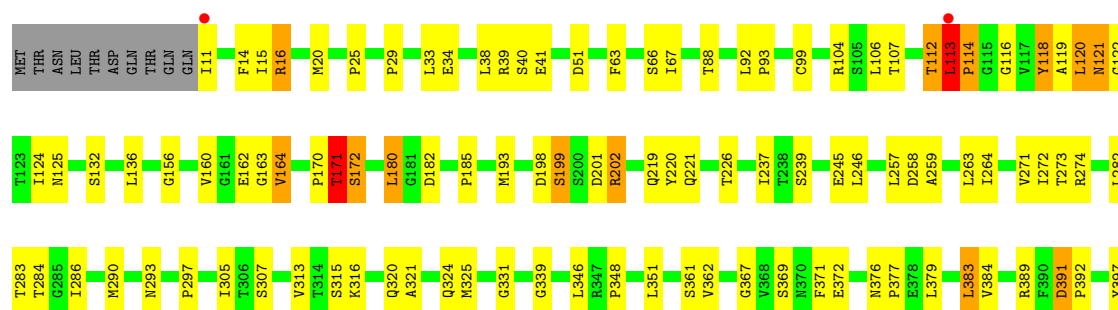
• Molecule 1: structural polypeptide VP2

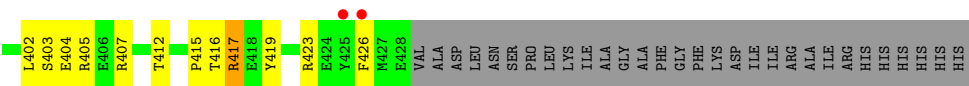
Chain S: 64% 23% 10%



• Molecule 1: structural polypeptide VP2

Chain T: 66% 22% 9%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	316.41Å 316.41Å 316.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.6 (40.00-2.60) 89.6 (40.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.165 , 0.215 0.166 , 0.215	Depositor DCC
R_{free} test set	14256 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	66956	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.20% 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 ⓘ

5.1 Standard geometry ⓘ

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

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.95	2/3226 (0.1%)	1.19	23/4407 (0.5%)
1	B	1.01	4/3213 (0.1%)	1.24	21/4389 (0.5%)
1	C	0.90	1/3180 (0.0%)	1.17	17/4342 (0.4%)
1	D	0.94	1/3179 (0.0%)	1.20	20/4340 (0.5%)
1	E	0.94	1/3192 (0.0%)	1.20	22/4359 (0.5%)
1	F	0.93	3/3175 (0.1%)	1.18	20/4335 (0.5%)
1	G	0.94	1/3172 (0.0%)	1.18	15/4331 (0.3%)
1	H	0.89	2/3179 (0.1%)	1.17	22/4341 (0.5%)
1	I	0.88	2/3180 (0.1%)	1.13	15/4342 (0.3%)
1	J	0.87	0/3163	1.15	16/4318 (0.4%)
1	K	0.87	1/3199 (0.0%)	1.18	20/4368 (0.5%)
1	L	0.92	0/3214	1.18	23/4390 (0.5%)
1	M	0.90	1/3172 (0.0%)	1.18	22/4331 (0.5%)
1	N	0.90	1/3171 (0.0%)	1.18	19/4329 (0.4%)
1	O	0.89	2/3171 (0.1%)	1.18	20/4330 (0.5%)
1	P	0.94	3/3200 (0.1%)	1.24	24/4369 (0.5%)
1	Q	0.88	3/3200 (0.1%)	1.16	19/4369 (0.4%)
1	R	0.97	1/3163 (0.0%)	1.19	15/4319 (0.3%)
1	S	0.92	1/3178 (0.0%)	1.18	22/4339 (0.5%)
1	T	0.97	0/3214	1.23	29/4390 (0.7%)
All	All	0.92	30/63741 (0.0%)	1.19	404/87038 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	3
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1
1	L	0	1
1	O	0	3
1	Q	0	1
All	All	0	11

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	325	MET	SD-CE	-10.06	1.54	1.79
1	P	20	MET	SD-CE	8.34	2.00	1.79
1	A	85	MET	SD-CE	-7.72	1.60	1.79
1	B	325	MET	SD-CE	-6.83	1.62	1.79
1	H	325	MET	SD-CE	-6.78	1.62	1.79

The worst 5 of 404 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	415	PRO	N-CA-C	-12.01	92.33	111.19
1	G	415	PRO	N-CA-C	-11.41	91.94	110.55
1	S	415	PRO	N-CA-C	-11.36	92.03	110.55
1	C	122	GLY	N-CA-C	11.25	126.45	111.72
1	K	415	PRO	N-CA-C	-11.17	92.35	110.55

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	TYR	Sidechain
1	D	206	TYR	Sidechain
1	D	397	TYR	Sidechain
1	D	45	TYR	Sidechain
1	J	397	TYR	Sidechain

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	3162	0	3141	118	0
1	B	3149	0	3125	107	0
1	C	3118	0	3097	95	0
1	D	3118	0	3099	65	0
1	E	3130	0	3111	106	0
1	F	3113	0	3094	91	0
1	G	3110	0	3086	116	0
1	H	3117	0	3095	96	0
1	I	3118	0	3097	72	0
1	J	3102	0	3077	91	0
1	K	3137	0	3115	103	0
1	L	3150	0	3127	102	0
1	M	3110	0	3086	98	0
1	N	3109	0	3086	96	0
1	O	3109	0	3084	85	0
1	P	3138	0	3117	107	0
1	Q	3138	0	3117	97	0
1	R	3101	0	3080	112	0
1	S	3116	0	3095	106	0
1	T	3150	0	3127	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	P	1	0	0	0	0
2	R	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
4	A	252	0	0	1	0
4	B	250	0	0	2	0
4	C	204	0	0	3	0
4	D	245	0	0	5	0
4	E	211	0	0	0	0
4	F	235	0	0	4	0
4	G	226	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	195	0	0	7	0
4	I	202	0	0	2	0
4	J	213	0	0	7	0
4	K	226	0	0	11	0
4	L	234	0	0	2	0
4	M	235	0	0	3	0
4	N	195	0	0	3	0
4	O	216	0	0	6	0
4	P	183	0	0	4	0
4	Q	201	0	0	1	0
4	R	226	0	0	4	0
4	S	226	0	0	9	0
4	T	270	0	0	5	0
All	All	66956	0	62056	1843	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 15.

The worst 5 of 1843 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)
4:J:512:HOH:O	1:P:121:ASN:HB3	1.32	1.23
1:T:417:ARG:HH11	1:T:417:ARG:HB2	1.07	1.15
1:R:379:LEU:HD23	1:R:383:LEU:HD22	1.28	1.14
1:G:279:ASP:HB3	1:K:286:ILE:HD11	1.31	1.12
1:D:379:LEU:HG	1:D:383:LEU:HD12	1.27	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/458 (91%)	397 (95%)	18 (4%)	3 (1%)	18	38
1	B	416/458 (91%)	399 (96%)	16 (4%)	1 (0%)	43	66
1	C	409/458 (89%)	390 (95%)	17 (4%)	2 (0%)	24	46
1	D	409/458 (89%)	387 (95%)	21 (5%)	1 (0%)	43	66
1	E	411/458 (90%)	392 (95%)	18 (4%)	1 (0%)	43	66
1	F	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	18	38
1	G	408/458 (89%)	389 (95%)	17 (4%)	2 (0%)	24	46
1	H	409/458 (89%)	390 (95%)	18 (4%)	1 (0%)	43	66
1	I	409/458 (89%)	388 (95%)	20 (5%)	1 (0%)	43	66
1	J	407/458 (89%)	387 (95%)	17 (4%)	3 (1%)	18	38
1	K	413/458 (90%)	391 (95%)	20 (5%)	2 (0%)	24	46
1	L	416/458 (91%)	396 (95%)	17 (4%)	3 (1%)	18	38
1	M	408/458 (89%)	388 (95%)	19 (5%)	1 (0%)	43	66
1	N	409/458 (89%)	388 (95%)	18 (4%)	3 (1%)	18	38
1	O	408/458 (89%)	386 (95%)	19 (5%)	3 (1%)	18	38
1	P	413/458 (90%)	388 (94%)	21 (5%)	4 (1%)	12	28
1	Q	413/458 (90%)	394 (95%)	17 (4%)	2 (0%)	24	46
1	R	407/458 (89%)	391 (96%)	15 (4%)	1 (0%)	43	66
1	S	410/458 (90%)	389 (95%)	19 (5%)	2 (0%)	24	46
1	T	416/458 (91%)	392 (94%)	23 (6%)	1 (0%)	43	66
All	All	8218/9160 (90%)	7810 (95%)	368 (4%)	40 (0%)	24	46

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	115	GLY
1	Q	115	GLY
1	A	220	TYR
1	G	321	ALA
1	J	220	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/385 (91%)	332 (94%)	20 (6%)	18	40
1	B	351/385 (91%)	327 (93%)	24 (7%)	14	32
1	C	349/385 (91%)	330 (95%)	19 (5%)	20	42
1	D	349/385 (91%)	333 (95%)	16 (5%)	24	49
1	E	350/385 (91%)	330 (94%)	20 (6%)	18	40
1	F	348/385 (90%)	323 (93%)	25 (7%)	13	30
1	G	348/385 (90%)	326 (94%)	22 (6%)	16	36
1	H	349/385 (91%)	329 (94%)	20 (6%)	18	40
1	I	349/385 (91%)	335 (96%)	14 (4%)	28	55
1	J	347/385 (90%)	330 (95%)	17 (5%)	22	47
1	K	350/385 (91%)	324 (93%)	26 (7%)	13	29
1	L	351/385 (91%)	326 (93%)	25 (7%)	13	31
1	M	348/385 (90%)	326 (94%)	22 (6%)	16	36
1	N	347/385 (90%)	324 (93%)	23 (7%)	15	34
1	O	348/385 (90%)	332 (95%)	16 (5%)	24	49
1	P	350/385 (91%)	322 (92%)	28 (8%)	11	25
1	Q	350/385 (91%)	327 (93%)	23 (7%)	15	34
1	R	347/385 (90%)	323 (93%)	24 (7%)	14	32
1	S	348/385 (90%)	332 (95%)	16 (5%)	24	49
1	T	351/385 (91%)	332 (95%)	19 (5%)	20	42
All	All	6982/7700 (91%)	6563 (94%)	419 (6%)	17	37

5 of 419 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	121	ASN
1	N	317	SER
1	S	383	LEU
1	L	286	ILE
1	M	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	130	GLN
1	R	303	GLN
1	S	324	GLN
1	H	293	ASN
1	H	233	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	420/458 (91%)	-0.61	3 (0%) 84 82	23, 33, 72, 105	0
1	B	418/458 (91%)	-0.56	9 (2%) 62 57	20, 32, 67, 106	0
1	C	413/458 (90%)	-0.52	7 (1%) 69 64	26, 37, 72, 105	0
1	D	413/458 (90%)	-0.64	5 (1%) 76 73	23, 34, 63, 106	0
1	E	415/458 (90%)	-0.39	12 (2%) 53 48	27, 36, 74, 114	0
1	F	413/458 (90%)	-0.63	6 (1%) 72 68	22, 35, 66, 98	0
1	G	412/458 (89%)	-0.59	3 (0%) 84 82	25, 37, 61, 106	0
1	H	413/458 (90%)	-0.50	6 (1%) 72 68	27, 39, 67, 114	0
1	I	413/458 (90%)	-0.52	5 (1%) 76 73	28, 38, 71, 107	0
1	J	411/458 (89%)	-0.53	5 (1%) 76 73	27, 38, 70, 99	0
1	K	417/458 (91%)	-0.52	6 (1%) 73 69	27, 38, 74, 108	0
1	L	418/458 (91%)	-0.58	4 (0%) 79 76	24, 34, 73, 103	0
1	M	412/458 (89%)	-0.53	4 (0%) 79 76	25, 38, 68, 105	0
1	N	413/458 (90%)	-0.49	4 (0%) 79 76	27, 38, 68, 104	0
1	O	412/458 (89%)	-0.56	4 (0%) 79 76	27, 37, 72, 104	0
1	P	417/458 (91%)	-0.37	11 (2%) 57 51	27, 39, 82, 112	0
1	Q	417/458 (91%)	-0.45	10 (2%) 59 54	27, 39, 77, 118	0
1	R	411/458 (89%)	-0.56	6 (1%) 72 68	26, 36, 56, 102	0
1	S	414/458 (90%)	-0.61	2 (0%) 87 85	25, 35, 65, 95	0
1	T	418/458 (91%)	-0.65	4 (0%) 79 76	23, 33, 62, 101	0
All	All	8290/9160 (90%)	-0.54	116 (1%) 73 69	20, 37, 70, 118	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	117	VAL	4.5
1	R	113	LEU	4.4
1	F	113	LEU	4.3
1	Q	113	LEU	4.3
1	N	113	LEU	4.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	I	5507	1/1	0.97	0.04	33,33,33,33	0
2	CL	G	5505	1/1	0.98	0.05	33,33,33,33	0
2	CL	H	5506	1/1	0.98	0.05	31,31,31,31	0
2	CL	B	5501	1/1	0.98	0.03	26,26,26,26	1
2	CL	R	5508	1/1	0.98	0.03	27,27,27,27	0
2	CL	A	5503	1/1	0.99	0.03	32,32,32,32	0
2	CL	P	5502	1/1	0.99	0.03	26,26,26,26	1
2	CL	C	5504	1/1	0.99	0.02	30,30,30,30	0
3	CA	P	5902	1/1	0.99	0.07	40,40,40,40	1
3	CA	B	5901	1/1	1.00	0.06	33,33,33,33	1
3	CA	C	5904	1/1	1.00	0.09	39,39,39,39	0
3	CA	G	5905	1/1	1.00	0.09	45,45,45,45	0
3	CA	H	5906	1/1	1.00	0.06	39,39,39,39	0
3	CA	I	5907	1/1	1.00	0.07	41,41,41,41	0
3	CA	A	5903	1/1	1.00	0.05	34,34,34,34	0
3	CA	R	5908	1/1	1.00	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.