



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:11 pm BST

PDB ID : 3P0S  
Title : Crystal structure of Bombyx mori densovirus 1 capsid  
Authors : Kaufmann, B.; Rossmann, M.G.  
Deposited on : 2010-09-29  
Resolution : 3.10 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

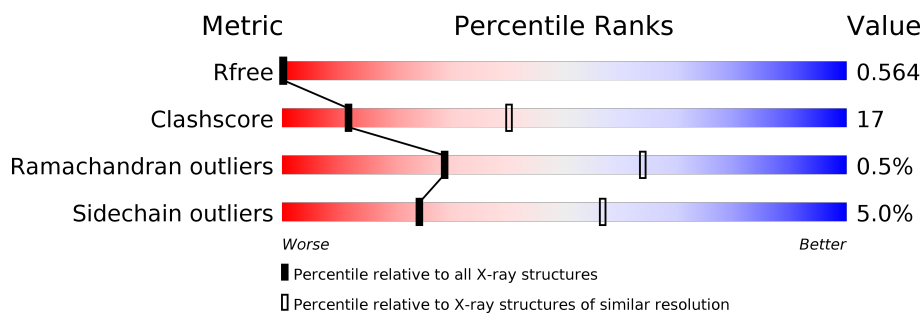
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	494	<div> <div>55%</div> <div>27%</div> <div>•</div> <div>17%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3290 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.

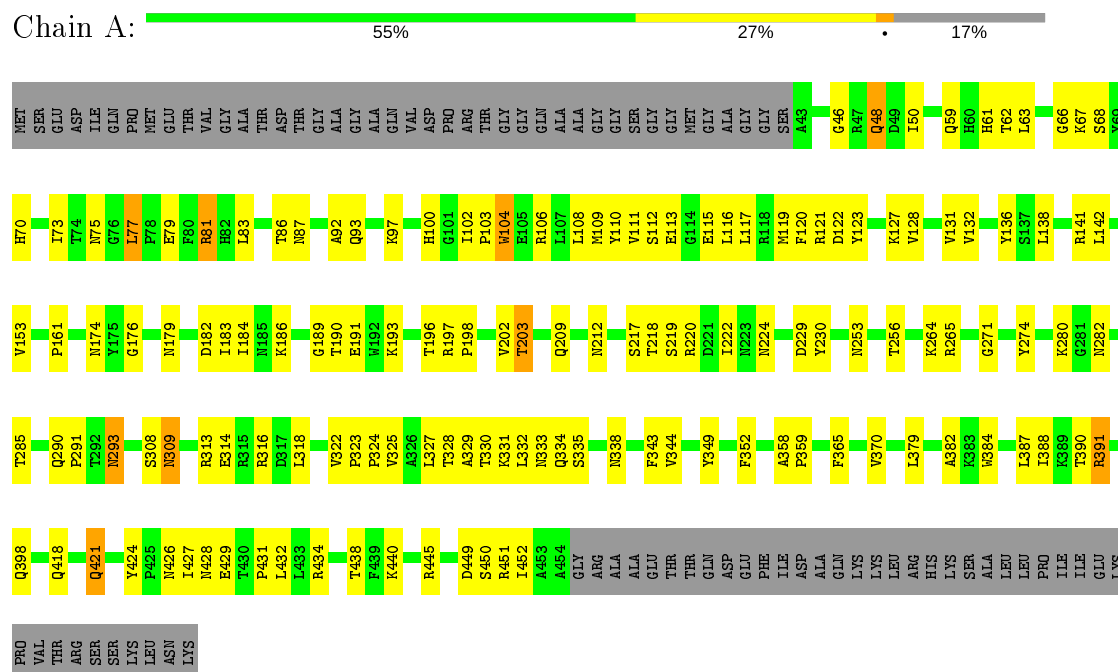
- Molecule 1 is a protein called Capsid protein VP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	3290	2090	568	620	12	0	0	0

### 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: Capsid protein VP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	245.40 Å   245.60 Å   245.70 Å 59.98°   67.93°   72.27°	Depositor
Resolution (Å)	45.00 – 3.10 45.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.00-3.10) 95.4 (45.58-3.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 3.12 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , (Not available) 0.564 , 0.564	Depositor DCC
$R_{free}$ test set	65671 reflections (8.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.11	EDS
Total number of atoms	3290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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, 0.333 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/3376	0.60	0/4599

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	3290	0	3207	113	0
All	All	3290	0	3207	113	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 17.

All (113) 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:A:81:ARG:HH11	1:A:93:GLN:HE22	1.13	0.92
1:A:81:ARG:HH11	1:A:93:GLN:NE2	1.69	0.90
1:A:111:VAL:HG13	1:A:115:GLU:HB2	1.54	0.89
1:A:141:ARG:HB3	1:A:153:VAL:HG12	1.55	0.86
1:A:190:THR:HG23	1:A:212:ASN:HD22	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:HG22	1:A:332:LEU:H	1.45	0.81
1:A:100:HIS:HD2	1:A:224:ASN:H	1.29	0.80
1:A:81:ARG:NH1	1:A:93:GLN:HE22	1.80	0.79
1:A:75:ASN:HD22	1:A:382:ALA:N	1.80	0.79
1:A:75:ASN:HD22	1:A:382:ALA:H	1.32	0.78
1:A:324:PRO:HG2	1:A:432:LEU:HD13	1.65	0.77
1:A:253:ASN:HD22	1:A:256:THR:H	1.29	0.76
1:A:161:PRO:HB2	1:A:370:VAL:HB	1.70	0.73
1:A:128:VAL:HG11	1:A:344:VAL:HG13	1.70	0.73
1:A:391:ARG:HG2	1:A:391:ARG:HH11	1.52	0.72
1:A:66:GLY:O	1:A:67:LYS:HD2	1.90	0.71
1:A:293:ASN:H	1:A:293:ASN:HD22	1.40	0.70
1:A:75:ASN:HB3	1:A:379:LEU:HD11	1.72	0.70
1:A:325:VAL:HG13	1:A:327:LEU:HG	1.73	0.69
1:A:318:LEU:HB2	1:A:323:PRO:HG3	1.75	0.67
1:A:330:THR:HG22	1:A:332:LEU:N	2.12	0.65
1:A:308:SER:HB3	1:A:313:ARG:HH11	1.63	0.64
1:A:66:GLY:C	1:A:67:LYS:HD2	2.19	0.63
1:A:329:ALA:HA	1:A:421:GLN:HG2	1.79	0.62
1:A:81:ARG:HD2	1:A:93:GLN:HE21	1.65	0.62
1:A:111:VAL:CG1	1:A:115:GLU:HB2	2.30	0.62
1:A:217:SER:O	1:A:218:THR:HG23	1.99	0.62
1:A:220:ARG:HH11	1:A:220:ARG:HG2	1.63	0.62
1:A:92:ALA:HB3	1:A:230:TYR:HB2	1.82	0.62
1:A:335:SER:H	1:A:338:ASN:HD22	1.50	0.60
1:A:293:ASN:HD22	1:A:293:ASN:N	2.00	0.59
1:A:131:VAL:HG11	1:A:344:VAL:HG11	1.83	0.59
1:A:59:GLN:HB2	1:A:398:GLN:HB2	1.84	0.59
1:A:182:ASP:OD1	1:A:186:LYS:HE3	2.03	0.59
1:A:432:LEU:HD12	1:A:449:ASP:O	2.02	0.59
1:A:81:ARG:HD2	1:A:93:GLN:NE2	2.19	0.58
1:A:426:ASN:HB3	1:A:429:GLU:HG2	1.86	0.58
1:A:106:ARG:HG3	1:A:184:ILE:HD11	1.84	0.58
1:A:176:GLY:HA3	1:A:179:ASN:HD22	1.69	0.57
1:A:314:GLU:OE1	1:A:316:ARG:HD3	2.04	0.57
1:A:128:VAL:HG11	1:A:344:VAL:CG1	2.35	0.56
1:A:77:LEU:HD13	1:A:379:LEU:HB2	1.87	0.56
1:A:330:THR:HG22	1:A:331:LYS:N	2.20	0.56
1:A:282:ASN:O	1:A:332:LEU:HD13	2.04	0.56
1:A:434:ARG:HH11	1:A:434:ARG:HG3	1.70	0.56
1:A:75:ASN:ND2	1:A:382:ALA:N	2.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:HG23	1:A:452:ILE:O	2.07	0.55
1:A:280:LYS:HE3	1:A:285:THR:O	2.08	0.54
1:A:138:LEU:O	1:A:141:ARG:NH2	2.40	0.54
1:A:426:ASN:HB3	1:A:429:GLU:CG	2.38	0.53
1:A:141:ARG:CB	1:A:153:VAL:HG12	2.34	0.53
1:A:63:LEU:N	1:A:63:LEU:HD12	2.23	0.53
1:A:391:ARG:HG2	1:A:391:ARG:NH1	2.22	0.53
1:A:75:ASN:CB	1:A:379:LEU:HD11	2.39	0.52
1:A:343:PHE:CD2	1:A:434:ARG:HG2	2.44	0.52
1:A:450:SER:O	1:A:452:ILE:N	2.42	0.52
1:A:220:ARG:NH1	1:A:220:ARG:HG2	2.25	0.52
1:A:112:SER:OG	1:A:115:GLU:HG3	2.10	0.51
1:A:324:PRO:CG	1:A:432:LEU:HD13	2.38	0.50
1:A:280:LYS:HE2	1:A:282:ASN:O	2.11	0.50
1:A:202:VAL:HG22	1:A:203:THR:N	2.27	0.49
1:A:79:GLU:CD	1:A:97:LYS:HD2	2.33	0.48
1:A:127:LYS:NZ	1:A:271:GLY:H	2.11	0.48
1:A:330:THR:OG1	1:A:427:ILE:HD11	2.13	0.48
1:A:121:ARG:NH1	1:A:122:ASP:OD1	2.47	0.48
1:A:308:SER:O	1:A:309:ASN:HB2	2.13	0.48
1:A:67:LYS:NZ	1:A:115:GLU:OE1	2.46	0.47
1:A:290:GLN:HB3	1:A:291:PRO:HD2	1.95	0.47
1:A:68:SER:HA	1:A:388:ILE:O	2.15	0.47
1:A:136:TYR:HB2	1:A:387:LEU:HB2	1.96	0.47
1:A:333:ASN:HB3	1:A:431:PRO:CG	2.45	0.46
1:A:191:GLU:OE2	1:A:193:LYS:HG3	2.15	0.46
1:A:391:ARG:CG	1:A:391:ARG:HH11	2.26	0.46
1:A:174:ASN:ND2	1:A:229:ASP:OD2	2.49	0.46
1:A:293:ASN:H	1:A:293:ASN:ND2	2.11	0.46
1:A:111:VAL:HG12	1:A:112:SER:O	2.17	0.45
1:A:197:ARG:HA	1:A:198:PRO:HD3	1.87	0.45
1:A:280:LYS:NZ	1:A:428:ASN:ND2	2.65	0.45
1:A:318:LEU:HB2	1:A:323:PRO:CG	2.46	0.45
1:A:116:LEU:C	1:A:116:LEU:HD23	2.37	0.45
1:A:110:TYR:CD1	1:A:390:THR:HB	2.52	0.45
1:A:189:GLY:HA2	1:A:212:ASN:ND2	2.32	0.44
1:A:325:VAL:HG13	1:A:327:LEU:CG	2.45	0.44
1:A:333:ASN:HB3	1:A:431:PRO:HG2	1.99	0.44
1:A:424:TYR:CZ	1:A:452:ILE:HG21	2.53	0.44
1:A:50:ILE:HD13	1:A:50:ILE:HA	1.84	0.44
1:A:103:PRO:O	1:A:109:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:SER:C	1:A:452:ILE:H	2.21	0.44
1:A:70:HIS:CE1	1:A:219:SER:HB2	2.53	0.44
1:A:352:PHE:HB2	1:A:418:GLN:O	2.17	0.43
1:A:93:GLN:HG2	1:A:229:ASP:OD1	2.18	0.43
1:A:86:THR:O	1:A:87:ASN:HB2	2.17	0.43
1:A:349:TYR:CD1	1:A:421:GLN:HB3	2.53	0.43
1:A:67:LYS:HD3	1:A:110:TYR:O	2.19	0.42
1:A:358:ALA:HA	1:A:359:PRO:HD3	1.88	0.42
1:A:73:ILE:HD11	1:A:384:TRP:CE3	2.55	0.42
1:A:102:ILE:N	1:A:102:ILE:HD12	2.35	0.42
1:A:322:VAL:HB	1:A:452:ILE:HG23	2.02	0.42
1:A:132:VAL:HG22	1:A:265:ARG:HG2	2.01	0.41
1:A:438:THR:HG22	1:A:438:THR:O	2.20	0.41
1:A:113:GLU:O	1:A:117:LEU:HG	2.20	0.41
1:A:48:GLN:CD	1:A:48:GLN:H	2.23	0.41
1:A:61:HIS:HD2	1:A:123:TYR:HE1	1.66	0.41
1:A:142:LEU:HD12	1:A:142:LEU:O	2.20	0.41
1:A:391:ARG:CG	1:A:391:ARG:NH1	2.83	0.41
1:A:111:VAL:HG11	1:A:119:MET:HE3	2.03	0.41
1:A:183:ILE:HG12	1:A:222:ILE:HB	2.02	0.41
1:A:142:LEU:HA	1:A:153:VAL:HG13	2.03	0.41
1:A:104:TRP:CH2	1:A:264:LYS:HB3	2.56	0.40
1:A:46:GLY:H	1:A:48:GLN:HE21	1.69	0.40
1:A:253:ASN:ND2	1:A:256:THR:HG23	2.36	0.40
1:A:274:TYR:HA	1:A:349:TYR:CE2	2.57	0.40
1:A:358:ALA:O	1:A:445:ARG:NH1	2.55	0.40

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	410/494 (83%)	379 (92%)	29 (7%)	2 (0%)	29 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	ARG
1	A	309	ASN

### 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	359/418 (86%)	341 (95%)	18 (5%)	24 57

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	62	THR
1	A	77	LEU
1	A	81	ARG
1	A	83	LEU
1	A	104	TRP
1	A	108	LEU
1	A	120	PHE
1	A	196	THR
1	A	203	THR
1	A	209	GLN
1	A	293	ASN
1	A	328	THR
1	A	334	GLN
1	A	365	PHE
1	A	391	ARG
1	A	421	GLN
1	A	440	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	61	HIS
1	A	75	ASN
1	A	87	ASN
1	A	93	GLN
1	A	100	HIS
1	A	159	GLN
1	A	174	ASN
1	A	179	ASN
1	A	212	ASN
1	A	253	ASN
1	A	282	ASN
1	A	293	ASN
1	A	311	GLN
1	A	333	ASN
1	A	334	GLN
1	A	338	ASN
1	A	360	GLN
1	A	377	ASN
1	A	413	GLN
1	A	421	GLN
1	A	428	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.