



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2017 – 02:57 PM EDT

PDB ID : 5A00  
Title : X-ray structure of a human Kobuvirus: Aichi virus A (AiV)  
Authors : Sabin, C.; Palkova, L.; Plevka, P.  
Deposited on : 2015-09-11  
Resolution : 2.10 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

<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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
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) : rb-20029077

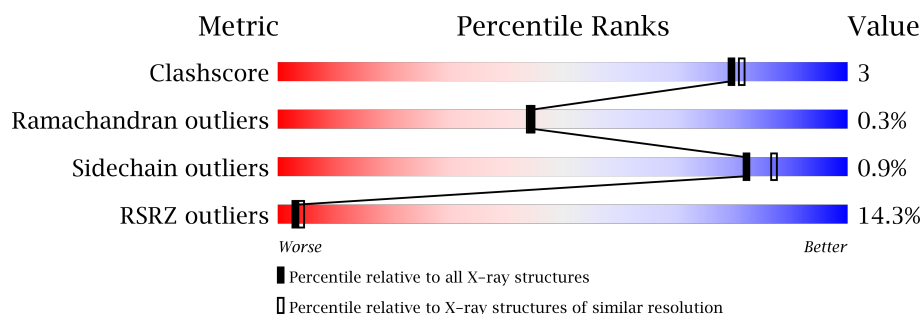
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	253	<div> <div>14%</div> <div>79%</div> <div>11%</div> <div>9%</div> </div>
2	B	370	<div> <div>10%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>
3	C	223	<div> <div>16%</div> <div>92%</div> <div>6%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5938 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 VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1746	1130	276	331	9			

- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2366	1506	390	464	6			

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total	C	N	O	S	0	0	0
			1679	1085	283	304	7			

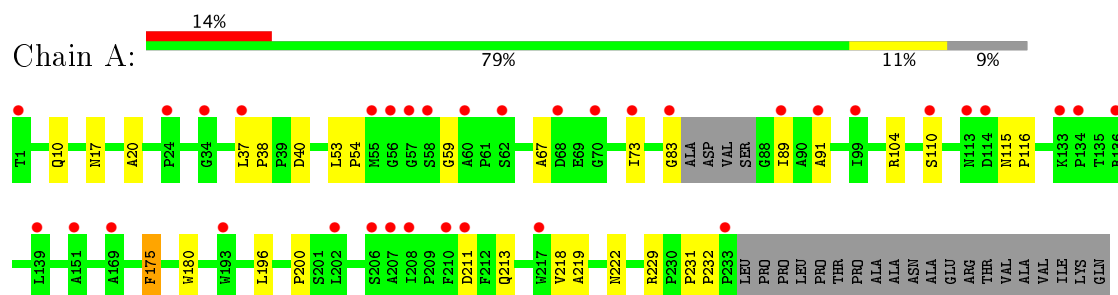
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	58	Total	O	0	0
			58	58		
4	C	37	Total	O	0	0
			37	37		

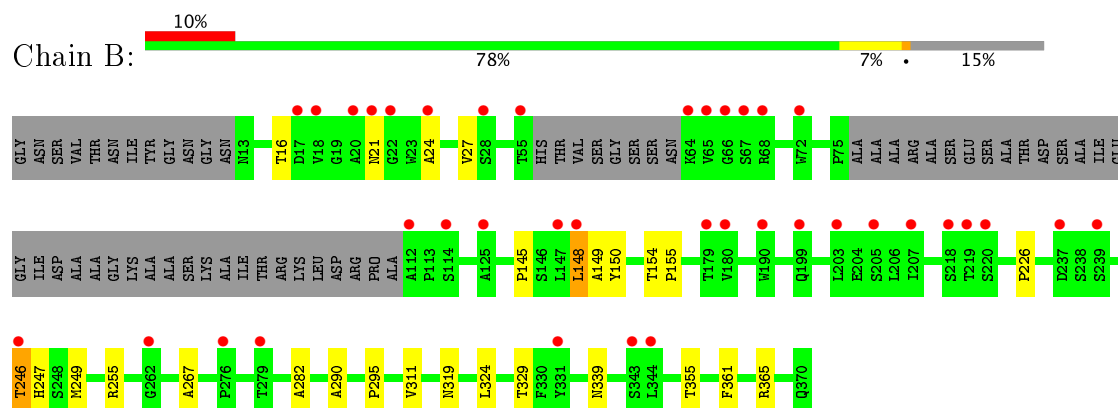
### 3 Residue-property plots [i](#)

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 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: VP0



#### • Molecule 2: VP1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	350.82Å 350.82Å 350.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.46 – 2.10 68.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (71.46-2.10) 89.6 (68.80-2.10)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1494.23 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.330 , (Not available) 0.361 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 18.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	5938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

### 5.1 Standard geometry

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	0.57	0/1806	0.60	0/2481
2	B	0.62	1/2448 (0.0%)	0.65	2/3379 (0.1%)
3	C	0.57	0/1736	0.63	0/2389
All	All	0.59	1/5990 (0.0%)	0.63	2/8249 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	246	THR	CB-CG2	-8.61	1.24	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	246	THR	CA-CB-CG2	-8.72	100.19	112.40
2	B	148	LEU	N-CA-C	-5.12	97.16	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1746	0	1681	17	0
2	B	2366	0	2246	20	0
3	C	1679	0	1635	7	0
4	A	52	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	58	0	0	0	0
4	C	37	0	0	0	0
All	All	5938	0	5562	36	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 3.

All (36) 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)
2:B:246:THR:HG22	2:B:246:THR:O	1.83	0.77
3:C:192:HIS:O	3:C:193:THR:HG22	1.96	0.66
2:B:149:ALA:CB	2:B:295:PRO:HB3	2.29	0.63
2:B:255:ARG:HB3	2:B:355:THR:HB	1.81	0.62
2:B:149:ALA:HB3	2:B:311:VAL:HG12	1.83	0.60
1:A:20:ALA:HB2	3:C:51:PRO:HG3	1.88	0.56
1:A:180:TRP:HA	2:B:324:LEU:HD21	1.89	0.54
1:A:110:SER:HB2	1:A:213:GLN:HB2	1.90	0.54
2:B:226:PRO:HA	2:B:329:THR:HG22	1.91	0.53
2:B:267:ALA:HB3	2:B:339:ASN:HB3	1.90	0.53
1:A:89:ILE:HD13	1:A:218:VAL:HG23	1.92	0.50
1:A:222:ASN:ND2	2:B:21:ASN:OD1	2.45	0.50
2:B:149:ALA:HB1	2:B:295:PRO:HB3	1.95	0.48
3:C:57:VAL:HG13	3:C:200:VAL:HB	1.95	0.48
1:A:231:PRO:HD2	2:B:290:ALA:HB1	1.96	0.47
1:A:229:ARG:HH21	2:B:282:ALA:HB2	1.80	0.46
1:A:91:ALA:HB1	1:A:232:PRO:HG3	1.97	0.46
2:B:247:HIS:CG	2:B:361:PHE:HB3	2.50	0.46
1:A:104:ARG:HB2	1:A:219:ALA:HB3	1.98	0.45
2:B:149:ALA:HB2	2:B:295:PRO:HB3	1.98	0.45
1:A:53:LEU:HD12	1:A:54:PRO:HD2	1.99	0.44
3:C:103:HIS:HB2	3:C:203:PHE:HB2	1.99	0.44
2:B:150:TYR:CD2	3:C:39:ALA:HB2	2.52	0.43
1:A:73:ILE:HG13	1:A:196:LEU:HB2	2.00	0.43
2:B:148:LEU:HG	2:B:150:TYR:O	2.17	0.43
3:C:99:GLU:HG3	3:C:155:PRO:HA	2.01	0.42
1:A:59:GLY:HA3	1:A:83:GLY:HA3	2.02	0.42
2:B:24:ALA:HB3	2:B:27:VAL:HG23	2.00	0.42
1:A:17:ASN:HA	2:B:145:PRO:HB3	2.02	0.42
1:A:115:ASN:HA	1:A:116:PRO:HD3	1.94	0.41
1:A:175:PHE:CD1	1:A:175:PHE:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:MET:HB2	2:B:319:ASN:HB3	2.01	0.41
1:A:67:ALA:HA	1:A:200:PRO:HG2	2.03	0.41
1:A:37:LEU:HA	1:A:38:PRO:HD3	1.96	0.40
2:B:154:THR:HA	2:B:155:PRO:HD3	1.92	0.40
2:B:16:THR:HA	3:C:18:ALA:HB2	2.03	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	225/253 (89%)	216 (96%)	9 (4%)	0	100	100
2	B	308/370 (83%)	295 (96%)	13 (4%)	0	100	100
3	C	218/223 (98%)	208 (95%)	8 (4%)	2 (1%)	20	14
All	All	751/846 (89%)	719 (96%)	30 (4%)	2 (0%)	44	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	146	ALA
3	C	218	PRO

### 5.3.2 Protein sidechains [i](#)

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	193/212 (91%)	189 (98%)	4 (2%)	59	64
2	B	264/302 (87%)	263 (100%)	1 (0%)	93	95
3	C	175/178 (98%)	174 (99%)	1 (1%)	89	92
All	All	632/692 (91%)	626 (99%)	6 (1%)	82	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	40	ASP
1	A	175	PHE
1	A	211	ASP
2	B	365	ARG
3	C	212	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
2	B	21	ASN
3	C	192	HIS

### 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 [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, 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	229/253 (90%)	1.29	35 (15%) 2 3	15, 22, 42, 51	0
2	B	314/370 (84%)	1.17	38 (12%) 5 6	15, 20, 39, 56	0
3	C	220/223 (98%)	1.17	36 (16%) 2 3	15, 20, 30, 42	0
All	All	763/846 (90%)	1.20	109 (14%) 3 4	15, 20, 39, 56	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ALA	9.8
2	B	21	ASN	8.1
2	B	112	ALA	6.8
3	C	79	ILE	6.5
1	A	206	SER	6.1
1	A	83	GLY	5.9
2	B	20	ALA	5.6
2	B	55	THR	5.2
1	A	208	ILE	5.0
1	A	58	SER	4.6
1	A	60	ALA	4.5
1	A	1	THR	4.3
2	B	343	SER	4.0
2	B	22	GLY	4.0
1	A	68	ASP	4.0
3	C	169	ASN	4.0
1	A	57	GLY	3.7
1	A	73	ILE	3.6
2	B	66	GLY	3.6
2	B	239	SER	3.6
1	A	202	LEU	3.5
3	C	192	HIS	3.4
1	A	133	LYS	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	147	LEU	3.4
2	B	17	ASP	3.4
2	B	28	SER	3.4
2	B	68	ARG	3.3
3	C	83	GLY	3.3
2	B	205	SER	3.2
3	C	72	PHE	3.2
2	B	65	VAL	3.2
3	C	9	GLY	3.2
1	A	151	ALA	3.2
1	A	233	PRO	3.1
3	C	8	PRO	3.1
2	B	148	LEU	3.1
3	C	132	GLN	3.0
3	C	82	THR	3.0
3	C	168	ASN	3.0
3	C	12	THR	2.9
2	B	207	ILE	2.9
2	B	180	VAL	2.9
2	B	190	TRP	2.9
2	B	179	THR	2.8
3	C	219	ALA	2.8
1	A	134	PRO	2.8
3	C	170	PRO	2.7
1	A	136	ARG	2.7
2	B	114	SER	2.7
3	C	104	LEU	2.7
2	B	67	SER	2.6
1	A	113	ASN	2.6
2	B	64	LYS	2.6
1	A	99	ILE	2.6
1	A	56	GLY	2.6
2	B	262	GLY	2.5
2	B	237	ASP	2.5
2	B	279	THR	2.5
1	A	24	PRO	2.5
1	A	62	SER	2.5
3	C	199	LEU	2.5
1	A	210	PHE	2.4
1	A	110	SER	2.4
1	A	34	GLY	2.4
2	B	219	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	160	SER	2.4
2	B	199	GLN	2.4
1	A	55	MET	2.4
3	C	77	SER	2.4
1	A	114	ASP	2.4
3	C	195	PRO	2.3
1	A	70	GLY	2.3
3	C	26	GLY	2.3
3	C	86	ILE	2.3
2	B	331	TYR	2.3
3	C	179	TYR	2.3
2	B	203	LEU	2.3
2	B	344	LEU	2.3
2	B	72	TRP	2.3
1	A	211	ASP	2.3
3	C	155	PRO	2.2
1	A	37	LEU	2.2
3	C	100	LEU	2.2
1	A	89	ILE	2.2
3	C	37	ILE	2.2
1	A	169	ALA	2.2
2	B	218	SER	2.2
2	B	246	THR	2.2
3	C	47	PHE	2.2
3	C	101	ALA	2.2
2	B	18	VAL	2.1
2	B	24	ALA	2.1
3	C	29	ALA	2.1
3	C	193	THR	2.1
2	B	220	SER	2.1
3	C	209	SER	2.1
3	C	6	ALA	2.1
3	C	181	SER	2.1
2	B	125	ALA	2.1
2	B	276	PRO	2.1
3	C	123	ALA	2.1
1	A	193	TRP	2.1
3	C	57	VAL	2.1
3	C	212	VAL	2.1
3	C	113	TYR	2.1
1	A	91	ALA	2.0
1	A	217	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	2.0
3	C	24	LEU	2.0

## 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.