



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2Z7J / pdb_00002z7j
Title : Structural insights into de multifunctional VP3 protein of birnaviruses:gold derivative
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Deposited on : 2007-08-23
Resolution : 2.40 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

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

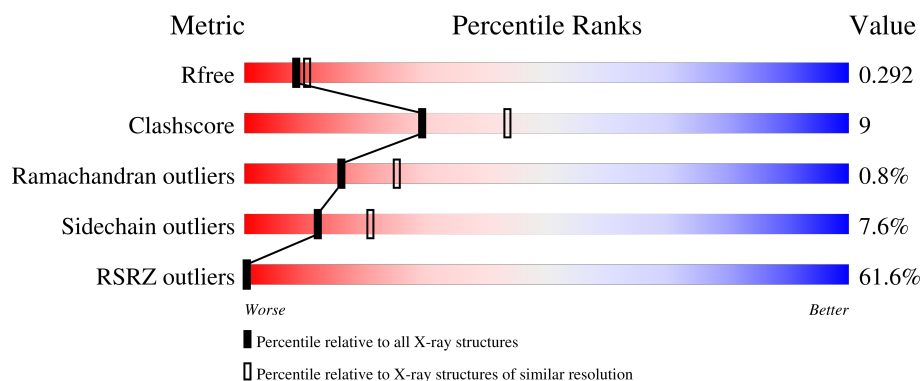
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	125	62% 81%13%6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1036 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 assembly protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1004	628	177	194	5			

- Molecule 2 is GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Au	0	0
			3	3		

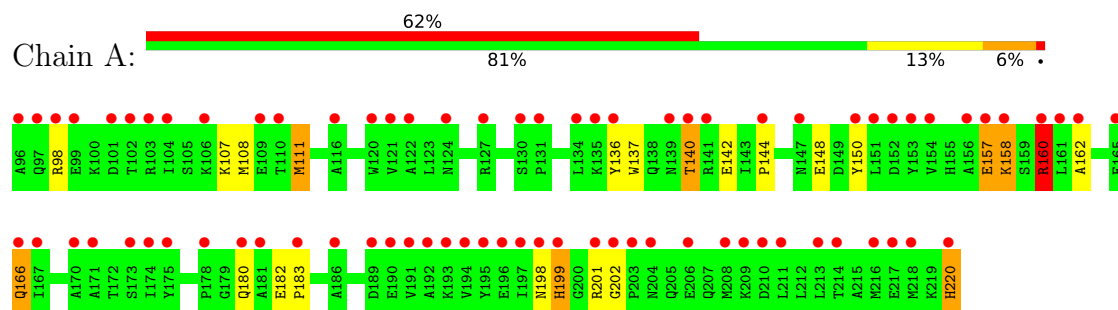
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		

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: Capsid assembly protein VP3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.75Å 69.75Å 71.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-2.40) 97.7 (20.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.285 0.277 , 0.292	Depositor DCC
R_{free} test set	329 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k 0.020 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	1036	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.84% 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](#)

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

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	0.55	0/1028	0.90	2/1389 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	166	GLN	CG-CD-NE2	6.67	126.41	116.40

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	1004	0	970	17	0
2	A	3	0	0	0	0
3	A	29	0	0	1	0
All	All	1036	0	970	17	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 9.

All (17) 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:220:HIS:OXT	1:A:220:HIS:ND1	2.32	0.63
1:A:162:ALA:HA	1:A:166:GLN:OE1	2.08	0.54
1:A:160:ARG:HD2	1:A:201:ARG:HA	1.91	0.52
1:A:136:TYR:O	1:A:140:THR:HB	2.08	0.52
1:A:160:ARG:CZ	1:A:202:GLY:H	2.22	0.52
1:A:98:ARG:NH2	3:A:225:HOH:O	2.28	0.51
1:A:140:THR:CG2	1:A:142:GLU:H	2.26	0.49
1:A:107:LYS:HG2	1:A:108:MET:HE2	1.97	0.46
1:A:140:THR:HG22	1:A:142:GLU:H	1.81	0.45
1:A:198:ASN:C	1:A:199:HIS:CG	2.95	0.44
1:A:148:GLU:HB3	1:A:150:TYR:CE1	2.53	0.43
1:A:182:GLU:HA	1:A:183:PRO:HD3	1.87	0.42
1:A:220:HIS:HD1	1:A:220:HIS:C	2.27	0.41
1:A:157:GLU:HB3	1:A:158:LYS:HE2	2.03	0.41
1:A:137:TRP:HB2	1:A:144:PRO:HG3	2.02	0.41
1:A:111:MET:HE2	1:A:111:MET:HB2	1.81	0.41
1:A:158:LYS:HG3	1:A:201:ARG:HH22	1.86	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	123/125 (98%)	120 (98%)	2 (2%)	1 (1%)	16	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ARG

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	105/105 (100%)	97 (92%)	8 (8%)	12	21

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	MET
1	A	140	THR
1	A	157	GLU
1	A	158	LYS
1	A	160	ARG
1	A	180	GLN
1	A	199	HIS
1	A	220	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 3 ligands modelled in this entry, 3 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	125/125 (100%)	2.32	77 (61%) 0 0	55, 64, 81, 86	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	HIS	6.0
1	A	96	ALA	4.6
1	A	201	ARG	4.4
1	A	161	LEU	4.1
1	A	99	GLU	4.1
1	A	217	GLU	4.0
1	A	158	LYS	4.0
1	A	175	TYR	3.9
1	A	116	ALA	3.8
1	A	101	ASP	3.8
1	A	192	ALA	3.7
1	A	157	GLU	3.7
1	A	120	TRP	3.6
1	A	106	LYS	3.6
1	A	160	ARG	3.6
1	A	165	GLU	3.4
1	A	153	TYR	3.4
1	A	110	THR	3.3
1	A	194	VAL	3.3
1	A	199	HIS	3.2
1	A	210	ASP	3.2
1	A	121	VAL	3.2
1	A	97	GLN	3.1
1	A	166	GLN	3.1
1	A	203	PRO	3.1
1	A	183	PRO	3.1
1	A	178	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	181	ALA	3.0
1	A	98	ARG	3.0
1	A	206	GLU	2.9
1	A	104	ILE	2.8
1	A	151	LEU	2.8
1	A	186	ALA	2.8
1	A	211	LEU	2.8
1	A	213	LEU	2.8
1	A	154	VAL	2.7
1	A	191	VAL	2.7
1	A	109	GLU	2.7
1	A	174	ILE	2.7
1	A	197	ILE	2.7
1	A	130	SER	2.7
1	A	102	THR	2.6
1	A	150	TYR	2.6
1	A	214	THR	2.6
1	A	127	ARG	2.6
1	A	140	THR	2.6
1	A	202	GLY	2.6
1	A	124	ASN	2.5
1	A	134	LEU	2.5
1	A	162	ALA	2.5
1	A	139	ASN	2.5
1	A	171	ALA	2.5
1	A	136	TYR	2.4
1	A	204	ASN	2.4
1	A	196	GLU	2.4
1	A	180	GLN	2.3
1	A	198	ASN	2.3
1	A	173	SER	2.3
1	A	167	ILE	2.3
1	A	209	LYS	2.3
1	A	216	MET	2.3
1	A	195	TYR	2.3
1	A	190	GLU	2.2
1	A	103	ARG	2.2
1	A	122	ALA	2.2
1	A	193	LYS	2.2
1	A	147	ASN	2.2
1	A	208	MET	2.1
1	A	152	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	135	LYS	2.1
1	A	141	ARG	2.1
1	A	144	PRO	2.1
1	A	170	ALA	2.1
1	A	156	ALA	2.0
1	A	189	ASP	2.0
1	A	131	PRO	2.0
1	A	218	MET	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 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($\text{\AA}^2$)	Q<0.9
2	AU	A	2	1/1	0.92	0.48	78,78,78,78	0
2	AU	A	3	1/1	0.95	0.20	133,133,133,133	1
2	AU	A	1	1/1	0.99	0.12	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.