



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 AM GMT

PDB ID : 2R72
Title : Crystal structure of infectious bursal disease virus VP1 polymerase, incubated with Mg²⁺ ion.
Authors : Garriga, D.; Navarro, A.; Querol-Audi, J.; Abaitua, F.; Rodriguez, J.F.; Verdaguier, N.
Deposited on : 2007-09-07
Resolution : 3.15 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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

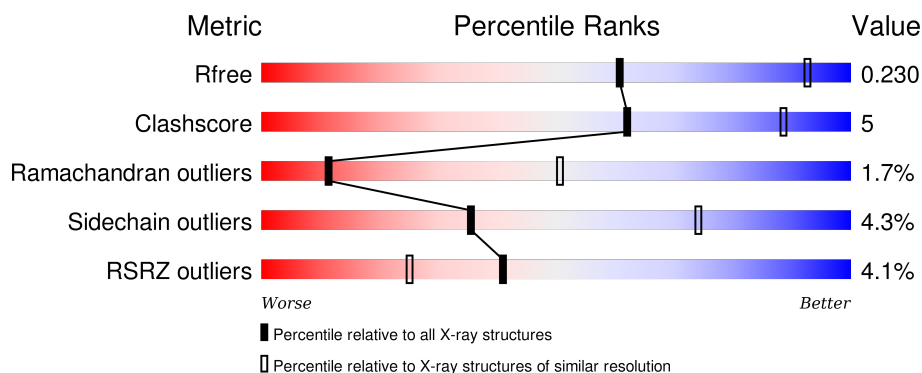
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	852	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	846	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	847	-	-	-	X
2	MG	A	848	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5921 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 INFECTIOUS BURSAL DISEASE VIRUS VP1 POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			5915	3787	1007	1099	22			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

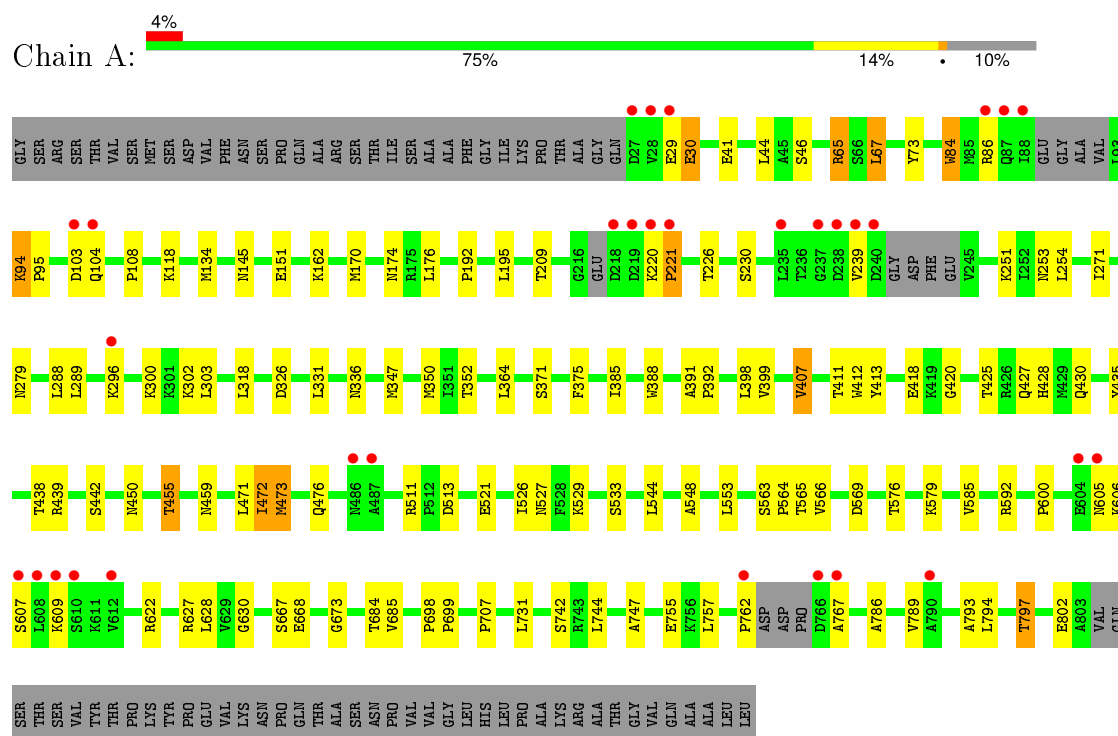
- Molecule 3 is water.

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

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 errors 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: INFECTIOUS BURSAL DISEASE VIRUS VP1 POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.84Å 122.84Å 354.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.15 20.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.15) 97.8 (20.00-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.235 0.206 , 0.230	Depositor DCC
R_{free} test set	1393 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 27545 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5921	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.32	0/6053	0.50	1/8231 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	762	PRO	N-CA-CB	5.82	110.28	103.30

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	5915	0	5861	64	0
2	A	3	0	0	0	0
3	A	3	0	0	0	0
All	All	5921	0	5861	64	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 5.

All (64) 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:230:SER:HB2	1:A:279:ASN:HD21	1.22	1.04
1:A:230:SER:HB2	1:A:279:ASN:ND2	2.04	0.69
1:A:427:GLN:HA	1:A:430:GLN:HG2	1.76	0.68
1:A:162:LYS:HA	1:A:326:ASP:HA	1.75	0.67
1:A:65:ARG:H	1:A:476:GLN:HE22	1.46	0.64
1:A:170:MET:O	1:A:174:ASN:HB2	1.98	0.64
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.81	0.63
1:A:41:GLU:HG2	1:A:118:LYS:HD2	1.81	0.62
1:A:435:TYR:CE2	1:A:439:ARG:HG3	2.34	0.61
1:A:103:ASP:O	1:A:104:GLN:HB2	2.00	0.61
1:A:375:PHE:CE1	1:A:385:ILE:HD13	2.37	0.60
1:A:459:ASN:O	1:A:797:THR:HG21	2.02	0.59
1:A:521:GLU:HB2	1:A:526:ILE:O	2.03	0.58
1:A:438:THR:O	1:A:442:SER:HB2	2.05	0.57
1:A:364:LEU:HD21	1:A:385:ILE:HD12	1.88	0.55
1:A:209:THR:O	1:A:371:SER:HB2	2.06	0.55
1:A:176:LEU:HD11	1:A:318:LEU:HD11	1.90	0.54
1:A:472:ILE:HG23	1:A:473:MET:H	1.72	0.53
1:A:230:SER:CB	1:A:279:ASN:HD21	2.09	0.53
1:A:318:LEU:HD22	1:A:336:ASN:HB3	1.91	0.53
1:A:65:ARG:H	1:A:476:GLN:NE2	2.05	0.53
1:A:44:LEU:HD12	1:A:170:MET:HA	1.91	0.53
1:A:303:LEU:HD21	1:A:744:LEU:HD13	1.92	0.52
1:A:170:MET:HG3	1:A:331:LEU:O	2.10	0.51
1:A:793:ALA:O	1:A:797:THR:HG22	2.10	0.51
1:A:565:THR:HG22	1:A:576:THR:HB	1.92	0.51
1:A:108:PRO:HB2	1:A:471:LEU:HD22	1.93	0.50
1:A:544:LEU:HD11	1:A:566:VAL:HG23	1.93	0.50
1:A:192:PRO:HA	1:A:195:LEU:HD12	1.95	0.49
1:A:418:GLU:HB2	1:A:527:ASN:HB2	1.95	0.47
1:A:303:LEU:HD11	1:A:744:LEU:HD22	1.95	0.47
1:A:220:LYS:N	1:A:221:PRO:HD3	2.29	0.47
1:A:254:LEU:HD22	1:A:271:ILE:HD11	1.97	0.46
1:A:548:ALA:HB3	1:A:579:LYS:HE3	1.98	0.45
1:A:226:THR:HG22	1:A:450:ASN:HB3	2.00	0.44
1:A:569:ASP:OD2	1:A:592:ARG:NH1	2.50	0.44
1:A:407:VAL:HA	1:A:411:THR:O	2.17	0.44
1:A:65:ARG:NH1	1:A:476:GLN:HE21	2.16	0.44
1:A:425:THR:H	1:A:428:HIS:HD2	1.66	0.44
1:A:667:SER:O	1:A:673:GLY:HA3	2.18	0.44
1:A:288:LEU:HD13	1:A:303:LEU:HD12	2.00	0.43
1:A:412:TRP:O	1:A:533:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD22	1:A:108:PRO:HG3	1.99	0.43
1:A:289:LEU:HD22	1:A:747:ALA:HB3	2.00	0.43
1:A:162:LYS:HG2	1:A:326:ASP:HB3	2.01	0.43
1:A:134:MET:HE1	1:A:151:GLU:HB3	2.00	0.42
1:A:347:MET:HA	1:A:350:MET:HE2	2.01	0.42
1:A:698:PRO:HA	1:A:699:PRO:HD3	1.91	0.42
1:A:553:LEU:HD13	1:A:585:VAL:HG21	2.00	0.42
1:A:742:SER:HA	1:A:786:ALA:HA	2.01	0.42
1:A:391:ALA:HA	1:A:392:PRO:HD3	1.91	0.42
1:A:65:ARG:HB2	1:A:476:GLN:HE22	1.85	0.42
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.91	0.42
1:A:627:ARG:HB3	1:A:685:VAL:HG11	2.02	0.42
1:A:425:THR:H	1:A:428:HIS:CD2	2.38	0.41
1:A:511:ARG:HD3	1:A:513:ASP:OD1	2.19	0.41
1:A:411:THR:HB	1:A:413:TYR:CE1	2.55	0.41
1:A:94:LYS:HA	1:A:95:PRO:HD3	1.89	0.41
1:A:731:LEU:HD11	1:A:755:GLU:HG2	2.02	0.41
1:A:628:LEU:HD13	1:A:685:VAL:HG22	2.04	0.40
1:A:84:TRP:C	1:A:86:ARG:H	2.24	0.40
1:A:385:ILE:O	1:A:388:TRP:HB3	2.21	0.40
1:A:563:SER:HA	1:A:564:PRO:HD3	1.95	0.40
1:A:289:LEU:HD11	1:A:455:THR:HG21	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	755/852 (89%)	705 (93%)	37 (5%)	13 (2%)	11 50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	767	ALA
1	A	221	PRO
1	A	473	MET
1	A	607	SER
1	A	609	LYS
1	A	94	LYS
1	A	472	ILE
1	A	605	ASN
1	A	239	VAL
1	A	420	GLY
1	A	84	TRP
1	A	630	GLY

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	626/730 (86%)	599 (96%)	27 (4%)	35 74

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	30	GLU
1	A	46	SER
1	A	65	ARG
1	A	67	LEU
1	A	73	TYR
1	A	145	ASN
1	A	251	LYS
1	A	253	ASN
1	A	296	LYS
1	A	300	LYS
1	A	302	LYS
1	A	352	THR
1	A	398	LEU

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Mol	Chain	Res	Type
1	A	399	VAL
1	A	407	VAL
1	A	455	THR
1	A	529	LYS
1	A	606	LYS
1	A	668	GLU
1	A	684	THR
1	A	707	PRO
1	A	757	LEU
1	A	789	VAL
1	A	794	LEU
1	A	797	THR
1	A	802	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	172	GLN
1	A	204	GLN
1	A	299	ASN
1	A	336	ASN
1	A	376	ASN
1	A	428	HIS
1	A	476	GLN
1	A	482	GLN
1	A	494	HIS
1	A	503	GLN
1	A	616	GLN

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

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

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 ⓘ

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	765/852 (89%)	-0.11	31 (4%) 41 25	51, 62, 80, 89	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	ASN	5.0
1	A	608	LEU	4.8
1	A	607	SER	4.7
1	A	28	VAL	4.4
1	A	238	ASP	4.4
1	A	237	GLY	4.3
1	A	219	ASP	4.2
1	A	27	ASP	4.1
1	A	766	ASP	4.0
1	A	240	ASP	3.9
1	A	88	ILE	3.7
1	A	87	GLN	3.4
1	A	609	LYS	3.4
1	A	487	ALA	3.4
1	A	218	ASP	3.4
1	A	29	GLU	3.2
1	A	605	ASN	3.1
1	A	612	VAL	3.1
1	A	221	PRO	2.9
1	A	296	LYS	2.8
1	A	235	LEU	2.7
1	A	104	GLN	2.7
1	A	86	ARG	2.6
1	A	762	PRO	2.5
1	A	220	LYS	2.4
1	A	790	ALA	2.4
1	A	767	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	610	SER	2.2
1	A	604	GLU	2.1
1	A	239	VAL	2.1
1	A	103	ASP	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	848	1/1	0.94	0.48	9.28	86,86,86,86	0
2	MG	A	846	1/1	0.57	0.44	3.18	71,71,71,71	0
2	MG	A	847	1/1	0.86	0.57	1.79	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.