



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:39 PM UTC

PDB ID : 2R70 / pdb_00002r70
Title : Crystal structure of infectious bursal disease virus VP1 polymerase, cocrystallized with an oligopeptide mimicking the VP3 C-terminus.
Authors : Garriga, D.; Navarro, A.; Querol-Audi, J.; Abaitua, F.; Rodriguez, J.F.; Verdaguier, N.
Deposited on : 2007-09-07
Resolution : 2.70 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

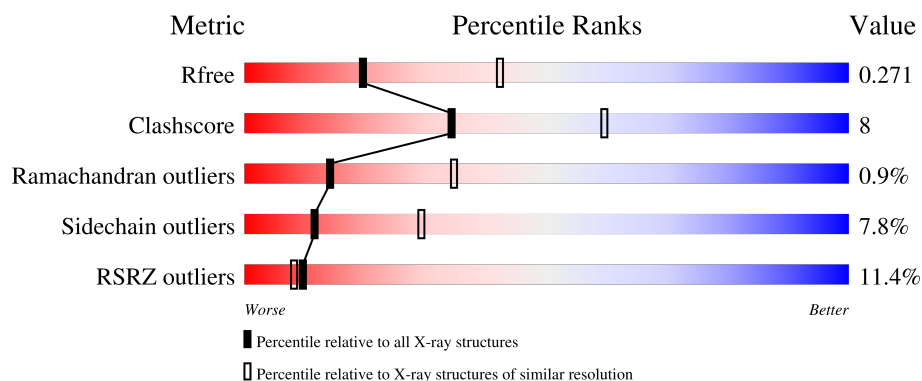
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	852	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5990 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 VIRUS VP1 POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	752	Total	C	N	O	S	0	0	0
			5853	3747	994	1090	22			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	137	Total	O	0	0
			137	137		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.80Å 123.80Å 361.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.9 (40.00-2.70) 93.9 (40.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.256 0.242 , 0.271	Depositor DCC
R_{free} test set	2195 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5990	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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](#)

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	0.56	0/5988	0.88	8/8136 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	LYS	N-CA-C	-9.98	101.19	113.97
1	A	302	LYS	N-CA-C	9.35	121.55	111.36
1	A	486	ASN	N-CA-C	7.44	119.92	110.33
1	A	634	TYR	CA-C-N	7.36	129.04	119.84
1	A	634	TYR	C-N-CA	7.36	129.04	119.84
1	A	323	GLU	N-CA-C	5.73	115.81	108.24
1	A	301	LYS	N-CA-C	5.69	120.21	113.16
1	A	362	ASN	N-CA-C	5.50	115.38	108.45

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	5853	0	5844	89	0
2	A	137	0	0	8	0
All	All	5990	0	5844	89	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 8.

All (89) 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:92:VAL:HG12	1:A:93:LEU:H	1.08	1.08
1:A:761:LYS:HB3	1:A:762:PRO:HA	1.42	1.02
1:A:92:VAL:HG12	1:A:93:LEU:N	1.72	1.01
1:A:595:CYS:SG	2:A:909:HOH:O	2.20	0.99
1:A:92:VAL:CG1	1:A:93:LEU:H	1.78	0.96
1:A:230:SER:HB2	1:A:279:ASN:HD21	1.33	0.94
1:A:85:MET:O	1:A:92:VAL:HG22	1.69	0.91
1:A:301:LYS:HG2	1:A:301:LYS:O	1.70	0.90
1:A:459:ASN:O	1:A:797:THR:HG21	1.81	0.79
1:A:229:PRO:HG3	1:A:350:MET:HE1	1.66	0.78
1:A:356:MET:CE	1:A:356:MET:HA	2.17	0.74
1:A:401:ALA:H	1:A:494:HIS:HD2	1.37	0.73
1:A:319:PHE:HD2	2:A:979:HOH:O	1.72	0.71
1:A:350:MET:HE3	1:A:453:TRP:HH2	1.56	0.70
1:A:704:VAL:HG21	1:A:708:VAL:HG22	1.74	0.69
1:A:482:GLN:HG2	1:A:486:ASN:HD21	1.56	0.69
1:A:296:LYS:NZ	2:A:937:HOH:O	2.25	0.68
1:A:761:LYS:HB3	1:A:762:PRO:CA	2.22	0.67
1:A:356:MET:HA	1:A:356:MET:HE2	1.77	0.67
1:A:589:ASP:HB3	1:A:592:ARG:HD2	1.77	0.66
1:A:600:PRO:HB3	1:A:622:ARG:HD2	1.77	0.65
1:A:319:PHE:CD2	2:A:979:HOH:O	2.48	0.65
1:A:92:VAL:CG1	1:A:93:LEU:N	2.43	0.64
1:A:65:ARG:HH11	1:A:476:GLN:HE21	1.47	0.61
1:A:294:GLY:HA2	1:A:299:ASN:ND2	2.16	0.61
1:A:793:ALA:O	1:A:797:THR:HG22	2.00	0.61
1:A:299:ASN:O	1:A:745:GLN:OE1	2.20	0.60
1:A:224:PRO:HB3	1:A:448:MET:HG3	1.84	0.59
1:A:227:ARG:HB2	1:A:232:MET:HE2	1.84	0.59
1:A:294:GLY:CA	1:A:299:ASN:ND2	2.67	0.57
1:A:482:GLN:CG	1:A:486:ASN:HD21	2.17	0.57
1:A:321:LYS:HA	2:A:979:HOH:O	2.04	0.57
1:A:425:THR:H	1:A:428:HIS:HD2	1.52	0.57
1:A:75:THR:HG1	1:A:95:PRO:C	2.14	0.56
1:A:421:GLU:HA	2:A:883:HOH:O	2.05	0.56
1:A:482:GLN:HG2	1:A:486:ASN:ND2	2.20	0.56
1:A:482:GLN:NE2	2:A:883:HOH:O	2.40	0.55
1:A:170:MET:O	1:A:174:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:OG1	1:A:95:PRO:O	2.23	0.54
1:A:318:LEU:HD22	1:A:336:ASN:HB3	1.89	0.53
1:A:401:ALA:H	1:A:494:HIS:CD2	2.24	0.53
1:A:299:ASN:O	1:A:745:GLN:NE2	2.41	0.53
1:A:93:LEU:O	1:A:94:LYS:O	2.27	0.53
1:A:229:PRO:HG3	1:A:350:MET:CE	2.38	0.52
1:A:339:SER:HB3	2:A:904:HOH:O	2.09	0.52
1:A:356:MET:HA	1:A:356:MET:HE3	1.92	0.52
1:A:451:GLN:NE2	1:A:451:GLN:HA	2.25	0.52
1:A:761:LYS:HE3	1:A:761:LYS:HA	1.92	0.51
1:A:321:LYS:HD3	1:A:337:ILE:HD11	1.92	0.51
1:A:450:ASN:HB3	1:A:452:THR:H	1.76	0.51
1:A:427:GLN:HA	1:A:430:GLN:HG2	1.93	0.50
1:A:230:SER:HB2	1:A:279:ASN:ND2	2.14	0.49
1:A:462:PRO:HB2	1:A:794:LEU:HD21	1.94	0.49
1:A:75:THR:OG1	1:A:95:PRO:C	2.55	0.49
1:A:757:LEU:O	1:A:760:SER:HB3	2.13	0.49
1:A:180:LYS:HG3	1:A:480:TYR:CZ	2.48	0.49
1:A:65:ARG:HH11	1:A:476:GLN:NE2	2.11	0.48
1:A:364:LEU:HD21	1:A:385:ILE:HD12	1.96	0.47
1:A:300:LYS:HE3	1:A:300:LYS:HB2	1.69	0.47
1:A:65:ARG:HD3	1:A:476:GLN:HE22	1.79	0.47
1:A:776:LEU:O	1:A:780:LEU:HG	2.15	0.46
1:A:716:VAL:O	1:A:720:LEU:HB2	2.16	0.45
1:A:65:ARG:H	1:A:476:GLN:HE22	1.65	0.45
1:A:482:GLN:CD	1:A:486:ASN:HD21	2.24	0.45
1:A:133:GLN:NE2	1:A:643:ASN:HD22	2.15	0.45
1:A:382:LEU:HD22	1:A:585:VAL:C	2.43	0.44
1:A:274:MET:HE2	1:A:274:MET:HB3	1.93	0.44
1:A:229:PRO:HG2	1:A:278:SER:HB2	1.99	0.44
1:A:301:LYS:HE2	1:A:301:LYS:HB3	1.24	0.44
1:A:616:GLN:HB2	1:A:652:LEU:HD21	2.00	0.44
1:A:299:ASN:O	1:A:745:GLN:CD	2.60	0.44
1:A:425:THR:H	1:A:428:HIS:CD2	2.35	0.43
1:A:133:GLN:HE21	1:A:643:ASN:HD22	1.67	0.43
1:A:482:GLN:OE1	1:A:486:ASN:ND2	2.50	0.43
1:A:37:TRP:CG	1:A:327:LYS:HE2	2.53	0.43
1:A:300:LYS:O	1:A:304:LEU:HG	2.18	0.43
1:A:138:PHE:HB2	1:A:636:LEU:HD11	2.00	0.43
1:A:437:LEU:HD23	1:A:441:TRP:CD1	2.53	0.42
1:A:52:LYS:O	1:A:56:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LYS:O	1:A:301:LYS:CG	2.51	0.42
1:A:295:THR:HA	1:A:296:LYS:HA	1.77	0.42
1:A:164:TYR:HA	1:A:323:GLU:O	2.19	0.41
1:A:424:CYS:HB3	1:A:482:GLN:HB2	2.03	0.41
1:A:34:PRO:HG2	1:A:159:ILE:HG22	2.02	0.41
1:A:93:LEU:O	1:A:94:LYS:C	2.62	0.40
1:A:199:PHE:CE1	1:A:430:GLN:HG3	2.56	0.40
1:A:170:MET:HG3	1:A:331:LEU:O	2.22	0.40
1:A:346:LEU:O	1:A:350:MET:HG3	2.21	0.40
1:A:377:PRO:HG3	1:A:573:TRP:CE2	2.57	0.40

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	740/852 (87%)	708 (96%)	25 (3%)	7 (1%)	14	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	LYS
1	A	767	ALA
1	A	468	SER
1	A	803	ALA
1	A	94	LYS
1	A	295	THR
1	A	685	VAL

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	628/730 (86%)	579 (92%)	49 (8%)	11	29

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	65	ARG
1	A	120	LYS
1	A	145	ASN
1	A	157	GLN
1	A	179	MET
1	A	251	LYS
1	A	252	ILE
1	A	286	SER
1	A	296	LYS
1	A	298	SER
1	A	300	LYS
1	A	301	LYS
1	A	318	LEU
1	A	356	MET
1	A	358	ASN
1	A	382	LEU
1	A	385	ILE
1	A	398	LEU
1	A	399	VAL
1	A	407	VAL
1	A	426	ARG
1	A	439	ARG
1	A	446	ASP
1	A	448	MET
1	A	451	GLN
1	A	455	THR
1	A	465	VAL
1	A	478	LYS
1	A	496	LEU

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Mol	Chain	Res	Type
1	A	501	LEU
1	A	523	LYS
1	A	532	ARG
1	A	560	GLU
1	A	562	SER
1	A	665	GLU
1	A	667	SER
1	A	700	LYS
1	A	704	VAL
1	A	706	ARG
1	A	718	ASN
1	A	720	LEU
1	A	741	ARG
1	A	761	LYS
1	A	772	ARG
1	A	777	SER
1	A	789	VAL
1	A	794	LEU
1	A	797	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	157	GLN
1	A	172	GLN
1	A	204	GLN
1	A	291	GLN
1	A	299	ASN
1	A	336	ASN
1	A	376	ASN
1	A	428	HIS
1	A	444	ASN
1	A	459	ASN
1	A	476	GLN
1	A	486	ASN
1	A	494	HIS
1	A	503	GLN
1	A	509	GLN
1	A	549	GLN
1	A	651	HIS
1	A	703	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](#)

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, 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	752/852 (88%)	0.72	86 (11%) 10 8	28, 46, 72, 94	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	VAL	7.5
1	A	86	ARG	7.1
1	A	88	ILE	6.8
1	A	604	GLU	5.4
1	A	28	VAL	5.1
1	A	236	THR	5.1
1	A	87	GLN	4.9
1	A	237	GLY	4.9
1	A	762	PRO	4.7
1	A	804	VAL	4.6
1	A	235	LEU	4.5
1	A	27	ASP	4.2
1	A	246	GLU	4.1
1	A	93	LEU	4.0
1	A	233	LEU	3.9
1	A	294	GLY	3.8
1	A	244	GLU	3.8
1	A	234	VAL	3.8
1	A	789	VAL	3.7
1	A	94	LYS	3.5
1	A	603	VAL	3.5
1	A	295	THR	3.4
1	A	766	ASP	3.4
1	A	85	MET	3.3
1	A	293	ALA	3.3
1	A	761	LYS	3.2
1	A	708	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	711	GLY	3.1
1	A	613	GLY	3.0
1	A	784	ASP	3.0
1	A	73	TYR	3.0
1	A	767	ALA	2.9
1	A	781	GLU	2.8
1	A	358	ASN	2.8
1	A	705	ASN	2.8
1	A	678	GLY	2.8
1	A	758	HIS	2.8
1	A	301	LYS	2.8
1	A	174	ASN	2.8
1	A	487	ALA	2.7
1	A	446	ASP	2.7
1	A	653	GLU	2.6
1	A	771	GLU	2.6
1	A	756	LYS	2.6
1	A	199	PHE	2.6
1	A	745	GLN	2.6
1	A	248	TYR	2.6
1	A	486	ASN	2.6
1	A	704	VAL	2.6
1	A	77	GLN	2.6
1	A	772	ARG	2.5
1	A	80	PRO	2.5
1	A	679	PHE	2.5
1	A	196	GLY	2.4
1	A	723	GLY	2.4
1	A	612	VAL	2.4
1	A	232	MET	2.4
1	A	450	ASN	2.4
1	A	245	VAL	2.4
1	A	179	MET	2.3
1	A	560	GLU	2.3
1	A	759	LYS	2.3
1	A	442	SER	2.3
1	A	319	PHE	2.3
1	A	754	ALA	2.3
1	A	522	ASP	2.3
1	A	707	PRO	2.3
1	A	485	GLY	2.3
1	A	299	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	444	ASN	2.2
1	A	724	ARG	2.2
1	A	76	ASP	2.2
1	A	783	ALA	2.2
1	A	229	PRO	2.2
1	A	746	ASP	2.2
1	A	490	PHE	2.2
1	A	726	ARG	2.2
1	A	84	TRP	2.1
1	A	379	ARG	2.1
1	A	251	LYS	2.1
1	A	727	ASN	2.1
1	A	731	LEU	2.1
1	A	119	GLU	2.1
1	A	722	THR	2.1
1	A	614	ILE	2.1
1	A	791	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.