



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:32 PM UTC

PDB ID : 2V8O / pdb_00002v8o
Title : Structure of the Murray Valley encephalitis virus RNA helicase to 1. 9A resolution
Authors : Mancini, E.J.; Assenberg, R.; Verma, A.; Walter, T.S.; Tuma, R.; Grimes, J.M.; Owens, R.J.; Stuart, D.I.
Deposited on : 2007-08-09
Resolution : 1.90 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

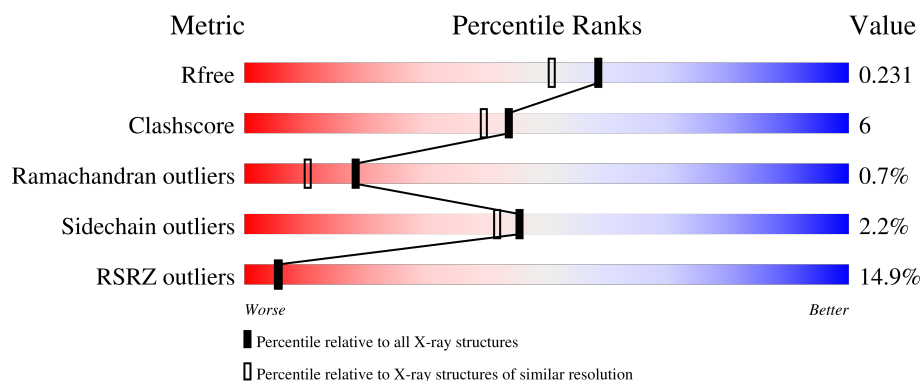
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	444	14% 84% 11% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3667 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 FLAVIVIRIN PROTEASE NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3383	2129	605	634	15			

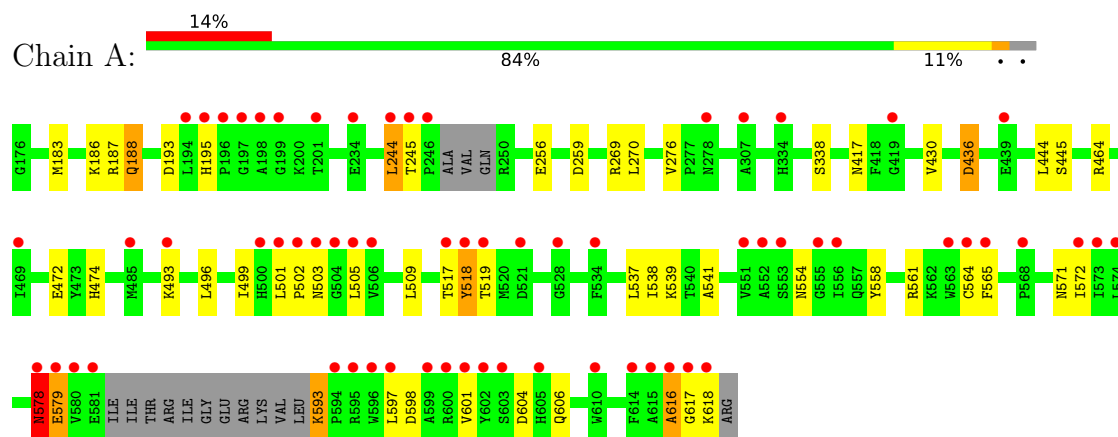
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	284	Total	O	0	0
			284	284		

3 Residue-property plots [i](#)

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: FLAVIVIRIN PROTEASE NS3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.52Å 76.41Å 70.61Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	70.53 – 1.90 70.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.53-1.90) 99.9 (70.53-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.223 0.188 , 0.231	Depositor DCC
R_{free} test set	1789 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3667	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 6.20% 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	0/3460	0.77	2/4693 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	436	ASP	N-CA-C	6.24	119.50	109.83
1	A	578	ASN	N-CA-C	5.03	121.52	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	ASP	Peptide
1	A	593	LYS	Peptide

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	3383	0	3338	41	0
2	A	284	0	0	1	0
All	All	3667	0	3338	41	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 6.

All (41) 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:616:ALA:HB3	1:A:617:GLY:HA3	1.42	1.02
1:A:417:ASN:HD22	1:A:464:ARG:HH12	1.05	0.96
1:A:616:ALA:CB	1:A:617:GLY:HA3	2.00	0.92
1:A:417:ASN:ND2	1:A:464:ARG:HH12	1.71	0.89
1:A:417:ASN:HD22	1:A:464:ARG:NH1	1.77	0.81
1:A:616:ALA:HB3	1:A:617:GLY:CA	2.21	0.69
1:A:564:CYS:O	1:A:593:LYS:CB	2.44	0.65
1:A:501:LEU:HD23	1:A:505:LEU:HB3	1.79	0.64
1:A:616:ALA:CB	1:A:617:GLY:CA	2.74	0.64
1:A:270:LEU:HD23	1:A:276:VAL:HG21	1.80	0.63
1:A:571:ASN:HA	1:A:597:LEU:HD11	1.80	0.63
1:A:517:THR:O	1:A:518:TYR:HB2	1.99	0.62
1:A:564:CYS:O	1:A:593:LYS:HB2	2.00	0.60
1:A:193:ASP:OD1	1:A:195:HIS:CE1	2.56	0.59
1:A:269:ARG:HG2	1:A:276:VAL:HG22	1.84	0.59
1:A:270:LEU:HB3	1:A:499:ILE:HG23	1.87	0.57
1:A:183:MET:HA	1:A:188:GLN:HG2	1.89	0.55
1:A:244:LEU:HD11	1:A:259:ASP:HB3	1.90	0.54
1:A:598:ASP:O	1:A:601:VAL:HG22	2.08	0.54
1:A:572:ILE:HG21	1:A:579:GLU:HG2	1.92	0.52
1:A:195:HIS:CE1	2:A:2021:HOH:O	2.63	0.52
1:A:244:LEU:CD1	1:A:259:ASP:HB3	2.41	0.52
1:A:564:CYS:O	1:A:593:LYS:HB3	2.09	0.52
1:A:472:GLU:OE1	1:A:474:HIS:HE1	1.93	0.51
1:A:430:VAL:HG13	1:A:445:SER:O	2.10	0.50
1:A:617:GLY:CA	1:A:618:LYS:C	2.83	0.50
1:A:244:LEU:N	1:A:244:LEU:HD12	2.28	0.48
1:A:417:ASN:ND2	1:A:464:ARG:NH1	2.47	0.48
1:A:565:PHE:HA	1:A:593:LYS:HB3	1.95	0.47
1:A:338:SER:OG	1:A:474:HIS:HD2	1.98	0.46
1:A:578:ASN:HB3	1:A:579:GLU:O	2.16	0.46
1:A:558:TYR:O	1:A:561:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LYS:HZ1	1:A:519:THR:HG23	1.81	0.45
1:A:430:VAL:CG1	1:A:444:LEU:HB3	2.48	0.43
1:A:186:LYS:O	1:A:187:ARG:HB2	2.19	0.42
1:A:496:LEU:HD22	1:A:509:LEU:HD23	2.01	0.42
1:A:493:LYS:NZ	1:A:519:THR:HG23	2.35	0.41
1:A:537:LEU:O	1:A:541:ALA:HB3	2.20	0.41
1:A:538:ILE:HG13	1:A:539:LYS:N	2.36	0.41
1:A:604:ASP:OD1	1:A:606:GLN:HG2	2.22	0.40
1:A:617:GLY:HA3	1:A:618:LYS:C	2.46	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	423/444 (95%)	405 (96%)	15 (4%)	3 (1%)	18	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	PRO
1	A	616	ALA
1	A	518	TYR

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	360/373 (96%)	352 (98%)	8 (2%)	45	42

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

Mol	Chain	Res	Type
1	A	188	GLN
1	A	244	LEU
1	A	245	THR
1	A	256	GLU
1	A	503	ASN
1	A	554	ASN
1	A	578	ASN
1	A	579	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	195	HIS
1	A	280	ASN
1	A	334	HIS
1	A	417	ASN
1	A	474	HIS
1	A	554	ASN
1	A	559	ASN
1	A	578	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 oligosaccharides 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 ⓘ

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	429/444 (96%)	0.86	64 (14%) 5 6	31, 42, 78, 100	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	ALA	5.0
1	A	563	TRP	4.4
1	A	500	HIS	4.2
1	A	580	VAL	4.0
1	A	485	MET	3.9
1	A	195	HIS	3.9
1	A	596	TRP	3.9
1	A	616	ALA	3.9
1	A	617	GLY	3.9
1	A	197	GLY	3.7
1	A	594	PRO	3.6
1	A	574	LEU	3.6
1	A	196	PRO	3.5
1	A	599	ALA	3.5
1	A	519	THR	3.4
1	A	618	LYS	3.4
1	A	556	ILE	3.4
1	A	501	LEU	3.4
1	A	602	TYR	3.3
1	A	568	PRO	3.3
1	A	246	PRO	3.3
1	A	565	PHE	3.3
1	A	597	LEU	3.2
1	A	505	LEU	3.1
1	A	504	GLY	3.0
1	A	551	VAL	3.0
1	A	573	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	601	VAL	2.9
1	A	502	PRO	2.9
1	A	572	ILE	2.8
1	A	194	LEU	2.8
1	A	518	TYR	2.7
1	A	199	GLY	2.7
1	A	603	SER	2.7
1	A	521	ASP	2.7
1	A	307	ALA	2.6
1	A	579	GLU	2.6
1	A	503	ASN	2.6
1	A	564	CYS	2.5
1	A	614	PHE	2.4
1	A	615	ALA	2.4
1	A	334	HIS	2.4
1	A	555	GLY	2.4
1	A	517	THR	2.4
1	A	278	ASN	2.3
1	A	245	THR	2.3
1	A	553	SER	2.2
1	A	534	PHE	2.2
1	A	506	VAL	2.2
1	A	201	THR	2.2
1	A	595	ARG	2.2
1	A	493	LYS	2.1
1	A	234	GLU	2.1
1	A	605	HIS	2.1
1	A	578	ASN	2.1
1	A	610	TRP	2.1
1	A	244	LEU	2.1
1	A	581	GLU	2.0
1	A	419	GLY	2.0
1	A	528	GLY	2.0
1	A	552	ALA	2.0
1	A	439	GLU	2.0
1	A	469	ILE	2.0
1	A	600	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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.