



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:18 AM UTC

PDB ID : 6J00 / pdb_00006j00
Title : The RNA-dependent RNA polymerase domain of dengue 3 NS5
Authors : Shimizu, H.; Sekine, S.
Deposited on : 2018-12-20
Resolution : 2.14 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

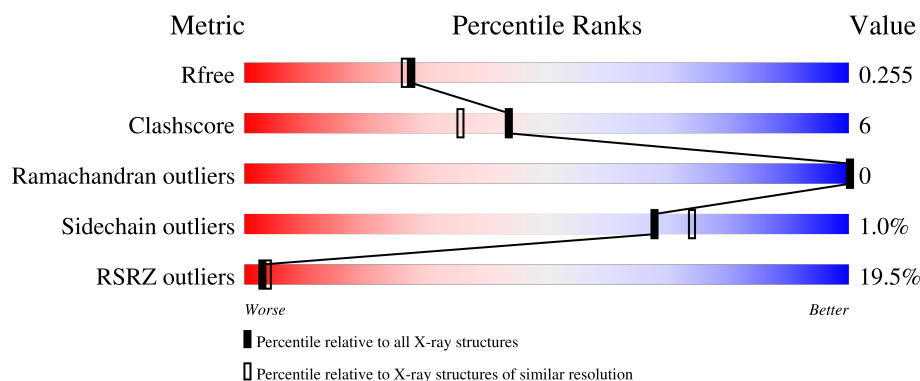
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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 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	647	17% 77% 12% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4905 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4678	2949	839	859	31			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

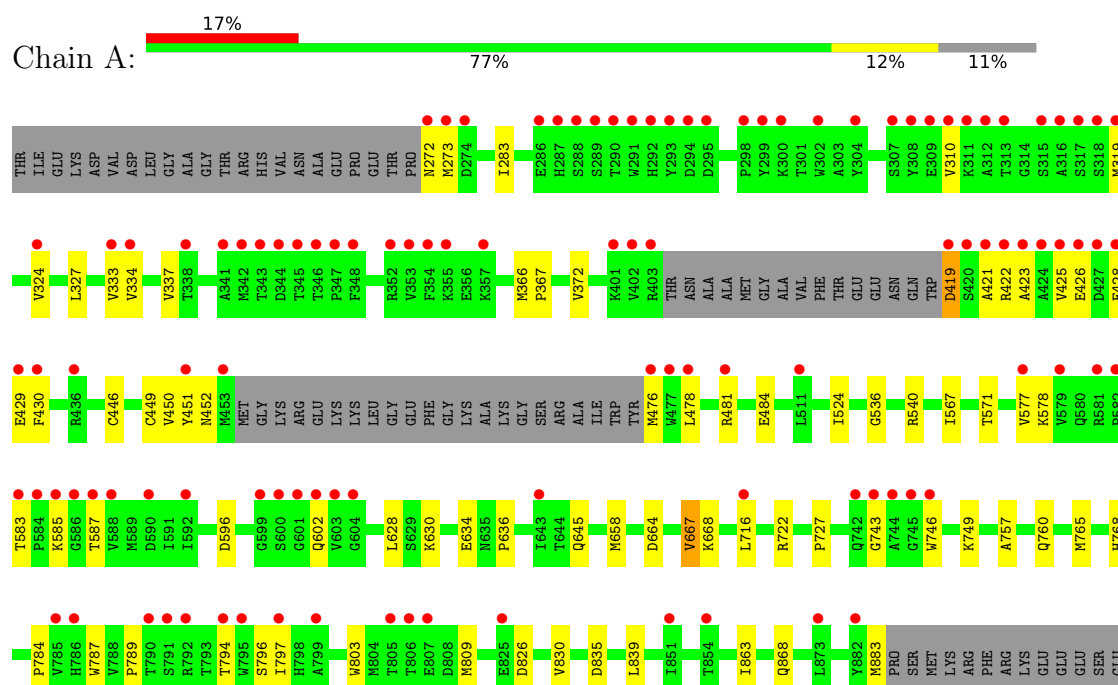
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	225	Total	O	0	0
			225	225		

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: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	161.52Å 177.36Å 58.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.52 – 2.14 51.52 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.8 (51.52-2.14) 99.8 (51.52-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.219 , 0.250 0.232 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4905	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

5.1 Standard geometry

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

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	0.13	0/4794	0.33	0/6488

There are no bond length outliers.

There are no bond angle outliers.

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	4678	0	4579	56	0
2	A	2	0	0	0	0
3	A	225	0	0	5	0
All	All	4905	0	4579	56	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 (56) 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:645:GLN:NE2	3:A:1001:HOH:O	1.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:MET:HE1	1:A:746:TRP:HD1	1.43	0.82
1:A:743:GLY:HA3	1:A:746:TRP:HZ2	1.52	0.74
1:A:883:MET:O	3:A:1002:HOH:O	2.07	0.73
1:A:596:ASP:OD2	3:A:1003:HOH:O	2.08	0.70
1:A:664:ASP:OD1	3:A:1004:HOH:O	2.10	0.70
1:A:421:ALA:HB1	1:A:425:VAL:HG11	1.73	0.69
1:A:422:ARG:HG3	1:A:423:ALA:H	1.56	0.69
1:A:868:GLN:NE2	3:A:1008:HOH:O	2.27	0.66
1:A:743:GLY:HA3	1:A:746:TRP:CZ2	2.33	0.64
1:A:583:THR:HG23	1:A:585:LYS:H	1.62	0.64
1:A:794:THR:HG22	1:A:796:SER:HB3	1.82	0.61
1:A:630:LYS:O	1:A:634:GLU:HG3	2.00	0.61
1:A:452:ASN:ND2	1:A:578:LYS:HB2	2.19	0.58
1:A:760:GLN:NE2	1:A:803:TRP:O	2.36	0.58
1:A:425:VAL:O	1:A:430:PHE:CD1	2.59	0.56
1:A:797:ILE:H	1:A:797:ILE:HD12	1.71	0.55
1:A:727:PRO:HG3	1:A:765:MET:HE3	1.89	0.55
1:A:283:ILE:HD11	1:A:450:VAL:HG11	1.89	0.54
1:A:419:ASP:OD1	1:A:419:ASP:N	2.40	0.54
1:A:722:ARG:HD3	1:A:826:ASP:HB3	1.91	0.53
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.91	0.51
1:A:451:TYR:HB3	1:A:577:VAL:HG22	1.93	0.51
1:A:366:MET:HE1	1:A:634:GLU:HG2	1.93	0.50
1:A:757:ALA:HB2	1:A:789:PRO:HB3	1.93	0.50
1:A:452:ASN:HD21	1:A:578:LYS:HE2	1.75	0.50
1:A:425:VAL:HG21	1:A:478:LEU:HD23	1.93	0.50
1:A:658:MET:HG2	1:A:667:VAL:HB	1.96	0.48
1:A:333:VAL:HG12	1:A:333:VAL:O	2.13	0.48
1:A:452:ASN:HD21	1:A:578:LYS:CE	2.27	0.48
1:A:422:ARG:CG	1:A:423:ALA:H	2.22	0.48
1:A:452:ASN:HD21	1:A:578:LYS:HB2	1.79	0.48
1:A:421:ALA:HB3	1:A:478:LEU:HB2	1.95	0.48
1:A:863:ILE:HG21	1:A:883:MET:HE2	1.97	0.47
1:A:476:MET:HE3	1:A:481:ARG:HG3	1.97	0.47
1:A:743:GLY:C	1:A:746:TRP:HE1	2.22	0.47
1:A:749:LYS:HD2	1:A:787:TRP:CE2	2.51	0.46
1:A:334:VAL:HG12	1:A:337:VAL:H	1.81	0.46
1:A:272:ASN:HB3	1:A:273:MET:H	1.67	0.44
1:A:536:GLY:O	1:A:540:ARG:HG2	2.17	0.44
1:A:484:GLU:OE2	1:A:602:GLN:HB3	2.18	0.44
1:A:716:LEU:HD21	1:A:839:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:MET:HE1	1:A:746:TRP:CD1	2.35	0.43
1:A:372:VAL:HG21	1:A:628:LEU:HD11	1.99	0.43
1:A:524:ILE:O	1:A:668:LYS:NZ	2.38	0.43
1:A:830:VAL:HG13	1:A:835:ASP:HB2	2.01	0.42
1:A:446:CYS:SG	1:A:449:CYS:HB2	2.59	0.42
1:A:567:ILE:O	1:A:571:THR:HB	2.20	0.42
1:A:768:HIS:CD2	1:A:768:HIS:H	2.38	0.41
1:A:428:GLU:OE1	1:A:429:GLU:N	2.53	0.41
1:A:784:PRO:HG2	1:A:787:TRP:CE2	2.55	0.41
1:A:422:ARG:HG3	1:A:423:ALA:N	2.31	0.41
1:A:426:GLU:H	1:A:426:GLU:CD	2.22	0.41
1:A:367:PRO:HB2	1:A:636:PRO:HA	2.03	0.41
1:A:310:VAL:O	1:A:587:THR:HB	2.20	0.40
1:A:426:GLU:OE1	1:A:426:GLU:N	2.34	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	569/647 (88%)	544 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	503/561 (90%)	498 (99%)	5 (1%)	68 74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	VAL
1	A	327	LEU
1	A	419	ASP
1	A	667	VAL
1	A	809	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	A	452	ASN
1	A	492	ASN
1	A	562	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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	575/647 (88%)	1.06	112 (19%) 3 4	26, 43, 94, 117	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	VAL	7.8
1	A	423	ALA	6.6
1	A	312	ALA	6.5
1	A	421	ALA	6.2
1	A	476	MET	6.0
1	A	333	VAL	5.8
1	A	794	THR	5.8
1	A	603	VAL	5.6
1	A	795	TRP	5.5
1	A	310	VAL	5.4
1	A	430	PHE	5.3
1	A	316	ALA	5.1
1	A	420	SER	4.9
1	A	422	ARG	4.8
1	A	426	GLU	4.8
1	A	451	TYR	4.7
1	A	348	PHE	4.7
1	A	343	THR	4.6
1	A	584	PRO	4.6
1	A	425	VAL	4.5
1	A	746	TRP	4.4
1	A	477	TRP	4.4
1	A	797	ILE	4.2
1	A	805	THR	4.2
1	A	293	TYR	4.1
1	A	579	VAL	4.1
1	A	588	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	311	LYS	4.0
1	A	601	GLY	3.9
1	A	274	ASP	3.9
1	A	453	MET	3.9
1	A	300	LYS	3.8
1	A	272	ASN	3.6
1	A	315	SER	3.6
1	A	318	SER	3.5
1	A	347	PRO	3.5
1	A	742	GLN	3.5
1	A	424	ALA	3.4
1	A	292	HIS	3.4
1	A	744	ALA	3.4
1	A	582	PRO	3.4
1	A	354	PHE	3.4
1	A	786	HIS	3.3
1	A	294	ASP	3.3
1	A	317	SER	3.2
1	A	341	ALA	3.2
1	A	342	MET	3.0
1	A	791	SER	3.0
1	A	403	ARG	3.0
1	A	402	VAL	3.0
1	A	604	GLY	3.0
1	A	299	TYR	2.9
1	A	743	GLY	2.9
1	A	345	THR	2.9
1	A	481	ARG	2.9
1	A	308	TYR	2.9
1	A	745	GLY	2.9
1	A	352	ARG	2.8
1	A	334	VAL	2.8
1	A	346	THR	2.7
1	A	790	THR	2.7
1	A	586	GLY	2.7
1	A	289	SER	2.7
1	A	290	THR	2.6
1	A	291	TRP	2.6
1	A	298	PRO	2.6
1	A	590	ASP	2.6
1	A	792	ARG	2.6
1	A	599	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	287	HIS	2.5
1	A	592	ILE	2.5
1	A	304	TYR	2.5
1	A	286	GLU	2.5
1	A	288	SER	2.5
1	A	313	THR	2.5
1	A	873	LEU	2.5
1	A	344	ASP	2.4
1	A	825	GLU	2.4
1	A	585	LYS	2.4
1	A	273	MET	2.4
1	A	401	LYS	2.4
1	A	587	THR	2.4
1	A	419	ASP	2.3
1	A	600	SER	2.3
1	A	309	GLU	2.3
1	A	785	VAL	2.3
1	A	295	ASP	2.3
1	A	355	LYS	2.3
1	A	338	THR	2.2
1	A	324	VAL	2.2
1	A	807	GLU	2.2
1	A	602	GLN	2.2
1	A	882	TYR	2.2
1	A	854	THR	2.2
1	A	428	GLU	2.1
1	A	716	LEU	2.1
1	A	806	THR	2.1
1	A	581	ARG	2.1
1	A	799	ALA	2.1
1	A	307	SER	2.1
1	A	478	LEU	2.1
1	A	319	MET	2.1
1	A	583	THR	2.1
1	A	851	ILE	2.1
1	A	577	VAL	2.1
1	A	357	LYS	2.1
1	A	427	ASP	2.1
1	A	643	ILE	2.1
1	A	302	TRP	2.1
1	A	511	LEU	2.0
1	A	429	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	436	ARG	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(Å ²)	Q<0.9
2	ZN	A	901	1/1	0.98	0.14	20,20,20,20	0
2	ZN	A	902	1/1	0.99	0.15	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.