



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:35 PM UTC

PDB ID : 5HN0 / pdb_00005hn0
Title : Dengue serotype 3 RNA-dependent RNA polymerase bound to compound 4
Authors : Noble, C.G.
Deposited on : 2016-01-17
Resolution : 2.05 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

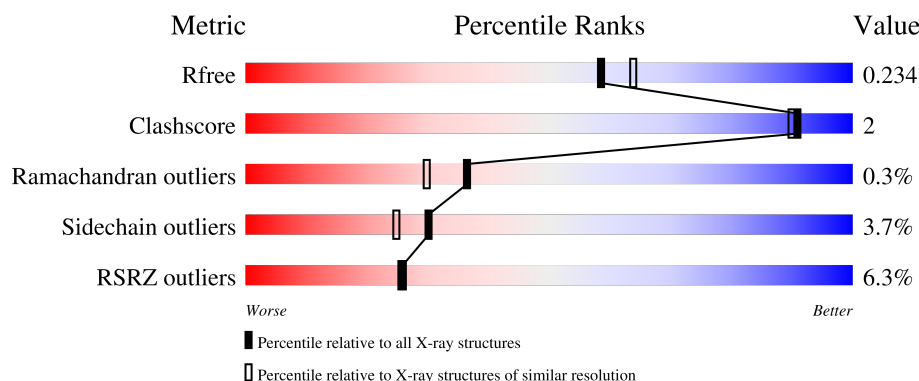
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	635	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5219 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 RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	1	0
			4769	3011	856	871	31			

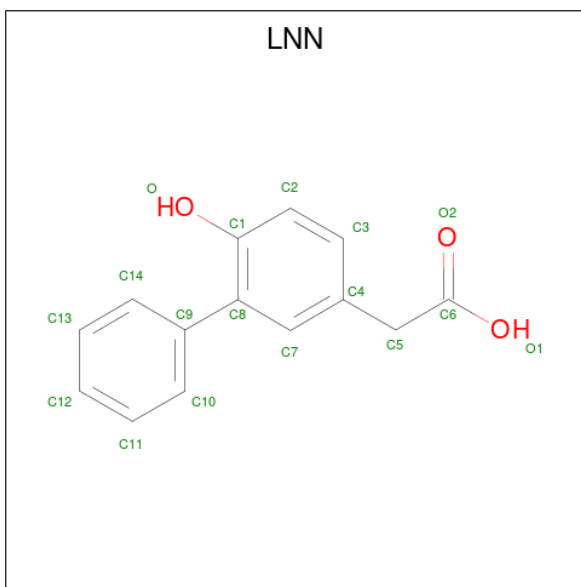
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLY	-	expression tag	UNP Q6DLV0
A	267	SER	-	expression tag	UNP Q6DLV0
A	268	HIS	-	expression tag	UNP Q6DLV0
A	269	MET	-	expression tag	UNP Q6DLV0
A	270	LEU	-	expression tag	UNP Q6DLV0
A	271	ASP	-	expression tag	UNP Q6DLV0
A	374	GLU	GLY	variant	UNP Q6DLV0

- 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 (6-hydroxybiphenyl-3-yl)acetic acid (CCD ID: LNN) (formula: C₁₄H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	14	3		

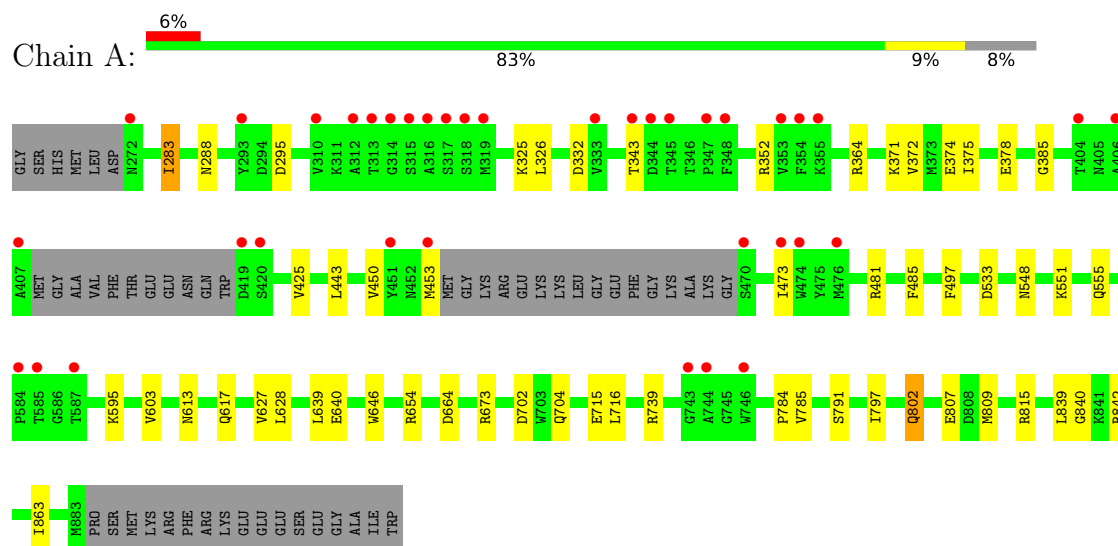
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	431	Total	O	0	0
			431	431		

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: RNA-directed RNA polymerase NS5



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	161.40Å 177.85Å 57.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.66 – 2.05 20.66 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.66-2.05) 99.9 (20.66-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.06Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.181 , 0.227 0.188 , 0.234	Depositor DCC
R_{free} test set	2676 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5219	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: LNN, 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	0.84	2/4893 (0.0%)	1.23	12/6627 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	809	MET	SD-CE	-5.65	1.65	1.79
1	A	863	ILE	CA-C	5.12	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	863	ILE	N-CA-CB	6.16	114.38	110.50
1	A	332	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	497	PHE	CA-CB-CG	-5.69	108.11	113.80
1	A	702	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	673	ARG	CA-C-N	5.55	127.98	120.38
1	A	673	ARG	C-N-CA	5.55	127.98	120.38
1	A	332	ASP	N-CA-C	-5.23	105.75	111.82
1	A	784	PRO	CA-C-N	5.07	127.68	120.53
1	A	784	PRO	C-N-CA	5.07	127.68	120.53
1	A	283	ILE	CA-C-N	5.05	127.01	120.44
1	A	283	ILE	C-N-CA	5.05	127.01	120.44
1	A	840	GLY	N-CA-C	-5.02	105.49	111.36

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	4769	0	4661	16	0
2	A	2	0	0	0	0
3	A	17	0	0	0	0
4	A	431	0	0	0	0
All	All	5219	0	4661	16	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 2.

All (16) 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:802:GLN:H	1:A:802:GLN:HE21	1.21	0.84
1:A:716:LEU:HD21	1:A:839:LEU:HD23	1.70	0.73
1:A:385:GLY:HA3	1:A:555:GLN:HE22	1.71	0.56
1:A:378:GLU:HG2	1:A:551:LYS:HD3	1.92	0.52
1:A:283:ILE:HD11	1:A:450:VAL:HG21	1.95	0.48
1:A:372:VAL:HG11	1:A:628:LEU:HD11	1.95	0.48
1:A:375:ILE:HD11	1:A:640:GLU:HG2	1.97	0.47
1:A:704:GLN:NE2	1:A:715:GLU:H	2.13	0.46
1:A:325:LYS:HG3	1:A:739:ARG:NH2	2.31	0.45
1:A:374:GLU:O	1:A:378:GLU:HG3	2.17	0.45
1:A:627:VAL:HG21	1:A:646:TRP:CD1	2.51	0.45
1:A:613:ASN:O	1:A:617:GLN:HG2	2.18	0.44
1:A:807:GLU:CD	1:A:815:ARG:HH22	2.27	0.42
1:A:548:ASN:HD22	1:A:551:LYS:HE2	1.84	0.42
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.55	0.42
1:A:485:PHE:HA	1:A:603:VAL:HG11	2.03	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	580/635 (91%)	565 (97%)	13 (2%)	2 (0%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	791	SER

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	511/552 (93%)	492 (96%)	19 (4%)	30	25

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	295	ASP
1	A	326	LEU
1	A	352	ARG
1	A	364	ARG
1	A	371	LYS
1	A	425	VAL
1	A	443	LEU
1	A	453	MET

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Mol	Chain	Res	Type
1	A	473	ILE
1	A	481	ARG
1	A	533	ASP
1	A	595	LYS
1	A	639	LEU
1	A	664	ASP
1	A	785	VAL
1	A	797	ILE
1	A	802	GLN
1	A	842	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	ASN
1	A	548	ASN
1	A	555	GLN
1	A	562	GLN
1	A	573	GLN
1	A	617	GLN
1	A	621	GLN
1	A	682	ASN
1	A	693	GLN
1	A	704	GLN
1	A	768	HIS
1	A	802	GLN
1	A	835	ASN
1	A	869	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	LNN	A	1003	-	18,18,18	1.19	1 (5%)	24,24,24	0.92	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LNN	A	1003	-	-	0/8/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	LNN	C8-C1	3.65	1.50	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	LNN	C9-C8-C1	-2.16	120.30	122.31

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	585/635 (92%)	0.04	37 (6%) 26 26	18, 36, 86, 112	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	VAL	4.8
1	A	473	ILE	4.1
1	A	343	THR	4.1
1	A	407	ALA	3.8
1	A	585	THR	3.4
1	A	347	PRO	3.3
1	A	345	THR	3.3
1	A	354	PHE	3.3
1	A	406	ALA	3.3
1	A	313	THR	3.1
1	A	312	ALA	3.1
1	A	348	PHE	3.0
1	A	584	PRO	3.0
1	A	453	MET	2.9
1	A	315	SER	2.8
1	A	318	SER	2.8
1	A	451	TYR	2.8
1	A	746	TRP	2.6
1	A	476	MET	2.6
1	A	316	ALA	2.6
1	A	743	GLY	2.5
1	A	744	ALA	2.5
1	A	420	SER	2.4
1	A	474	TRP	2.4
1	A	333	VAL	2.4
1	A	355	LYS	2.4
1	A	470	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	587	THR	2.3
1	A	293	TYR	2.3
1	A	344	ASP	2.3
1	A	404	THR	2.3
1	A	419	ASP	2.3
1	A	314	GLY	2.2
1	A	317	SER	2.2
1	A	310	VAL	2.1
1	A	319	MET	2.0
1	A	272	ASN	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
3	LNN	A	1003	17/17	0.88	0.10	46,49,51,51	0
2	ZN	A	1002	1/1	0.99	0.03	41,41,41,41	0
2	ZN	A	1001	1/1	1.00	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.