



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1YKS / pdb_00001yks
Title : Crystal structure of yellow fever virus NS3 helicase
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Deposited on : 2005-01-18
Resolution : 1.80 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

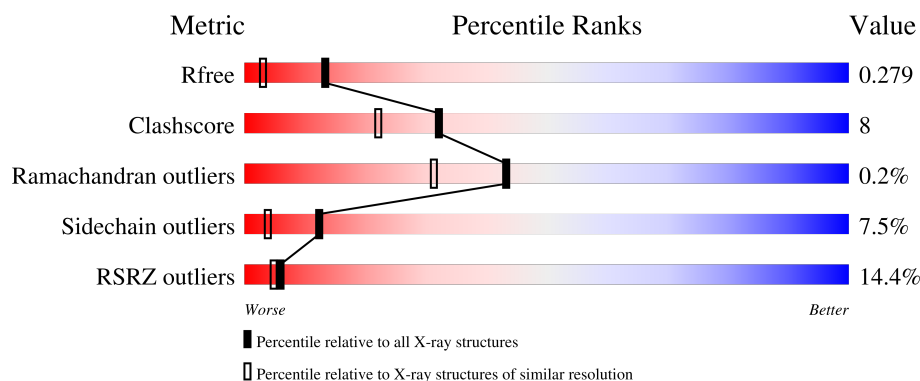
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	440	14% 80% 15% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3643 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 [contains: Flavivirin protease NS3 catalytic subunit].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3382	2115	626	619	22			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLY	-	cloning artifact	UNP P19901
A	185	SER	-	cloning artifact	UNP P19901
A	186	HIS	-	cloning artifact	UNP P19901

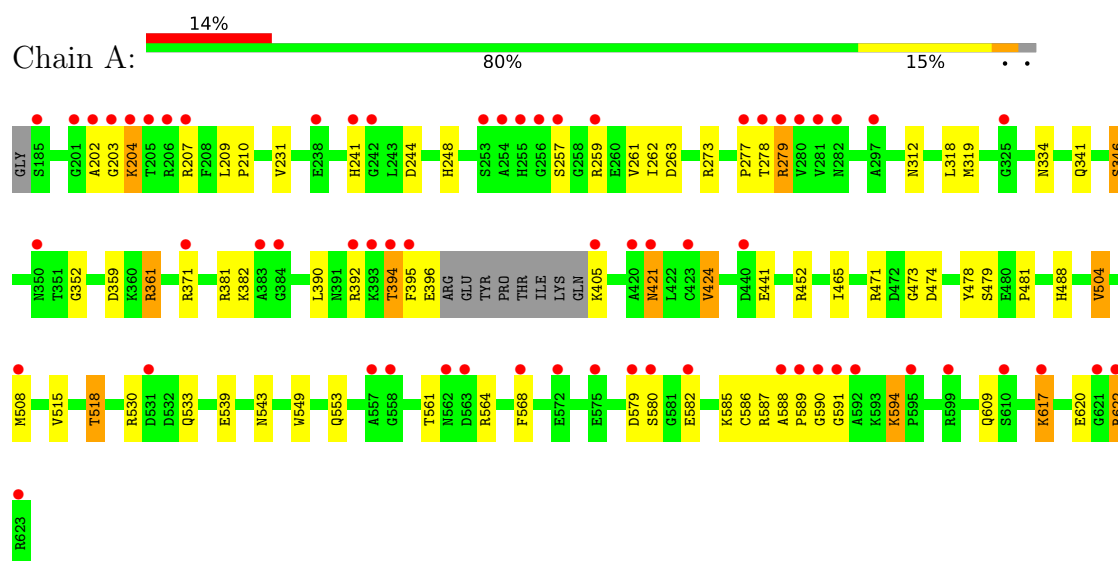
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	261	Total	O	0	0
			261	261		

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 polyprotein [contains: Flavivirin protease NS3 catalytic subunit]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.02Å 43.80Å 93.07Å 90.00° 104.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.80) 97.6 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.193 , 0.238 0.251 , 0.279	Depositor DCC
R_{free} test set	1994 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 54.7	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	3643	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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	0.70	1/3458 (0.0%)	0.89	4/4678 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	MET	SD-CE	-6.22	1.64	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ARG	N-CA-C	5.66	117.94	107.99
1	A	352	GLY	N-CA-C	5.38	122.74	115.32
1	A	590	GLY	N-CA-C	-5.10	107.50	114.64
1	A	346	SER	N-CA-C	-5.06	106.51	113.30

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	3382	0	3357	54	0
2	A	261	0	0	12	0
All	All	3643	0	3357	54	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 (54) 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:508:MET:SD	2:A:839:HOH:O	2.35	0.84
1:A:204:LYS:HD2	2:A:809:HOH:O	1.82	0.80
1:A:564:ARG:HH22	1:A:622:ARG:HH21	1.27	0.78
1:A:568:PHE:CE1	1:A:588:ALA:HA	2.19	0.78
1:A:568:PHE:CZ	1:A:588:ALA:HA	2.19	0.77
1:A:203:GLY:O	1:A:207:ARG:HB2	1.85	0.77
1:A:479:SER:HB3	2:A:802:HOH:O	1.90	0.70
1:A:421:ASN:H	1:A:421:ASN:HD22	1.40	0.69
1:A:504:VAL:HG21	2:A:875:HOH:O	1.94	0.68
1:A:568:PHE:CZ	1:A:588:ALA:CA	2.80	0.64
1:A:539:GLU:HG2	1:A:561:THR:HG21	1.79	0.63
1:A:346:SER:HB2	2:A:807:HOH:O	1.98	0.62
1:A:361:ARG:NH2	1:A:473:GLY:O	2.32	0.62
1:A:568:PHE:CE2	1:A:588:ALA:HB2	2.36	0.61
1:A:202:ALA:HB2	1:A:334:ASN:HD21	1.66	0.60
1:A:488:HIS:H	1:A:488:HIS:CD2	2.19	0.60
1:A:394:THR:HG22	1:A:395:PHE:HD2	1.66	0.58
1:A:421:ASN:H	1:A:421:ASN:ND2	2.02	0.58
1:A:539:GLU:CD	1:A:543:ASN:HD22	2.17	0.52
1:A:381:ARG:HD3	2:A:674:HOH:O	2.08	0.52
1:A:515:VAL:O	1:A:518:THR:HB	2.10	0.52
1:A:424:VAL:HG12	1:A:465:ILE:CG2	2.41	0.51
1:A:568:PHE:CD2	1:A:588:ALA:HB2	2.46	0.51
1:A:371:ARG:NE	2:A:769:HOH:O	2.44	0.50
1:A:568:PHE:CD2	1:A:594:LYS:HB2	2.47	0.50
1:A:549:TRP:O	1:A:553:GLN:HG2	2.12	0.49
1:A:278:THR:OG1	2:A:866:HOH:O	2.20	0.49
1:A:471:ARG:HD2	1:A:474:ASP:OD1	2.14	0.48
1:A:277:PRO:HD3	2:A:832:HOH:O	2.13	0.48
1:A:209:LEU:HB3	1:A:210:PRO:HD3	1.95	0.47
1:A:588:ALA:HB1	1:A:589:PRO:CD	2.45	0.47
1:A:568:PHE:CZ	1:A:588:ALA:HB2	2.50	0.47
1:A:568:PHE:CE1	1:A:588:ALA:CA	2.95	0.46
1:A:248:HIS:HE1	1:A:263:ASP:OD1	1.98	0.46
1:A:359:ASP:OD1	1:A:361:ARG:HD3	2.16	0.46
1:A:587:ARG:HG3	1:A:591:GLY:HA2	1.98	0.45
1:A:530:ARG:HG2	1:A:533:GLN:OE1	2.16	0.45
1:A:568:PHE:CE1	1:A:588:ALA:CB	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HG13	1:A:262:ILE:HG13	2.00	0.44
1:A:588:ALA:HB1	1:A:589:PRO:HD2	2.00	0.43
1:A:341:GLN:HG3	1:A:478:TYR:CE1	2.54	0.42
1:A:394:THR:HG22	1:A:395:PHE:CD2	2.52	0.42
1:A:568:PHE:CZ	1:A:588:ALA:CB	3.03	0.42
1:A:488:HIS:CD2	2:A:877:HOH:O	2.73	0.41
1:A:203:GLY:O	1:A:207:ARG:CB	2.64	0.41
1:A:508:MET:HE3	1:A:508:MET:HB3	1.83	0.41
1:A:587:ARG:CG	1:A:591:GLY:HA2	2.50	0.41
1:A:568:PHE:CE1	1:A:589:PRO:HD3	2.55	0.41
1:A:564:ARG:HA	1:A:564:ARG:HD3	1.89	0.41
1:A:452:ARG:CZ	1:A:481:PRO:HG2	2.50	0.41
1:A:586:CYS:HB2	1:A:620:GLU:OE1	2.20	0.40
1:A:617:LYS:HD2	1:A:622:ARG:O	2.22	0.40
1:A:259:ARG:NH1	2:A:811:HOH:O	2.40	0.40
1:A:231:VAL:HG23	2:A:797:HOH:O	2.20	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	427/440 (97%)	406 (95%)	20 (5%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	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	359/368 (98%)	332 (92%)	27 (8%)	12 4

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

Mol	Chain	Res	Type
1	A	204	LYS
1	A	241	HIS
1	A	244	ASP
1	A	273	ARG
1	A	279	ARG
1	A	312	ASN
1	A	318	LEU
1	A	361	ARG
1	A	382	LYS
1	A	390	LEU
1	A	392	ARG
1	A	394	THR
1	A	396	GLU
1	A	405	LYS
1	A	421	ASN
1	A	424	VAL
1	A	441	GLU
1	A	504	VAL
1	A	518	THR
1	A	579	ASP
1	A	580	SER
1	A	582	GLU
1	A	585	LYS
1	A	594	LYS
1	A	609	GLN
1	A	617	LYS
1	A	622	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	248	HIS
1	A	334	ASN
1	A	341	GLN
1	A	391	ASN
1	A	421	ASN
1	A	488	HIS

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	431/440 (97%)	0.89	62 (14%) 6 5	5, 17, 38, 69	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	PHE	6.3
1	A	277	PRO	5.5
1	A	257	SER	5.2
1	A	621	GLY	5.0
1	A	592	ALA	4.8
1	A	591	GLY	4.7
1	A	394	THR	4.4
1	A	242	GLY	4.3
1	A	278	THR	3.9
1	A	393	LYS	3.6
1	A	205	THR	3.6
1	A	421	ASN	3.4
1	A	580	SER	3.2
1	A	383	ALA	3.2
1	A	202	ALA	3.1
1	A	203	GLY	3.0
1	A	282	ASN	3.0
1	A	423	CYS	3.0
1	A	204	LYS	3.0
1	A	617	LYS	2.9
1	A	568	PHE	2.9
1	A	582	GLU	2.9
1	A	280	VAL	2.8
1	A	253	SER	2.8
1	A	297	ALA	2.8
1	A	622	ARG	2.8
1	A	254	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	206	ARG	2.8
1	A	279	ARG	2.7
1	A	255	HIS	2.7
1	A	575	GLU	2.7
1	A	588	ALA	2.7
1	A	256	GLY	2.7
1	A	558	GLY	2.7
1	A	259	ARG	2.7
1	A	562	ASN	2.7
1	A	590	GLY	2.7
1	A	420	ALA	2.6
1	A	623	ARG	2.6
1	A	610	SER	2.6
1	A	201	GLY	2.6
1	A	350	ASN	2.6
1	A	563	ASP	2.6
1	A	185	SER	2.6
1	A	440	ASP	2.5
1	A	371	ARG	2.4
1	A	572	GLU	2.4
1	A	281	VAL	2.4
1	A	589	PRO	2.3
1	A	595	PRO	2.3
1	A	238	GLU	2.2
1	A	579	ASP	2.2
1	A	325	GLY	2.2
1	A	207	ARG	2.2
1	A	557	ALA	2.2
1	A	599	ARG	2.2
1	A	508	MET	2.1
1	A	531	ASP	2.1
1	A	392	ARG	2.1
1	A	405	LYS	2.1
1	A	384	GLY	2.1
1	A	241	HIS	2.1

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.