



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:08 PM EDT

PDB ID : 2DVP / pdb_00002dvp
Title : Structure of NTPase from Pyrococcus horikoshii
Authors : Lokanath, N.K.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-07-31
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

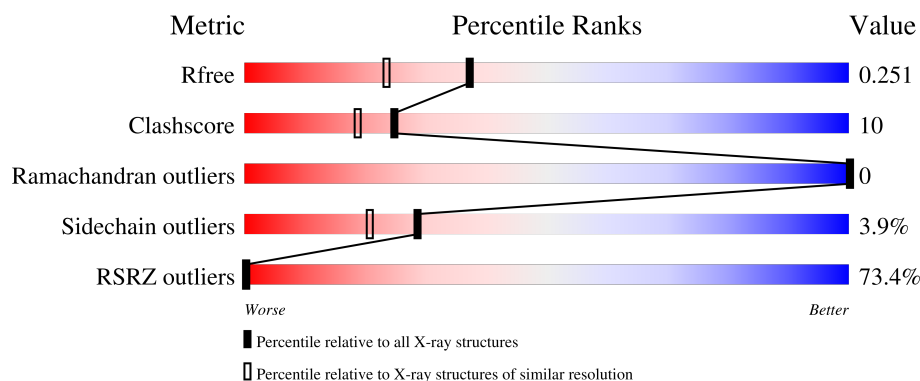
1 Overall quality at a glance

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	186	73% 82% 16% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1587 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 Hypothetical protein PH1917.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1480	972	238	266	4			

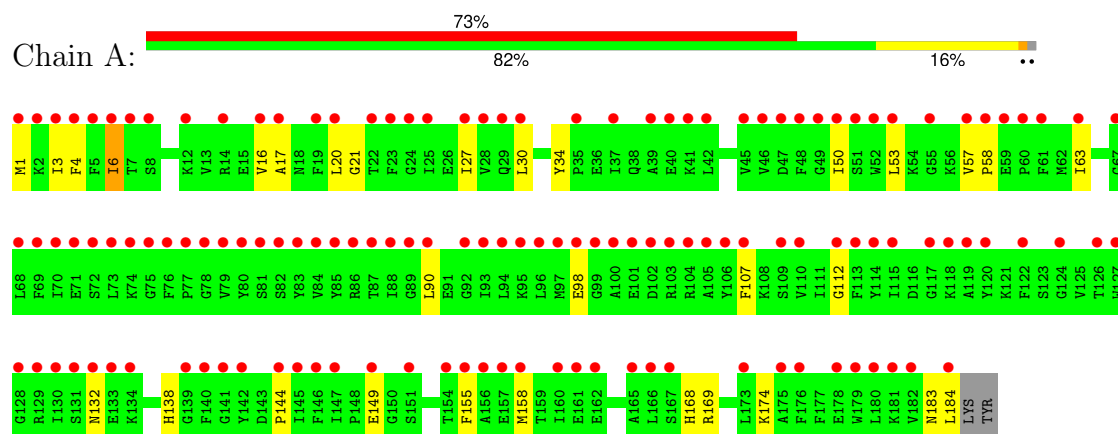
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	107	Total	O	0	0
			107	107		

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: Hypothetical protein PH1917



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	71.52Å 71.52Å 78.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (40.00-1.90) 96.1 (40.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.276 0.249 , 0.251	Depositor DCC
R_{free} test set	846 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	1587	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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	0.77	0/1519	0.90	0/2042

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 [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	1480	0	1477	29	0
2	A	107	0	0	2	0
All	All	1587	0	1477	29	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 10.

All (29) 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:16:VAL:HG12	1:A:27:ILE:CD1	1.70	1.20
1:A:6:ILE:CD1	1:A:53:LEU:HD13	1.76	1.16
1:A:20:LEU:HD12	1:A:27:ILE:HD11	1.34	1.08
1:A:6:ILE:HD12	1:A:53:LEU:HD13	1.42	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG12	1:A:27:ILE:HD13	1.44	0.99
1:A:16:VAL:HG12	1:A:27:ILE:HD12	1.57	0.86
1:A:6:ILE:HD13	1:A:53:LEU:HD13	1.63	0.78
1:A:16:VAL:CG1	1:A:27:ILE:HD13	2.12	0.78
1:A:16:VAL:CG1	1:A:27:ILE:CD1	2.58	0.77
1:A:20:LEU:CD1	1:A:27:ILE:HD11	2.24	0.58
1:A:50:ILE:HD11	1:A:112:GLY:HA3	1.87	0.57
1:A:98:GLU:OE2	2:A:279:HOH:O	2.18	0.55
1:A:183:ASN:O	1:A:184:LEU:HD23	2.08	0.53
1:A:6:ILE:HD13	1:A:53:LEU:CD1	2.36	0.52
1:A:6:ILE:HD13	1:A:53:LEU:HD22	1.90	0.52
1:A:6:ILE:CD1	1:A:53:LEU:CD1	2.69	0.51
1:A:34:TYR:CD2	1:A:53:LEU:HD11	2.47	0.50
1:A:1:MET:HE1	1:A:3:ILE:HD11	1.94	0.49
1:A:4:PHE:HB3	1:A:30:LEU:HD12	1.94	0.49
1:A:107:PHE:HB3	1:A:168:HIS:CG	2.50	0.46
1:A:57:VAL:CG2	1:A:58:PRO:HD2	2.48	0.44
1:A:6:ILE:HD12	1:A:53:LEU:CD1	2.29	0.44
1:A:169:ARG:CZ	1:A:169:ARG:HB2	2.49	0.42
1:A:138:HIS:O	2:A:285:HOH:O	2.22	0.41
1:A:90:LEU:HD11	1:A:144:PRO:HG2	2.03	0.41
1:A:1:MET:HE3	1:A:3:ILE:HG13	2.02	0.41
1:A:17:ALA:O	1:A:21:GLY:N	2.53	0.41
1:A:6:ILE:H	1:A:6:ILE:HG13	1.71	0.40
1:A:6:ILE:HD12	1:A:63:ILE:CG2	2.52	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	182/186 (98%)	176 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	155/157 (99%)	149 (96%)	6 (4%)	28 21

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	132	ASN
1	A	149	GLU
1	A	155	PHE
1	A	158	MET
1	A	174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	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

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	184/186 (98%)	2.83	135 (73%) 0 0	40, 49, 58, 65	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	LEU	7.6
1	A	180	LEU	6.2
1	A	184	LEU	5.7
1	A	113	PHE	5.6
1	A	74	LYS	5.5
1	A	73	LEU	5.4
1	A	96	LEU	5.3
1	A	88	ILE	5.2
1	A	154	THR	5.2
1	A	127	TRP	5.2
1	A	69	PHE	5.1
1	A	70	ILE	5.1
1	A	52	TRP	5.1
1	A	106	TYR	4.9
1	A	100	ALA	4.8
1	A	93	ILE	4.7
1	A	76	PHE	4.6
1	A	75	GLY	4.5
1	A	145	ILE	4.4
1	A	57	VAL	4.3
1	A	134	LYS	4.3
1	A	105	ALA	4.3
1	A	53	LEU	4.2
1	A	87	THR	4.2
1	A	117	GLY	4.1
1	A	79	VAL	4.1
1	A	139	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	4.1
1	A	97	MET	4.0
1	A	90	LEU	4.0
1	A	41	LYS	4.0
1	A	61	PHE	4.0
1	A	39	ALA	3.9
1	A	50	ILE	3.8
1	A	45	VAL	3.8
1	A	77	PRO	3.8
1	A	49	GLY	3.8
1	A	120	TYR	3.6
1	A	126	THR	3.6
1	A	40	GLU	3.6
1	A	114	TYR	3.6
1	A	6	ILE	3.6
1	A	37	ILE	3.6
1	A	24	GLY	3.5
1	A	72	SER	3.5
1	A	60	PRO	3.5
1	A	46	VAL	3.5
1	A	92	GLY	3.5
1	A	80	TYR	3.5
1	A	3	ILE	3.5
1	A	4	PHE	3.5
1	A	140	PHE	3.5
1	A	55	GLY	3.4
1	A	103	ARG	3.4
1	A	27	ILE	3.4
1	A	130	ILE	3.4
1	A	160	ILE	3.4
1	A	104	ARG	3.3
1	A	182	VAL	3.3
1	A	102	ASP	3.3
1	A	131	SER	3.3
1	A	84	VAL	3.3
1	A	85	TYR	3.2
1	A	149	GLU	3.2
1	A	118	LYS	3.1
1	A	89	GLY	3.1
1	A	83	TYR	3.1
1	A	142	TYR	3.1
1	A	179	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.0
1	A	181	LYS	2.9
1	A	58	PRO	2.9
1	A	157	GLU	2.9
1	A	63	ILE	2.9
1	A	119	ALA	2.9
1	A	42	LEU	2.9
1	A	19	PHE	2.8
1	A	23	PHE	2.8
1	A	48	PHE	2.8
1	A	178	GLU	2.8
1	A	17	ALA	2.8
1	A	110	VAL	2.8
1	A	81	SER	2.8
1	A	156	ALA	2.8
1	A	78	GLY	2.8
1	A	151	SER	2.7
1	A	25	ILE	2.7
1	A	47	ASP	2.7
1	A	165	ALA	2.7
1	A	107	PHE	2.7
1	A	141	GLY	2.6
1	A	176	PHE	2.6
1	A	146	PHE	2.6
1	A	173	LEU	2.6
1	A	71	GLU	2.6
1	A	155	PHE	2.6
1	A	122	PHE	2.5
1	A	144	PRO	2.5
1	A	7	THR	2.5
1	A	22	THR	2.5
1	A	98	GLU	2.5
1	A	133	GLU	2.5
1	A	162	GLU	2.5
1	A	2	LYS	2.5
1	A	67	GLY	2.5
1	A	5	PHE	2.4
1	A	30	LEU	2.4
1	A	161	GLU	2.4
1	A	20	LEU	2.4
1	A	35	PRO	2.4
1	A	29	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	132	ASN	2.4
1	A	112	GLY	2.4
1	A	115	ILE	2.4
1	A	158	MET	2.4
1	A	51	SER	2.4
1	A	14	ARG	2.3
1	A	28	VAL	2.3
1	A	59	GLU	2.3
1	A	68	LEU	2.3
1	A	82	SER	2.3
1	A	101	GLU	2.3
1	A	167	SER	2.2
1	A	175	ALA	2.2
1	A	166	LEU	2.2
1	A	12	LYS	2.2
1	A	124	GLY	2.2
1	A	147	ILE	2.1
1	A	129	ARG	2.1
1	A	95	LYS	2.0
1	A	128	GLY	2.0
1	A	16	VAL	2.0
1	A	86	ARG	2.0
1	A	8	SER	2.0
1	A	109	SER	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.