



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:12 PM UTC

PDB ID : 4FVM / pdb\_00004fvm  
Title : Crystal structure of yeast DNA polymerase alpha  
Authors : Perera, R.L.; Pellegrini, L.  
Deposited on : 2012-06-29  
Resolution : 2.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

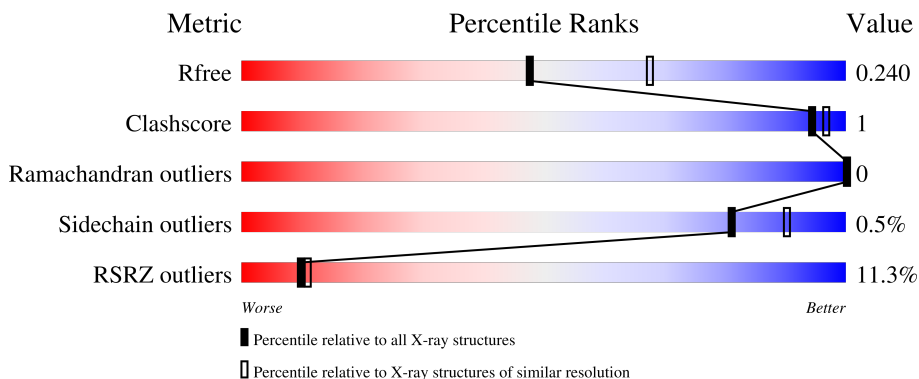
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	910	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13690 atoms, of which 6791 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 DNA polymerase alpha catalytic subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	829	13474	4229	6791	1158	1248	48	0	12	0

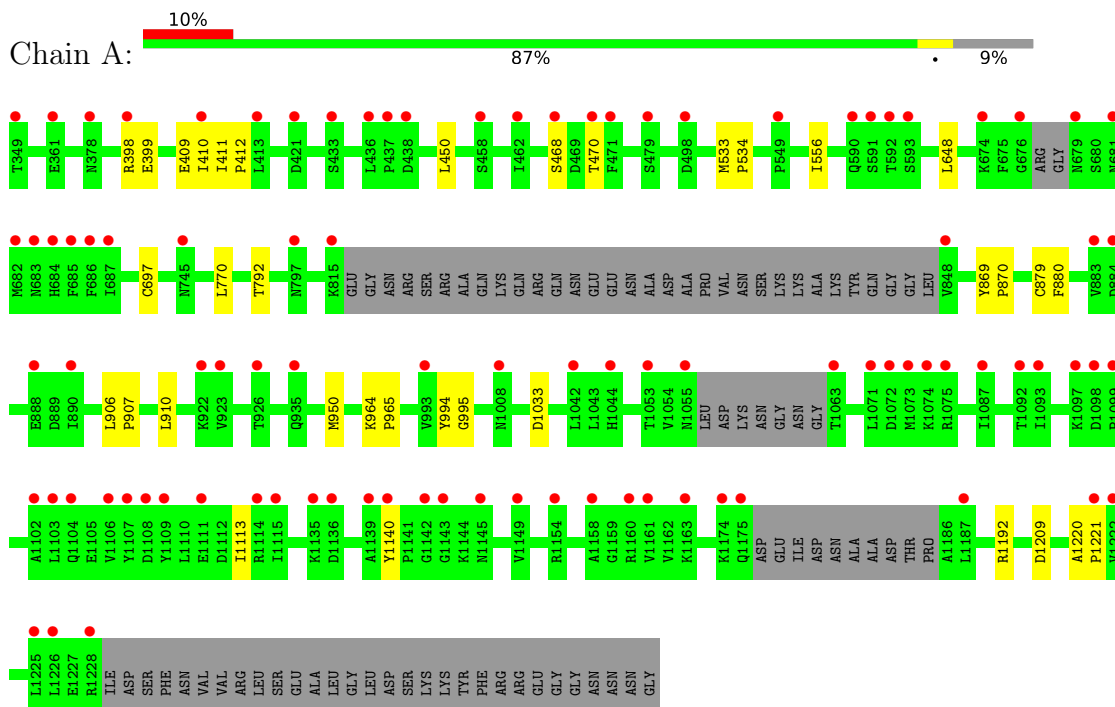
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	216	Total	O	0	0
			216	216		

### 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: DNA polymerase alpha catalytic subunit A



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.38Å 127.14Å 74.57Å 90.00° 104.78° 90.00°	Depositor
Resolution (Å)	36.51 – 2.30 36.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.51-2.30) 99.0 (36.51-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1078)	Depositor
R, $R_{free}$	0.205 , 0.236 0.210 , 0.240	Depositor DCC
$R_{free}$ test set	2974 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.861	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.022 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.27	0/6843	0.62	0/9253

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	6683	6791	6743	17	0
2	A	216	0	0	1	0
All	All	6899	6791	6743	17	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 1.

All (17) 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:792:THR:O	2:A:1444:HOH:O	2.09	0.70
1:A:906:LEU:HB3	1:A:907:PRO:HD3	1.89	0.53
1:A:411:ILE:HB	1:A:412:PRO:HD3	1.90	0.53
1:A:398:ARG:NH2	1:A:468:SER:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:HD12	1:A:411:ILE:N	2.26	0.51
1:A:1220:ALA:HB3	1:A:1221:PRO:HD3	1.95	0.49
1:A:409:GLU:OE1	1:A:470:THR:OG1	2.34	0.46
1:A:697:CYS:SG	1:A:770:LEU:HD23	2.55	0.46
1:A:964:LYS:N	1:A:965:PRO:CD	2.79	0.46
1:A:869:TYR:N	1:A:870:PRO:HD2	2.32	0.44
1:A:1192:ARG:NH2	1:A:1209:ASP:OD2	2.52	0.43
1:A:994:TYR:CG	1:A:995:GLY:N	2.87	0.42
1:A:556:ILE:HD11	1:A:648:LEU:HA	2.01	0.42
1:A:879:CYS:SG	1:A:880:PHE:N	2.93	0.41
1:A:910:LEU:HD21	1:A:950:MET:HG3	2.03	0.41
1:A:398:ARG:HG3	1:A:399:GLU:N	2.36	0.41
1:A:533:MET:HB2	1:A:534:PRO:HD2	2.03	0.41

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	831/910 (91%)	809 (97%)	22 (3%)	0	<b>100</b> <b>100</b>

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	764/818 (93%)	760 (100%)	4 (0%)	81 90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	LEU
1	A	1033	ASP
1	A	1113	ILE
1	A	1140	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	653	HIS
1	A	721	GLN
1	A	728	HIS
1	A	741	GLN
1	A	1024	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 [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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	829/910 (91%)	0.79	94 (11%) <b>10</b> <b>11</b>	23, 63, 107, 147	7 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1072	ASP	5.7
1	A	1145	ASN	4.9
1	A	676	GLY	4.8
1	A	1139	ALA	4.5
1	A	848	VAL	4.5
1	A	1099	PRO	4.5
1	A	683	ASN	4.3
1	A	1044[A]	HIS	4.2
1	A	1107	TYR	4.1
1	A	1108	ASP	4.0
1	A	1109	TYR	3.8
1	A	1142	GLY	3.7
1	A	1161	VAL	3.7
1	A	679	ASN	3.6
1	A	1225	LEU	3.6
1	A	470	THR	3.5
1	A	1063	THR	3.5
1	A	922	LYS	3.5
1	A	685	PHE	3.5
1	A	1187	LEU	3.4
1	A	1008	ASN	3.4
1	A	1140	TYR	3.2
1	A	797	ASN	3.1
1	A	1160	ARG	3.0
1	A	413	LEU	3.0
1	A	1111	GLU	3.0
1	A	1106	VAL	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	890	ILE	2.9
1	A	1071	LEU	2.9
1	A	684	HIS	2.9
1	A	1158	ALA	2.9
1	A	433	SER	2.9
1	A	1073	MET	2.8
1	A	682	MET	2.8
1	A	349	THR	2.8
1	A	745[A]	ASN	2.8
1	A	591	SER	2.8
1	A	687	ILE	2.8
1	A	1104	GLN	2.8
1	A	1075	ARG	2.8
1	A	686	PHE	2.7
1	A	1098	ASP	2.7
1	A	593	SER	2.7
1	A	1143	GLY	2.7
1	A	888	GLU	2.6
1	A	438	ASP	2.6
1	A	471	PHE	2.6
1	A	1042	LEU	2.6
1	A	498	ASP	2.6
1	A	1092	THR	2.6
1	A	410	ILE	2.6
1	A	1102	ALA	2.5
1	A	1136	ASP	2.5
1	A	1175	GLN	2.5
1	A	1115	ILE	2.4
1	A	1135	LYS	2.4
1	A	1154	ARG	2.4
1	A	592	THR	2.4
1	A	462	ILE	2.4
1	A	883	VAL	2.4
1	A	815	LYS	2.4
1	A	1226	LEU	2.4
1	A	884	ASP	2.4
1	A	437	PRO	2.4
1	A	549	PRO	2.4
1	A	436	LEU	2.4
1	A	378	ASN	2.4
1	A	1149	VAL	2.3
1	A	1114	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1228	ARG	2.3
1	A	993	VAL	2.3
1	A	681	ASN	2.3
1	A	1097	LYS	2.3
1	A	1055	ASN	2.2
1	A	398	ARG	2.2
1	A	361	GLU	2.2
1	A	468	SER	2.2
1	A	479	SER	2.2
1	A	674	LYS	2.2
1	A	1174	LYS	2.2
1	A	1053	THR	2.2
1	A	421	ASP	2.2
1	A	1221	PRO	2.2
1	A	1222	VAL	2.1
1	A	1074	LYS	2.1
1	A	926	THR	2.1
1	A	1163	LYS	2.1
1	A	1087	ILE	2.1
1	A	923	VAL	2.1
1	A	590	GLN	2.1
1	A	935	GLN	2.1
1	A	1093	ILE	2.0
1	A	458	SER	2.0
1	A	1103	LEU	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.