



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:47 pm GMT

PDB ID : 3A2F  
Title : Crystal Structure of Pyrococcus furiosus DNA polymerase/PCNA monomer mutant complex  
Authors : Nishida, H.; Ishino, Y.; Morikawa, K.  
Deposited on : 2009-05-15  
Resolution : 2.67 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

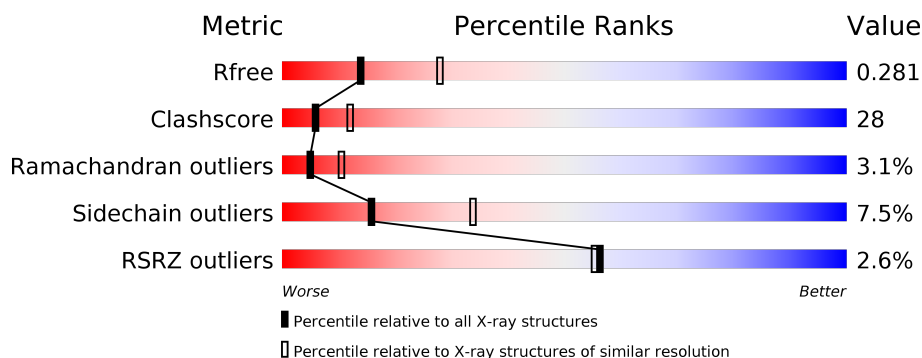
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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))
$R_{free}$	100719	3050 (2.70-2.66)
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (2.70-2.66)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	775	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>42%</div> <div>6%</div> </div> </div>
2	B	248	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>36%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8254 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 DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	Se	0	0	0
			6204	4016	1029	1145	4	10			

- Molecule 2 is a protein called DNA polymerase sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	247	Total	C	N	O	Se	0	0	0
			1924	1234	306	376	8			

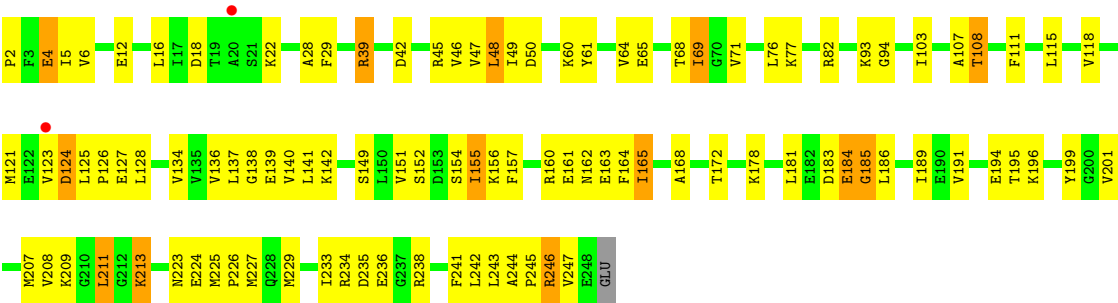
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	LEU	MET	ENGINEERED	UNP O73947
B	143	ALA	ASP	ENGINEERED	UNP O73947
B	147	ALA	ASP	ENGINEERED	UNP O73947

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	24	Total	O	0	0
			24	24		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.35Å 90.45Å 186.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.67 46.55 – 2.67	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.55-2.67) 99.0 (46.55-2.67)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.241 , 0.284 0.237 , 0.281	Depositor DCC
$R_{free}$ test set	1867 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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	0.38	0/6338	0.65	3/8566 (0.0%)
2	B	0.43	0/1942	0.67	1/2606 (0.0%)
All	All	0.39	0/8280	0.65	4/11172 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	ASP	CB-CA-C	-7.44	95.52	110.40
2	B	185	GLY	N-CA-C	-6.43	97.03	113.10
1	A	337	VAL	N-CA-C	-5.48	96.19	111.00
1	A	364	ARG	N-CA-C	-5.13	97.14	111.00

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	6204	0	6122	358	0
2	B	1924	0	1967	99	0
3	A	102	0	0	6	0
3	B	24	0	0	2	0
All	All	8254	0	8089	449	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 28.

The worst 5 of 449 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:541:ASP:OD1	1:A:542:THR:CG2	1.83	1.25
1:A:541:ASP:OD1	1:A:542:THR:HG22	1.47	1.13
1:A:541:ASP:OD1	1:A:542:THR:HG23	1.53	1.05
1:A:188:ARG:HG3	1:A:228:ILE:HD11	1.41	1.01
1:A:2:ILE:HG23	1:A:128:PRO:HA	1.45	0.98

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	771/775 (100%)	667 (86%)	75 (10%)	29 (4%)	4	7
2	B	245/248 (99%)	227 (93%)	15 (6%)	3 (1%)	15	34
All	All	1016/1023 (99%)	894 (88%)	90 (9%)	32 (3%)	5	10

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	100	VAL
1	A	302	GLY
1	A	542	THR
1	A	693	LYS



### 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	639/671 (95%)	590 (92%)	49 (8%)	15	32
2	B	211/208 (101%)	196 (93%)	15 (7%)	17	37
All	All	850/879 (97%)	786 (92%)	64 (8%)	16	34

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	THR
1	A	542	THR
2	B	184	GLU
1	A	418	ASN
1	A	484	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	462	GLN
1	A	484	GLN
2	B	173	GLN
1	A	440	HIS
1	A	737	GLN

### 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 carbohydrates 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	763/775 (98%)	0.13	24 (3%)	49	48	29, 63, 101, 109	0
2	B	239/248 (96%)	-0.05	2 (0%)	86	86	38, 60, 83, 97	0
All	All	1002/1023 (97%)	0.09	26 (2%)	56	55	29, 62, 99, 109	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	4.5
1	A	773	LYS	4.1
1	A	55	THR	4.0
1	A	671	LEU	3.5
1	A	48	ILE	3.3

### 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 carbohydrates 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.