



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 07:55 AM EDT

PDB ID : 6P4F  
Title : Crystal structure of the XPB-Bax1-forked DNA ternary complex  
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Deposited on : 2019-05-27  
Resolution : 3.55 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 : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

## 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 3.55 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 14208 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-dependent ATPase XPBII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	435	Total	C	N	O	S	0	0	0
			3295	2137	537	618	3			
1	C	436	Total	C	N	O	S	0	0	0
			3266	2107	535	620	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q970I2
A	1	SER	MET	conflict	UNP Q970I2
C	0	GLY	-	expression tag	UNP Q970I2
C	1	SER	MET	conflict	UNP Q970I2

- Molecule 2 is a protein called Endonuclease Bax1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	373	Total	C	N	O	S	0	0	0
			2877	1898	464	512	3			
2	D	373	Total	C	N	O	S	0	0	0
			2871	1895	460	514	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	insertion	UNP Q970I1
D	1	GLY	-	insertion	UNP Q970I1

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*TP\*GP\*AP\*CP\*TP\*CP\*AP\*AP\*CP\*AP\*TP\*CP\*CP\*TP\*TP\*TP\*GP\*CP\*TP\*AP\*CP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	24	Total	C	N	O	P	0	0	0
			481	233	82	143	23			
3	G	24	Total	C	N	O	P	0	0	0
			481	233	82	143	23			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*TP\*GP\*TP\*AP\*GP\*GP\*TP\*TP\*TP\*CP\*CP\*AP\*TP\*GP\*TP\*TP\*GP\*AP\*GP\*TP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	22	Total	C	N	O	P	0	0	0
			453	217	77	137	22			
4	H	21	Total	C	N	O	P	0	0	0
			433	207	75	130	21			

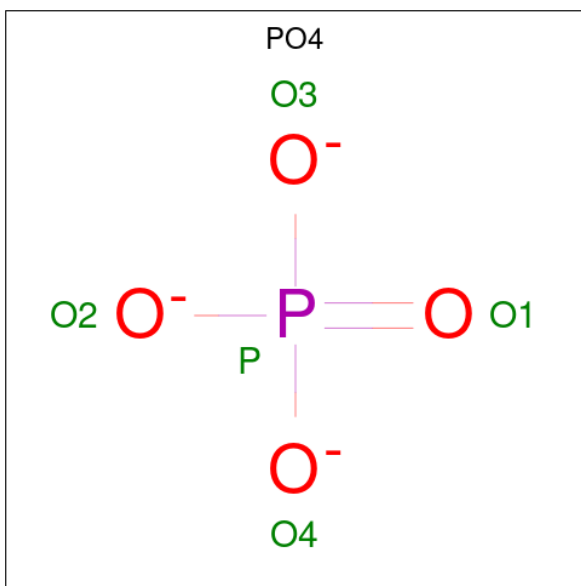
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Mg	0	0
			6	6		
5	B	6	Total	Mg	0	0
			6	6		
5	C	5	Total	Mg	0	0
			5	5		
5	D	4	Total	Mg	0	0
			4	4		
5	E	2	Total	Mg	0	0
			2	2		
5	F	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Cl	0	0
			4	4		
6	B	5	Total	Cl	0	0
			5	5		
6	D	1	Total	Cl	0	0
			1	1		
6	G	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.69Å 92.15Å 172.13Å 90.00° 132.24° 90.00°	Depositor
Resolution (Å)	39.73 – 3.55	Depositor
% Data completeness (in resolution range)	93.5 (39.73-3.55)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.22	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.15.2-3472	Depositor
R, $R_{free}$	0.250 , 0.272	Depositor
Wilson B-factor (Å <sup>2</sup> )	104.0	Xtrriage
Anisotropy	0.128	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 36 are monoatomic - leaving 3 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	$\# Z  > 2$
7	PO4	F	101	-	4,4,4	1.03	0	6,6,6	0.37	0
7	PO4	D	401	-	4,4,4	0.94	0	6,6,6	0.45	0
7	PO4	B	401	-	4,4,4	0.96	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers

EDS failed to run properly - this section is therefore empty.