

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 2, 2023 – 01:19 AM EDT

ontaining DNA complex

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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	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 (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.75 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 4 unique types of molecules in this entry. The entry contains 4112 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Р	187	Total	С	Ν	0	S	0	0	0
	I D	107	1472	959	250	255	8	0	0	
1	Λ	187	Total	С	Ν	0	S	0	0	0
1 A	187	1470	959	248	255	8	0	0	0	

• Molecule 1 is a protein called TATA-box-binding protein 1.

Chain	Residue	Modelled	Actual	Comment	Reference
В	-19	MET	-	initiating methionine	UNP P28147
В	-18	GLY	-	expression tag	UNP P28147
В	-17	SER	-	expression tag	UNP P28147
В	-16	SER	-	expression tag	UNP P28147
В	-15	HIS	-	expression tag	UNP P28147
В	-14	HIS	-	expression tag	UNP P28147
В	-13	HIS	-	expression tag	UNP P28147
В	-12	HIS	-	expression tag	UNP P28147
В	-11	HIS	-	expression tag	UNP P28147
В	-10	HIS	-	expression tag	UNP P28147
В	-9	SER	-	expression tag	UNP P28147
В	-8	SER	-	expression tag	UNP P28147
В	-7	GLY	-	expression tag	UNP P28147
В	-6	LEU	-	expression tag	UNP P28147
В	-5	VAL	-	expression tag	UNP P28147
В	-4	PRO	-	expression tag	UNP P28147
В	-3	ARG	-	expression tag	UNP P28147
В	-2	GLY	-	expression tag	UNP P28147
В	-1	SER	-	expression tag	UNP P28147
В	0	HIS	-	expression tag	UNP P28147
А	-19	MET	-	initiating methionine	UNP P28147
А	-18	GLY	-	expression tag	UNP P28147
А	-17	SER	-	expression tag	UNP P28147
А	-16	SER	-	expression tag	UNP P28147
А	-15	HIS	-	expression tag	UNP P28147

There are 40 discrepancies between the modelled and reference sequences:

Continued on next page...



Chain	Residue	Modelled	Actual Comment		Reference
А	-14	HIS	-	expression tag	UNP P28147
А	-13	HIS	-	expression tag	UNP P28147
A	-12	HIS	-	expression tag	UNP P28147
А	-11	HIS	-	expression tag	UNP P28147
А	-10	HIS	-	expression tag	UNP P28147
А	-9	SER	-	expression tag	UNP P28147
А	-8	SER	-	expression tag	UNP P28147
А	-7	GLY	-	expression tag	UNP P28147
А	-6	LEU	-	expression tag	UNP P28147
А	-5	VAL	-	expression tag	UNP P28147
А	-4	PRO	-	expression tag	UNP P28147
А	-3	ARG	-	expression tag	UNP P28147
А	-2	GLY	-	expression tag	UNP P28147
А	-1	SER	-	expression tag	UNP P28147
А	0	HIS	-	expression tag	UNP P28147

Continued from previous page...

• Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*CP\*TP\*AP\*TP\*AP\*AP\*AP\*CP\*GP\*GP\*GP\*CP\*A)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
0	Е	1.4	Total	С	Ν	Ο	Р	0	0	0
	14	287	137	58	79	13	0	0	0	
0	С	14	Total	С	Ν	Ο	Р	0	0	0
	14	287	137	58	79	13	0	0	0	

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Б	1.4	Total	С	Ν	Ο	Р	0	0	0
5 F	14	281	136	47	85	13	0	0	0	
2	Л	1.4	Total	С	Ν	Ο	Р	0	0	0
5 D	14	281	136	47	85	13	0	0	0	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	7	Total O 7 7	0	0
4	Е	2	Total O 2 2	0	0

Continued on next page...

0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	3	Total O 3 3	0	0
4	А	13	Total O 13 13	0	0
4	С	3	Total O 3 3	0	0
4	D	6	Total O 6 6	0	0

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



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	41.30Å 57.97Å 149.75Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $96.50^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	148.79 - 2.75	Depositor
% Data completeness	97.1 (148.79-2.75)	Depositor
(in resolution range)		-
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$< I/\sigma(I) > 1$	$1.98 (at 2.73 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
$R, R_{free}$	0.230 , $0.278$	Depositor
Wilson B-factor $(Å^2)$	50.6	Xtriage
Anisotropy	0.566	Xtriage
L-test for twinning <sup>2</sup>	$<  L  > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.124 for h,-k,-h-l	Xtriage
Total number of atoms	4112	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 13.62% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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)

There are no ligands in this entry.

#### 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 (i)

## 5.1 Protein, DNA and RNA chains (i)

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

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

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

## 5.3 Carbohydrates (i)

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

## 5.4 Ligands (i)

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

### 5.5 Other polymers (i)

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

