

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 01:54 AM EDT

PDB ID : 6N62

Title : Escherichia coli RNA polymerase sigma70-holoenzyme bound to upstream fork

promoter DNA

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Deposited on : 2018-11-24

Resolution : 3.80 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 (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 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-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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 9 unique types of molecules in this entry. The entry contains 29075 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-directed RNA polymerase subunit alpha.

	\mathbf{Mol}	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
Ī	1	Λ	228	Total	С	N	О	S	0	0	0
	1	Α		1750	1088	312	344	6	0		
	1	D	217	Total	С	N	О	S	0	0	0
	1	Ъ	217	1667	1041	293	327	6	0	U	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z6
A	236	VAL	-	expression tag	UNP P0A7Z6
A	237	LEU	-	expression tag	UNP P0A7Z6
A	238	PHE	-	expression tag	UNP P0A7Z6
A	239	GLN	-	expression tag	UNP P0A7Z6
В	235	GLU	-	expression tag	UNP P0A7Z6
В	236	VAL	-	expression tag	UNP P0A7Z6
В	237	LEU	-	expression tag	UNP P0A7Z6
В	238	PHE	-	expression tag	UNP P0A7Z6
В	239	GLN	_	expression tag	UNP P0A7Z6

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	С	1337	Total 10545	C 6616	N 1838	O 2048	S 43	0	0	0

• Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	D	1226	Total 9557	C 6006	N 1714	O 1791	S 46	0	0	0

There are 3 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP P0A8T8
D	1408	LEU	-	expression tag	UNP P0A8T8
D	1409	GLU	-	expression tag	UNP P0A8T8

• Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	Е	79	Total 627	C 382	N 118	O 126	S 1	0	0	0

• Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
5	F	471	Total	С	N	О	S	0	0	0
		411	3839	2405	684	727	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	$\operatorname{conflict}$	UNP Q0P6L9

• Molecule 6 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	29	Total 595	C 284	N 106	O 176	P 29	0	0	0

• Molecule 7 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Т	24	Total	С	N	О	Р	0	0	0
'	_	24	492	233	94	141	24			Ü

 \bullet Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Mg 1 1	0	0

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	2	Total Zn 2 2	0	0

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



3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	173.77Å 173.77Å 388.77Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	
Resolution (Å)	24.88 - 3.80	Depositor
% Data completeness	99.7 (24.88-3.80)	Depositor
(in resolution range)		
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.08 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.286 , 0.334	Depositor
Wilson B-factor (A^2)	171.7	Xtriage
Anisotropy	0.039	Xtriage
L-test for twinning ²	$ < L > = 0.45, < L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29075	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities 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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 (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.

