

wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 - 03:14 am BST

PDB ID	:	4RNP
Title	:	BACTERIOPHAGE T7 RNA POLYMERASE, HIGH SALT CRYSTAL
		FORM, LOW TEMPERATURE DATA, ALPHA-CARBONS ONLY
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Deposited on		
Resolution	:	3.00 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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.11

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 3.00 Å.

141614

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	Percen	Percentile Ranks				
Clashscore			0			
V	lorse	Bette	?r			
I	Percentile relative to all X-ray stru	uctures				
Percentile relative to X-ray structures of similar resolution						
	1					
Metric	Whole archive	Similar resolu	ution			
	(#Entries)	(#Entries, resolution range)				

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 >=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 <=5%

2416(3.00-3.00)

Note EDS was not executed.

Clashscore

Mol	Chain	Length	Quality of chain			
1	А	883	88%	12%		
1	В	883	88%	12%		
1	С	883	88%	12%		



4RNP

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2340 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	А	780	Total C 780 780	0	0	780
1	В	780	Total C 780 780	0	0	780
1	С	780	Total C 780 780	0	0	780

• Molecule 1 is a protein called RNA POLYMERASE.



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

- Chain A: 88% 12% LYS VAL GLU GLU GLU GLU CLEU LEU LYS LYS LYS VAL CYS VAL VAL VAL VAL AET ASN THR ASN TLE JLN JLYS JLYS JLV ALAASP ALAASP ALAASP ALAASN ALA ALA ALA ALA VAL THR ALEU TYR JLY SER CYS SER VAL LYS ASP LYS LYS LYS THR • Molecule 1: RNA POLYMERASE Chain B: 88% 12% VAL VAL 3LU 3LU 3LU 3LU CEU VAL CYS VAL 7LYS VAL 7LYS VAL 7LYS VAL 3LN ASN ALA 3LY VAL VAL VAL GLU VAL LYS ASP ASP LYS LYS THR GLY GLY THR LEU ALA TYR GLY GLU GLV GLV LEU PHE GLY GLN • Molecule 1: RNA POLYMERASE Chain C: 88% 12% ASN ASN THR THR THR THR THR THR THR THR ALA ASP ASN LEU LEU HH ALEA
- Molecule 1: RNA POLYMERASE









4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	112.27Å 137.68Å 122.57Å	Depositor	
a, b, c, α , β , γ	90.00° 96.36° 90.00°	Depositor	
Resolution (Å)	(Not available) - 3.00	Depositor	
% Data completeness	(Not available) ((Not available)-3.00)	Depositor	
(in resolution range)		Depositor	
R_{merge}	(Not available)	Depositor	
R_{sym}	0.14	Depositor	
Refinement program		Depositor	
R, R_{free}	(Not available) , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2340	wwPDB-VP	
Average B, all atoms $(Å^2)$	12.0	wwPDB-VP	



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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	А	780	0	0	0	0
1	В	780	0	0	0	0
1	С	780	0	0	0	0
All	All	2340	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.



5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

