



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1ARO / pdb\_00001aro  
Title : T7 RNA POLYMERASE COMPLEXED WITH T7 LYSOZYME  
Authors : Steitz, T.; Jeruzalmi, D.  
Deposited on : 1997-08-08  
Resolution : 2.80 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

<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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

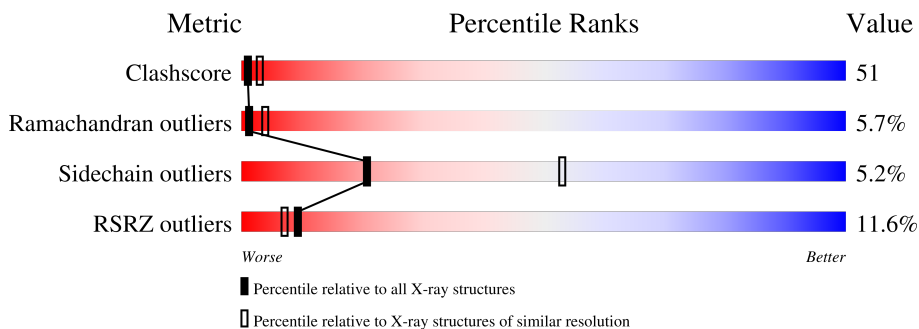
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7314 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 T7 RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	P	774	6124	3912	1065	1115	32	161	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	347	SER	CYS	conflict	UNP P00573
P	723	SER	CYS	engineered mutation	UNP P00573
P	839	SER	CYS	engineered mutation	UNP P00573

- Molecule 2 is a protein called T7 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	149	1183	742	220	216	5	23	0	0

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	6	Total	Hg	0	0
			6	6		
3	L	1	Total	Hg	0	0
			1	1		

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	273.38Å 95.61Å 63.58Å 90.00° 101.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (30.00-2.80) 91.3 (30.00-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.54 (at 2.76Å)	Xtrriage
Refinement program	CNS, X-PLOR	Depositor
R, $R_{free}$	0.262 , 0.309 0.274 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.0	Xtrriage
Anisotropy	0.523	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 77.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	P	0.93	19/6261 (0.3%)	1.50	118/8460 (1.4%)
2	L	0.67	0/1210	1.15	10/1630 (0.6%)
All	All	0.90	19/7471 (0.3%)	1.45	128/10090 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	10
2	L	0	1
All	All	0	11

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	559	VAL	C-N	-22.22	1.02	1.33
1	P	499	ASN	C-N	-17.02	1.09	1.33
1	P	74	ILE	N-CA	14.89	1.74	1.46
1	P	497	LEU	C-N	-14.72	1.13	1.33
1	P	58	GLN	C-O	13.39	1.39	1.23

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	559	VAL	O-C-N	-26.88	94.25	121.94
1	P	8	LYS	O-C-N	-20.31	90.50	123.00
1	P	559	VAL	CA-C-N	19.52	158.83	121.54
1	P	559	VAL	C-N-CA	19.52	158.83	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	P	8	LYS	CA-C-N	15.61	151.35	121.54

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	162	PHE	Sidechain
1	P	497	LEU	Mainchain
1	P	74	ILE	Mainchain
1	P	8	LYS	Peptide,Mainchain
1	P	9	ASN	Mainchain

## 4.2 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	P	6124	0	6086	618	1
2	L	1183	0	1156	97	0
3	L	1	0	0	0	0
3	P	6	0	0	2	0
All	All	7314	0	7242	709	1

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 51.

The worst 5 of 709 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:P:74:ILE:CB	1:P:74:ILE:CA	1.75	1.55
1:P:73:LEU:C	1:P:74:ILE:HA	1.18	1.50
1:P:74:ILE:CA	1:P:74:ILE:N	1.74	1.45
1:P:74:ILE:N	1:P:75:THR:H	1.10	1.40
1:P:74:ILE:N	1:P:75:THR:N	1.82	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:233:ASN:OD1	1:P:838:SER:O[1_554]	1.63	0.57

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

#### 4.3.1 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	P	760/828 (92%)	591 (78%)	120 (16%)	49 (6%)	<b>1</b> <b>3</b>
2	L	-	110 (75%)	34 (23%)	3 (2%)	<b>6</b> <b>21</b>
All	All	907/828 (110%)	701 (77%)	154 (17%)	52 (6%)	<b>1</b> <b>4</b>

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	94	ALA
1	P	197	GLY
1	P	498	GLU
1	P	554	VAL
1	P	584	ALA

#### 4.3.2 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	P	642/680 (94%)	609 (95%)	33 (5%)	<b>21</b> 54
2	L	-	117 (94%)	7 (6%)	<b>19</b> 50
All	All	766/680 (113%)	726 (95%)	40 (5%)	<b>21</b> 53

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	720	ARG
2	L	1034	GLN
1	P	728	VAL
1	P	851	ASP
2	L	1049	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	790	HIS
2	L	1025	GLN
1	P	811	HIS
1	P	857	GLN
2	L	1036	HIS

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

There are no RNA molecules in this entry.

#### 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 oligosaccharides in this entry.

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

Of 7 ligands modelled in this entry, 7 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	P	7

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	73:LEU	C	74:ILE	N	3.03
1	P	58:GLN	C	59:LEU	N	2.01
1	P	8:LYS	C	9:ASN	N	1.19
1	P	9:ASN	C	10:ASP	N	1.17
1	P	497:LEU	C	498:GLU	N	1.13

## 5 Fit of model and data [i](#)

### 5.1 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(Å <sup>2</sup> )	Q<0.9
1	P	723/828 (87%)	0.74	87 (12%) <b>9</b> <b>6</b>	19, 74, 110, 123	39 (5%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	538	GLY	16.7
1	P	539	SER	7.1
1	P	233	ASN	6.0
1	P	712	ASP	5.3
1	P	241	SER	4.9

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

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

### 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HG	P	909	1/1	0.93	0.10	199,199,199,199	0
3	HG	P	908	1/1	0.94	0.20	199,199,199,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HG	P	906	1/1	0.95	0.06	136,136,136,136	0
3	HG	P	907	1/1	0.97	0.21	159,159,159,159	0
3	HG	P	904	1/1	0.99	0.04	87,87,87,87	0
3	HG	P	905	1/1	0.99	0.03	83,83,83,83	0
3	HG	L	903	1/1	0.99	0.03	113,113,113,113	0

## 5.5 Other polymers [i](#)

There are no such residues in this entry.