



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9OAV / pdb\_00009oav  
Title : TNA polymerase, 8-64, binary complex  
Authors : Lee, J.J.; Maola, V.A.; Chim, N.; Chaput, J.C.  
Deposited on : 2025-04-21  
Resolution : 2.50 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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

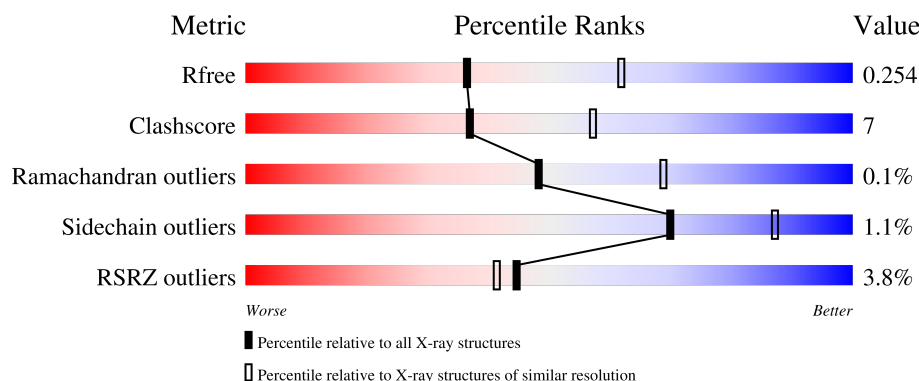
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	775	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>
2	T	18	<div> <div>6%</div> <div>56%</div> <div>44%</div> </div>
3	P	13	<div> <div>54%</div> <div>38%</div> <div>8%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6980 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 8-64, TNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	1	0
			6240	4018	1058	1149	15			

- Molecule 2 is a DNA chain called Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	18	Total	C	N	O	P	0	0	0
			370	175	71	106	18			

- Molecule 3 is a DNA chain called Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			265	124	51	77	13			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		

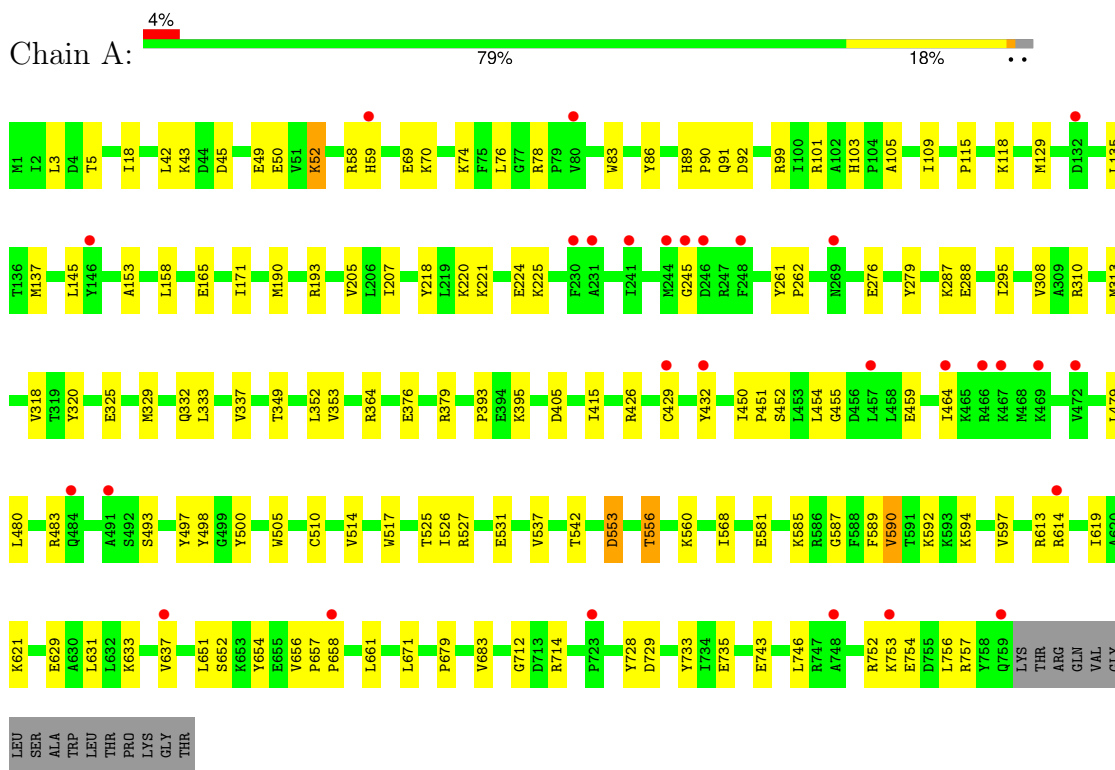
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	T	11	Total	O	0	0
			11	11		
5	P	4	Total	O	0	0
			4	4		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: 8-64, TNA polymerase



- Molecule 2: Template



- Molecule 3: Primer



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.39Å 108.03Å 123.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 2.50 49.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.50-2.50) 99.9 (49.50-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.51Å)	Xtriage
Refinement program	PHENIX v1.20.1_4487	Depositor
R, $R_{free}$	0.229 , 0.255 0.229 , 0.254	Depositor DCC
$R_{free}$ test set	2000 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 25.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6980	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TFT, MG, FA2

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	A	0.12	0/6385	0.28	0/8618
2	T	0.20	0/415	0.39	0/638
3	P	0.19	0/253	0.32	0/388
All	All	0.13	0/7053	0.29	0/9644

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

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	A	6240	0	6267	89	0
2	T	370	0	202	6	0
3	P	265	0	142	3	0
4	A	3	0	0	0	0
5	A	87	0	0	1	0
5	P	4	0	0	0	0
5	T	11	0	0	0	0
All	All	6980	0	6611	95	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 7.

The worst 5 of 95 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:O	1:A:78:ARG:NH1	2.08	0.87
1:A:288:GLU:OE2	1:A:310:ARG:NH2	2.15	0.80
1:A:592:LYS:HD3	2:T:10:DG:H5''	1.75	0.69
1:A:3:LEU:HD23	1:A:129:MET:HE1	1.77	0.67
1:A:429:CYS:HB3	1:A:432[A]:TYR:CZ	2.31	0.65

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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	A	758/775 (98%)	741 (98%)	16 (2%)	1 (0%)	48 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	THR

### 5.3.2 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	A	658/670 (98%)	651 (99%)	7 (1%)	70 87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	THR
1	A	590	VAL
1	A	671	LEU
1	A	652	SER
1	A	553	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	437	GLN
1	A	520	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
3	FA2	P	13	3,2	15,22,23	3.08	9 (60%)	14,32,35	1.53	2 (14%)
3	TFT	P	12	3,2	17,20,21	3.32	12 (70%)	23,29,32	1.87	5 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '–' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FA2	P	13	3,2	-	0/1/21/22	0/3/3/3
3	TFT	P	12	3,2	-	0/5/21/22	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	12	TFT	O3T-C3T	-8.37	1.31	1.45
3	P	13	FA2	C2-N3	7.08	1.43	1.32
3	P	12	TFT	C1T-N1	5.12	1.62	1.47
3	P	13	FA2	C4-N3	4.52	1.41	1.35
3	P	13	FA2	O4'-C4'	4.51	1.53	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	12	TFT	C5-C4-N3	5.31	119.94	115.32
3	P	12	TFT	C4-N3-C2	-4.47	121.48	127.34
3	P	13	FA2	N3-C2-N1	-3.26	124.25	128.67
3	P	13	FA2	O2'-C2'-C3'	-3.10	102.17	111.08
3	P	12	TFT	C5M-C5-C6	2.95	126.84	122.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	12	TFT	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 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.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

### 6.1 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	A	759/775 (97%)	0.44	29 (3%) 44 41	32, 49, 75, 124	1 (0%)
2	T	18/18 (100%)	0.29	1 (5%) 31 29	44, 53, 123, 125	0
3	P	11/13 (84%)	0.41	0 100 100	52, 62, 94, 98	0
All	All	788/806 (97%)	0.44	30 (3%) 44 41	32, 49, 79, 125	1 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	472	VAL	4.4
1	A	59	HIS	3.9
1	A	753	LYS	3.4
1	A	457	LEU	3.4
1	A	637	VAL	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	FA2	P	13	20/21	0.91	0.11	44,48,51,53	0
3	TFT	P	12	19/20	0.94	0.09	46,47,50,53	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 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
4	MG	A	802	1/1	0.85	0.24	52,52,52,52	0
4	MG	A	803	1/1	0.89	0.23	42,42,42,42	0
4	MG	A	801	1/1	0.98	0.05	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.