



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9TCA / pdb\_00009tca  
Title : Crystal Structure of a tRNA acceptor stem mimic at 1.94 Å resolution  
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Deposited on : 2025-11-20  
Resolution : 1.94 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 : 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



## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 933 atoms, of which 290 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.

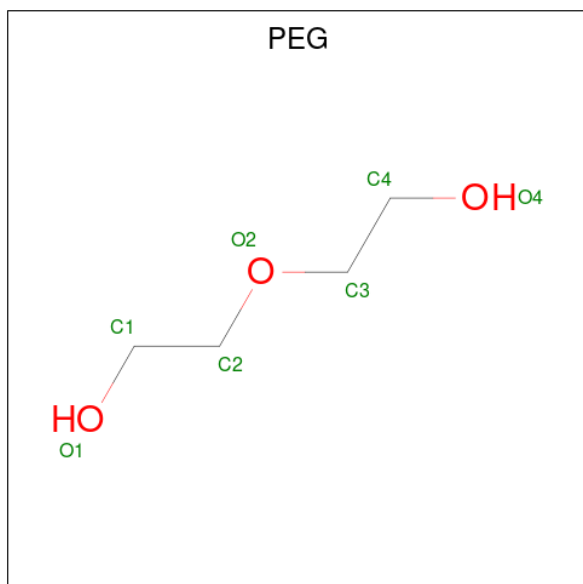
- Molecule 1 is a RNA chain called RNA (5'-R(P\*AP\*GP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				P
1	A	5	Total 160	C 49	H 50	N 23	O 33	P 5	0	0	0
1	C	5	Total 160	C 49	H 50	N 23	O 33	P 5	0	0	0

- Molecule 2 is a RNA chain called RNA (5'-R(\*UP\*CP\*GP\*CP\*UP\*UP\*UP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				P
2	B	9	Total 266	C 82	H 86	N 25	O 65	P 8	0	0	0
2	D	10	Total 298	C 92	H 96	N 30	O 71	P 9	0	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			15	4	8	3		

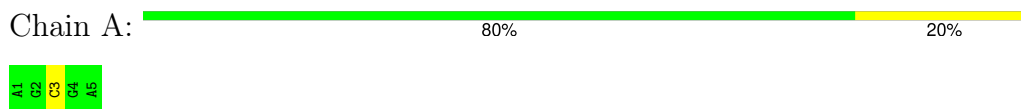
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	14	Total	O	0	0
			14	14		
4	C	5	Total	O	0	0
			5	5		
4	D	14	Total	O	0	0
			14	14		

### 3 Residue-property plots

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: RNA (5'-R(P\*AP\*GP\*CP\*GP\*A)-3')



- Molecule 1: RNA (5'-R(P\*AP\*GP\*CP\*GP\*A)-3')

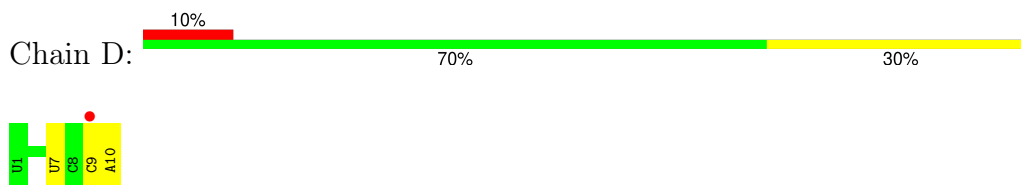


There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(\*UP\*CP\*GP\*CP\*UP\*UP\*UP\*CP\*C)-3')



- Molecule 2: RNA (5'-R(\*UP\*CP\*GP\*CP\*UP\*UP\*UP\*CP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	28.82Å 32.38Å 78.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.05 – 1.94 27.05 – 1.94	Depositor EDS
% Data completeness (in resolution range)	96.5 (27.05-1.94) 96.4 (27.05-1.94)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, $R_{free}$	0.247 , 0.277 0.249 , 0.286	Depositor DCC
$R_{free}$ test set	290 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	933	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4291e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.61	0/123	1.20	1/190 (0.5%)
1	C	0.61	0/123	1.07	0/190
2	B	0.67	0/198	1.62	3/305 (1.0%)
2	D	0.66	0/223	1.22	1/344 (0.3%)
All	All	0.65	0/667	1.32	5/1029 (0.5%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	C	O3'-P-O5'	-9.86	89.22	104.00
2	B	3	G	C4'-C3'-O3'	-8.91	99.63	113.00
2	B	3	G	C2'-C3'-O3'	8.64	126.67	113.70
1	A	3	C	O3'-P-O5'	-6.62	94.08	104.00
2	D	7	U	O3'-P-O5'	-5.07	96.39	104.00

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	A	110	50	56	0	0
1	C	110	50	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	180	86	97	0	0
2	D	202	96	108	0	0
3	D	7	8	10	0	0
4	A	1	0	0	0	0
4	B	14	0	0	0	0
4	C	5	0	0	0	0
4	D	14	0	0	0	0
All	All	643	290	327	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 molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	4/5 (80%)	0	0
1	C	4/5 (80%)	0	0
2	B	8/10 (80%)	1 (12%)	0
2	D	9/10 (90%)	2 (22%)	1 (11%)
All	All	25/30 (83%)	3 (12%)	1 (4%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	C
2	D	9	C
2	D	10	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	9	C

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	PEG	D	101	-	6,6,6	0.45	0	5,5,5	0.29	0

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	PEG	D	101	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	101	PEG	O1-C1-C2-O2
3	D	101	PEG	O2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

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	5/5 (100%)	0.37	0 100 100	41, 52, 59, 61	0
1	C	5/5 (100%)	0.43	0 100 100	40, 46, 55, 59	0
2	B	9/10 (90%)	0.28	0 100 100	34, 41, 66, 105	0
2	D	10/10 (100%)	0.36	1 (10%) 12 14	35, 43, 67, 146	0
All	All	29/30 (96%)	0.35	1 (3%) 48 54	34, 50, 67, 146	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	9	C	3.1

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

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

### 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
3	PEG	D	101	7/7	0.78	0.15	51,53,56,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.