



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:26 am GMT

PDB ID : 1X9S
Title : T7 DNA polymerase in complex with a primer/template DNA containing a disordered N-2 aminofluorene on the template, crystallized with dideoxy-CTP as the incoming nucleotide.
Authors : Dutta, S.; Li, Y.; Johnson, D.; Dzantiev, L.; Richardson, C.C.; Romano, L.J.; Ellenberger, T.
Deposited on : 2004-08-24
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

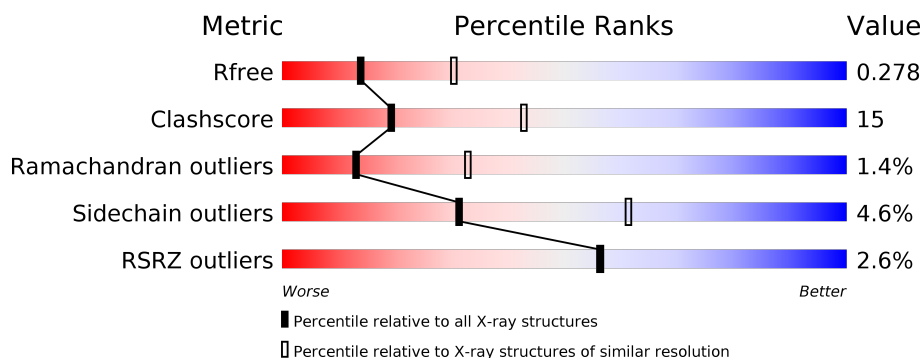
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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. 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	P	22	
2	T	26	
3	A	698	
4	B	108	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	A	3001	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6462 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 DNA chain called 5'-D(*GP*GP*AP*GP*AP*GP*TP*GP*AP*TP*T*GP*GP*TP*AP*GP*TP*GP*TP*GP*AP*(2DT))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	11	Total	C	N	O	P	0	0	0
			228	110	43	65	10			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*(AFG)P*AP*TP*CP*AP*CP*AP*C*P*TP*AP*CP*CP*AP*AP*TP*CP*AP*CP*TP*CP*TP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	11	Total	C	N	O	P	0	0	0
			219	105	39	64	11			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	673	Total	C	N	O	S	0	0	0
			5189	3313	887	965	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP P00581
A	?	-	ARG	DELETION	UNP P00581
A	?	-	PHE	DELETION	UNP P00581
A	?	-	GLY	DELETION	UNP P00581
A	?	-	SER	DELETION	UNP P00581
A	?	-	HIS	DELETION	UNP P00581

- Molecule 4 is a protein called Thioredoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	105	Total	C	N	O	S	0	0	0
			774	500	121	150	3			

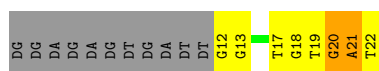
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total 43	O 43	0	0
6	B	2	Total 2	O 2	0	0
6	T	6	Total 6	O 6	0	0

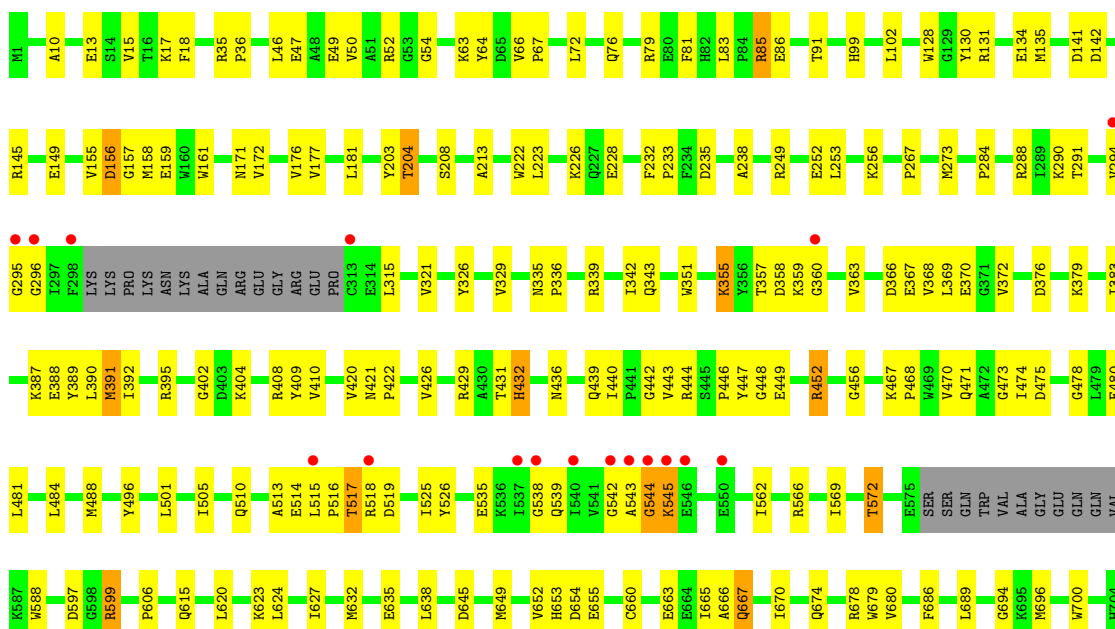
- Molecule 1: 5'-D(*GP*GP*AP*GP*AP*GP*TP*GP*AP*TP*T*GP*GP*TP*AP*GP*TP*GP*TP*GP*AP*(2DT))-3'



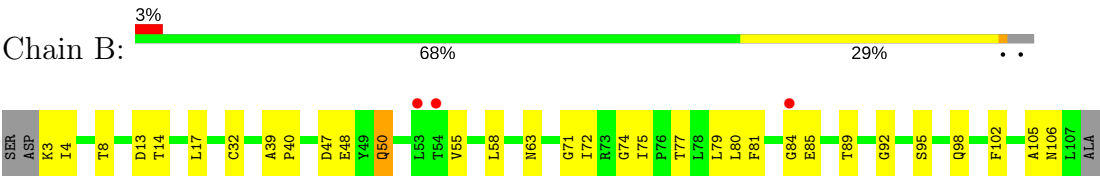
Chain T: 



Chain A: 



● Molecule 4: Thioredoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.58Å 211.10Å 51.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.64 – 2.70 46.64 – 2.58	Depositor EDS
% Data completeness (in resolution range)	95.1 (46.64-2.70) 92.8 (46.64-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.40 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.279 0.225 , 0.278	Depositor DCC
R_{free} test set	1624 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6462	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 2DT, MG

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	0.41	0/235	0.85	0/363
2	T	0.52	0/244	0.81	0/372
3	A	0.39	0/5318	0.59	0/7226
4	B	0.34	0/789	0.60	0/1078
All	All	0.39	0/6586	0.62	0/9039

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	2
2	T	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	20	DG	Sidechain
1	P	21	DA	Sidechain
2	T	7	DC	Sidechain

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	P	228	0	127	12	0
2	T	219	0	124	6	0
3	A	5189	0	4909	152	0
4	B	774	0	750	18	0
5	A	1	0	0	0	0
6	A	43	0	0	1	0
6	B	2	0	0	0	0
6	T	6	0	0	1	0
All	All	6462	0	5910	179	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 15.

The worst 5 of 179 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)
3:A:624:LEU:HD12	3:A:680:VAL:HG22	1.49	0.92
3:A:645:ASP:HB3	3:A:665:ILE:HD13	1.52	0.90
3:A:624:LEU:HD11	3:A:679:TRP:HZ3	1.39	0.87
1:P:21:DA:H2'	1:P:22:2DT:H73	1.58	0.86
3:A:674:GLN:NE2	3:A:678:ARG:HH11	1.77	0.81

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	
3	A	667/698 (96%)	620 (93%)	37 (6%)	10 (2%)	12	30
4	B	103/108 (95%)	94 (91%)	8 (8%)	1 (1%)	18	43
All	All	770/806 (96%)	714 (93%)	45 (6%)	11 (1%)	13	33

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	156	ASP
3	A	544	GLY
3	A	545	LYS
3	A	518	ARG
3	A	515	LEU

5.3.2 Protein sidechains ⓘ

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	
3	A	511/579 (88%)	488 (96%)	23 (4%)	32	62
4	B	78/87 (90%)	74 (95%)	4 (5%)	28	56
All	All	589/666 (88%)	562 (95%)	27 (5%)	31	61

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	444	ARG
3	A	514	GLU
4	B	58	LEU
3	A	452	ARG
3	A	204	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	266	GLN

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Mol	Chain	Res	Type
3	A	335	ASN
3	A	347	GLN
3	A	439	GLN
3	A	502	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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$
1	2DT	P	22	1,2	12,20,21	1.19	2 (16%)	12,28,31	4.82	3 (25%)

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
1	2DT	P	22	1,2	-	0/3/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	22	2DT	C6-C5	-2.14	1.34	1.40
1	P	22	2DT	C4-N3	2.99	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	22	2DT	C5-C4-N3	-9.02	115.30	125.24
1	P	22	2DT	C5M-C5-C6	2.13	122.92	118.67
1	P	22	2DT	C4-N3-C2	13.73	127.17	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	22	2DT	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [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, 95th 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 ²)	Q<0.9
1	P	10/22 (45%)	0.03	0 100 100	29, 41, 91, 98	0
2	T	11/26 (42%)	0.16	1 (9%) 10 7	18, 32, 57, 73	0
3	A	673/698 (96%)	-0.12	17 (2%) 58 58	9, 27, 66, 83	0
4	B	105/108 (97%)	0.12	3 (2%) 52 52	20, 35, 53, 64	0
All	All	799/854 (93%)	-0.08	21 (2%) 56 56	9, 29, 65, 98	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	545	LYS	5.0
3	A	543	ALA	4.5
3	A	544	GLY	4.3
3	A	294	VAL	3.8
3	A	298	PHE	3.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
1	2DT	P	22	19/20	0.97	0.17	-	22,26,27,29	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
5	MG	A	3001	1/1	0.94	0.28	10.84	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.