



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 05:23 am BST

PDB ID : 1QLN
Title : STRUCTURE OF A TRANSCRIBING T7 RNA POLYMERASE INITIATION COMPLEX
Authors : Cheetham, G.M.T.; Steitz, T.A.
Deposited on : 1999-09-01
Resolution : 2.40 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

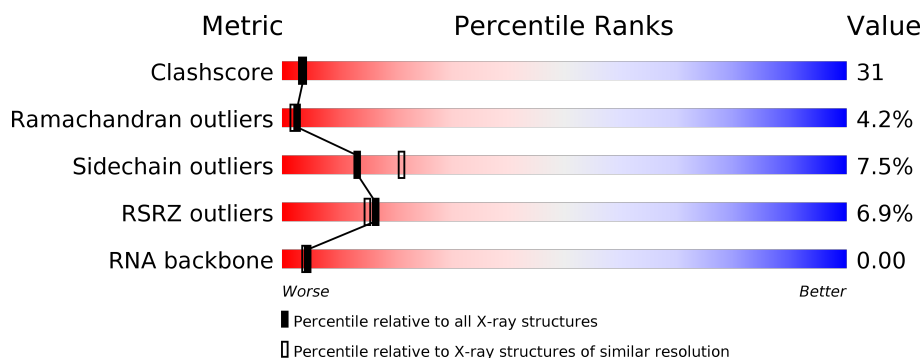
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 $\leq 5\%$. 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	883	
2	N	17	
3	R	3	
4	T	22	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7992 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 BACTERIOPHAGE T7 RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	0	0
			6696	4269	1167	1224	36			

- Molecule 2 is a DNA chain called DNA (5-D(P*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*TP*A)-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	14	Total	C	N	O	P	0	0	0
			283	136	50	83	14			

- Molecule 3 is a RNA chain called RNA (5- R(PPP*GP*GP*G)-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	3	Total	C	N	O	P	0	0	0
			78	30	15	28	5			

- Molecule 4 is a DNA chain called DNA (5- D (P*CP*TP*CP*CP*CP*TP*AP*TP*AP*GP*TP*GP*AP*GP*TP*CP*GP*TP* AP*TP*TP*A)-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	22	Total	C	N	O	P	0	0	0
			448	215	76	135	22			

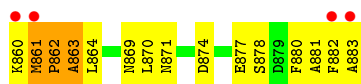
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	429	Total	O	0	0
			429	429		
5	N	21	Total	O	0	0
			21	21		
5	R	2	Total	O	0	0
			2	2		

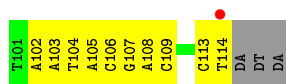
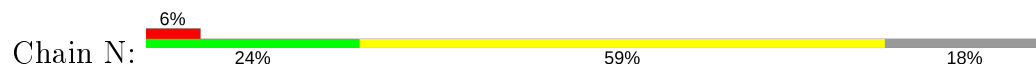
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	T	35	Total	O	0	0
			35	35		



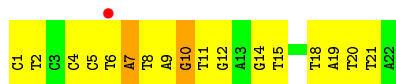
- Molecule 2: DNA (5-D(P*TP*AP*AP*TP*AP*CP*GP*AP*CP*TP*CP*AP*CP*TP*A)-3)



- Molecule 3: RNA (5- R(PPP*GP*GP*G)-3)



- Molecule 4: DNA (5- D (P*CP*TP*CP*CP*CP*TP*AP*TP*AP*GP*TP*GP*AP*GP*TP*C P*GP*TP* AP*TP*TP*A)-3)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	221.20 Å 73.60 Å 80.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 39.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.00-2.40) 97.5 (39.79-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.39 Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.223 , 0.267 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7992	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: GTP

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	0.58	0/6851	0.78	4/9281 (0.0%)
2	N	0.83	0/316	0.96	0/484
3	R	0.79	0/51	0.75	0/78
4	T	0.79	0/500	0.93	0/769
All	All	0.61	0/7718	0.80	4/10612 (0.0%)

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
4	T	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	VAL	N-CA-C	-5.83	95.26	111.00
1	A	715	THR	N-CA-C	-5.71	95.60	111.00
1	A	346	HIS	N-CA-C	-5.52	96.10	111.00
1	A	181	ALA	N-CA-C	-5.41	96.41	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	T	10	DG	Sidechain
4	T	7	DA	Sidechain

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	6696	0	6561	416	0
2	N	283	0	159	13	0
3	R	78	0	34	2	0
4	T	448	0	251	42	0
5	A	429	0	0	17	0
5	N	21	0	0	0	0
5	R	2	0	0	0	0
5	T	35	0	0	2	0
All	All	7992	0	7005	451	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 31.

The worst 5 of 451 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:713:LYS:HD3	1:A:714:LYS:H	1.05	1.11
1:A:710:VAL:HG11	1:A:720:ARG:H	1.03	1.10
1:A:710:VAL:HG11	1:A:720:ARG:N	1.65	1.08
4:T:4:DC:H2'	4:T:5:DC:O4'	1.54	1.08
1:A:298:ARG:HD2	4:T:6:DT:H5'	1.35	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	858/883 (97%)	734 (86%)	88 (10%)	36 (4%)	3 2

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	168	GLU
1	A	169	GLN
1	A	175	GLY
1	A	178	TYR

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
1	A	680/729 (93%)	629 (92%)	51 (8%)	13 21

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	TRP
1	A	539	SER
1	A	831	THR
1	A	506	ASP
1	A	540	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	ASN
1	A	437	ASN
1	A	786	GLN
1	A	406	ASN
1	A	411	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	1/3 (33%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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$
3	GTP	R	1	3,4	26,34,34	1.30	5 (19%)	33,54,54	3.60	9 (27%)

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	GTP	R	1	3,4	-	8/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	GTP	C6-N1	3.92	1.39	1.33
3	R	1	GTP	PG-O2G	2.42	1.64	1.54
3	R	1	GTP	C8-N7	-2.16	1.30	1.34
3	R	1	GTP	PG-O3G	2.07	1.62	1.54
3	R	1	GTP	O4'-C1'	2.04	1.43	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	1	GTP	O3G-PG-O3B	14.53	153.38	104.64
3	R	1	GTP	C5-C6-N1	-8.49	111.82	123.43
3	R	1	GTP	O3B-PG-O1G	-5.81	78.97	111.19
3	R	1	GTP	C6-N1-C2	5.74	125.06	115.93
3	R	1	GTP	PA-O3A-PB	4.64	148.75	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	1	GTP	C5'-O5'-PA-O3A
3	R	1	GTP	O4'-C4'-C5'-O5'
3	R	1	GTP	C3'-C4'-C5'-O5'
3	R	1	GTP	C5'-O5'-PA-O1A
3	R	1	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	GTP	2	0

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](#)

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	A	862/883 (97%)	0.32	60 (6%) 16 15	18, 41, 85, 105	0
2	N	14/17 (82%)	0.18	1 (7%) 16 14	31, 49, 71, 108	0
3	R	2/3 (66%)	0.16	0 100 100	59, 59, 59, 61	0
4	T	22/22 (100%)	0.19	1 (4%) 33 31	39, 51, 95, 101	0
All	All	900/925 (97%)	0.32	62 (6%) 16 15	18, 42, 86, 108	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	MET	10.1
1	A	175	GLY	8.0
1	A	599	ASP	7.9
1	A	601	ASN	6.5
1	A	600	GLU	6.5

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, 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	B-factors(Å ²)	Q<0.9
3	GTP	R	1	32/32	0.56	0.32	81,92,115,115	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.