



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:29 PM EDT

PDB ID : 6UU7 / pdb_00006uu7
Title : E. coli sigma-S transcription initiation complex with a 6-nt RNA and an NTP ("Old" crystal soaked with UTP, CTP, ddGTP, and dinucleotide ApG for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
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

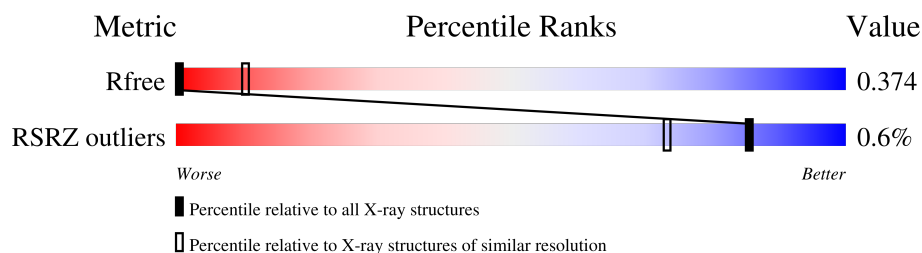
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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))
R_{free}	180053	1088 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.94Å 153.77Å 232.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 4.40 49.15 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.15-4.40) 99.2 (49.15-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.344 , 0.390 0.334 , 0.374	Depositor DCC
R_{free} test set	1464 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	179.5	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 336.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	28934	wwPDB-VP
Average B, all atoms (Å ²)	304.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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.

3 Model quality [i](#)

3.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

Of 1 non-standard protein/DNA/RNA residues modelled in this entry, 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	333	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	333	19:U	O3'	101:DDG	P	1.80

4 Fit of model and data ⓘ

4.1 Protein, DNA and RNA chains ⓘ

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	AAA	230/242 (95%)	-0.34	4 (1%) 69 55	235, 332, 394, 420	0
1	BBB	228/242 (94%)	-0.18	3 (1%) 75 60	219, 299, 405, 493	0
2	CCC	1341/1342 (99%)	-0.38	13 (0%) 79 64	135, 265, 411, 503	0
3	DDD	1362/1407 (96%)	-0.46	1 (0%) 92 87	138, 283, 458, 547	0
4	EEE	79/90 (87%)	-0.63	0 100 100	208, 315, 468, 542	0
5	FFF	270/336 (80%)	-0.38	2 (0%) 84 71	263, 376, 482, 500	0
6	111	29/50 (58%)	-0.21	0 100 100	304, 372, 557, 600	0
7	222	32/50 (64%)	-0.07	0 100 100	256, 367, 577, 639	0
8	333	5/6 (83%)	-0.45	0 100 100	340, 354, 386, 388	0
All	All	3576/3765 (94%)	-0.40	23 (0%) 85 73	135, 295, 457, 639	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	43	LEU	4.5
2	CCC	127	ILE	4.1
1	AAA	217	ILE	3.6
2	CCC	587	LEU	3.4
2	CCC	124	MET	3.4
2	CCC	1180	MET	3.2
1	AAA	205	MET	3.1
2	CCC	333	ILE	3.1
2	CCC	571	LEU	3.0
1	BBB	224	LEU	2.9
2	CCC	533	LEU	2.8
3	DDD	253	VAL	2.7
1	BBB	50	SER	2.6
5	FFF	116	LEU	2.6
2	CCC	870	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	43	LEU	2.5
2	CCC	663	VAL	2.5
2	CCC	239	MET	2.5
2	CCC	530	ILE	2.3
5	FFF	120	ILE	2.3
2	CCC	164	THR	2.1
1	AAA	221	ALA	2.1
2	CCC	230	PHE	2.1

MODRES-RSR INFOmissingINFO

4.2 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

4.3 Other polymers [i](#)

There are no such residues in this entry.