



wwPDB X-ray Structure Validation Summary Report

Apr 27, 2026 – 07:38 PM EDT

PDB ID : 2A68 / pdb_00002a68
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic rifabutin
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-01
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

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)
Xtrriage (Phenix) : 2.0
EDS : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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 2.50 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 61089 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 DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	B	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	K	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	L	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1119	Total 8829	C 5581	N 1577	O 1647	S 24	0	0	0
2	M	1119	Total 8829	C 5581	N 1577	O 1647	S 24	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1392	Total 10797	C 6819	N 1925	O 2020	S 33	0	0	0
3	N	1392	Total 10797	C 6819	N 1925	O 2020	S 33	0	0	0

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	95	Total 769	C 488	N 133	O 144	S 4	0	0	0
4	O	95	Total 769	C 488	N 133	O 144	S 4	0	0	0

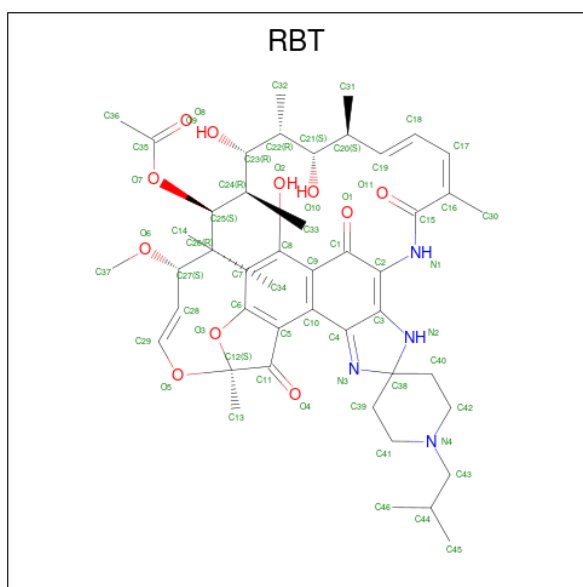
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	345	2771	1744	504	519	4	0	0	0
5	P	345	2771	1744	504	519	4	0	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total 31	Mg 31	0	0
6	B	23	Total 23	Mg 23	0	0
6	C	81	Total 81	Mg 81	0	0
6	D	137	Total 137	Mg 137	0	0
6	E	10	Total 10	Mg 10	0	0
6	F	31	Total 31	Mg 31	0	0
6	K	21	Total 21	Mg 21	0	0
6	L	25	Total 25	Mg 25	0	0
6	M	69	Total 69	Mg 69	0	0
6	N	108	Total 108	Mg 108	0	0
6	O	6	Total 6	Mg 6	0	0
6	P	20	Total 20	Mg 20	0	0

- Molecule 7 is RIFABUTIN (CCD ID: RBT) (formula: C₄₆H₆₂N₄O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			61	46	4	11		
7	M	1	Total	C	N	O	0	0
			61	46	4	11		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	253	Total	O	0	0
			253	253		
9	B	307	Total	O	0	0
			307	307		
9	C	1000	Total	O	0	0
			1000	1000		
9	D	1418	Total	O	0	0
			1418	1418		
9	E	112	Total	O	0	0
			112	112		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	456	Total 456	O 456	0	0
9	K	213	Total 213	O 213	0	0
9	L	237	Total 237	O 237	0	0
9	M	998	Total 998	O 998	0	0
9	N	1357	Total 1357	O 1357	0	0
9	O	117	Total 117	O 117	0	0
9	P	377	Total 377	O 377	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.50Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.257	Depositor
Wilson B-factor (Å ²)	45.1	Xtrriage
Anisotropy	0.178	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.499 for -h,-k,l 0.085 for h,-h-k,-l 0.085 for -k,-h,-l	Xtrriage
Total number of atoms	61089	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 568 ligands modelled in this entry, 566 are monoatomic - leaving 2 for Mogul analysis.

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$
7	RBT	M	8002	-	61,66,66	2.97	26 (42%)	87,101,101	1.99	18 (20%)
7	RBT	C	8001	6	61,66,66	2.98	24 (39%)	87,101,101	1.92	20 (22%)

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
7	RBT	M	8002	-	-	18/59/116/116	0/5/6/6
7	RBT	C	8001	6	-	18/59/116/116	0/5/6/6

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	8001	RBT	C9-C8	8.95	1.58	1.41
7	M	8002	RBT	C9-C8	8.64	1.57	1.41
7	M	8002	RBT	C8-C7	7.67	1.54	1.40
7	C	8001	RBT	C5-C6	7.48	1.48	1.39
7	C	8001	RBT	C8-C7	7.32	1.54	1.40

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RBT	C42-C40-C38	7.50	122.58	112.55
7	C	8001	RBT	C42-C40-C38	7.48	122.55	112.55
7	M	8002	RBT	C41-C39-C38	7.31	122.32	112.55
7	C	8001	RBT	C41-C39-C38	7.22	122.20	112.55
7	C	8001	RBT	O3-C6-C5	-5.43	111.08	114.34

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	8001	RBT	C16-C17-C18-C19
7	C	8001	RBT	C26-C27-C28-C29
7	C	8001	RBT	C26-C27-O6-C37

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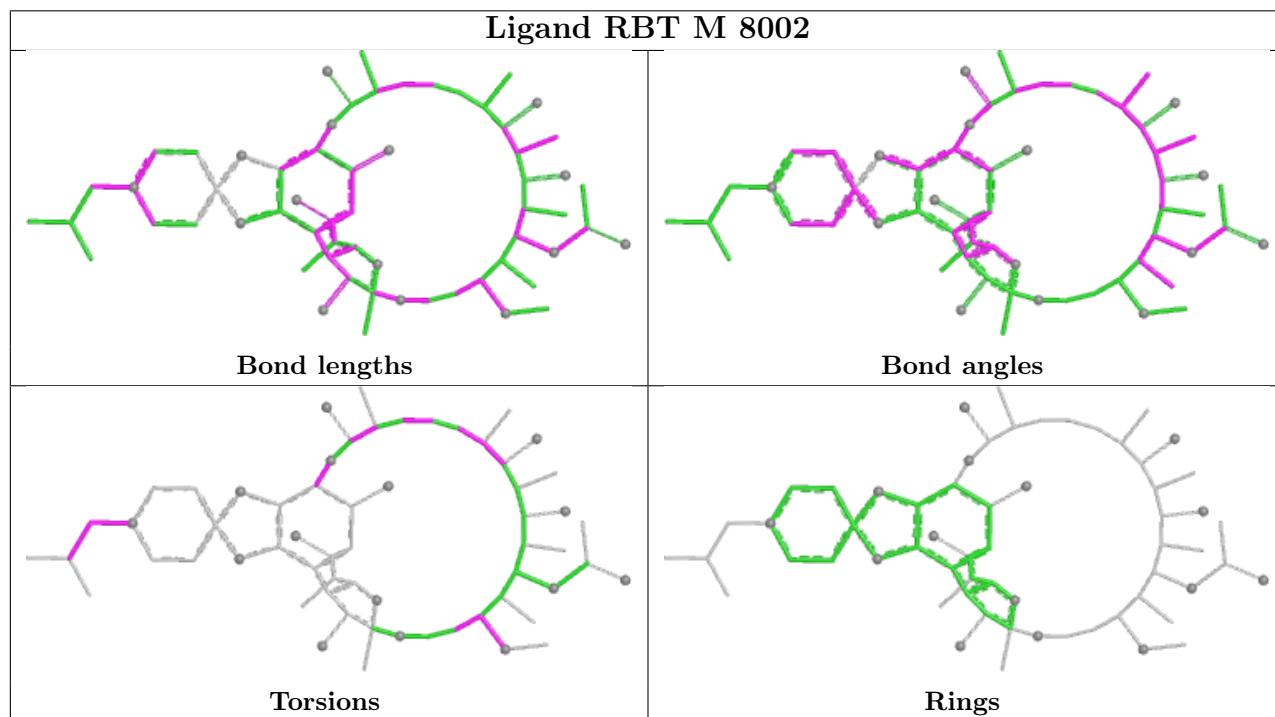
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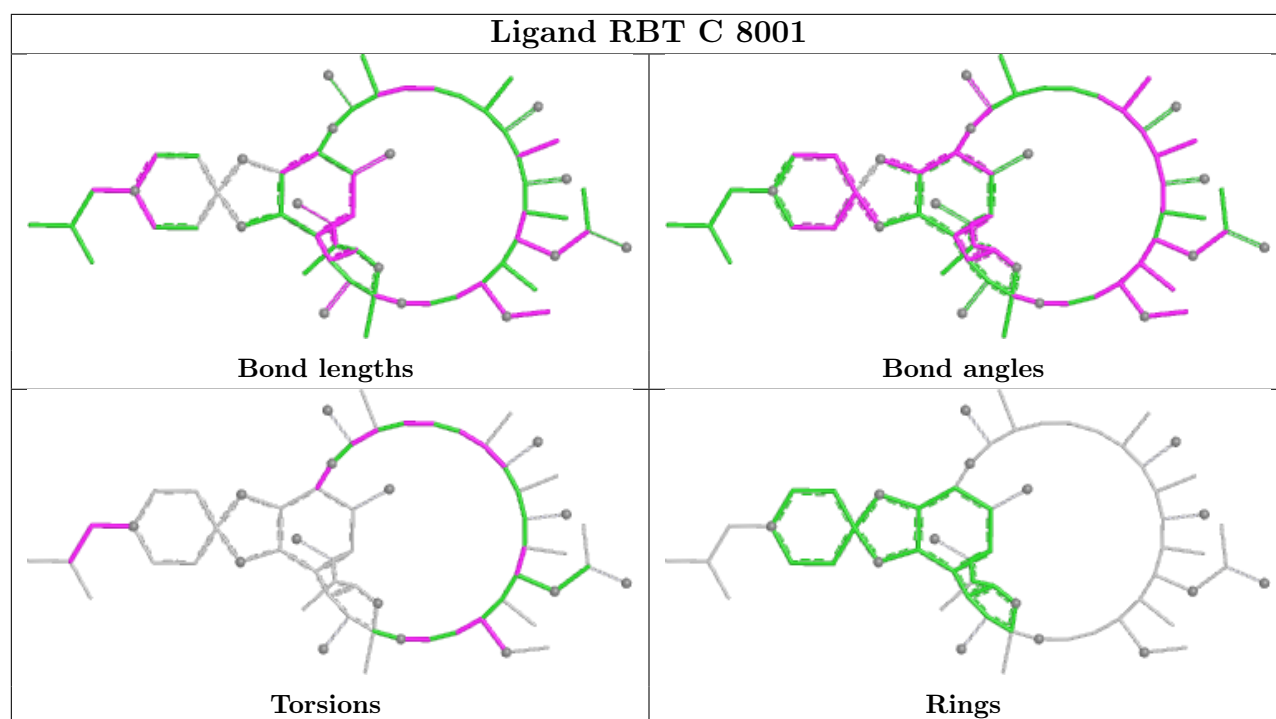
Mol	Chain	Res	Type	Atoms
7	M	8002	RBT	C3-C2-N1-C15
7	M	8002	RBT	C26-C27-O6-C37

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

5.1 Protein, DNA and RNA chains [i](#)

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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