

# Full wwPDB EM Validation Report (i)

Mar 6, 2024 – 12:06 PM JST

PDB ID : 1X18

Title : Contact sites of ERA GTPase on the THERMUS THERMOPHILUS 30S SUB-

UNIT

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Deposited on : 2005-04-02

Resolution : 13.50 Å(reported)

Based on initial models : 1EGA, 1FJF

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*A user guide is available at
<a href="https://www.wwpdb.org/validation/2017/EMValidationReportHelp">https://www.wwpdb.org/validation/2017/EMValidationReportHelp</a>
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

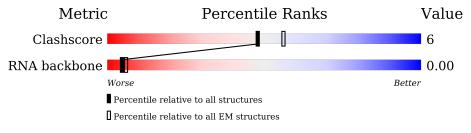
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 13.50 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 $(\# \mathrm{Entries})$	${ m EM~structures} \ (\#{ m Entries})$	
Clashscore	158937	4297	
RNA backbone	4643	859	

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain	
1	A	11	100%	-
2	В	31	100%	
3	С	20	90% 10%	
4	D	24	92% 8%	
5	Е	231	100%	
6	F	154	100%	_
7	G	119	99%	•
8	Н	73	99%	•
9	X	292	98%	



# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 955 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 5'-R(P\*CP\*GP\*AP\*UP\*GP\*GP\*CP\*GP\*AP\*AP\*G)-3'.

Mol	Chain	Residues	Atom	ıs	AltConf	Trace
1	A	11	Total 11	P 11	0	11

• Molecule 2 is a RNA chain called RNA (31-MER).

Mol	Chain	Residues	Atoms	AltConf	Trace
2	В	31	Total P 31 31	0	31

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

Mol	Chain	Residues	Atoms	AltConf	Trace
3	С	20	Total P 20 20	0	20

• Molecule 4 is a RNA chain called 5'-R(P\*UP\*GP\*UP\*UP\*GP\*GP\*GP\*UP\*UP\*AP\*AP\* GP\*UP\*CP\*CP\*GP\*AP\*AP\*AP\*CP\*GP\*AP\*AP\*G)-3'.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	D	24	Total P 24 24	0	24

• Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	E	231	Total C 231 231	0	231

• Molecule 6 is a protein called 30S ribosomal protein S7.



Mol	Chain	Residues	Ato	ms	AltConf	Trace
6	F	154	Total 154	C 154	0	154

• Molecule 7 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	G	119	Total C 119 119	0	119

• Molecule 8 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	Н	73	Total C 73 73	0	73

• Molecule 9 is a protein called GTP-binding protein era.

Mol	Chain	Residues	Ato	ms	AltConf	Trace
9	X	292	Total 292	C 292	0	292



## 3 Residue-property plots (i)

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. 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. 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.

9	nout any outlier are shown as a g	red = 3 or more. Stretches of 2 or more green connector. Residues present in the
• Molecule 1: 5'-R(P*CF	P*GP*AP*UP*GP*GP*CP*GP*	'AP*AP*G)-3'
Chain A:	100%	
There are no outlier resid	dues recorded for this chain.	
• Molecule 2: RNA (31-1	MER)	
Chain B:	100%	
There are no outlier resid	dues recorded for this chain.	
• Molecule 3: 5'-R(P*UI CP*GP*C)-3'	P*UP*CP*CP*CP*GP*GP*	*CP*CP*UP*GP*GP*GP*GP*CP*CP
Chain C:	90%	10%
080 0839 0834 0834		
• Molecule 4: 5'-R(P*UI CP*AP*AP*CP*GP*AI		*UP*AP*AP*GP*UP*CP*CP*GP
Chain D:	92%	8%
C100 A101 A101 A101 A101 A101 A101 A101		
• Molecule 5: 30S riboso	omal protein S2	
Chain E:	100%	
There are no outlier resid	dues recorded for this chain.	
• Molecule 6: 30S riboso	omal protein S7	
Chain F:	100%	
There are no outlier resid	dues recorded for this chain	

There are no outlier residues recorded for this cha

• Molecule 7: 30S ribosomal protein S11



Chain G:	99%		
K11 S129 S129			
• Molecule 8: 30S ribosomal protein S18			
Chain H:	99%		
A20 K88			
• Molecule 9: GTP-binding protein era			
Chain X:	98%		
M.132 M.132 M.285 M.286 M.286 M.286			



# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	1.00Å 1.00Å 1.00Å	Donogitor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	(Not available) – 13.50	Depositor	
% Data completeness	(Not available) ((Not available)-13.50)	Depositor	
(in resolution range)	, , ,	Depositor	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
Refinement program	unknown	Depositor	
$R, R_{free}$	(Not available) , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	955	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP	



## 5 Model quality (i)

### 5.1 Standard geometry (i)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	11	0	0	0	0
2	В	31	0	0	0	0
3	С	20	0	0	2	0
4	D	24	0	0	2	0
5	Е	231	0	0	0	0
6	F	154	0	0	0	0
7	G	119	0	0	1	0
8	Н	73	0	0	1	0
9	X	292	0	0	6	0
All	All	955	0	0	6	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 6.

All (6) 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)
8:H:20:ALA:CA	9:X:181:PRO:CA	1.89	1.46
4:D:101:A:P	9:X:132:LYS:CA	2.48	1.01
3:C:930:C:P	9:X:285:TRP:CA	2.52	0.96
4:D:100:C:P	9:X:135:LEU:CA	2.81	0.69
7:G:92:GLU:CA	9:X:271:ALA:CA	2.87	0.51
3:C:929:G:P	9:X:286:ALA:CA	3.09	0.41

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

#### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/11	-	-
2	В	0/31	-	-
3	С	0/20	-	-
4	D	0/24	-	-
All	All	0/86	-	-

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 (i)

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

### 5.5 Carbohydrates (i)

There are no monosaccharides 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.

