Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Mar 2, 2017 – 11:05 am GMT

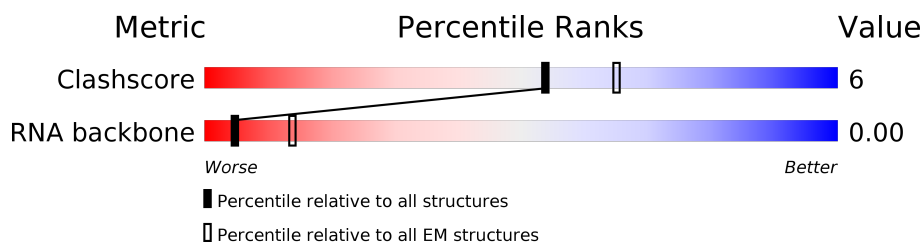|		
PDB ID	:	1X18
Title	:	Contact sites of ERA GTPase on the THERMUS THERMOPHILUS 30S SUBUNIT
Authors	:	Sharma, M.R.; Barat, C.; Agrawal, R.K.
Deposited on	:	2005-04-02
Resolution	:	13.50 Å(reported)
Based on PDB ID	:	1FJF, 1EGA

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
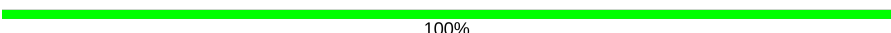*ELECTRON MICROSCOPY*
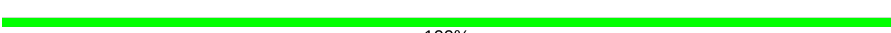
The reported resolution of this entry is 13.50 Å.

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	Percentile Ranks	Value
Clashscore		6
RNA backbone		0.00

Worse   *Better*

▮ Percentile relative to all structures

❘ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	11	100%
2	B	31	100%
3	C	20	90% 10%
4	D	24	92% 8%
5	E	231	100%
6	F	154	100%
7	G	119	99% •
8	H	73	99% •
9	X	292	98% •

2 Entry composition ⓘ

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	Atoms		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	B	31	Total 31	P 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*GP*CP*CP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	20	Total 20	P 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*CP*GP*CP*AP*AP*CP*GP*AP*G)-3'.

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

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

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

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

Mol	Chain	Residues	Atoms	AltConf	Trace
6	F	154	Total C 154　　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	H	73	Total C 73　　73	0	73

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

Mol	Chain	Residues	Atoms	AltConf	Trace
9	X	292	Total C 292　　292	0	292

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.

• Molecule 1: 5'-R(P*CP*GP*AP*UP*GP*GP*CP*GP*AP*AP*G)-3'

Chain A:

There are no outlier residues recorded for this chain.

• Molecule 2: RNA (31-MER)

Chain B:

There are no outlier residues recorded for this chain.

• Molecule 3: 5'-R(P*UP*UP*CP*CP*CP*GP*GP*GP*CP*CP*UP*GP*GP*GP*GP*CP*CP*CP*GP*C)-3'

Chain C:
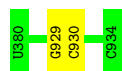
• Molecule 4: 5'-R(P*UP*GP*UP*UP*GP*GP*GP*UP*UP*AP*AP*GP*UP*CP*CP*CP*GP*CP*AP*AP*CP*GP*AP*G)-3'

Chain D:

• Molecule 5: 30S ribosomal protein S2

Chain E:

There are no outlier residues recorded for this chain.

• Molecule 6: 30S ribosomal protein S7

Chain F:

There are no outlier residues recorded for this chain.

• Molecule 7: 30S ribosomal protein S11

Chain G:

99%

K11 E92 S129

• Molecule 8: 30S ribosomal protein S18

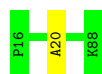Chain H:

99%

P16 A20 K88

• Molecule 9: GTP-binding protein era

Chain X:

98%

D4 K132 L135 P181 A271 W285 A286 L295

4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of 3D-MAPS by wiener filtration	Depositor
Microscope	FEI TECANI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	2000	Depositor
Minimum defocus (nm)	1180	Depositor
Maximum defocus (nm)	3940	Depositor
Magnification	49696	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 ⓘ

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	B	31	0	0	0	0
3	C	20	0	0	2	0
4	D	24	0	0	2	0
5	E	231	0	0	0	0
6	F	154	0	0	0	0
7	G	119	0	0	1	0
8	H	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 ⓘ

5.3.1 Protein backbone ⓘ

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

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/11	-	-
2	B	0/31	-	-
3	C	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 ⓘ

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

5.5 Carbohydrates ⓘ

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.