Molecular Cell, ***Volume 31***

Supplemental Data

Molecular Mechanism of Sequence-Directed DNA Loading and Translocation by FtsK

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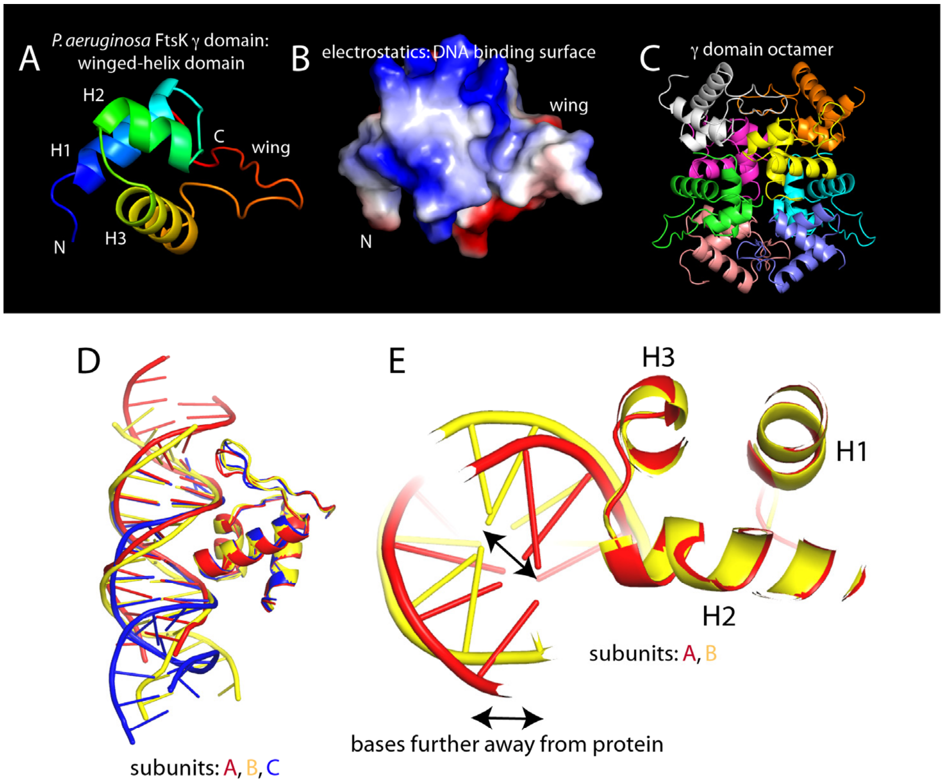


Figure 1 supplement, Löwe *et al.*

Crystal structure of unbound *Pseudomonas aeruginosa* FtsKγ.

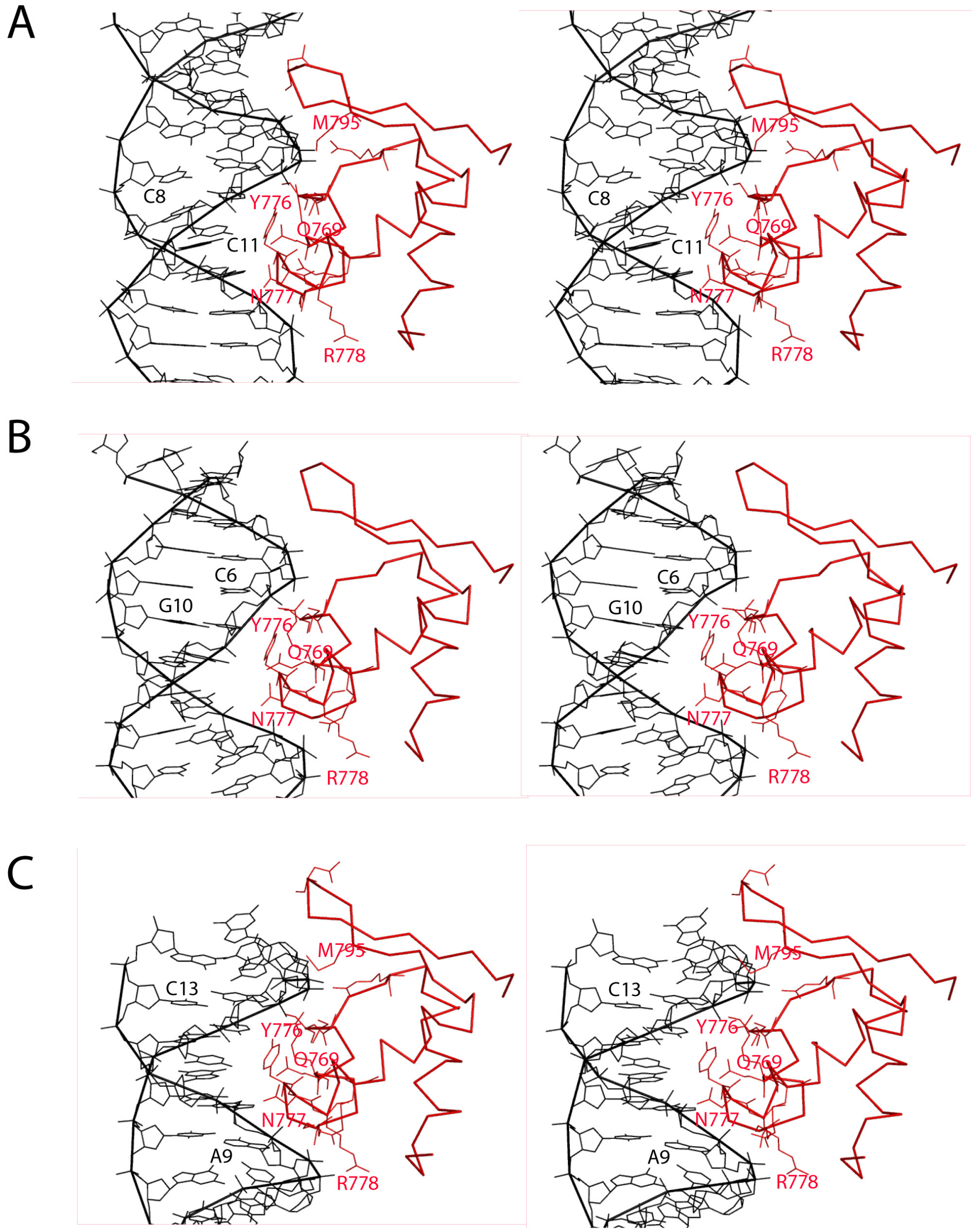
A) *Pseudomonas aeruginosa* FtsKγ (GSS-742-811) is a winged helix domain (WHD). The very common fold consists of three helices (H1-H3) and a wing with some residues in β sheet conformation. Reviewed in (Gajiwala and Burley, 2000).

B) The electrostatic potential of isolated PaFtsKγ shows strong positive charge around the tips of helices H2 and H3, making this the likely DNA-binding surface, as previously determined by NMR (Sivanathan et al., 2006).

C) In the crystals of PaFtsKγ, the protein forms a very tight octamer with 222 point symmetry of unknown biological significance.

D) Superposition of the three γ domains bound to DNA. A is in red, B is in yellow and C is in blue. All three subunits share a very similar binding mode.

E) Subunit B is further away from the bases than subunit A and C. Only subunits A and B are shown for clarity and it becomes apparent that the DNA twists away locally from subunit B allowing different bases to be recognised.



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chain I 5': G5 - G6 - G7 - C8 - A9 - G10- G11- G12
             |    |    |    |    |    |    |    |
chain J 3': C12- C11- C10- G9 - T8 - C7 - C6 - C5
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Figure 2 supplement, Löwe *et al.*

Detailed stereo views of the γ domains A, B and C bound to KOPS DNA. The residues in contact with the DNA are summarised in table 1 supplement. Subunit B differers in binding mode from A and C because it recognises a different sequence on the DNA. All specific contacts with the DNA are through water molecules (not shown for clarity, see table 1 supplement).

Table 1 supplement

DNA-protein interactions for the three gamma domains

subunit A

R762	backbone
I765	sugar
Q769	sequence specific (NE2:O6 of G6 via water 49) (OE1:N4 of C10 via water 67)
R770	backbone
K773	backbone
Y776	stacks against bases
N777	sequence specific (OD1:N4 of C12 via water 43)
R778	backbone
R781	distant backbone

wing:

M795	sugar
N798	backbone

subunit B

I765	sugar
S766	sequence specific (OG:N4 of C7 via water 4)
Q769	sequence specific (NE2:O4 of T8 via water) (OE1:N6 of A9 via water 81)
Y776	stacks against bases
R778	backbone
R781	backbone

wing:

no sidechains contact

subunit C

R762	backbone
I765	sugar
S766	sequence specific (OG:N7 of G4 via water)
Q769	sequence specific (NE2:O6 of G11 via water 139) (OE1:N4 of C5 via water 203)
R770	backbone
K773	backbone
Y776	stacks against bases
N777	sequence specific (OD1:N4 of C7 via water 56)
R778	backbone
R781	backbone

wing:

M795	sugar