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Topical Perspectives

# Dynamic characteristics of a flagellar motor protein analyzed using an elastic network model

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ABSTRACT

At the base of a flagellar motor, its rotational direction and speed are regulated by the interaction between rotor and stator proteins. A switching event occurs when the cytoplasmic rotor protein, called C-ring, changes its conformation in response to binding of the CheY signal protein. The C-ring structure consists of FliG, FliM, and FliN proteins and its conformational changes in FliM and FliG including $Helix_{MC}$ play an important role in switching the motor direction. Therefore, clarifying their dynamic properties as well as conformational changes is a key to understanding the switching mechanism of the motor protein. In this study, to elucidate dynamic characteristics of the C-ring structure, both harmonic (intrinsic vibration) and anharmonic (transition pathway) analyses are conducted by using the symmetry-constrained elastic network model. As a result, the first three normal modes successfully capture the essence of transition pathway from wild type to CW-biased state. Their cumulative square overlap value reaches up to 0.842. Remarkably, it is also noted from the transition pathway that the cascade of interactions from the signal protein to FliM to FliG, highlighted by the major mode shapes from the first three normal modes, induces the reorientation ($\sim 100^{\circ}$ rotation of $FliG_{C5}$) of FliG C-terminal that directly interacts with the stator protein. Presumably, the rotational direction of the motor protein is switched by this substantial change in the stator-rotor interaction.

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## 1. Introduction

The flagellar motor is an important organelle in many bacteria because it propels the bacteria in a liquid environment so that it can find a suitable place for survival [1]. Counterclockwise (CCW) rotation of all flagellar motors propels the cell body forward. When flagellar motors change their rotational direction to the clockwise (CW) direction, the cell tumbles and it changes swimming direction in a liquid media [2]. In this way, the cell can move towards a more favorable environment and escapes from unfavorable conditions.

In Fig. 1, the base of a basal body is embedded in the cell membrane and consists of two major parts: stator proteins and the rotor proteins (MS-ring, Cytoplasmic-ring, hook, filament, and other proteins) [3,4]. The MS-ring, which is an assembly of 26 copies of the FliF proteins, transmits torque to the filament directly [3,5]. The stator proteins and C-ring electrostatically interact each other [6]. The core of the stator proteins is composed of $MotA_4MotB_2$ complexes and located in the peptidoglycan layer [7–9]. The C-ring is composed of FliG, FliM, and FliN proteins [3]. The C-terminal domain of FliG electrostatically interacts with the cytoplasmic loop of the MotA stator protein. This interaction can generate torque on the motor and also change the rotational direction of the flagellar motor [9]. Switching of the motor is regulated by a chemotactic regulator, the CheY signal protein, which binds between the FliM and FliN, inducing conformational changes of the FliG proteins and allowing the motor to rotate in the CW direction [10,11]. For the rotational direction, the switch between CW and CCW takes milliseconds with no significant change in rotational speed [12,13]. This effective switching mechanism could be attributed to the cooperativity of the motor [14].

Although the entire structure of C-ring has not yet been elucidated, structures related to the FliG and FliM proteins have been revealed in Fig. 2. The middle and C-terminal domain of FliG and the middle domain of FliM ($FliG_{MC}$-$FliM_M$) in *Thermotoga maritime* (TM) form a complex (PDB ID: 4FHR), as shown in Fig. 2A, and its structure was revealed by X-ray diffraction [15]. In this protein complex, the C-terminal domain of FliG can be divided into two subdomains: the armadillo repeated motif (ARM) and the bundle of six helices

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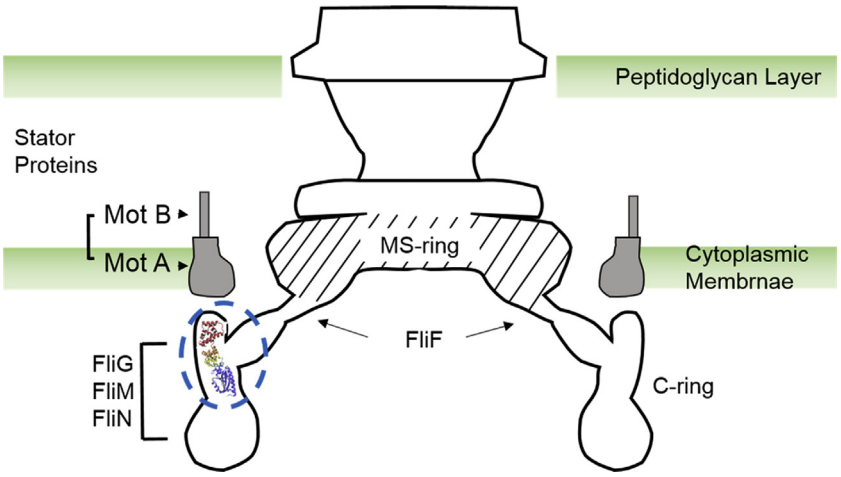


**Fig. 1.** The flagellar motor exists in the cell membrane. Torque is generated by a proton motive force, which is a flow of ions across the cytoplasmic membrane. The MS-ring, which is composed of FliF proteins, transmits torque from the cytoplasmic ring (C-ring) to the helical filament. The C-ring consists of three proteins: FliG, FliM, and FliN. Interaction between FliG in the C-ring and a stator protein produces torque energy, and the rotational direction of the motor can be regulated by the switching mechanism. The unit model proposed in this study is indicated by the blue circle.

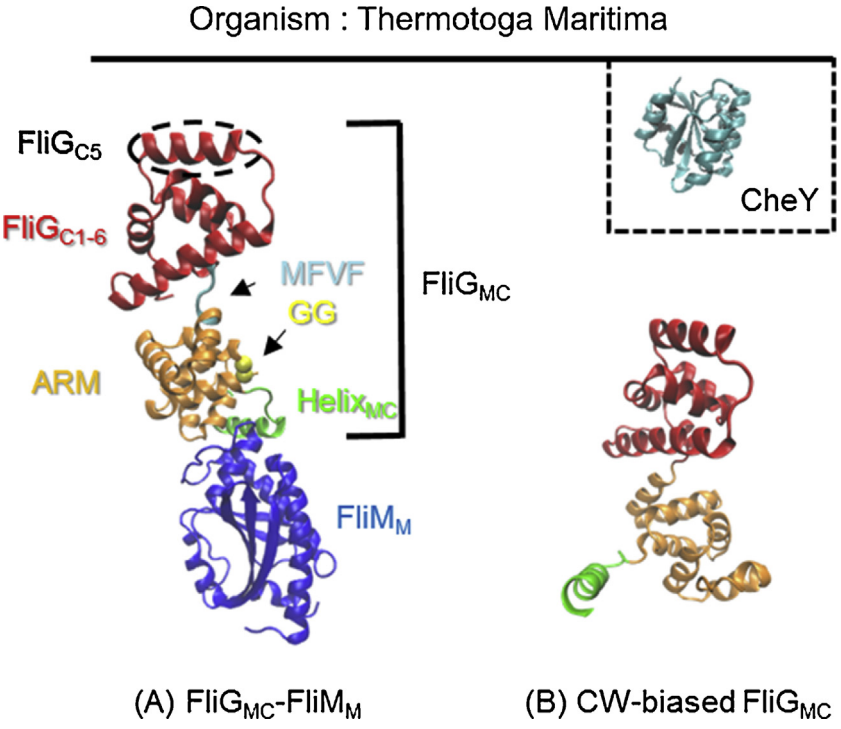


**Fig. 2.** Various domains and motifs of FliG. Each name matches with its corresponding part in the PDB structure by color. The signal protein CheY is inserted in the dotted box. (A) $FliG_{MC}$-$FliM_{M}$ complex including conserved motifs GG and MFVF (PDB ID: 4FHR) (B) Clockwise-biased $FliG_{MC}$ (PDB ID: 3AJC).

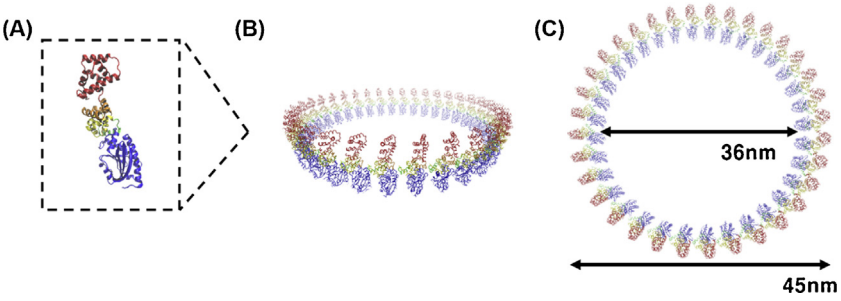


**Fig. 3.** $FliG_{MC}$-$FliM_{M}$ (PDB ID: 4FHR) is used for constructing the unit model. A total of 34 copies of the unit model constructs the C-ring, and its diameter agrees well with previous research. (A) The unit model of the C-ring. (B) Side view of the ring structure. (C) Top view of the ring structure.

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