

Volume 77 (2021)

Supporting information for article:

Structure of a dimer of the Sulfolobus solfataricus MCM N-terminal domain reveals a potential role in MCM ring opening

Martin Meagher, Madison N. Spence and Eric J. Enemark

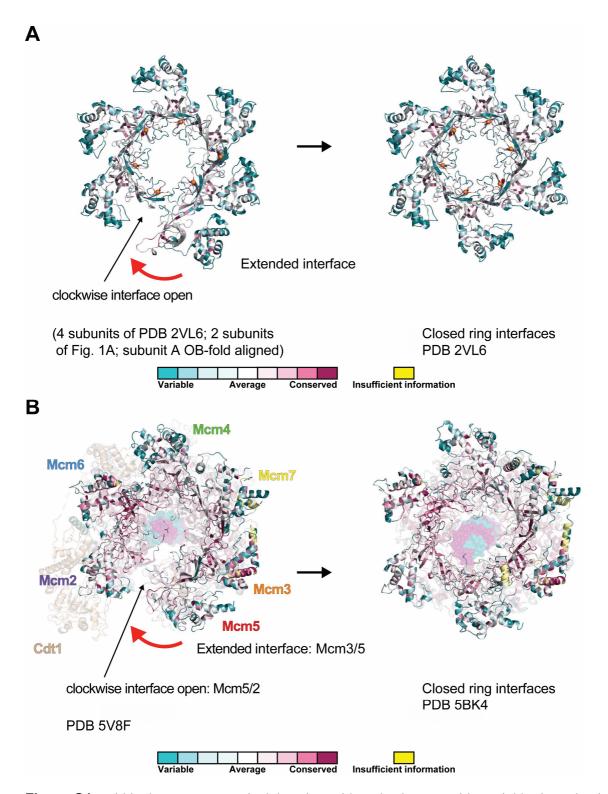


Figure S1 Within the MCM N-terminal domain, residues that interact with a neighboring subunit or with Cdt1 are generally not well-conserved. Each residue of SsoMCM (A) or eukaryotic MCM (B) is shaded according to its conservation score in ConSurf-DB (Ben Chorin et al., 2020; Goldenberg et al., 2009). The illustrations are otherwise identical to those of Figure 4 with the cylinders removed for clarity. The color scheme is as defined by ConSurf graded from highly conserved in magenta to highly variable in teal and residues with insufficient information in yellow. Please provide a brief description

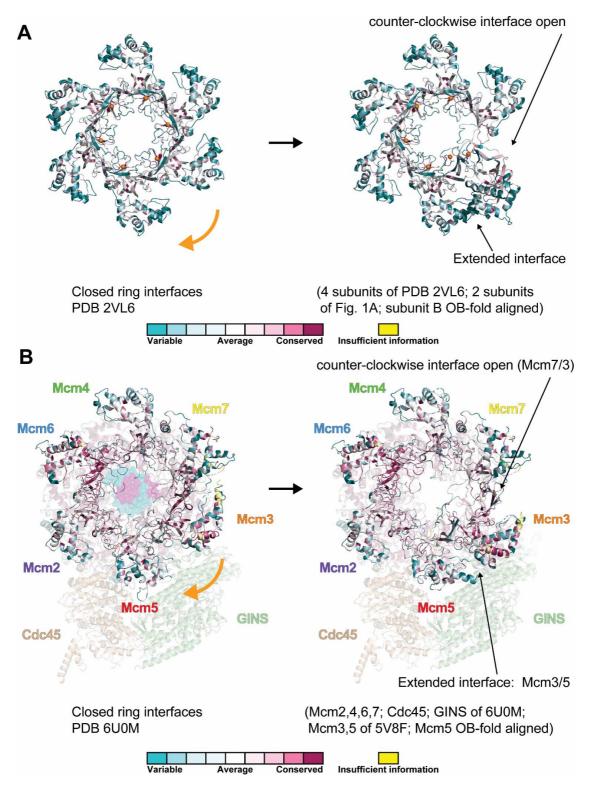


Figure S2 Within the MCM N-terminal domain, residues that interact with a neighboring subunit, Cdc45, or GINS are generally not well-conserved. Each residue of SsoMCM (A) or eukaryotic MCM (B) is shaded according to its conservation score in ConSurf-DB (Ben Chorin et al., 2020; Goldenberg et al., 2009). The illustrations are otherwise identical to those of Figure 5 with the cylinders removed for clarity. The color scheme is as defined by ConSurf graded from highly conserved in magenta to highly variable in teal and residues with insufficient information in yellow.

Video S1 Open-to-closed ring transformations of MCM loading as depicted in Figure 4. An extended interface stabilizes an open interface to the clockwise side. Views are from the N-terminal side of the complex. The structures and orientations of the OB-fold β -barrels are emphasized with a cyan tube with a magenta stripe. Left) The open ring structure consists of the closed ring SsoMCM-N hexamer (PDB 2VL6 (Liu et al., 2008)) with two subunits replaced by the dimer structure of this study superimposed based on the OB-fold of chain A (as in Figure 4A, left). The closed ring structure is the closed ring SsoMCM-N hexamer (PDB 2VL6 (Liu et al., 2008)). Right) Transformation between two bona-fide species of MCM loading. The open ring structure is the cryo-EM structure of OOCM bound to DNA (PDB 5V8F; (Yuan et al., 2017)). Orc1-6:Cdc6 are excluded for clarity. The closed ring structure is one Mcm2-7 hexamer of the cryo-EM structure of the Mcm2-7 double-hexamer encircling DNA (PDB 5BK4; (Noguchi et al., 2017)). An extended interface between Mcm3 and Mcm5 correlates with a gap at the Mcm5/2 gate.

Video S2 Proposed closed-to-open MCM ring transformations of MCM activation as depicted in Figure 5. An extended interface stabilizes an open interface to the counter-clockwise side. Views are from the N-terminal side of the complex. The structures and orientations of the OB-fold β -barrels are emphasized with a cyan tube with a magenta stripe. Left) The closed ring structure is the closed ring SsoMCM-N hexamer (PDB 2VL6 (Liu et al., 2008)). The open ring structure consists of the closed ring SsoMCM-N hexamer (PDB 2VL6 (Liu et al., 2008)) with two subunits replaced by the dimer structure of this study superimposed based on the OB-fold of chain B (as in Figure 5A, right). Right) The closed ring structure is the cryo-EM structure of CMG encircling DNA (PDB 6U0M; (Yuan et al., 2020)). An open ring model was generated by replacing CMG subunits Mcm3 and Mcm5 by those of open ring OOCM (PDB 5V8F; (Yuan et al., 2017)) which had been superimposed onto CMG based on the OB-fold of Mcm5 (see Figure 5B, right). The model has a gap in the ring between Mcm7 and Mcm3, the proposed interface for strand exit during MCM activation