

Supplementary Tables and Figures

Supplementary Table S1. Coordination distances between metal ion and donor atoms in *SaFtsZf*-GDP and *SaFtsZt*-GDP

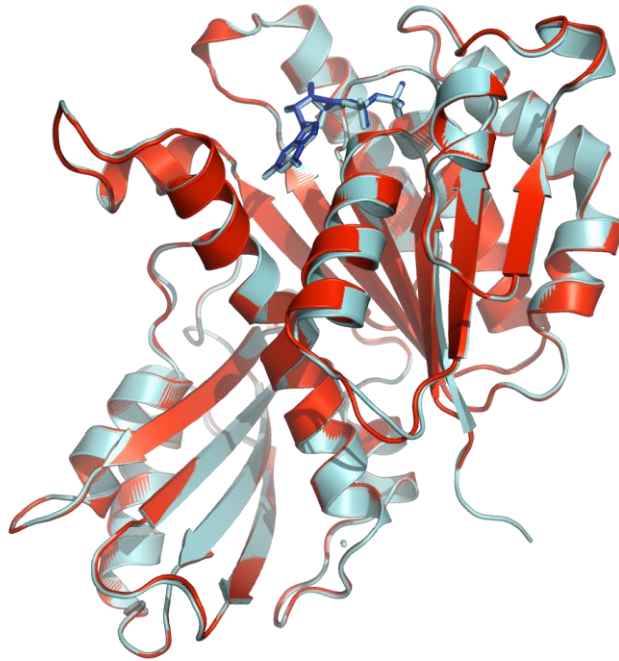
	<i>SaFtsZf</i> mol A	<i>SaFtsZf</i> mol B	<i>SaFtsZt</i>
Coordination distances ^a			
Leu200	2.31	2.39	2.26
Val203	2.29	2.27	2.35
Asn208 CO [□]	2.40	2.44	2.36
Leu209	2.43	2.44	2.36
H ₂ O	2.45	2.46	2.41
H ₂ O	2.46	2.55	2.45
Structural condition of the calcium ion			
Occupancy	0.87	0.75	0.66

^a Coordination distances were determined using *Coot* (Emsley & Cowtan, 2004).

Supplementary Table S2. RMS conformational differences between asymmetric molecules in apo-form^a.

	mol A	mol B	mol C	mol D
mol A	-	0.48 Å	0.58 Å	0.51 Å
mol B	-	-	0.67 Å	0.54 Å
mol C	-	-	-	0.77 Å

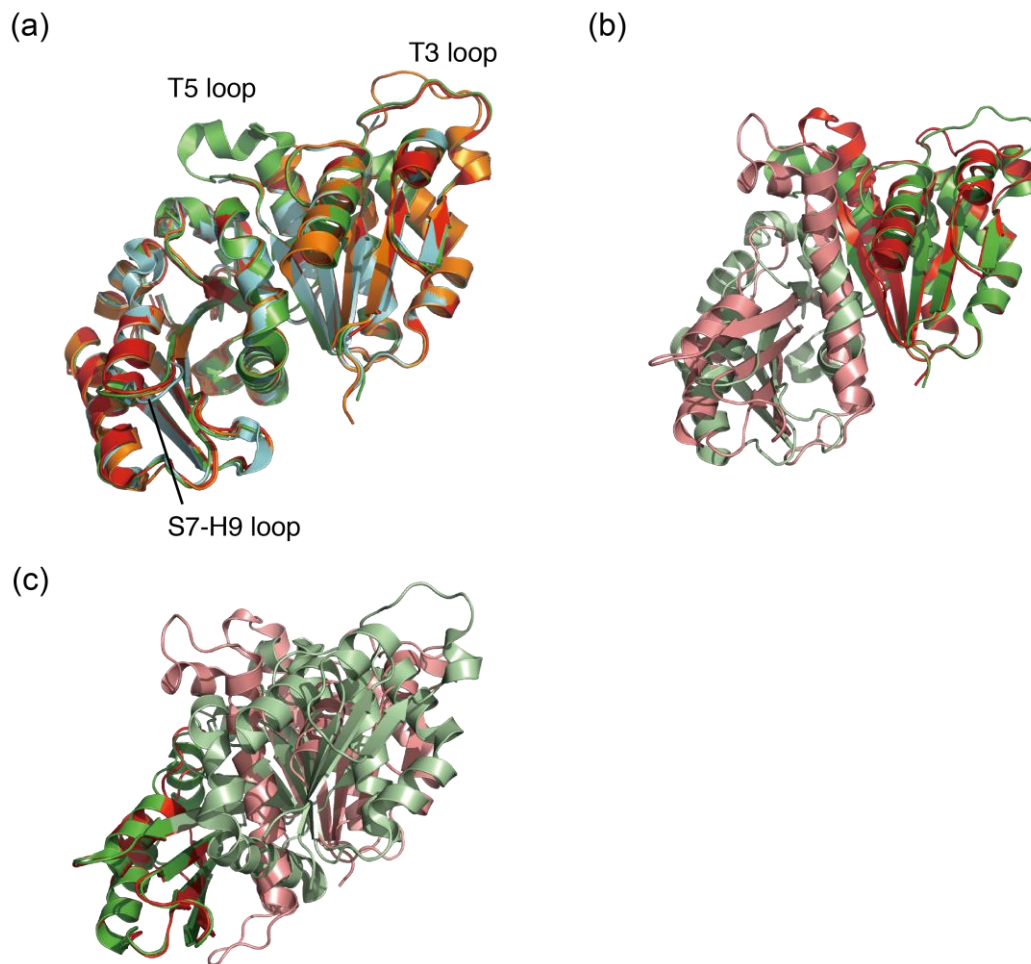
^aThe conformational differences of the four independent molecules in the apo-form, except for the residues in disordered and highly flexible loops (residues 31 – 38, 52 – 54, 67 – 73, 137 – 146, 217 – 223, 231 – 237) were calculated from the C α coordinates in the calculation region using *PyMOL* (Schrödinger, 2010).



Supplementary Figure S1. Structure comparison between *SaFtsZf*-GDP and *SaFtsZt*-GDP. *SaFtsZf*-GDP and *SaFtsZt*-GDP are colored red and cyan, respectively. GDPs bound to *SaFtsZf*-GDP and *SaFtsZt*-GDP are represented as blue and cyan sticks, respectively. The divalent cations coordinated to *SaFtsZf*-GDP and *SaFtsZt*-GDP are represented as green and cyan spheres, respectively.

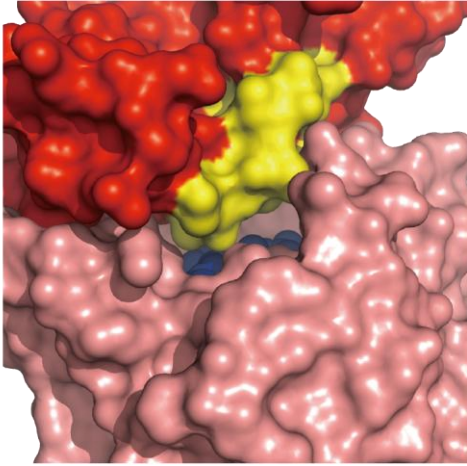


Supplementary Figure S2. Structure comparison between Native *SaFtsZt* (mol C) and SeMet *SaFtsZt* (mol C). Native and SeMet proteins are colored green and orange, respectively. These two molecules were superposed well with root mean square deviations (rmsd) of 0.42 Å for backbone C α atoms.

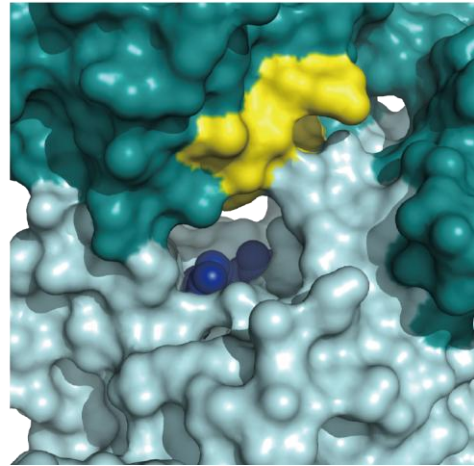


Supplementary Figure S3. Structural comparisons of the apo-form. (a) Four asymmetric molecules are compared, and are colored green, cyan, magenta, and orange, respectively. The conformations of the T3 loop (residues 66 – 75) and the S7 – H9 loop (residues 231 – 236) were flexible, and the H1 – S2 loop (residues 31 – 37) and the T5 loop (residues 136 – 146) were disordered except for mol C. (b) – (c) These figures show the structural comparisons between GDP-form and apo-form. The GDP-form and apo-form are colored red and green, respectively. Panels (b) and (c) show the best-fitting superpositions of N-terminal subdomain (residues 12 – 161) and C-terminal subdomain (residues 230 – 310), respectively. The regions not superposed in each structure are shown in pale color.

(a)

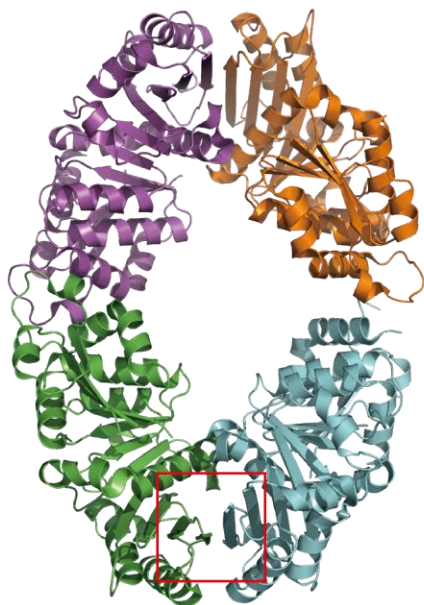


(b)

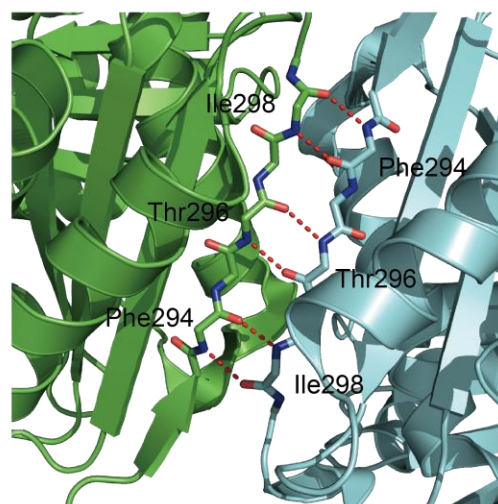


Supplementary Figure S4. Structural comparison between the nucleotide-binding pockets in the GDP-form and in *MjFtsZ* (PDB ID: 1W5A). (a) *SaFtsZ* and its contacting molecule are represented in red and pink, respectively. (b) Dimer molecules of *MjFtsZ* are represented in teal and cyan, respectively. These figures are viewed from the same directions. Yellow surfaces show the T7 loop. GDP bound to the GDP-form and GTP bound to *MjFtsZ* are represented as blue spheres.

(a)



(b)



Supplementary Figure S5. Crystal structures of the apo-form. (a) This figure shows the four asymmetric molecules of apo-form in an asymmetric unit. Four molecules are indicated in orange, green, magenta, and cyan, respectively. (b) An anti-parallel β -sheet is formed between mol A and mol B. This interaction is marked by the red box in (a). Hydrogen bonds are indicated as red dotted lines. The distances between Phe294 N and Ile298 CO, Phe294 CO and Ile298 N, Thr296 N and Thr296 CO, Thr296 CO and Thr296 N, Ile298 N and Phe294 CO, and Ile298 CO and Phe294 N are 3.1, 2.7, 2.9, 2.9, 2.6, 3.0 Å, respectively.



Supplementary Figure S6. *Fo-Fc* map of PC190723 complex. *SaFtsZ*, calcium ion, and GDP are represented as blue cartoon, green sphere, and blue sticks, respectively. Chlorine, nitrogen, oxygen, sulfur, fluorine and carbon atoms of PC190723 are colored green, blue, red, yellow, sky-blue, and cyan, respectively. Orange mesh represents the *Fo-Fc* map. *Fo-Fc* maps are displayed over 3.0σ .

(a)

lane No.	1	2	3	4	5	6	7
NaCl (mM)		-	5	25	50	100	200
1 mM GTP		+	+	+	+	+	+
SaFtsZf							

(b)

lane No.	1	2	3	4	5	6	7
KCl (mM)		-	5	25	50	100	200
1 mM GTP		+	+	+	+	+	+
SaFtsZf							

Supplementary Figure S7. The sedimentation assay using sodium and potassium ions. These procedures are the same as the sedimentation assay in the main article, except for the sedimentation buffer (20 mM HEPES-KOH, pH 7.5 and 1 mM MgCl₂). Sodium and potassium ions cannot polymerize *SaFtsZ*.

References

- Emsley, P. & Cowtan, K. (2004). *Acta crystallographica. Section D, Biological crystallography* **60**, 2126-2132.
- Schrödinger, L. L. C. (2010). *The PyMOL Molecular Graphics System, Version 1.3*.