Supporting Information

Free Energy Analysis of a Conformational Change of Heme ABC Transporter BhuUV-T

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Table S1. Selected atoms for tMD and the string method calculation

simulation	selected atoms[†]
targeted MD & string method	((((segid:PRA or segid:PRB) and not rno:22-28 and not rno:356-362 and \ not rno:49-55 and \ not rno:133-144 and \ not rno:167-172 and \ not rno:282-289 and \ not rno:330-336) or \ ((segid:PRC or segid:PRD) and not rno:1-7 and not rno:267-273 and \ not rno:10-16 and \ not rno:49-61 and \ not rno:91-95 and \ not rno:165-174 and \ not rno:109-120)) and \ (an:CA)) or \ ((segid:PRC or segid:PRD) and (rno:90 and an:CD)) or \ ((segid:PRC or segid:PRD) and (rno:90 and an:OE1)) or \ ((segid:PRC or segid:PRD) and (rno:90 and an:NE2)) or \ ((segid:PRC or segid:PRD) and (rno:36 and an:CG)) or \ ((segid:PRC or segid:PRD) and (rno:36 and an:ND2)) or \ ((segid:PRC or segid:PRD) and (rno:40 and an:NZ)) or \ ((segid:PRC or segid:PRD) and (rno:41 and an:OG)) or \ ((segid:PRC or segid:PRD) and (rno:42 and an:OG1)) or \ ((segid:PRC or segid:PRD) and (rno:147 and an:CB)) or \ ((segid:PRC or segid:PRD) and (rno:147 and an:OG)) or \ ((segid:PRC or segid:PRD) and (rno:180 and an:CG)) or \ ((segid:PRC or segid:PRD) and (rno:181 and an:CD)) or \ ((segid:PRC or segid:PRD) and (rno:185 and an:O)) or \ ((segid:PRC or segid:PRD) and (rno:214 and an:ND1)) or \ ((segid:PRC or segid:PRD) and (rno:214 and an:NE2)) or \ ((segid:PRC or segid:PRD) and (rno:214 and an:CG)) or \

((segid:PRA or segid:PRB) and (rno:108 and an:CG)) or \

((segid:PRA or segid:PRB) and (rno:108 and an:ND2)) or \

((segid:PRA or segid:PRB) and (rno:110 and an:CG))

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† Atom selections are described in the GENESIS selection format (https://www.r-ccs.riken.jp/labs/cbrt/). "PRX" denotes the protomer X. Protomer A and B correspond to the TMDs, while protomer C and D to the NBDs. Atom names follow the PDB nomenclature.

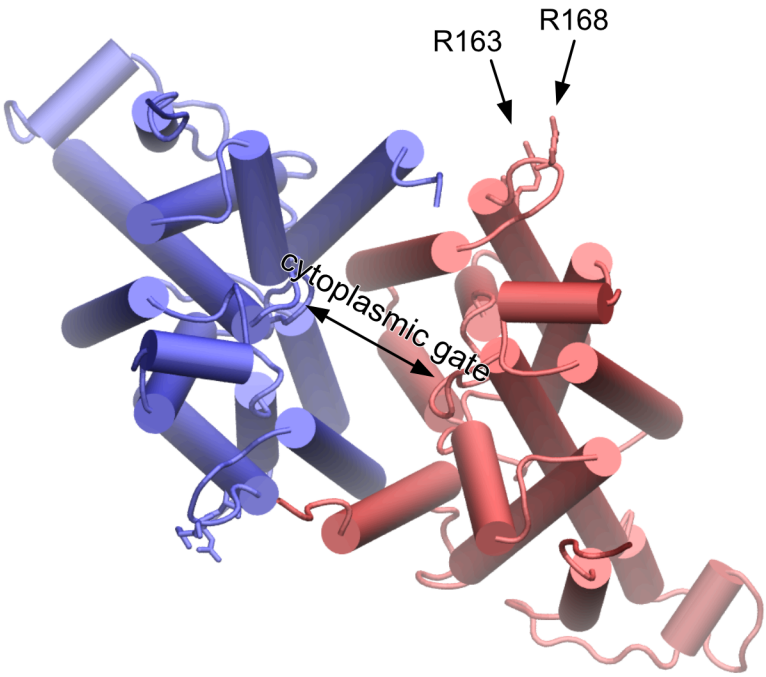

Figure S1. Residues that could be labeled by dyes. The protein (BhuUs only) is shown from the cytoplasmic side. The side chains of R163 and R168 are shown in a stick representation.

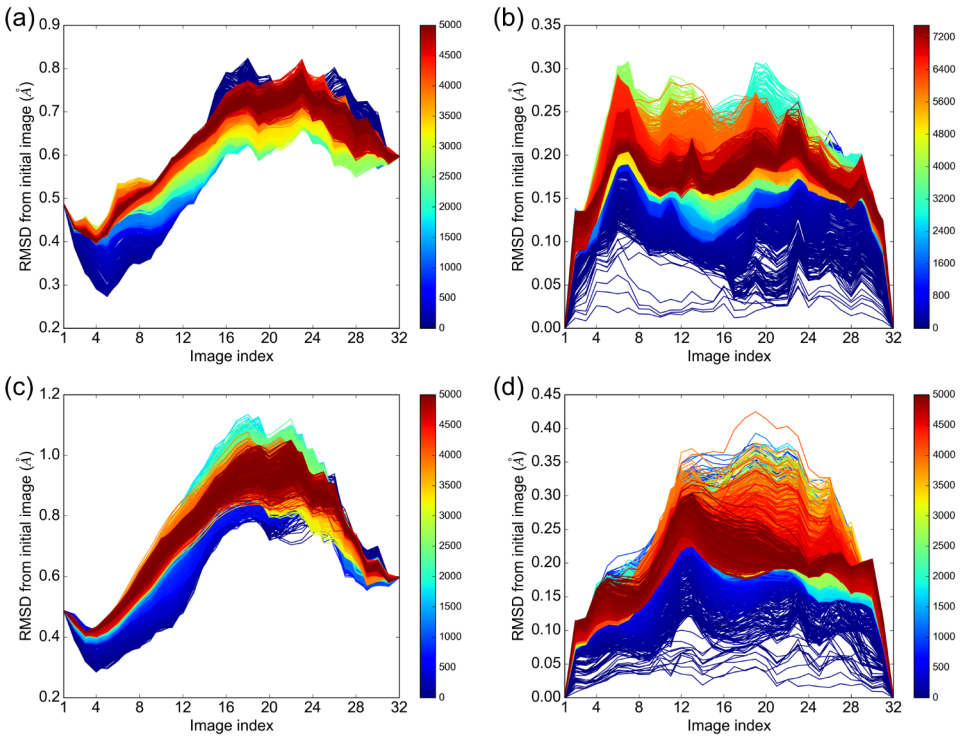

Figure S2. Convergence of the string calculations. The RMSD from the initial image was calculated for each cycle and plotted according to the color bar on the right side. (a-d) The evolution of RMSD of the second (a), third (b), fourth (c), and fifth (d) string calculations. Note that the terminal images (image 1 and 32) were fixed.