Supplementary Material

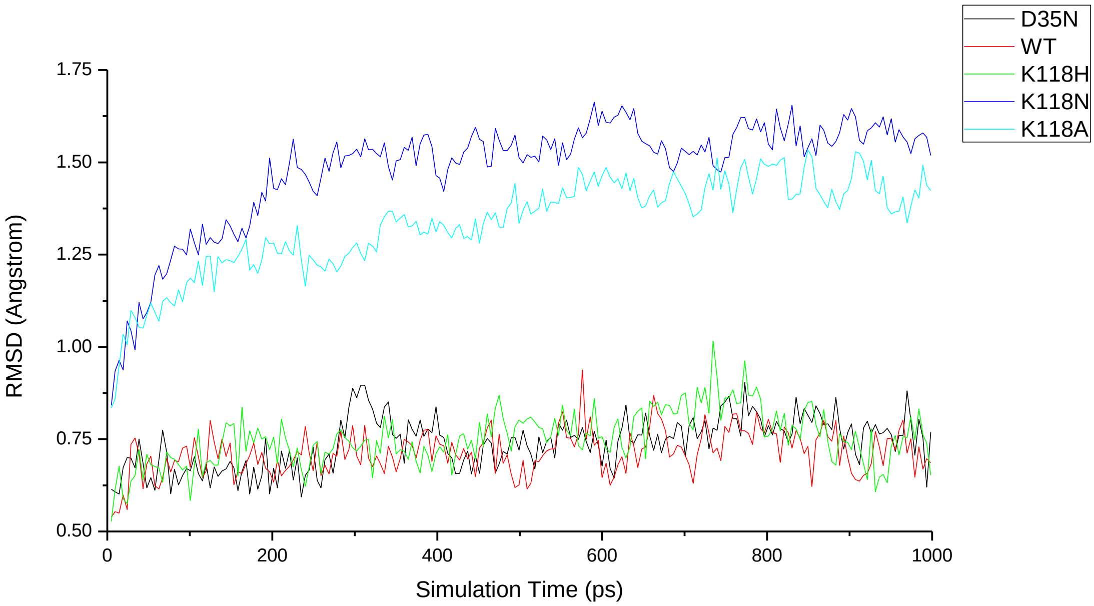

Figure S1. R.m.s.d. of Cα (residues 2-206) during the course of MD simulation compared with the corresponding equilibration structure.

Table S1. Bacterial strains, plasmids, and primers used in *entB* deletion

Strain, plasmid, or primer	Relevant characteristics	Source (reference)
Strains		
BL21 (DE3)	An *E.coli* B strain with DE3 , a λ prophage carrying the T7 RNA polymerase gene and lacI^q	Reference (20)
BL21 (DE3) *ΔentB-ICL*	BL21 (DE3) mutant deleted of *entB-ICL* gene	This work
Plasmids		
pET-21b/*vibB-ISC*	Ap^r; *vibB-ICL gene* cloned into pET-21b	This work
pET-21b/*entB-ICL*	Ap^r; *entB-ICL gene* cloned into pET-21b	This work
pET-21b/*vibB-ISC-K118N*	Ap^r; mutated *vibB-ISC gene (K118N)* cloned into pET-21b	This work
pET-21b/*vibB-ISC-K118H*	Ap^r; mutated *vibB-ISC gene (K118H)* cloned into pET-21b	This work
pET-21b/*vibB-ISC-K118A*	Ap^r; mutated *vibB-ISC gene (K118A)* cloned into pET-21b	This work
pET-21b/*vibB-ISC-D35N*	Ap^r; mutated *vibB-ISC gene (D35N)* cloned into pET-21b	This work
pKD46	Ap^r, Red recombinase expression plasmid	Reference (19)
pKD4	Ap^r, Kan^r; FRT-flanked *kan* cassette-bearing plasmid; oriR6K origin; template for PCR primers K1 and K2	Reference (19)

Primers	**Sequence (5' to 3')**
K1	5'-CCTGCGTGAACAGGGTATTGCCGAATTTAAATTACCGGATCGCGTGGAGTGTGTAGGCTGGAGCTGCTTC-3'
K2	5'-CACTTCGGTCGCAAAGGGATATTGCTCCTGAGTGAACGCTTGATCAAAACCATATGAATATCCTCCTTAG-3'
K3	5'-CCAGCGCCTTTGATGCCAAC-3'
K4	5'-GCCGATTGTCTGTTGTGCCC-3'

Table S2. RMSD for the complex structures of wild-type VibB-ISC and Lys118 mutants

RMSD (Å) for the complex structures

	WT	K118H	K118N	K118A
CA	0.711 (0.076)	0.749 (0.089)	0.887 (0.119)	0.740 (0.081)
total [a]	1.335 (0.145)	1.290 (0.155)	1.475 (0.182)	1.328 (0.157)
active site [b]	0.503(0.129)	0.715 (0.170)	0.571 (0.209)	0.511 (0.125)

[a] Not including isochorismate and solvent water.

[b] Including residue 35, residue 118, isochorismate, and the two water molecules adjacent to the active site.

Table S3. Structure validation with QMEAN and ProQ

	Ligand-bound VibB-ISC	Wild type VibB-ISC
QMEAN score	0.808	0.818
ProQ score		
LGscore	6.820	6.357
MaxSub	0.342	0.279