SUPPLEMENTAL DATA

Crystal Structure of the Peptidase Domain of *Streptococcus* ComA, a Bifunctional ATP-binding Cassette Transporter Involved in Quorum Sensing Pathway

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FIGURE S1. **Time Course of Rmsd of C_α Atoms from the Corresponding Atoms of the Initial Structure during the MD Simulation.** The rmsd's of the MuPEP1–MuComC complex from the initial structure were calculated every 2 ps.

FIGURE S2. **Rms Positional Fluctuations of Each C_α Atom of the MuPEP1–MuComC Complex.** *A*, Rms positional fluctuations of each C_α atom of MuPEP1 (residues from 5 to141) in the MD simulation during 0.4 ns–1.0 ns from the corresponding atom at 0.4 ns. Residue numbers corresponding to major peaks and troughs are shown. *B*, Rms positional fluctuations of each C_α atom of MuComC (residues from –25 to –1) in the MD simulation during 0.4 ns–1.0 ns from the corresponding atom at 0.4 ns. The rmsd's of MuComC were calculated after rigid body alignment against the MuPEP1 component of the complex.

FIGURE S3. **Putative Hydrophobic Concaves of MuPEP1 (left) and PPEP (right).** Surface representation of the result from the HotPatch program. The hydrophilic region is colored in red and hydrophobic region is in blue. The regions enclosed by the orange oval lines indicate the hydrophobic concaves adjacent to the active site cleft. The two structures are aligned based on the least-squares superimposition of the C_α atoms. The hydrophobic concave of MuPEP1 consists of Thr50, Ala51, Leu52, Val55, His87, Leu94, Gln95, Thr132, Leu134, and Ile136, and that of PPEP consists of Thr50, Ala51, Leu52, Val55, His87, Val88, Leu89, Leu94, Leu95, Thr132, Val134, and Leu136.

TABLE S1. **X-ray Data Collection and Refinement Statistics**

Data set	Native	Se-Remote	Se-Peak	Se-Edge
Wavelength (Å)	1.000	0.9000	0.9789	0.9795
Space group	$P4_32_12$		$P4_32_12$	
Unit cell parameters (Å)	$a = b = 58.61$, $c = 112.1$ $\alpha=\beta=\gamma = 90°$		$a = b = 59.03$, $c = 112.5$ $\alpha=\beta=\gamma = 90°$	
Molecules per asymmetric unit	1		1	
Resolution range (Å)	50–1.9	50–1.9	50–1.9	50–1.9
Reflections observed / unique	214,295/16,136	218,026/16,371	217,224/16,358	187,538/14,121
Completeness (%)	100.0 (100.0)	100.0 (100.0)	100.0 (100.0)	100.0 (100.0)
Redundancy	13.3	13.3	13.3	13.3
Average $I/\sigma I$	45.0 (10.2)	40.7 (7.0)	43.5 (7.7)	41.5 (8.8)
R_{merge} (%)[a]	6.4 (29.9)	6.9 (33.7)	7.5 (30.2)	6.7 (29.4)
Refinement				
Resolution range (Å)	41–1.9			
Total reflections	16,053			
R_{work} (%)[b] / R_{free} (%)[c]	21.2/23.4			
Number of protein atoms/water atoms	1,092/95			
Rmsd[d] bond length (Å)	0.005			
Rmsd[d] angle (°)	1.20			
Average B-factor (Å^2)	25.7			
Ramachandran plot				
Most favored (%)	91.7			
Additional (%)	6.7			
Disallowed (%)	1.7			

Values in parentheses are for the highest resolution shell.

[a] $R_{merge} = \sum_h\sum_i|I_{h,i} - \langle I_h\rangle|/\sum_h\sum_i I_{h,i}$ where $I_{h,i}$ is the ith observation of reflection h and $\langle I_h\rangle$ is the mean intensity of reflection h.

[b] $R_{work} = \sum||F_{obs}| - |F_{calc}||/\sum|F_{obs}|$ where F_{obs} and F_{calc} are the observed and calculated structure factors, respectively.

[c] R_{free} is calculated in the same manner as R_{work}, except that F_{obs} corresponds to 10% of the reflections not used in the refinement.

[d] Rmsd, root-mean-square deviation.

TABLE S2. **Oligonucleotides Used for the Site-directed Mutagenesis**

Name	Sequence
T50Sf	5’-GACCATGGATGGGACGTCGGCTTTGGGCTTGGTC-3’
T50Sr	5’-GACCAAGCCCAAAGCCGACGTCCCATCCATGGTC-3’
A51Wf	5’-CCATGGATGGGACGACGTGGTTGGGCTTGGTCAAGG-3’
A51Wr	5’-CCTTGACCAAGCCCAACCACGTCGTCCCATCCATGG-3’
L52Af	5’-GATGGGACGACGGCTGCGGGCTTGGTCAAGGTG-3’
L52Ar	5’-CACCTTGACCAAGCCCGCAGCCGTCGTCCCATC-3’
V55Af	5’-CGGCTTTGGGCTTGGCCAAGGTGGCAGAGGA-3’
V55Ar	5’-TCCTCTGCCACCTTGGCCAAGCCCAAAGCCG-3’
L52A/V55Af	5’-CGACGGCTGCGGGCTTGGCCAAGGTGGCAGAGGAG-3’
L52A/V55Ar	5’-CTCCTCTGCCACCTTGGCCAAGCCCGCAGCCGTCG-3’
A67Wf	5’-GATTGGTTTTGAGACGCGATGGATTAAGGCAGATATGACG-3’
A67Wr	5’-CGTCATATCTGCCTTAATCCATCGCGTCTCAAAACCAATC-3’
L94Af	5’-CTTAAGGAAGGGAAAGCGCTCCACTACTATGTG-3’
L94Ar	5’-CACATAGTAGTGGAGCGCTTTCCCTTCCTTAAG-3’
V134Af	5’-GAAGAATGGACAGGAGCGACTCTTTTTATGGCAC-3’
V134Ar	5’-GTGCCATAAAAAGAGTCGCTCCTGTCCATTCTTC-3’

FIGURE S1

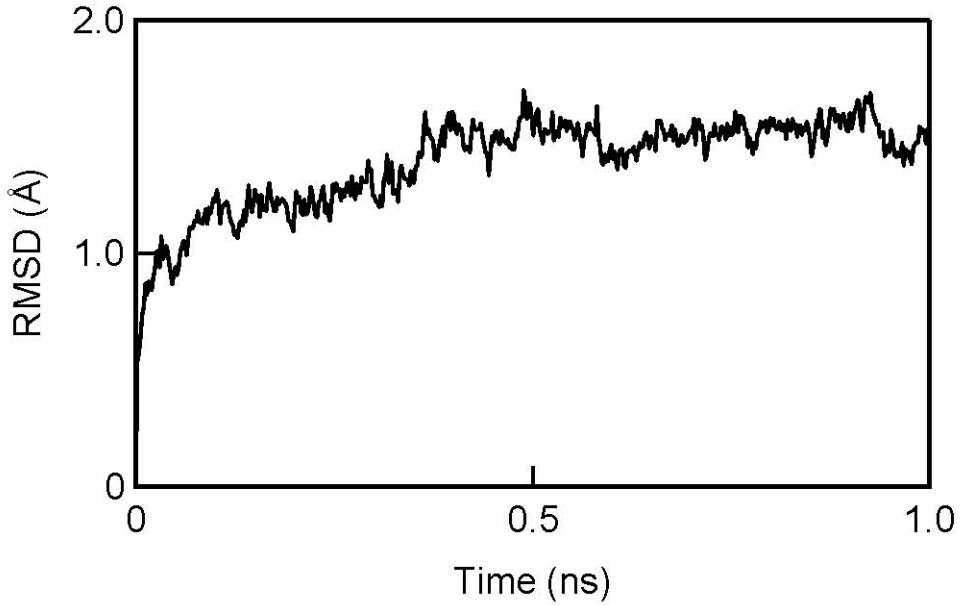

FIGURE S2

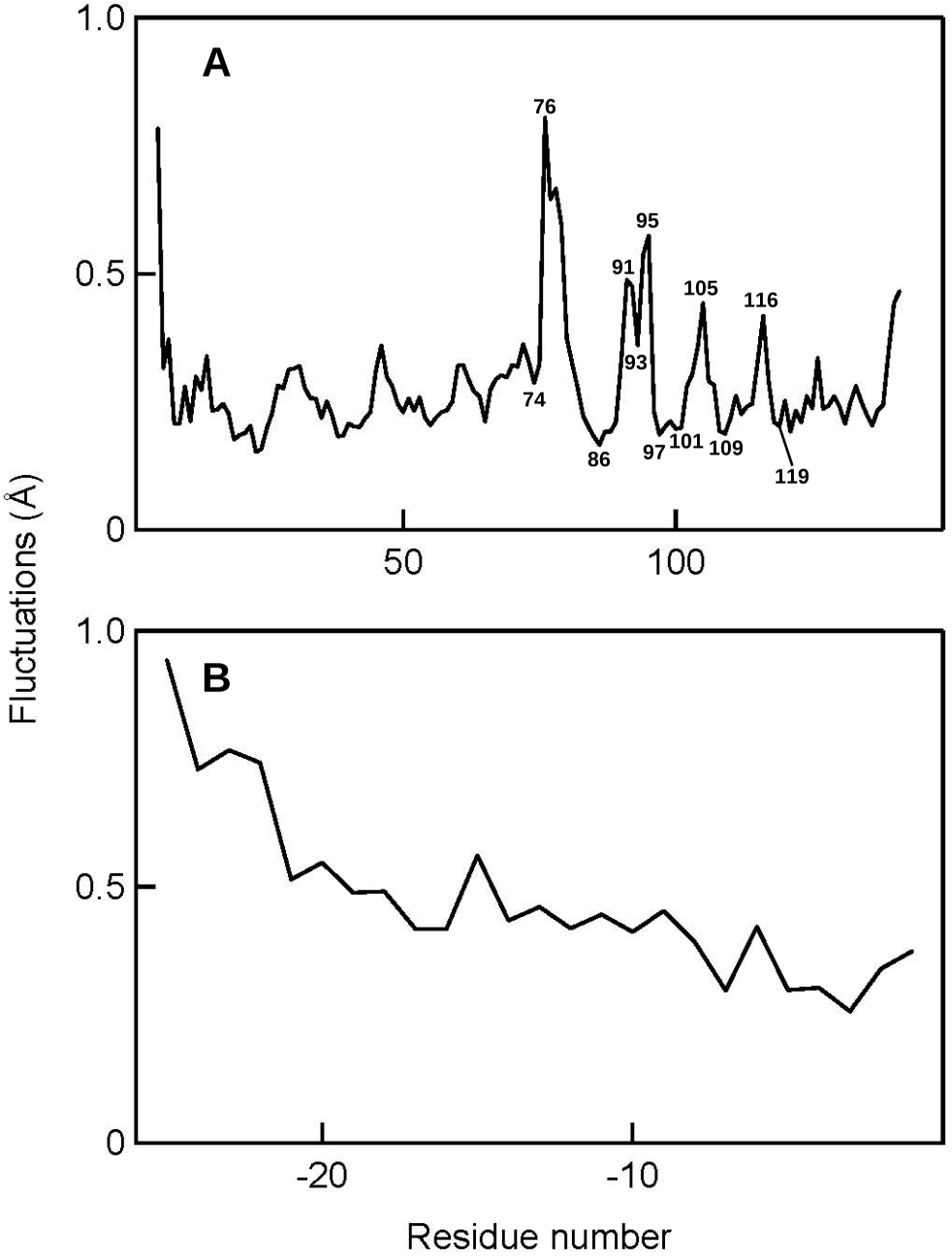
A
B
1.0
0.5
0
50
100
-20
-10
Fluctuations (Å)
Residue number
76
74
86
91
93
95
97
101
105
109
116
119

FIGURE S3