

Supplemental materials

TABLE S1. Data collection and refinement statistics

	Native TLA-3	Avibactam complex	OP0595 complex
Data collection			
Beam line	BL2S1 (AichiSR)	BL2S1 (AichiSR)	BL2S1 (AichiSR)
Wavelength (Å)	1.12	1.12	1.12
Resolution range (Å)	55.18–1.59 (1.68–1.59) ^a	55.48–1.59 (1.68–1.59) ^a	55.22–2.00 (2.11–2.00) ^a
Space group	<i>C</i> 2	<i>C</i> 2	<i>C</i> 2
Cell dimensions			
<i>a</i> (Å)	94.8	95.9	95.2
<i>b</i> (Å)	67.9	68.1	67.9
<i>c</i> (Å)	45.1	45.3	45.3
α (°)	90.0	90.0	90.0
β (°)	94.2	94.5	94.6
γ (°)	90.0	90.0	90.0
No. of unique reflections	38203 (5557) ^a	38600 (5528) ^a	18894 (2688) ^a
Redundancy	7.1 (6.9) ^a	7.1 (7.0) ^a	7.5 (7.6) ^a
Completeness (%)	99.8 (99.6) ^a	98.8 (97.7) ^a	97.0 (95.6) ^a
R_{merge} (%)	5.1 (18.1) ^a	4.4 (20.4) ^a	7.4 (29.5) ^a
mean $I/\sigma(I)$	24.7 (9.4) ^a	28.1 (8.8) ^a	20.0 (6.6) ^a
Refinement			
R_{working} (%)	13.5	15.9	16.1
R_{free} (%)	16.0	19.2	20.9
Ramachandran statistics (%)			
Favored	98.2	98.5	96.3
Allowed	1.8	1.5	3.7
Disallowed	0	0	0
Average <i>B</i>-factors (Å²)			
Protein	13.6	17.5	20.5
Ligand/ion	26.3	24.8	36.2
Water	26.3	29.3	25.0
r.m.s.d.			
Bond lengths (Å)	0.012	0.011	0.013
Bond angles (°)	1.506	1.470	1.477

^aValues in parentheses are for the highest-resolution shell.

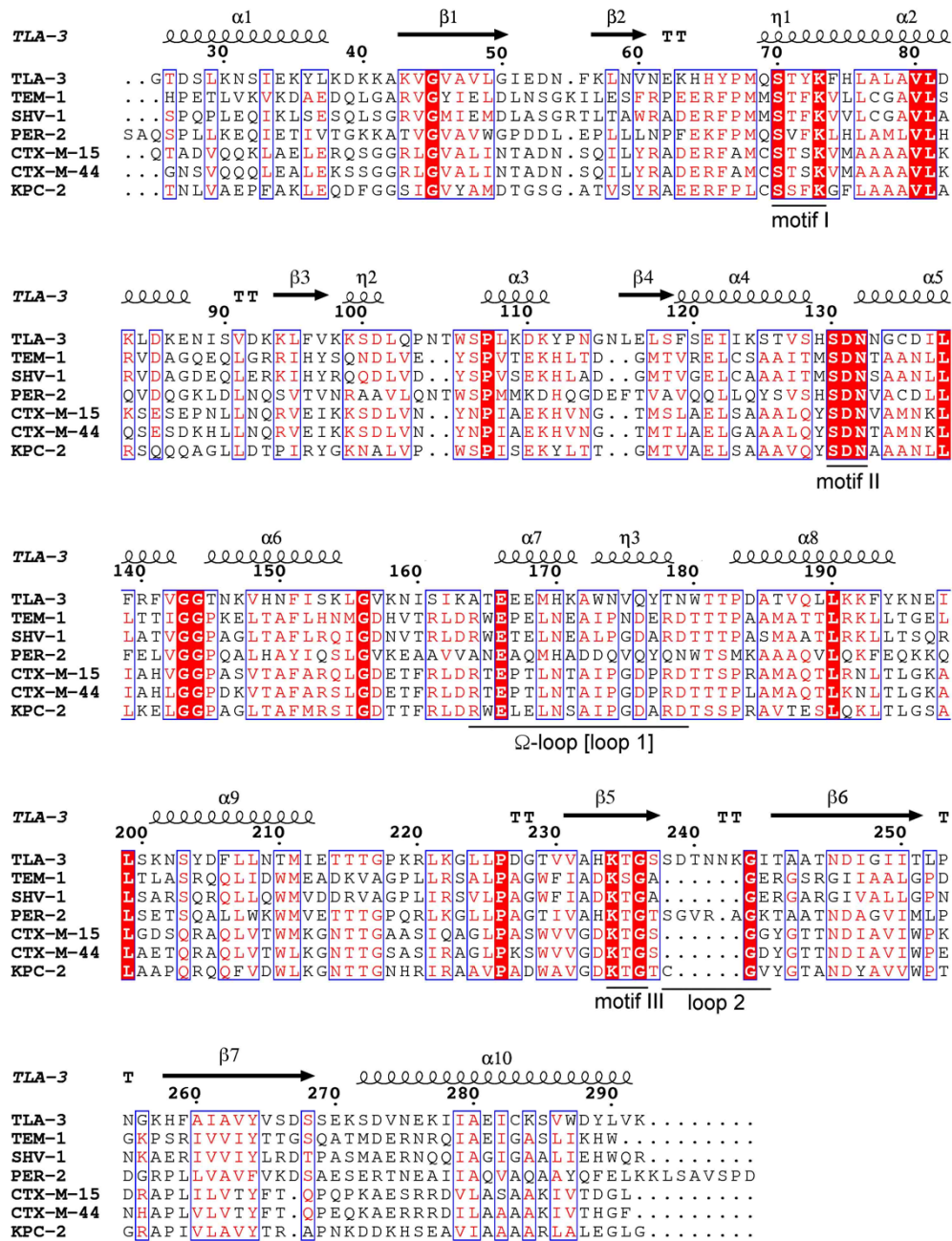


Fig. S2

Figure S2. Amino acid alignments of class A β-lactamases for which three-dimensional structures have been determined. The strictly conserved amino acid residues are boxed in red. Physicochemically similar amino acids are shown in red. The secondary structure elements of TLA-3 are shown above the alignments. The figure was prepared using ClustalW (<http://clustalw.ddbj.nig.ac.jp>) and ESPrift 3.0 (<http://esprift.ibcp.fr/ESPrift/ESPrift/>).