

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	C2	C2	C2
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 (Å ²)			
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.

1 20 30 33
MKKHLIVIAF CALFASAFAA**A** **KGTD**SLKNS**A** **KGTDSLKNSI** EKYLKD**KKAK**
51
VGVAVLGIED NFKLNVNEKH HYPMQSTYKF HLALAVLDKL DKENISVDKK
101
LFVKKSDLQP NTWSPLKDKY PNGNLELSFS EIIKSTVSHS DNNNGCDILFR
151
FVGGTNKVHN FISKLGVKNI SIKATEEEEMH KAWNQYTNW TTPDATVQLL
201
KKFYKNEILS KNSYDFLLNT MIETTGPKR LKGLLPDGTV VAHKTGSSDT
251
NNKGITAATN DIGIITLPNG KHFIAIAYVS DSSEKSDVNE KIIAEICKSV
301
WDYLVKD**GK**

Fig. S1

Figure S1. Amino acid sequence of immature TLA-3 β -lactamase. The duplicated amino acid sequence in the N-terminus is highlighted in yellow and cyan. The N-terminal amino acids determined using Edman degradation are shown in red letters. Amino acids included in the TLA-3 structural model are underlined.

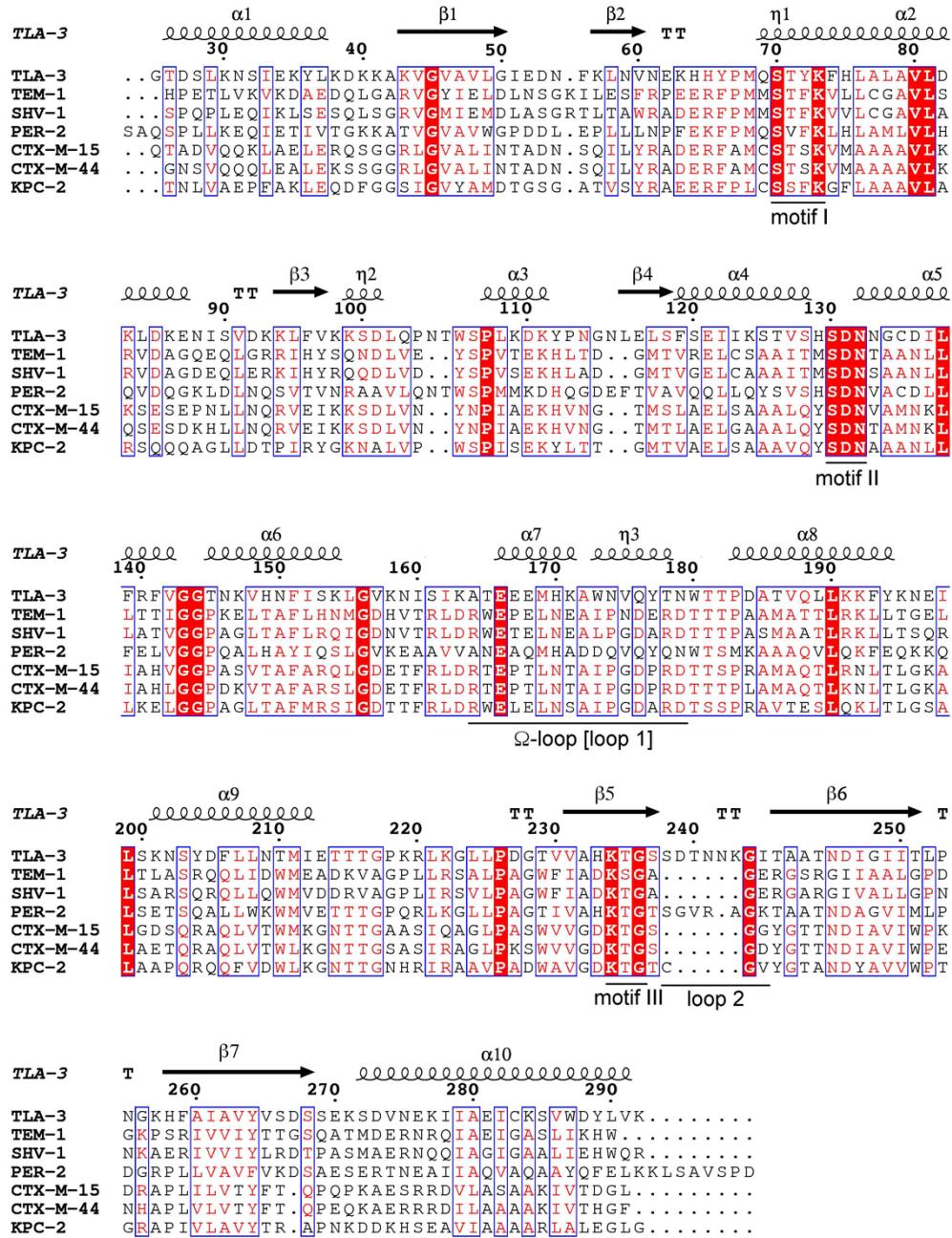


Fig. S2

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 ESPript 3.0 (<http://escript.ibcp.fr/ESPript/ESPript/>).