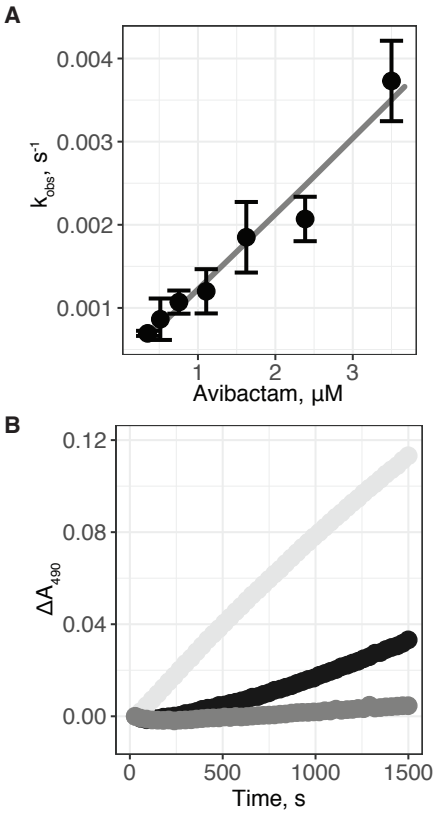

Figure S1. On and off-rate determination of avibactam to VCC-1. **A)** Plot of avibactam concentration vs k_{obs} in on-rate experiments. Error bars represent the SD of three separate experiments. **B)** Time course of recovery of VCC-1 activity against following dilution in reaction buffer containing nitrocefin. 1 μM VCC-1 was incubated in the absence (light grey) and presence (black) of 5 μM avibactam, parallel experiment was performed maintaining the initial avibactam concentration (grey).

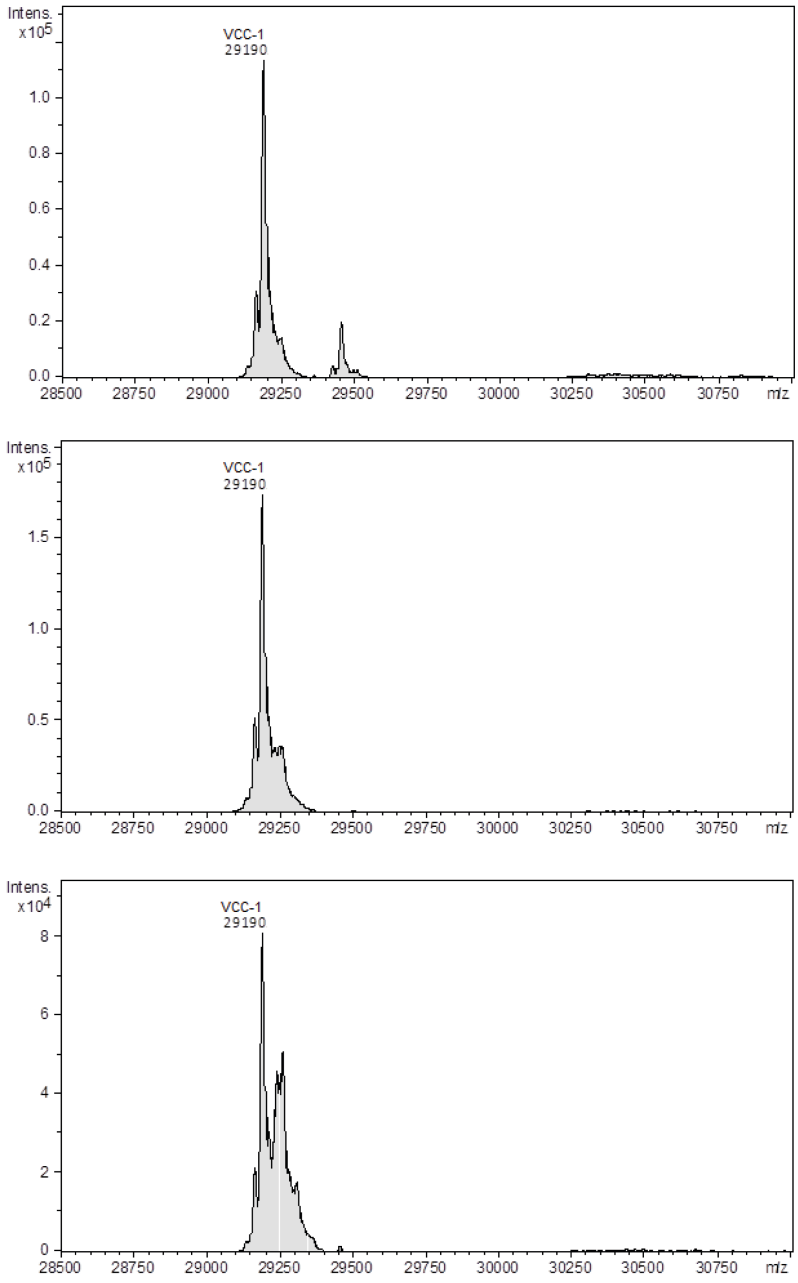

Figure S2. Reconstructed ESI-MS spectra of unbound VCC-1 (no avibactam). The mass of unbound VCC-1 is identical the mass of a species that appears over a 32 hr when VCC-1 is incubated with avibactam (Fig. 2). MS measurements were taken in the same time frame (1 hour (top), 10 hours (middle) and 32 hours (bottom)) as shown in Fig 2. The peak at 29,190 amu corresponds to that of recombinant VCC-1 (expected mass = 29,193 amu).

Table S1: Crystallographic and refinement statistics for apo and avibactam-bound VCC-1.		
Data collection	**VCC-1**	**VCC-1 – avibactam**
X-ray source	CLS 08B1-1	Rigaku MicroMax 007HF
Space group	C2	$P4_32_12$
Unit cell dimensions	*a* = 209.93 Å, *b* = 46.65 Å, *c* = 113.61 Å, α = γ = 90°, β = 99.28°	*a* = *b* = 62.06 Å, *c* = 134.35 Å, α =β= γ = 90°
Wavelength (Å)	0.9795	1.54
Resolution (Å)	56.06 – 1.70 (1.73 – 1.70)*	56.34 – 1.90 (1.94 – 1.90)
Total observations	549396 (26644)	124852 (6986)
Unique observations	119395 (5879)	21085 (1236)
Multiplicity	4.6 (4.5)	5.9 (5.7)
R_{merge}	0.052 (0.303)	0.126 (0.636)
CC(1/2)	0.999 (0.970)	0.995 (0.827)
I / σI	13.8 (3.2)	9.3 (2.3)
Completeness (%)	99.5 (98.9)	98.0 (91.1)
Refinement		
R_{work} / R_{free}	0.16 / 0.20	0.16 / 0.20
Reflections used for R-free	1466 (143)	1999 (180)
Total non-hydrogen atoms	9367	2274
Macromolecules	8026	2013
Avibactam	-	17
Solvent	1341	248
Average B-factor (Å^2)	26.42	20.64
Macromolecules	24.81	19.57
Avibactam	-	20.94
Solvent	36.01	29.35
RMSD bond lengths (Å) /angles (°)	0.009/1.28	0.007/0.88
Ramachandran plot favoured/allowed/outliers (%)	97.10/2.90/0.00	96.92/3.08/0.00
* Values for the highest resolution shell are shown in parentheses		