

1 **Supplemental Material**

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3 **Antibacterial spectrum of a tetrazole-based reversible inhibitor of**
4 **serine β -lactamases**

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Table S1. X-ray Data Collection and Refinement Statistics		
	CTX-M-14 S237A with compound 1	CTX-M-27 with compound 1
Data Collection		
Space group	P2 ₁	P2 ₁
Cell dimensions		
a, b, c (Å)	45.19, 107.13, 47.85	44.96, 107.24, 47.79
α , β , γ (°)	90, 101.52, 90	90, 101.86, 90
Resolution (Å)	34.13 – 1.05 (1.11 – 1.05)	35.95 – 1.15 (1.21 – 1.15)
No. of unique reflections	204,404 (28,335)	156,537 (22,838)
R _{merge} (%)	6.4 (24.0)	10.4 (60.4)
I/ σ (I)	11.4 (4.1)	7.5 (2.2)
Completeness (%)	98.8 (93.9)	100 (100)
Multiplicity	3.5 (3.0)	3.6 (3.5)
Refinement		
Resolution (Å)	29.40 – 1.05	35.95 – 1.15
R _{work} (%)	12.61	14.09
R _{free} (%)	14.66	16.60
No. atoms		
Protein	4,073	4,039
Ligand/Ion	108	138
Water	908	890
B-factors (Å ²)		
protein	9.46	9.37
ligand/ion	19.11	16.12
water	28.68	26.90
RMS deviations		
Bond lengths (Å)	0.008	0.009
Bond angles (°)	1.33	1.35
Ramachandran plot		
favored (%)	98.07	98.08
allowed (%)	1.54	1.54
outliers (%)	0.39	0.38
PDB code	6BT6	6BU3

22 *Statistics for the highest-resolution shell are shown in parentheses