

Supporting Information for

NXL104 Irreversibly Inhibits the β -Lactamase from *Mycobacterium tuberculosis*

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Table S1. Summary of protein-ligand interactions.

Protein (BlaC)			Clav	Dist ^a	Protein (BlaC)			NXL104	Dist ^a
Residue	Atom name	Atom name			Residue	Atom name	Atom name		
Ser84	N	OAH	2.8		Ser70	N	OAC	2.6	
Thr253	N	OAH	2.9		Ser128	OG	OAL	3.0	
Asn186	ND2	NAK	3.5		Thr237	OG1	OAE	3.0	
Glu182	OE1	NAK	4.4		Thr237	OG1	OAG	3.3	
Ile117	N	NAK	5.6		Thr239	O	NAA	3.1	
PO ₄ 309	O4	OAN	4.1		Thr239	O	OAC	2.8	
PO ₄ 309	O3	OAN	4.4		Thr239	N	OAC	2.8	
PO ₄ 308	O2	OAQ	3.1		Thr239	OG1	OAE	3.5	
Asp255	N	OAQ	3.6		Thr239	OG1	OAD	2.9	
PO ₄ 308	O1	OAQ	4.1		HOH492	O	NAK	3.2	
HOH516	O	OAN	2.4		HOH508	O	OAD	3.5	

HOH583	O	NAK	3.1	HOH508	O	OAG	3.1
				HOH541	O	CAN	2.8
				HOH541	O	O	2.9
				HOH541	O	N	3.1
				HOH541	O	OAC	3.1
				HOH772	O	OAC	3.2
				HOH772	O	OAE	1.7
				HOH772	O	OAL	2.3
				HOH737	O	OAE	3.4
				HOH737	O	OAG	2.6

^a Distance (Å) between the ligand and protein atoms
