Supplementary Tables

Table S1. Details of the antimycobacterial drugs used in this study.

Name	PubChem CID	Molecular Weight	Molecular Formula
Delamanid	6480466	534.491	$C_{25}H_{25}F_3N_4O_6$
Pretomanid	456199	359.26	$C_{14}H_{12}F_3N_3O_5$
Clofazimine	2794	473.407	$C_{27}H_{22}Cl_2N_4$
Bedaquiline	5388906	555.516	$C_{32}H_{31}BrN_2O_2$
Terizidone	65720	302.29	$C_{14}H_{14}N_4O_4$
Amithiozone	9568512	236.3	$C_{10}H_{12}N_4OS$
Dapsone	2955	248.307	$C_{12}H_{12}N_2O_2S$
Morinamide	70374	222.248	$C_{10}H_{14}N_4O_2$
Protionamide	666418	180.276	$C_9H_{12}N_2S$
Isoniazid	3767	137.142	$C_6H_7N_3O$
Ethionamide	2761171	166.249	$C_8H_{10}N_2S$
Pyrazinamide	1046	123.115	$C_5H_5N_3O$
Ethambutol	14052	204.314	$C_{10}H_{24}N_2O_2$
Cycloserine	6234	102.093	$C_3H_6N_2O_2$

Table S2. Details of the target proteins of *P. aeruginosa* used in this study.

S. No.	Protein	PDB ID	Size of Grid			Centre of Grid		
			x	y	z	x	y	z
1.	LasA	3IT7	46	38	46	23.512	4.315	-11.282
2.	LasI	1RO5	50	46	46	39.183	-11.983	-11.794
3.	LasR	2UV0	34	50	46	25.471	35.493	42.516
4.	PqsR	4JVI	50	46	48	-27.568	62.524	10.084
5.	RhlR	8DQ1	52	56	66	131.366	138.844	165.832

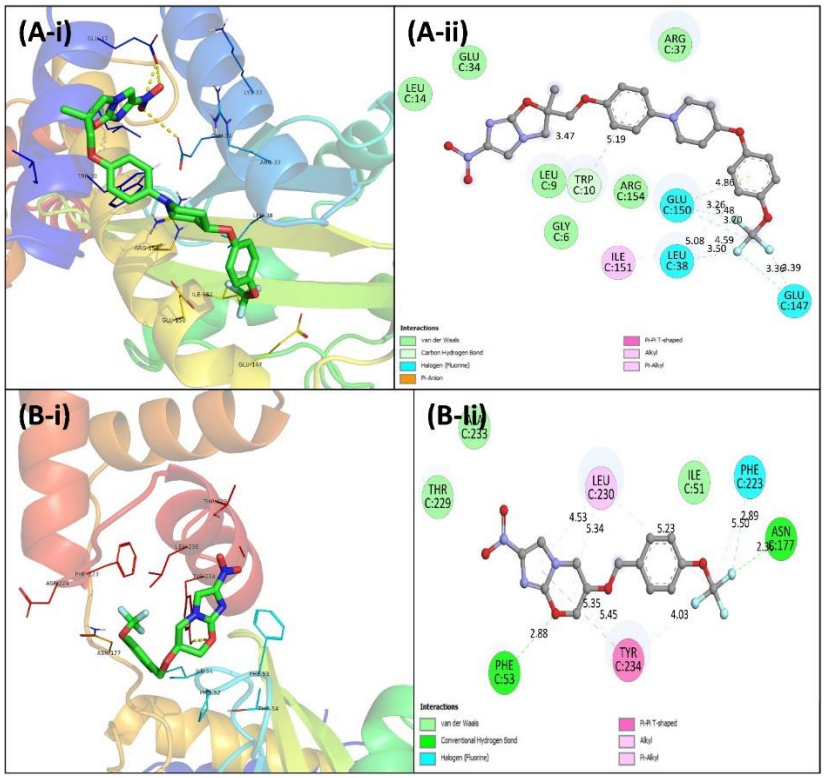

Figure S1. (A) Docked pose of the RhlR-delamanid complex. (A-i) Three-dimensional representation of the RhlR-delamanid complex; delamanid is shown as sticks. RhlR is shown as a coloured ribbon in which interacting residues are heighted. (A-ii) Two-dimensional representation of the RhlR-delamanid complex prepared using Discovery Studio 2021. (B) Docked pose of the RhlR-pretomanid complex. (B-i) Three-dimensional representation of the RhlR-pretomanid complex; pretomanid is shown as sticks. RhlR is shown as a coloured ribbon in which interacting residues are heighted. (A-ii) Two-dimensional representation of the RhlR-pretomanid complex prepared using Discovery Studio 2021.

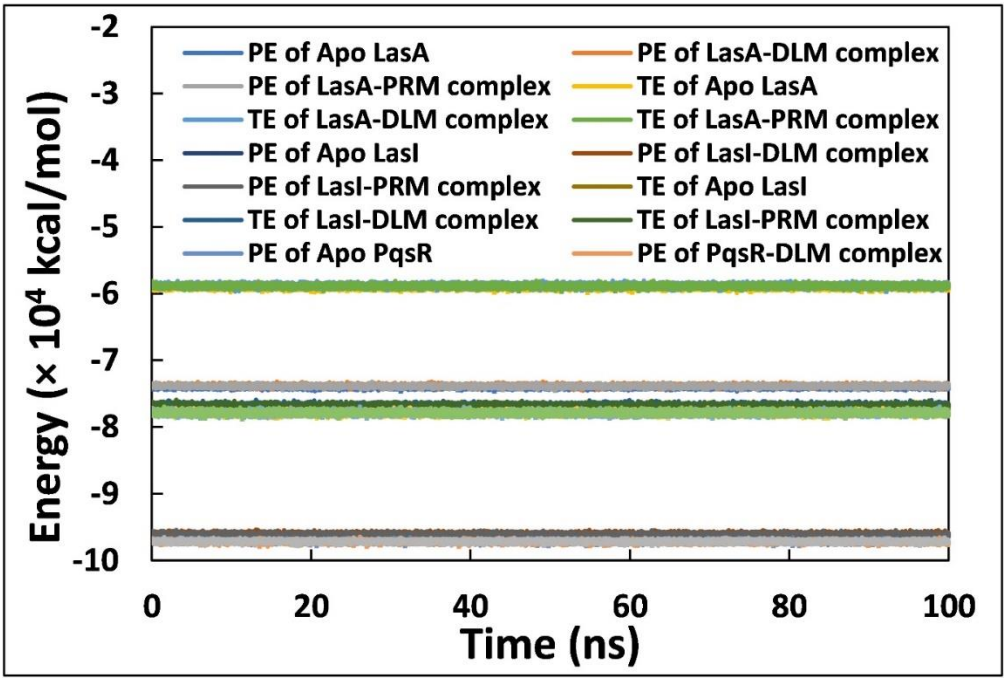

Figure S2. Total energy and potential energy of apo LasA, LasA-delamanid complex, LasA-pretomanid complex, apo LasI, LasI-delamanid complex, LasI-pretomanid complex, apo PqsR, PqsR-delamanid complex, and PqsR-pretomanid complex as a function of time.

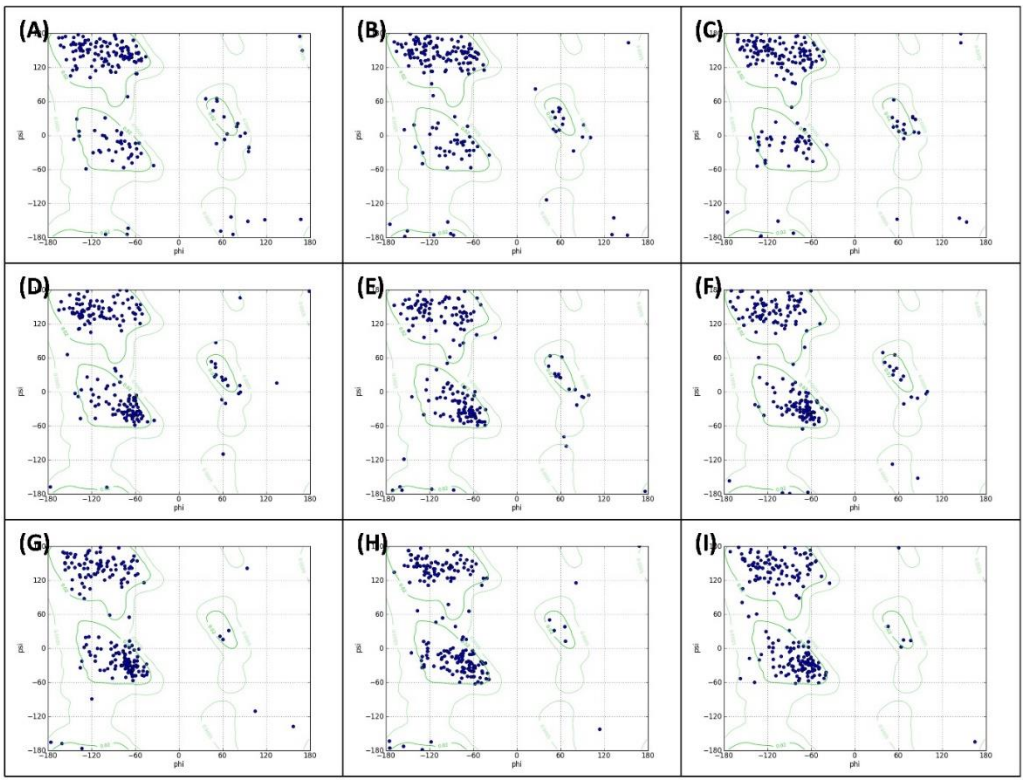

Figure S3. (A) Ramachandran plot of energy minima structure of apo LasA. (B) Ramachandran plot of energy minima structure of LasA-delamanid complex. (C) Ramachandran plot of energy minima structure of LasA-pretomanid complex. (D) Ramachandran plot of energy minima structure of apo LasI. (E) Ramachandran plot of energy minima structure of LasI-delamanid complex. (F) Ramachandran plot of energy minima structure of LasI-pretomanid complex. (G) Ramachandran plot of energy minima structure of apo PqsR. (H) Ramachandran plot of energy minima structure of PqsR-delamanid complex. (I) Ramachandran plot of energy minima structure of PqsR-pretomanid complex.