

SUPPORTING INFORMATION

Antimicrobial resistance conferred by OXA-48 β - lactamases: towards a detailed mechanistic understanding

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Available OXA-48 structures in the Protein Data Bank

Structures include apoenzyme structures (APO) and complexes with clinically used β -lactam antibiotics and inhibitors (AE = covalent acyl-enzyme complex, P = hydrolyzed product complex).

Table S1. List of crystal structures of OXA-48-like β -lactamases in the Protein Data Bank.

ENZYME	PDB ID	RES. (Å)	ADD. INFO
OXA-48			
APO	3HBR	1.90	
APO	6P96	1.60	
APO	4S2P	1.70	

APO	6RJ7	1.73	
IMIPENEM (AE)	6P97	1.80	
IMIPENEM (AE)	6PTU	2.00	
IMIPENEM (AE)	5QB4	1.95	
IMIPENEM (AE)	7KH9	2.29	K73A
IMIPENEM (P)	6PK0	1.75	
MEROPENEM (AE)	6P98	1.75	
MEROPENEM (AE)	6PT1	2.00	
MEROPENEM (AE)	7KHQ	2.00	K73A
ERTAPENEM (AE)	6P99	2.25	
DORIPENEM (AE)	6P9C	1.90	
DORIPENEM (AE)	6PXX	1.50	K73A
FAROPENEM (AE)	6PSG	2.13	
CEFTAZIDIME (AE)	6Q5F	2.50	P68A
CEFOTAXIME (AE)	6PQI	2.05	
CEFOXITIN (AE)	6PT5	2.30	
AVIBACTAM (AE)	6Q5B	2.22	P68A
AVIBACTAM (AE)	4WMC	2.30	
AVIBACTAM (AE)	4S2J	2.54	pH 6.5
AVIBACTAM (AE)	4S2K	2.10	pH 7.5
AVIBACTAM (AE)	4S2N	2.00	pH 8.5
OXA-163			
APO	4S2L	1.72	
APO	4S2M	2.87	Iodide complex
APO	5ODZ	2.07	
IMIPENEM (AE)	7KHZ	2.04	K73A
MEROPENEM (AE)	7KHY	1.84	K73A
OXA-181			
APO	5OE0	2.05	
OXA-245			
APO	5OE2	2.20	