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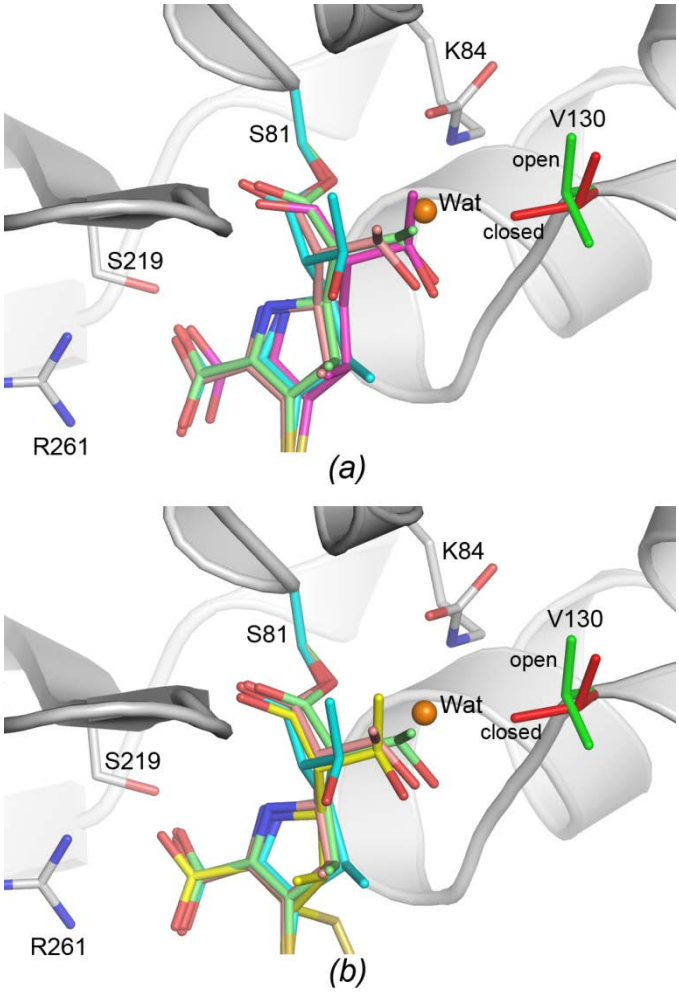
Supporting information for article:

Role of conserved surface hydrophobic residues in the carbapenemase activity of the class D β-lactamases

Marta Toth, Clyde A. Smith, Nuno T. Antunes, Nichole K. Stewart, Lauren Maltz and Sergei B. Vakulenko

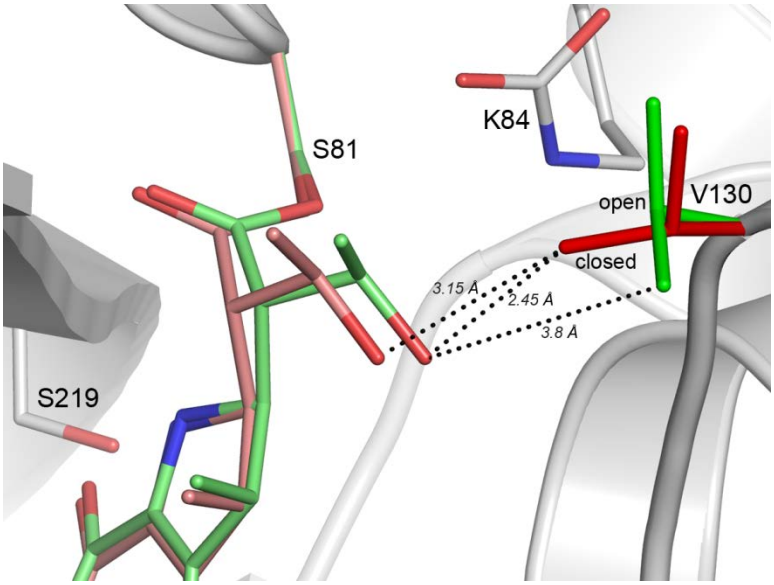
Supplementary Figures



Supplementary Figure S1

Ligand docking of meropenem and doripenem. (*a*), Doripenem docked to the three receptor models, OXA-143^{open} (green Val130 and green doripenem), OXA-143^{closed} (red Val130 and pink doripenem) and OXA-143$^{open+water}$ (green Val130, orange Wat, and cyan doripenem). The location of the doripenem observed in the K84D mutant OXA-24/40 structure is also shown as magenta sticks for comparison. (*b*), Meropenem docked to the three receptor models, OXA-143^{open} (green Val130 and green meropenem), OXA-143^{closed} (red Val130 and pink meropenem)

and OXA-143$^{open+water}$ (green Val130, orange Wat, and cyan meropenem). The location of the meropenem observed in the OXA-23 structure is also shown as yellow sticks for comparison.



Supplementary Figure S2

Docking of doripenem to OXA-143. The positions of doripenem in the OXA-143^{open} receptor (green Val130, green doripenem), and in the OXA-143^{closed} receptor (red Val130, pink doripenem) is shown. The black dotted lines indicate the closest approach distances between the oxygen atom of the 6α-hydroxyethyl group of the doripenem in the two poses, and the Val130 residue. The minimum carbon-oxygen non-bonded distance is approximately 3.2 Å (Bondi, 1964). Meropenem (not shown for clarity) docks in an almost identical fashion to the OXA-143^{open} and OXA-143^{closed} receptors.

Supplementary Tables

Supplementary Table S1

Sequence identities and *rmsd*s of the known OXA structures with OXA-143

Structure	Source	Sequence identity (%)	*rmsd* (Å) †	PDB code ‡
OXA-1	*E. coli*	24.2	1.53 (224)	1M6K
OXA-10	*P. aeruginosa*	38.5	1.39 (226)	1EWZ
OXA-13	*P. aeruginosa*	36.6	1.43 (224)	1H8Z
OXA-23	*A. baumannii*	66.1	0.72 (239)	4JF6
OXA-24/40	*A. baumannii*	89.6	0.70 (240)	3G4P
OXA-46	*P. aeruginosa*	30.9	1.44 (207)	3IF6
OXA-48	*K. pneumoniae*	34.1	1.31 (226)	3HBR
OXA-51	*A. baumannii*	68.8	0.71 (240)	4ZDX
OXA-58	*A. baumannii*	54.6	1.20 (238)	4OH0

† The numbers of matching C_α atoms used in the superposition are given in parentheses. ‡ From http://www.rcsb.org (Berman *et al.*, 2000).

Supplementary Table S2

Ligand docking results[†]

Antibiotic	Receptor	Score[‡]	Energy (kcal/mol)		
			Hydrogen bonding	Hydrophobic interactions	Van der Waals
Meropenem	OXA-143$^{open+water}$	-27.5	-12.4	-6.2	-15.2
	OXA-143^{open}	-44.3	-14.2	-6.0	-27.5
	OXA-143^{closed}	-35.5	-12.3	-6.1	-23.4
Doripenem	OXA-143$^{open+water}$	-26.3	-12.0	-5.5	-17.5
	OXA-143^{open}	-45.0	-14.0	-5.4	-31.1
	OXA-143^{closed}	-36.3	-12.8	-5.5	-24.9

[†]Averaged over 5 docking runs for each receptor/substrate pair. [‡] Calculated by ICM-Pro 3.8-5 (Abagyan & Totrov, 1994, Abagyan *et al.*, 1994). The score has no units. More negative numbers are indicative of stronger binding.

Supplementary references

Abagyan, R. A. & Totrov, M. M. (1994). *J. Mol. Biol.* **235**, 983-1002.

Abagyan, R. A., Totrov, M. M. & Kuznetsov, D. A. (1994). *J. Comp. Chem.* **15**, 488-506.

Berman, H. M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T. N., Weissig, H., Shindyalov, I. N. & Bourne, P. E. (2000). *Nucleic Acids Res.* **28**, 235-242.

Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.