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Supporting information for article:

Crystal structure of vancomycin bound to the resistance determinant d-alanine-d-serine

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Table S1 Structural similarity between the ten vancomycin monomers within the asymmetric unit. Pairwise superpositions were carried out for all vancomycin monomers in the asymmetric unit (denoted as chains A-J). Shown are RMSD values (Å) for all non-hydrogen atoms within the vancomycin aglycon after superposition. Carbohydrate moieties were omitted from the superposition and RMSD calculations.

Chain	A	B	C	D	E	F	G	H	I	J
A	---									
B	0.59	---								
C	0.30	0.55	---							
D	0.54	0.62	0.62	---						
E	0.44	0.52	0.49	0.20	---					
F	0.58	0.63	0.63	0.08	0.23	---				
G	0.58	0.09	0.55	0.60	0.50	0.62	---			
H	0.58	0.12	0.56	0.61	0.50	0.62	0.07	---		
I	0.60	0.11	0.57	0.62	0.51	0.63	0.08	0.12	---	
J	0.53	0.61	0.61	0.18	0.26	0.20	0.60	0.60	0.62	---

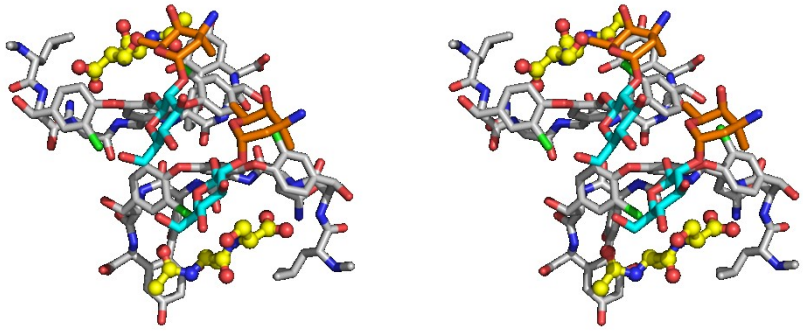

Figure S1 Divergent stereo view of a back-to-back vancomycin dimer bound to D-Ala-D-Ser. This figure uses the same color scheme as Figure 1(*e*); the view is rotated by 90° about a horizontal axis relative to that of Figure 1(*e*). An approximate two-fold axis of symmetry perpendicular to the plane of the page relates the two vancomycin aglycon moieties; the carbohydrate groups do not obey this symmetry.

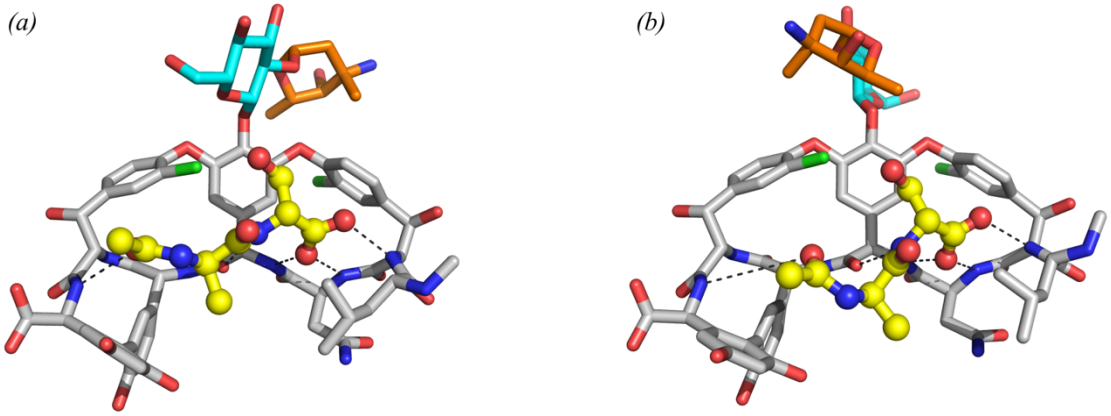

Figure S2 Views looking into the ligand-binding site for the two conformations of the vancomycin carbohydrate group. (*a*) Binding site overhung by glucose; (*b*) binding site overhung by vancosamine. Dashed lines show hydrogen bonds between the ligand and the antibiotic. This figure uses the same color scheme as Figure 1(*e*).