Table S1. Data collection and refinement statistics

	Apo	Ampicillin	Carbenicillin
Data collection			
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions (Å)			
a, b, c (Å)	84.6 / 127.8 / 54.9	84.7 / 128.3 / 54/7	84.8 / 127.8 / 54.7
Resolution (Å)	20 - 2.0	30 - 2.1	30 – 2.0
R_{merge} [b] (%)	5.9 (32.7)	6.6 (32.2)	6.4 (30.3)
I/σ (I)	19.2 (2.5)	27.3 (4.5)	24.9 (4.1)
Completeness (%)	92.7 (64.02)	98.5 (88.3)	97.2 (85.2)
Redundancy	4.2 (11.9)	5.5 (3.7)	4.8 (2.9)
Structure refinement			
Resolution (Å)	20 - 2.0	30 - 2.1	30 – 2.0
No. of reflections	36557	35202	35006
R_{work} [c] / R_{free}	19.8 / 24.9	19.2 / 23.3	18.5 / 22.6
No. atoms, Proteins/ Water	3768 / 74	3773 / 121	3790 / 114
No. molecules, Glycerol	1	3	3
R.m.s.d., bond lengths (Å) / angles (°)	0.008/1.15	0.009/1.08	0.008/1.15
Average B-factor (Å^2)	47.7	25.8	45.5
Ramachandran plot			
Most favored region	89.7	88.3	90.5
Additional allowed region	10.3	11.7	9.3
Generally allowed region	0	0	0.2

[a] The numbers in parentheses are statistics from the highest resolution shell.

[b] $R_{merge} = \Sigma |I_{obs} - I_{avg}| / I_{obs}$, where I_{obs} is the observed intensity of individual reflection and I_{avg} is average over symmetry equivalents.

[c] $R_{work} = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$, where $|F_o|$ and $|F_c|$ are the observed and calculated structure factor amplitudes, respectively. R_{free} was calculated with 5% of the data.

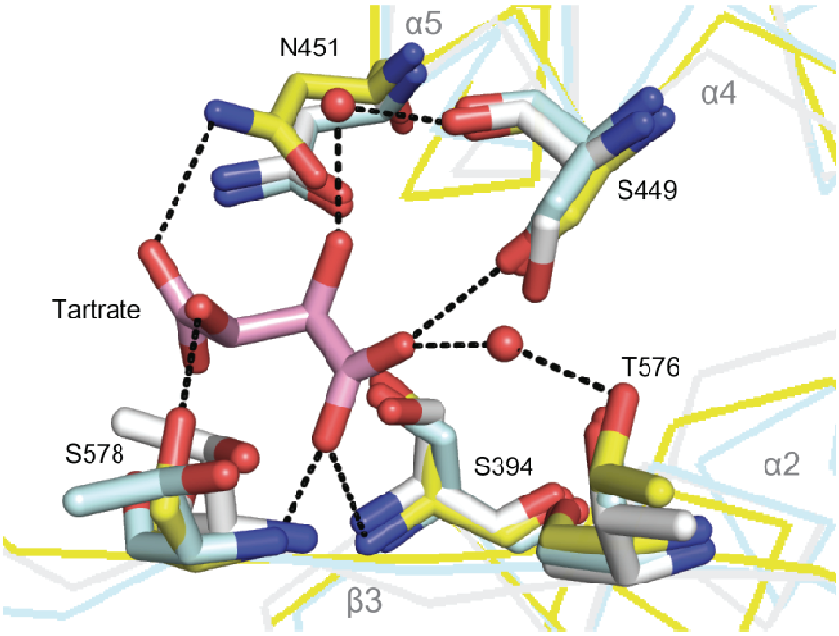

Figure S1. Structural superimposition of the active site of *Lm*PBP4 bound to tartrate on two other PBPs. The residues interacting with tartrate (pink) of *Lm*PBP4 are shown in yellow bonds and the corresponding residues of *S. aureus* PBP2 (PDB code 3DWK) are colored in gray, and those of *P. aeruginosa* PBP3 (PDB code 3OCL) are colored in pale cyan. The secondary structures of these PBPs are presented as a ribbon model. Water molecules are shown as red spheres, and hydrogen bonds are shown as black dashed lines.