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Supporting information for article:

Structure of P46, an immunodominant surface protein from *Mycoplasma hyopneumoniae*: interaction with a monoclonal antibody

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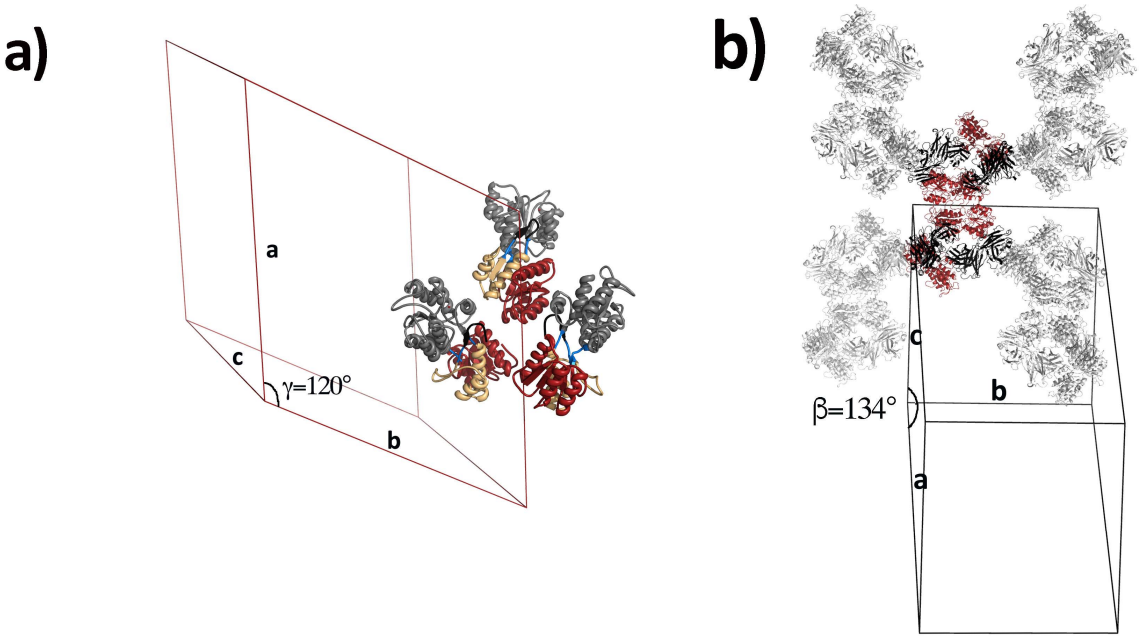

Figure S1 Asymmetric unit cell content and crystal packing. a) The three molecules found in the asymmetric unit of the P46 crystals do not present any common pattern of interactions between them. b) View down a local two-fold axis that relates pairs of the P46-FabP46 complexes found in the crystal asymmetric unit of these complexes. P46 is depicted in brown and the FabP46 in black. Neighbour molecules, surrounding the reference asymmetric unit, are also depicted (in grey) to give an overview of the crystal packing interactions.

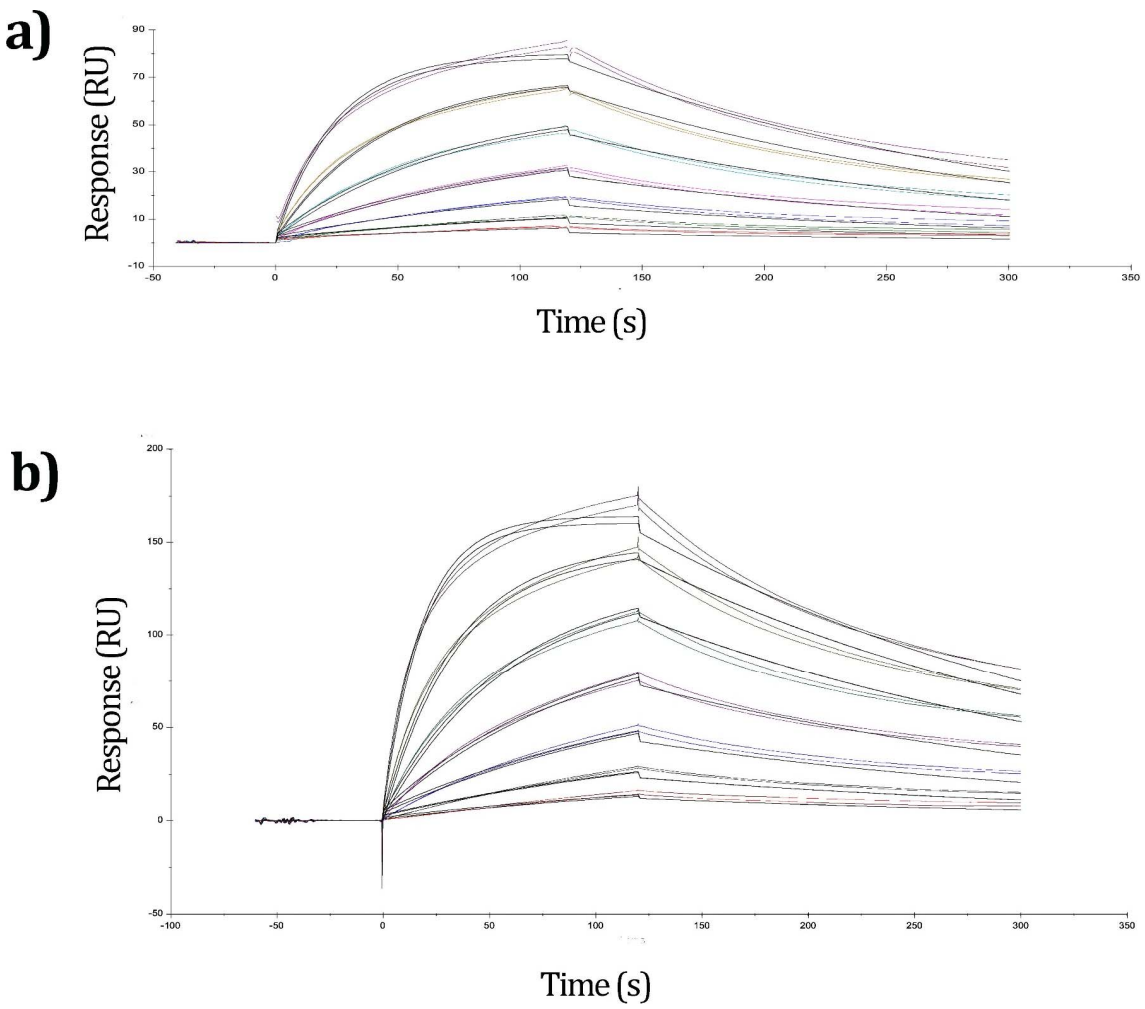

Figure S2 BIAcore SPR kinetic analyses of the binding between FabP46 and P46. Sensorgrams for immobilized P46 as a ligand to bind FabP46 were analyzed with BiaEvaluation software (BIAcore). The binding curves were fitted to a 1:1 model (low density ligand). a) Sensorgrams of P46 binding to increasing concentrations of FabP46 (from 3 to 200 nM, in each step the concentration is double), giving a K_D value of 29 nM. b) Same as (a) adding 1 uM of xylose, giving a KD value of 16nM.

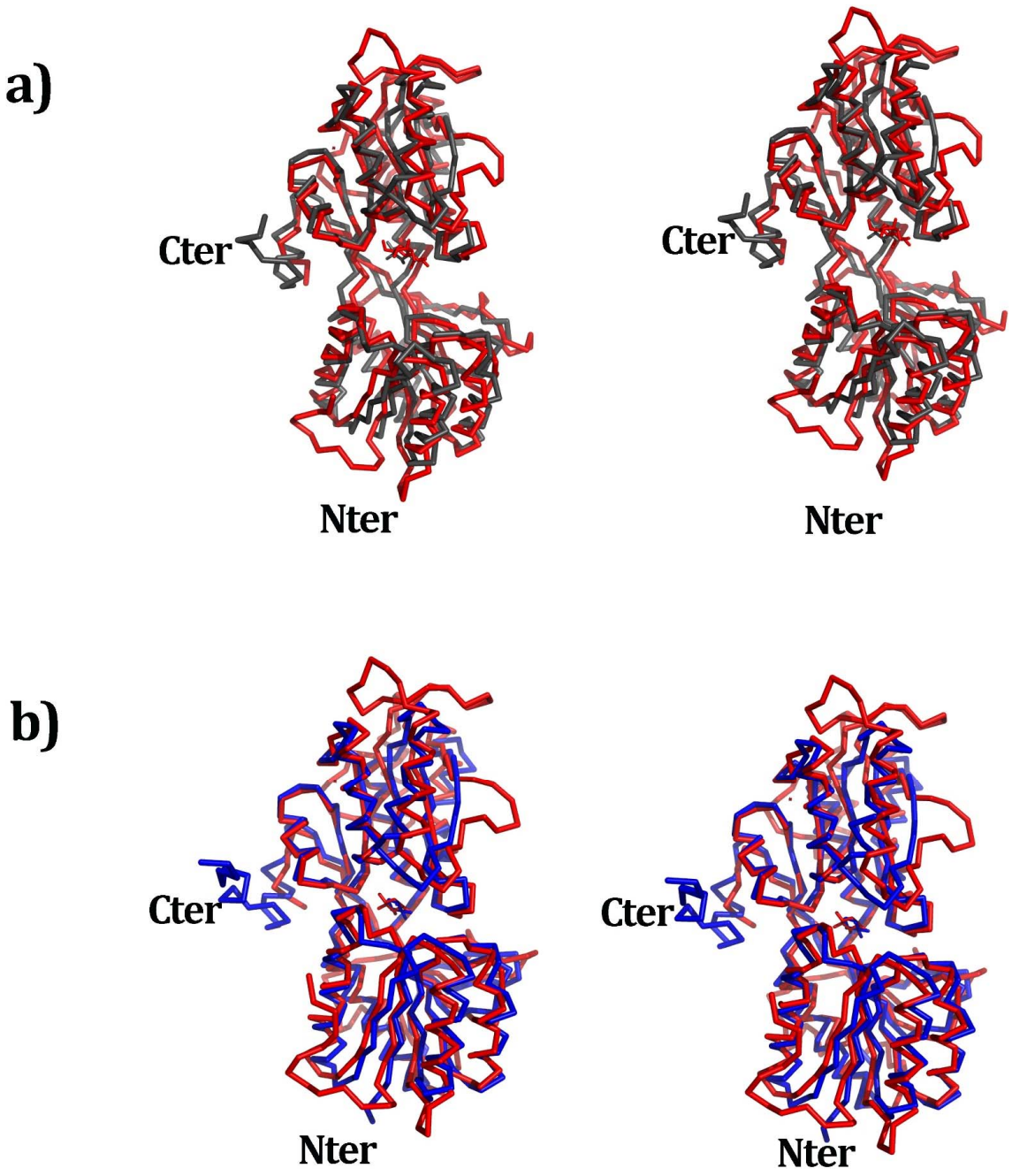

Figure S3 Superposition of closed and open structures. Stereo views of the superposition of P46 (in red) with the corresponding structures of the Xylose Binding Protein (XBP) from E. coli. The P46 and XBP structures have a bound ligand, respectively maltose and xylose ligand, in the same location. The top panel (a) corresponds to the superposition of the "open" conformations, with a RMSD of 2.0 Å for 305 residues (the PDB code of the XBP protein is 3m9x (in grey)). Panel (b) corresponds to the superposition of the "closed" conformations, with a RMSD of 1.8 Å for 313 residues" (the PDB code of the XBP protein is 3ma0 (in blue)). In both structures, P46 and XBP, there is a xylose bound in the same location.

Table S1 Interactions between P46 and FabP46 fragment

P46	FabP46 L (1)	Interface area Å^2 (2)	ΔG Kcal/mol	Hydrogen bonds	Salt Bridge
A	M	436	-2.9	6	
B	Q	420	-2.6	7	
S	C	417	-2.6	8	
T	I	422	-2.9	7	
P46	FabP46 H (1)				
A	N	387	2.3	7	3
B	R	393	0.4	8	4
S	D	390	0.9	8	4
T	E	405	-0.5	8	4

(1) specific interactions with the CDR regions

(2)Calculated with PISA (Krissinel & Henrick, 2007), as difference in total accessible areas of isolated and interfacing structures divided by two