Fig. S1

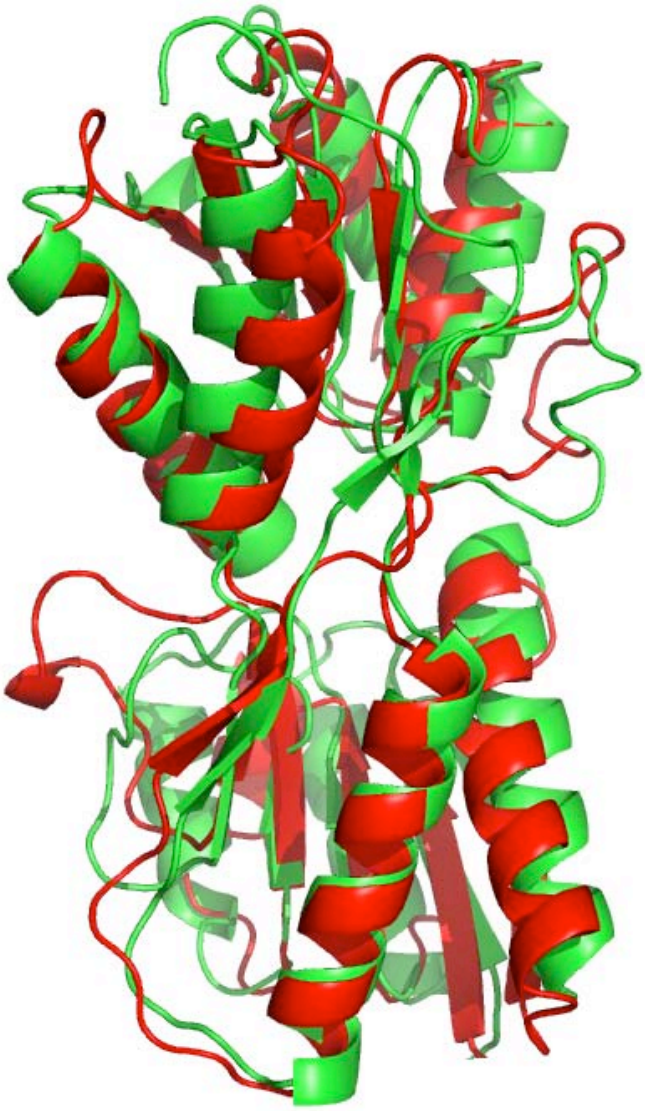

Fig. S1: Superimposition of the periplasmic binding protein fold of XylR (red) onto that of PurR (green). This overlay results in a root mean squared deviation of 2.5 Å for 212 corresponding Cα atoms.

Fig. S2

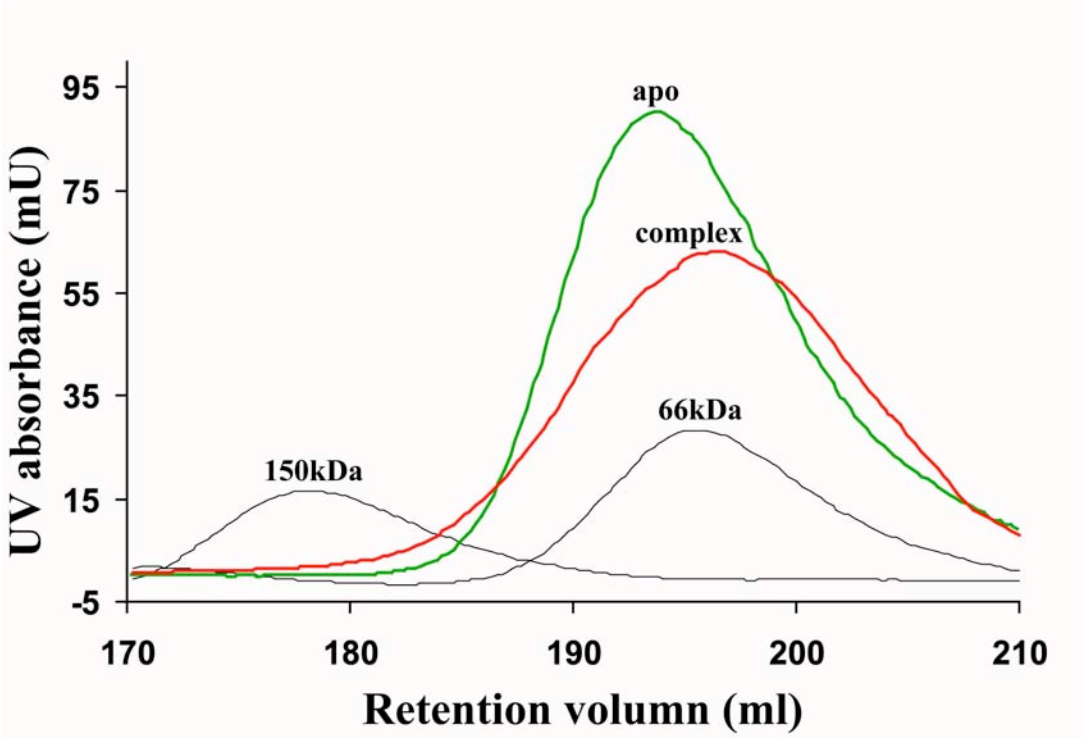

Fig. S2: Representative gel filtration characterization of XylR. All samples and protein standards were in the same buffer (25 mM Tris 7.5, 150 mM NaCl, 5% glycerol) and loaded onto a Superdex 200 26/60 column. Apo XylR (green curve), XylR-D-xylose complex (red) and standards (black) of alcohol dehyrogenase (150 kDa) and Bovine serum albumin (66 kDa). The molecular weights were determined by comparing ratio of V_e/V_o of protein samples and protein standards. Size exclusion chromatography experiments typically revealed molecular weights (MW) of between 70-75 kDa for XylR samples (the predicted values of for XylR monomer and dimer are 43 kDa and 87 kDa).

Fig. S3

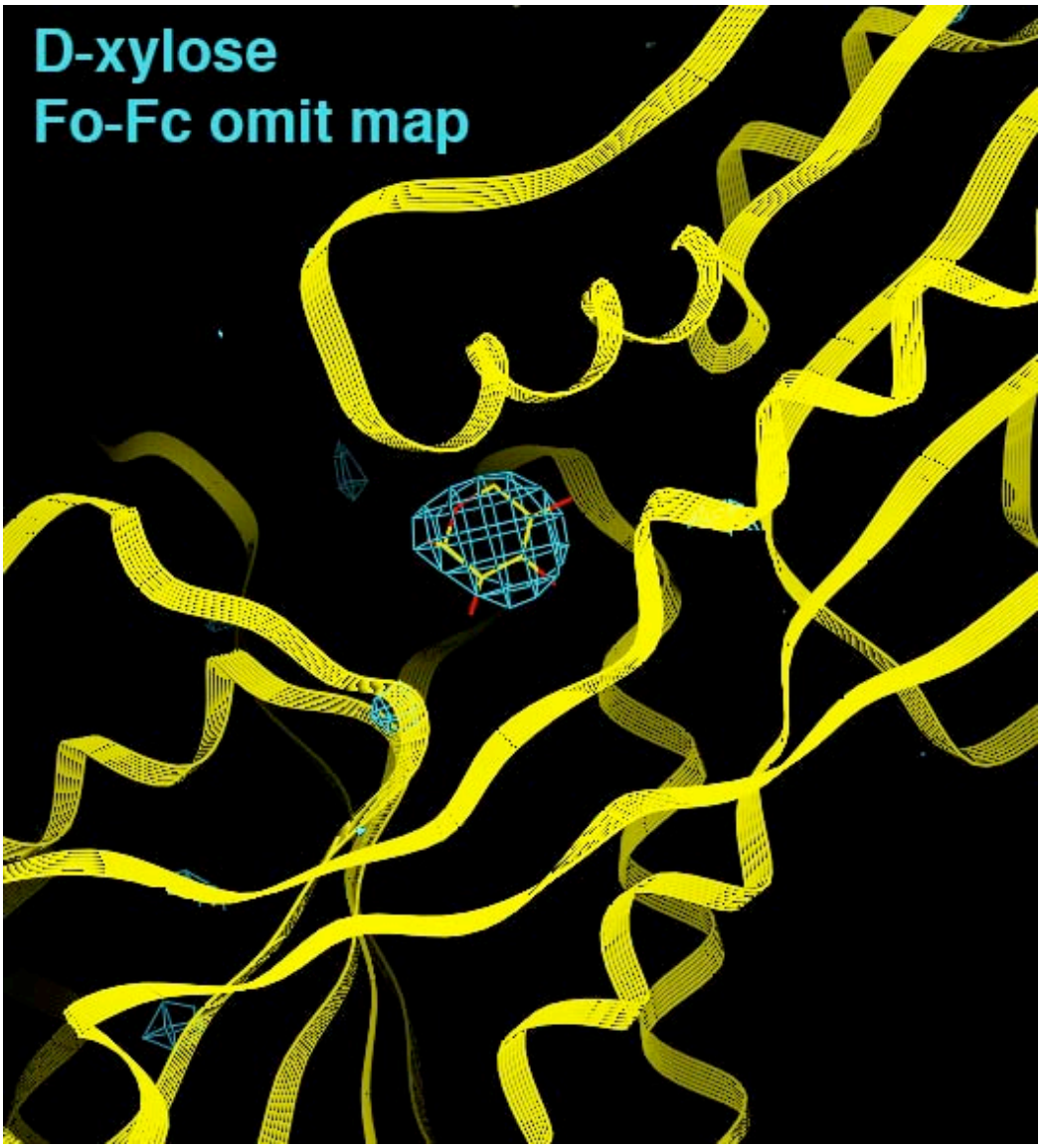

Fig. S3: Fo-Fc omit map contoured at 3.8 σ. This map was calculated by first removing the D-xylose and then refining the structure by simulated annealing. The D-xylose is shown as a stick with carbon and oxygen atoms colored yellow and red, respectively. The protein is shown as yellow ribbons and the map is represented as a blue mesh.

Fig. S4

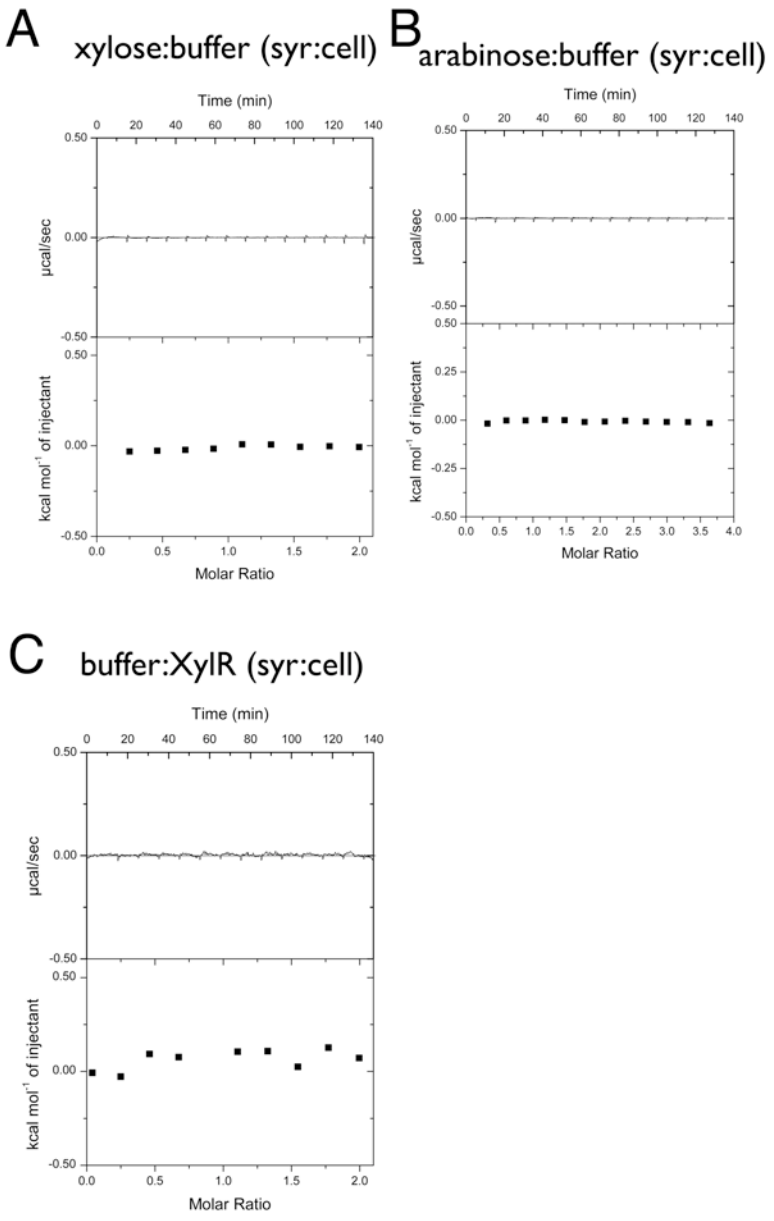

Fig. S4: ITC control experiments in which D-xylose and L-arabinose binding to XylR was analysed. (A) The titration of D-xylose into the reaction buffer produced minimal heats of dilution. (B) Titration experiment of L-arabinose into reaction buffer. The lack of discernable peak confirms that the solution containing the sugars and that containing the protein was well matched. (C) Titration experiment of buffer into XylR also revealed no significant signal.

Fig. S5

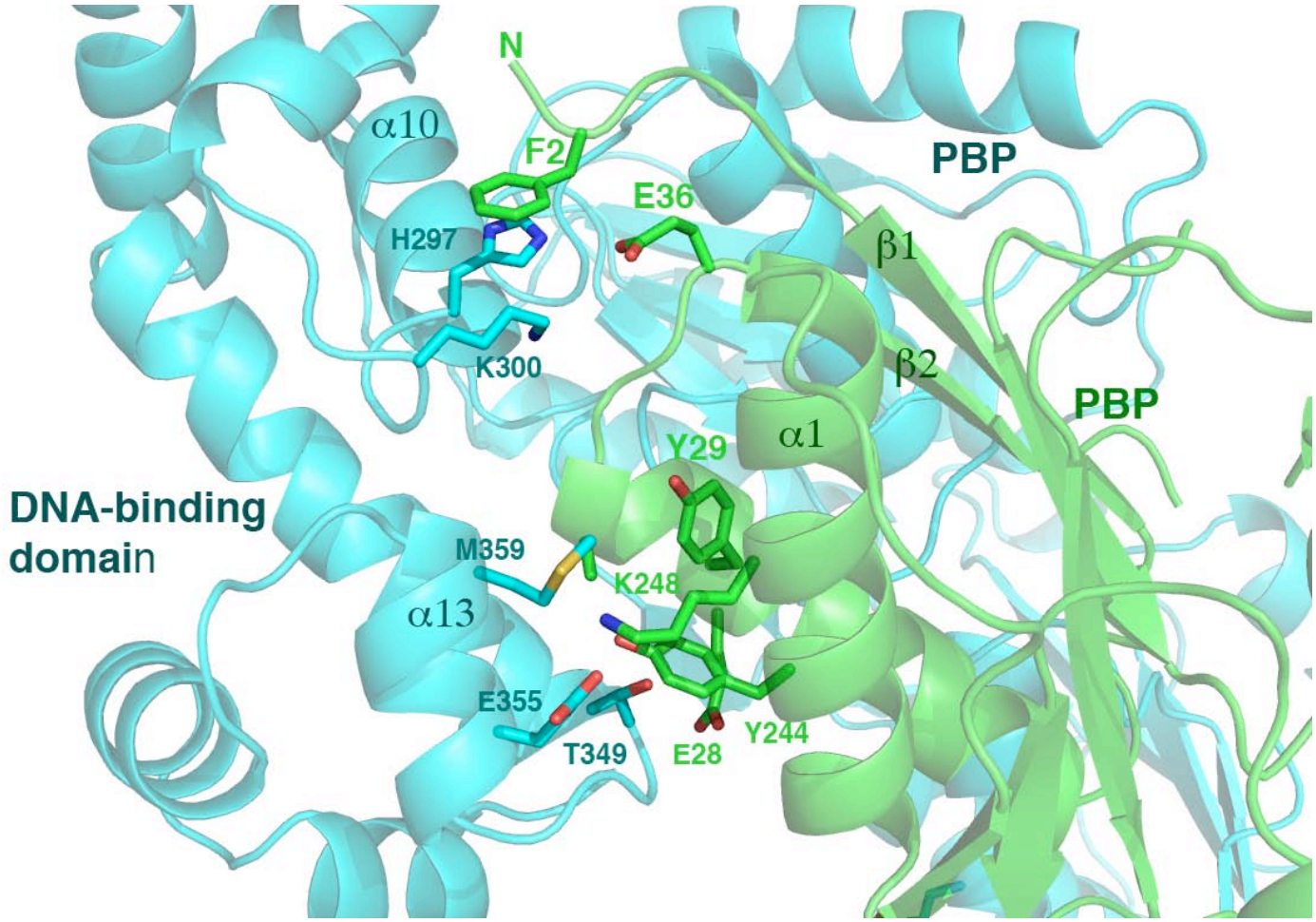

Fig. S5: Ribbon diagram of the XylR interface formed between the DNA-binding domain of one subunit (cyan) with the PBP fold of the other subunit (green).

Fig. S6

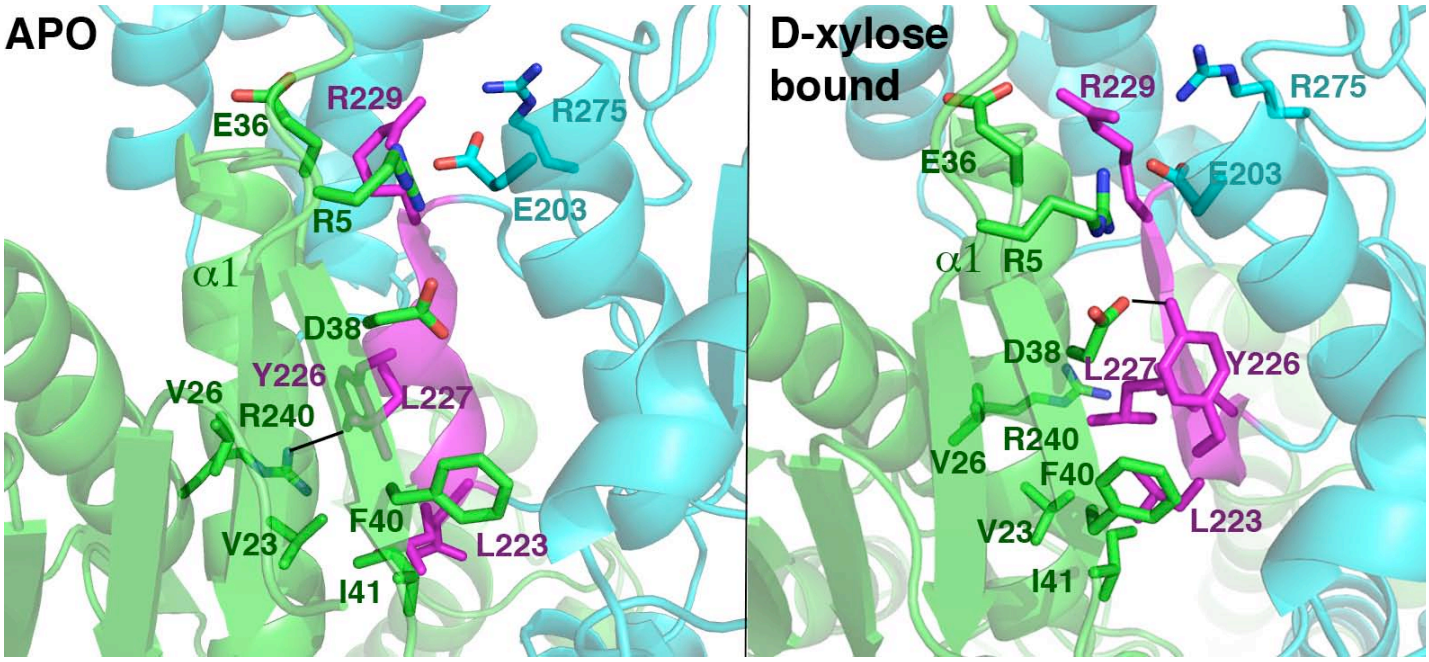

Fig. S6: Ribbon diagram of the XylR interface formed between the PBP domains of XylR. To the left is shown the interface in the apo form where residues 221-229, which undergo a helix to strand change upon D-xylose binding, are colored magneta. To the right is the same interface in the D-xylose bound form.

Fig. S7

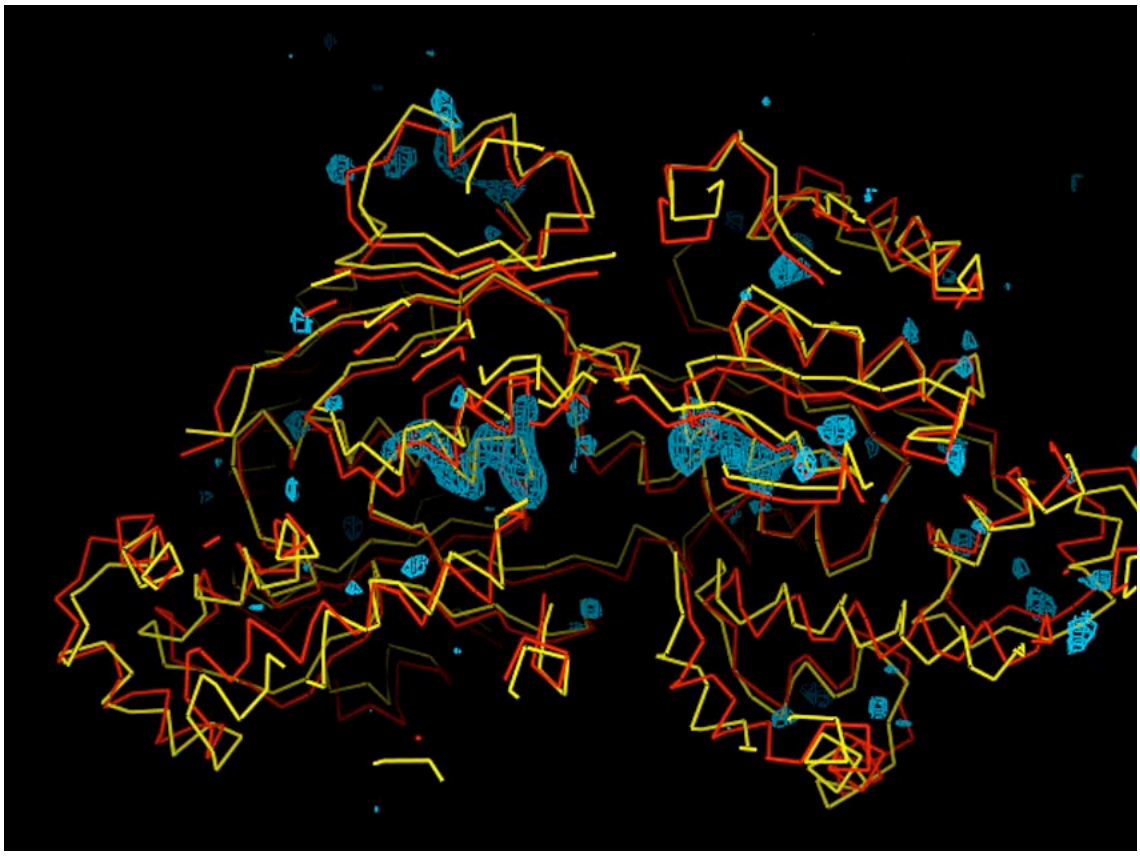

Fig. S7. Superimposition of the D-xylose bound (red) XylR structure onto the apo (yellow) XylR structure showing the initial Fo-Fc map (after Molecular replacement using the D-xylose structure as a model followed by rigid body refinement) contoured at 3.4 σ. A large shift in the conformation of residues 221-229 is observed (central helices) wherein these amino acids undergo a strand to helix transition. This is quite clear despite the relatively low resolution of the apo structure (3.4 Å).

Fig. S8

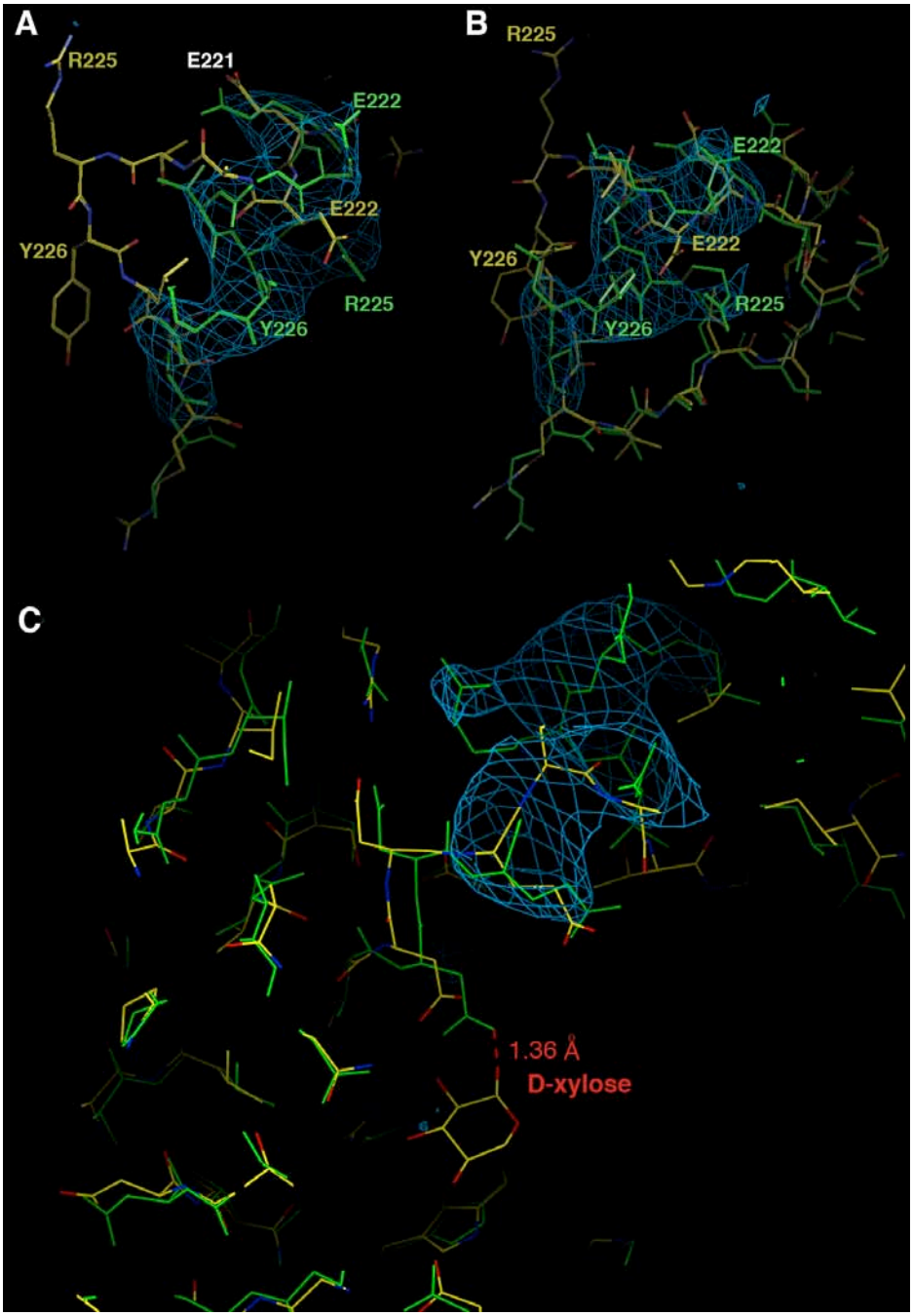

Fig. S8. Close up view of the transition region of XylR (A-B) Close up of a superimposition of the D-xylose bound (yellow) XylR structure onto the apo (green) XylR structure around residues 221-229, which undergoes a helix to strand transition upon D-xylose binding. The blue mesh corresponds to the initial Fo-Fc map (after Molecular replacement using the D-xylose structure as a model followed by rigid body refinement) contoured at 3.6 σ. The folding of residues 221-229 into a helixcal conformation is clear, again, despite the relatively low resolution of the apo structure (3.4 Å). (C) Same region showing the location of the D-xylose in the complex structure underscoring the resulting clash between the D-xylose and apo form, which is proposed to trigger the helix to coil transition.

Fig. S9

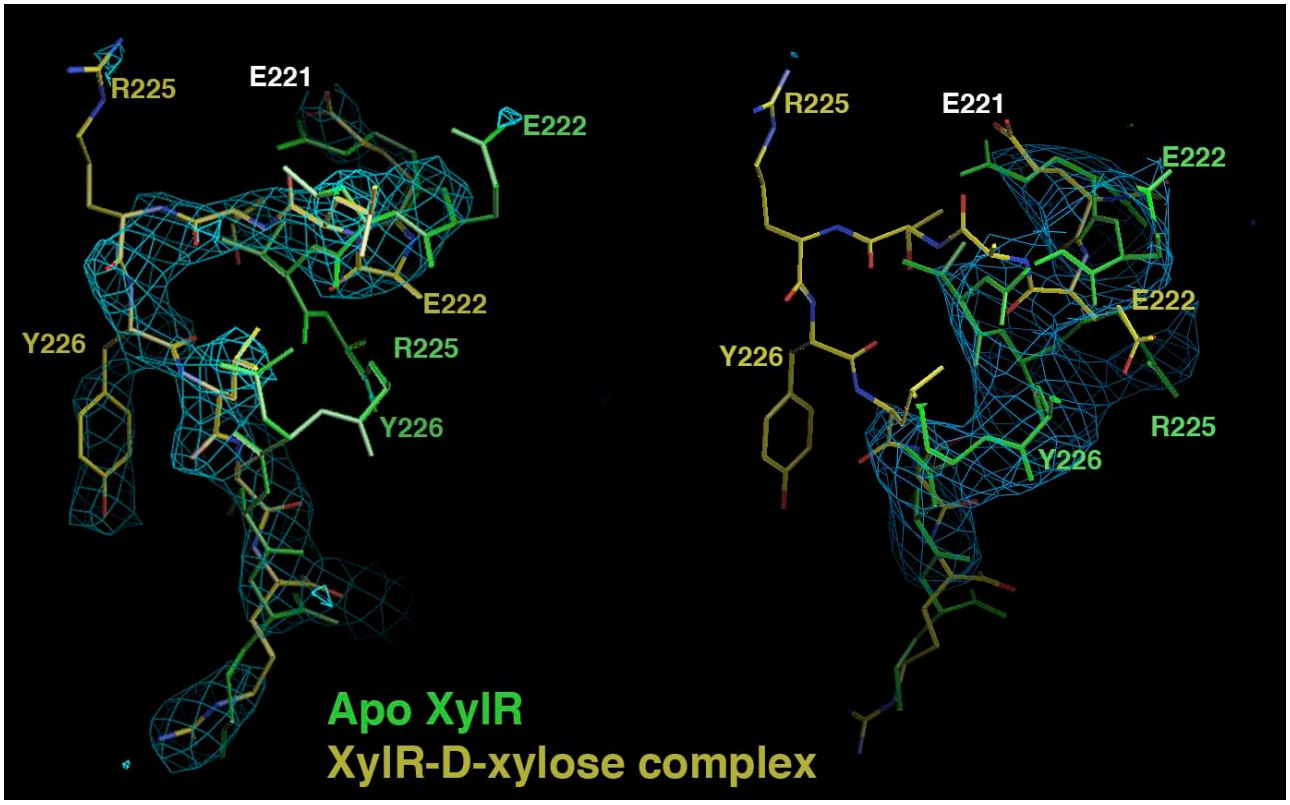

Fig. S9. Close up comparison of omit Fo-Fc map of residues 221-229 of the XylR-D-xylose bound structure (green) and the initial Fo-Fc map (after Molecular replacement using the D-xylose structure as a model followed by rigid body refinement) of the apo XylR structure (yellow). Both maps are contoured at 3.6 σ. Superimpositions of each structure onto the other structure with map included highlights the conformational change in this region.