SUPPLEMENTAL DATA

MECHANISTIC INSIGHTS INTO THE ALLOSTERIC REGULATION OF BACTERIAL ADP-GLUCOSE PYROPHOSPHORYLASES

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1. SUPPLEMENTAL TABLE

Table 1. *Ec*AGPase•R130A data collection and refinement statistics.

	***Ec*AGPase R130A**
Beamline / PDB code	I04 DLS / 5MNI
Wavelength (Å)	0.9795
Resolution range (Å)	73.8 - 3.09 (3.201 - 3.09)
Space group	$P\ 2_1$
Unit cell	94.2243 147.603 125.572 90 91.5238 90
Total reflections	210464 (21224)
Unique reflections	62893 (6268)
Multiplicity	3.3 (3.4)
Completeness (%)	0.99 (1.00)
Mean I/sigma (I)	8.86 (1.23)
Wilson B-factor	84.78
R-merge	0.08515 (0.9436)
R-meas	0.1016 (1.122)
CC1/2	0.997 (0.524)
CC*	0.999 (0.829)
Reflections used in refinement	62619 (6176)
Reflections used for R-free	3163 (321)
R-work	0.2356 (0.3831)
R-free	0.2727 (0.4124)
R.m.s. coordinates error (Å) Luzzati plot	0.6528
Number of non-hydrogen atoms	23701
Macromolecules	23701
Ligands	-
Protein residues	3182
RMS (bonds)	0.005
RMS (angles)	0.68
Ramachandran favored (%)	95
Ramachandran outliers (%)	0.22
Rotamer outliers (%)	0.8
Clashscore	4.13
Average B-factor	82.52
Macromolecules	82.52
Ligands	-
Solvent	-

Statistics for the highest-resolution shell are shown in parentheses. Atom count do not consider hydrogen atoms.
* Friedel mates were averaged when calculating reflection statistics.

2. SUPPLEMENTAL FIGURES

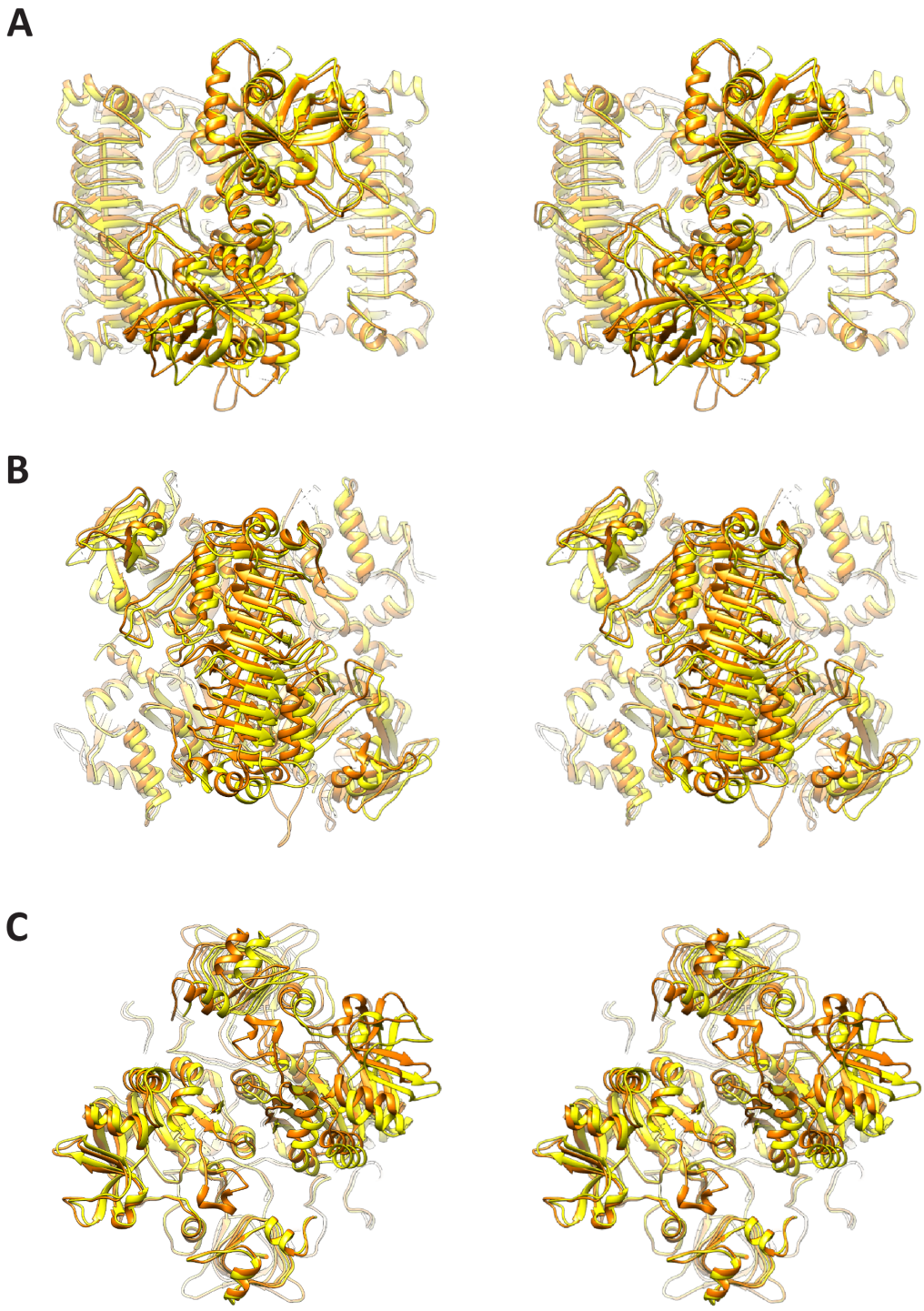

Figure S1. The crystal structure of *Ec*AGPase•R130A. *A-B*. Two stereo views of the structural superposition between the *Ec*AGPase•R130A (yellow) and *Ec*AGPase•FBP (orange) tetramers, based on the alignment of LβH domains pairs as shown in Figure 8. *C*. Stereo view of the *Ec*AGPase•R130A structure (protomer D: yellow) centred at the sensory motif, superimposed with an *Ec*AGPase•AMP•SUC protomer (orange), revealing the prominent conformational changes leading the SM motif to partially occupy the AMP binding site. The other *Ec*AGPase•R130A protomers of the asymmetric unit appear superposed in grey scale, showing variability in the RL1, RL2 regions and the G-rich loop.

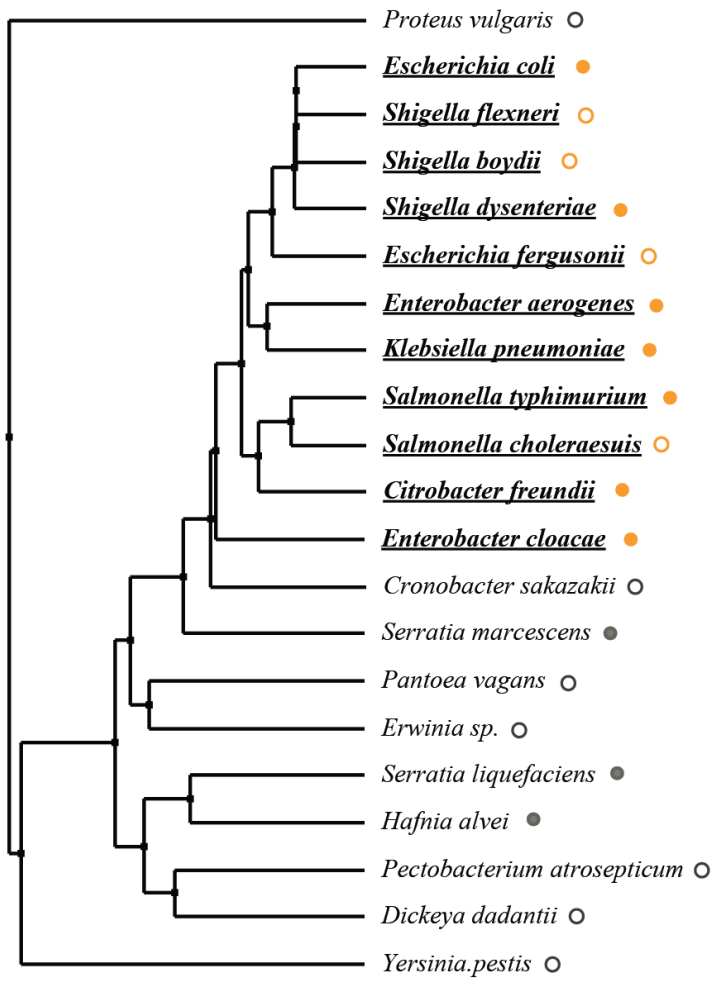

Figure S2. Evolution of the FBP regulatory site within the enterobacteriaceae family of AGPases. Middle distance BLOSUM62 tree. The species known to use FBP are marked with an orange spot and those proposed to use it, based on the conservation of the C-terminus, with an empty orange spot. The species reported not to be regulated by this metabolite are marked with a grey spot and those proposed not to be with an empty grey spot.