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**Supporting information for article:**

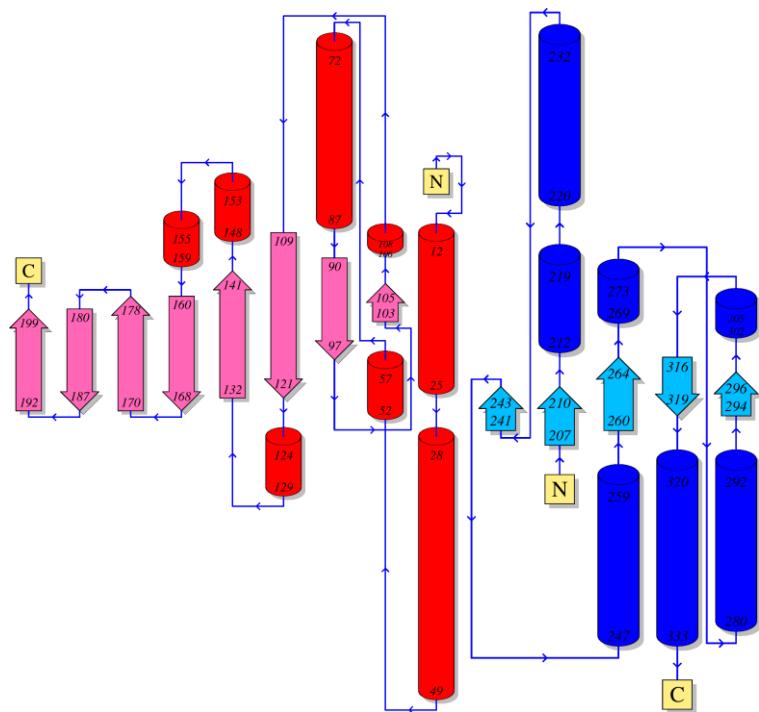
**Structures of the *Mycobacterium tuberculosis* GlpX protein (class II fructose-1,6-bisphosphatase): implications for the active oligomeric state, catalytic mechanism and citrate inhibition**

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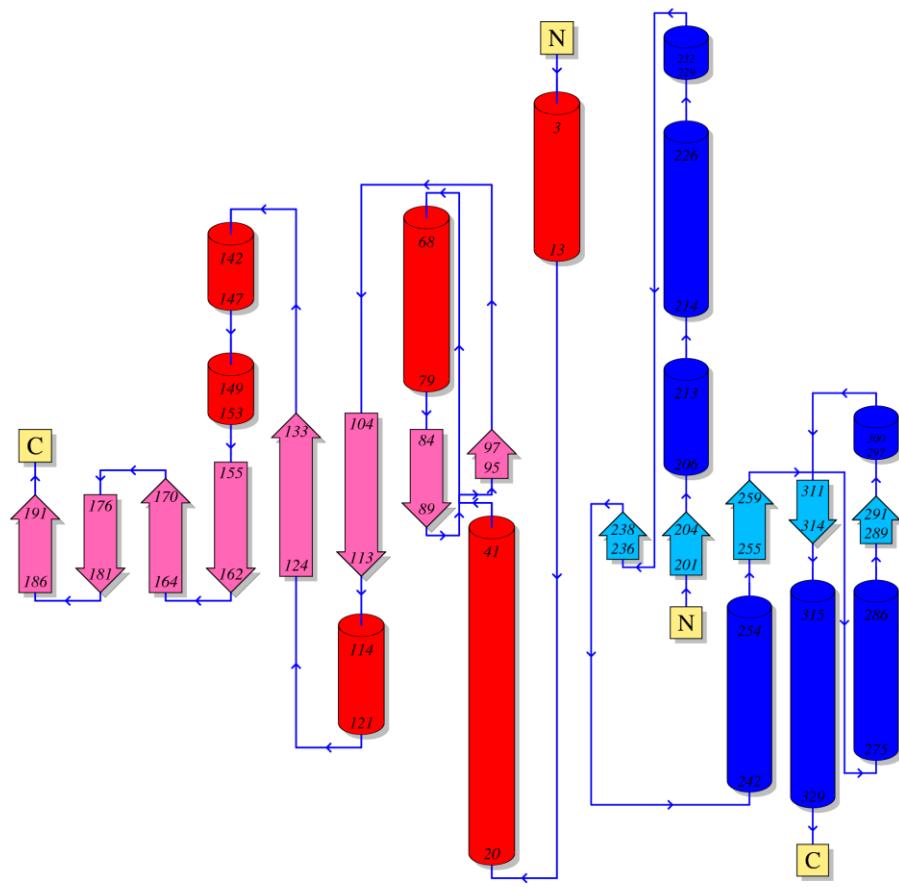
**Figure S1** Boundaries of  $\beta$ -strands in the different  $\beta$ -sheets present in Class I and Class II FBPases. Definition of the  $\beta$ -sheets (A, B) and the boundaries of the component  $\beta$ -strands in the structures of previously published Class I FBPase from pig kidney (4fbp, Table S1a) and *E.coli* (2q8m, Table S1b), compared with the *E. coli* Class II FBPase (3d1r, Table S1c). The overall topologies of the corresponding domain structures are presented in Figs. S1(a), S1(b) and S1(c) respectively (domains 1, 2 in red and blue respectively). Tables and figures were prepared with PDBSum ([www.ebi.ac.uk/thornton-srv/databases/pdbsum/](http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/)).

**Table S1(a).** 4fbp Pig kidney (*Sus scrofa*) (Class I)

No.	Start	End	Sheet	resid	No.	Sequence	
						Edge	
1.	Thr91	Thr96	A	6	No	TCVLVLT	
2.	Ile103	Ile104	A	2	Yes	II	
3.	Arg110	Asp121	A	12	No	RGKYVVCFDPLD	
4.	Ile132	Arg140	A	9	No	IGTIFGIYR	
5.	Ala161	Tyr167	A	7	No	AAGYALY	
6.	Thr171	Met177	A	7	No	TMLVLAM	
7.	Gly180	Asp187	A	8	No	GVNCFMLD	
8.	Glu192	Arg198	A	7	Yes	EFILVDR	
9.	Ile208	Ser210	B	3	No	IYS	
10.	Gly241	Ala242	B	2	Yes	GA	
11.	Ile261	Tyr264	B	4	No	IFMY	
12.	Leu294	Thr296	B	3	Yes	LAT	
13.	Ile316	Gly319	B	4	No	IILG	

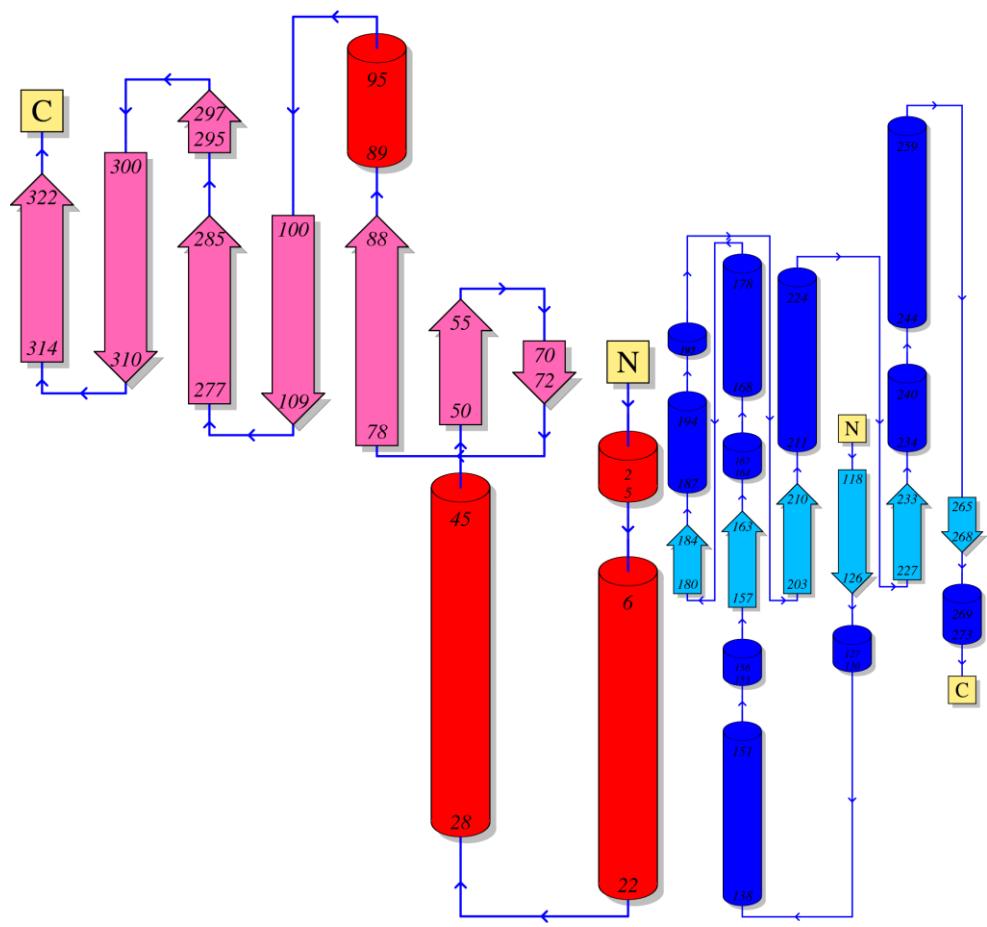
**Figure S1(a)****Table S1(b).** 2q8m (*E. coli*) Class I

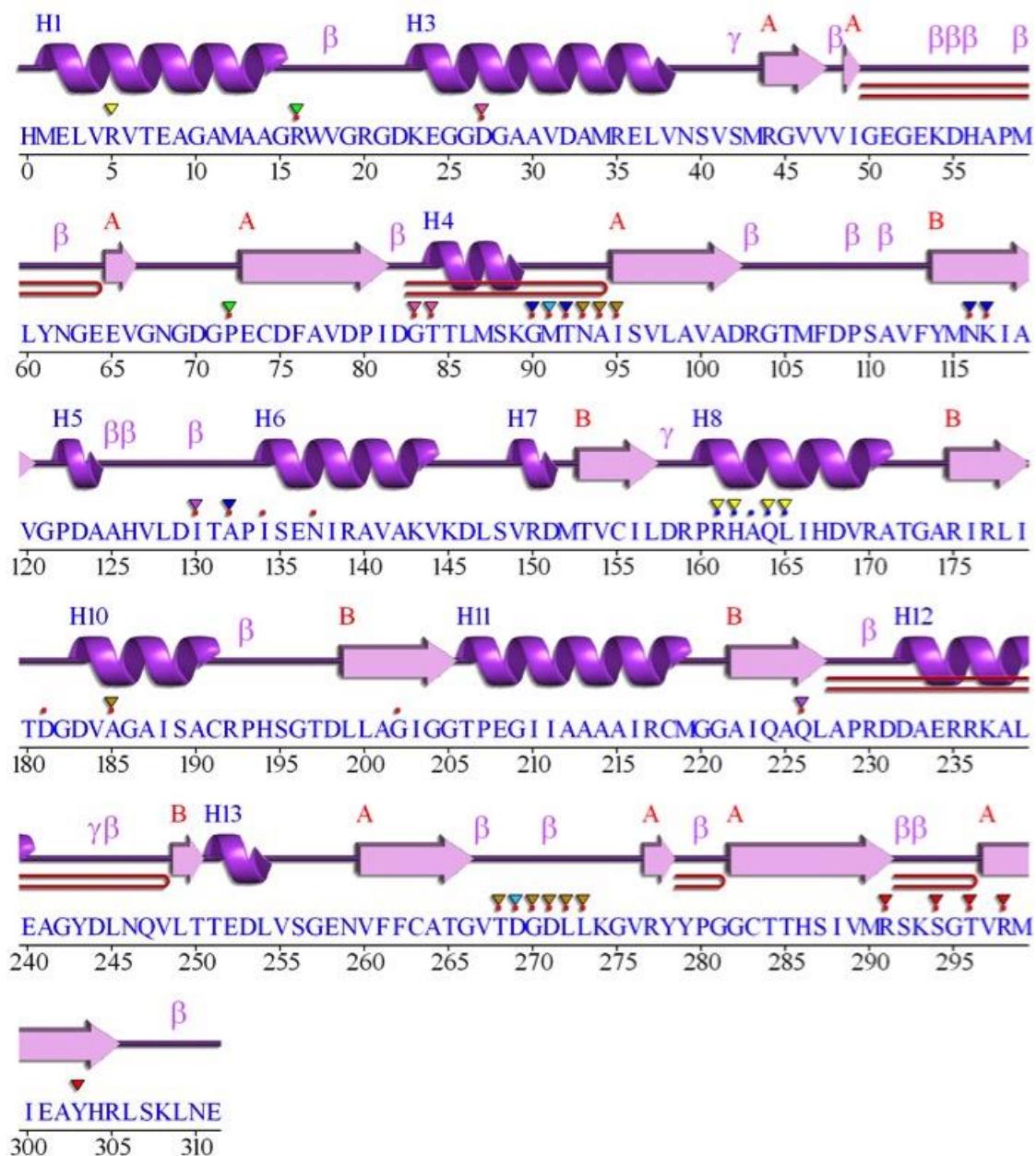
No.	Start	End	Sheet	resid	No.		Sequence
					Edge	Sequence	
1.	Gly85	Ser88	A	4	No	GIAS	
2.	Val95	Val96	A	2	Yes	VV	
3.	Tyr105	Asp113	A	9	No	YVVL-DPLD	
4.	Val124	Arg132	A	9	No	VGTIFSIYR	
5.	Ala155	Tyr161	A	7	No	AAGYVVY	
6.	Thr165	Thr170	A	6	No	T-LVYT	
7.	Val175	Tyr180	A	6	No	VHAFTY	
8.	Phe187	Unk194	A	8	Yes	FCLCQER-	
9.	Thr202	Ser204	B	3	No	TYS	
10.	Thr236	Ser237	B	2	Yes	TS	
11.	Ile256	Tyr259	B	4	No	IYLY	
12.	Lys289	Ser291	B	3	Yes	KAS	
13.	Phe311	Gly314	B	4	No	FFVG	

**Figure S1(b)**

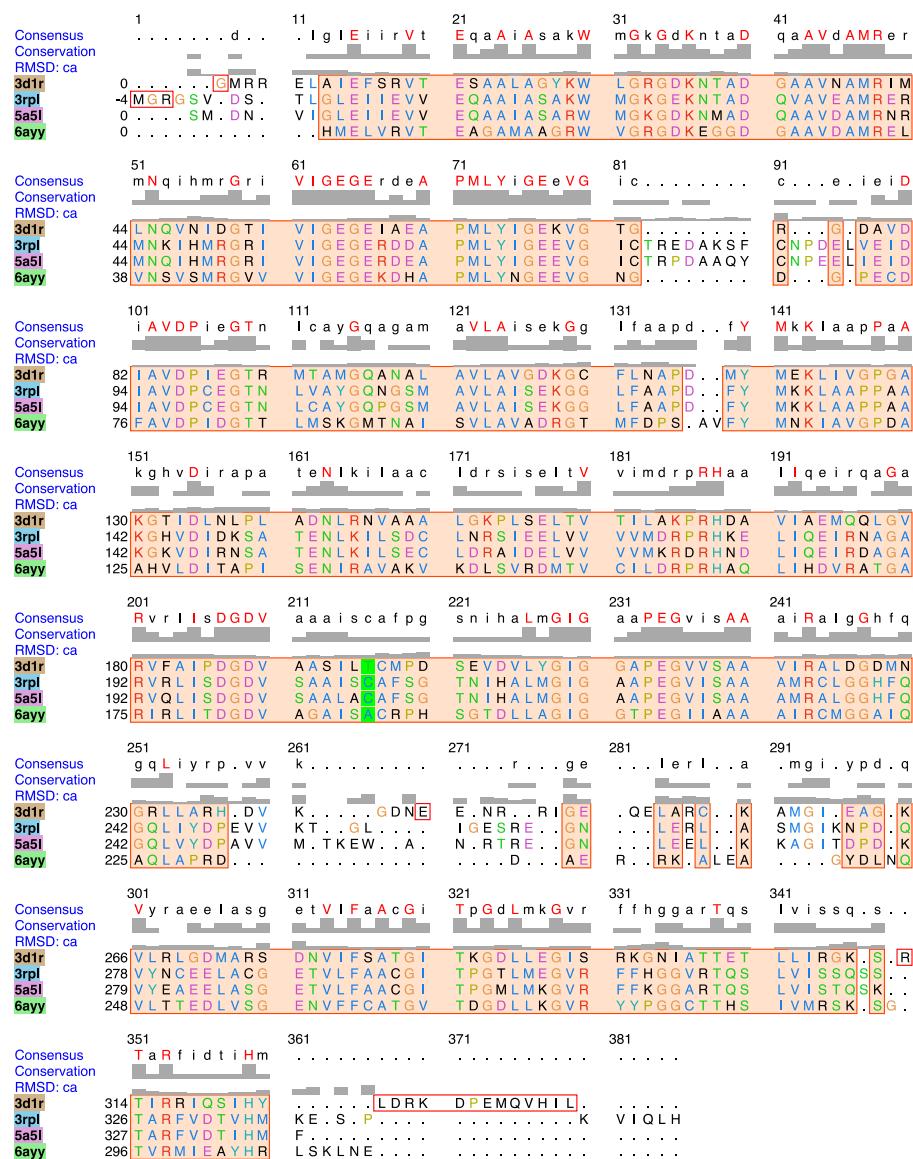
**Table S1(c).** 3d1r (*E. coli*) (Class II)

No.	Start	End	Sheet	resid	No.	Sequence
					Edge	
1.	Asp50	Ile55	A	6	No	DGTIVI
2.	Lys71	Val72	A	2	Yes	KV
3.	Ala79	Glu88	A	10	No	AVDIAVDPIE
4.	Leu101	Asp108	A	8	No	LAVLAVGD
5.	Tyr119	Val125	B	7	No	YMEKLIV
6.	Thr158	Leu162	B	5	No	TVTIL
7.	Arg180	Ile184	B	5	Yes	RVFAI
8.	Val204	Gly210	B	7	No	VLYGIGG
9.	Asp227	Leu233	B	7	No	DMNGRLL
10.	Val266	Arg268	B	3	Yes	VLR
11.	Val278	Gly284	A	7	No	VIFSATG
12.	Ser295	Lys297	A	3	Yes	SRK
13.	Ile300	Arg309	A	10	No	IATTETLLIR
14.	Ile315	His322	A	8	Yes	IRRIQSIH

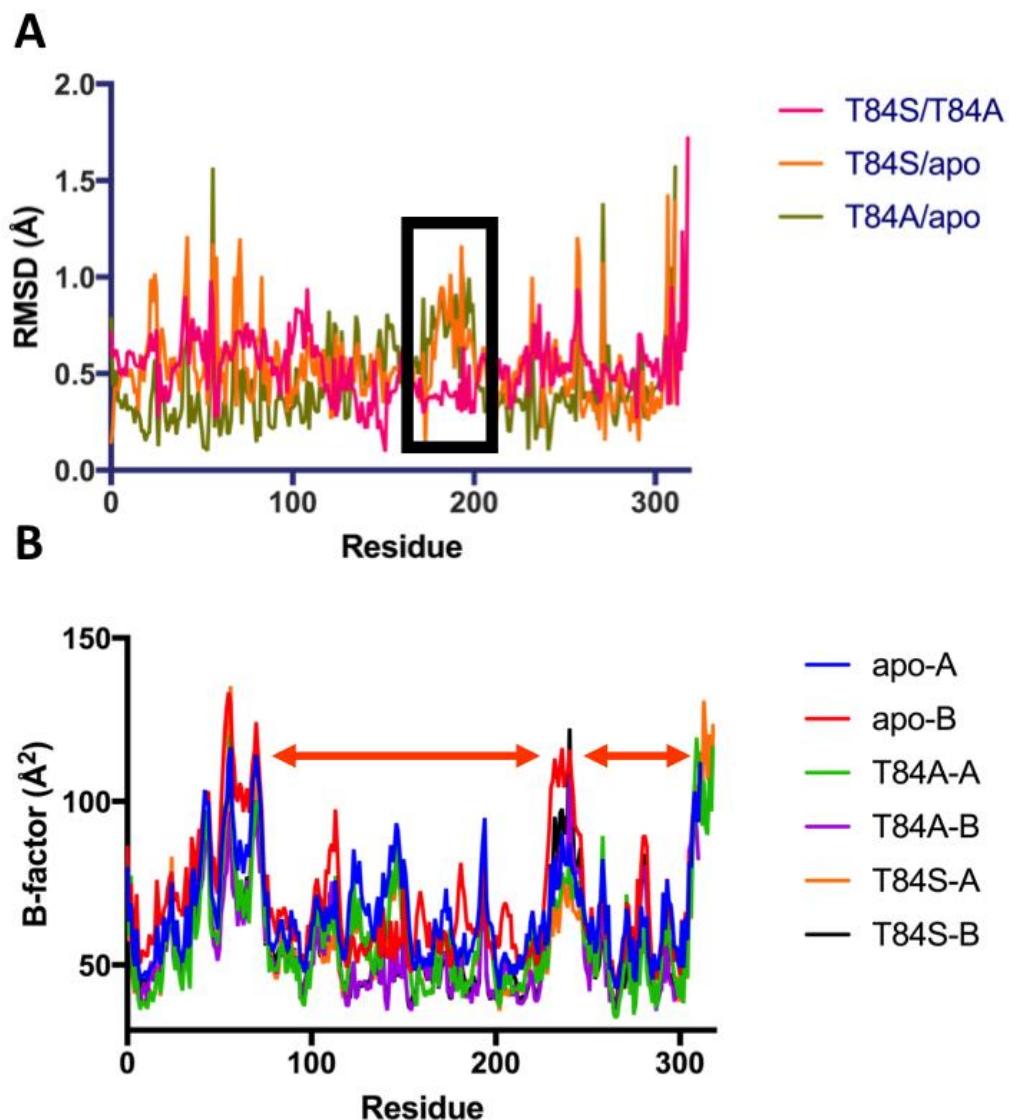
**Figure S1(c)**



**Figure S2** Secondary structure of *MtFPBaseII*. The secondary structure for *MtFPBaseII* is represented as  $\alpha$ -helices (H1-H13) and  $\beta$ -sheets (A or B), prepared by PDBsum (Laskowski, 2001). Turns are defined as either  $\beta$  or  $\gamma$ . Red squares indicated residue contacts to a ligand and blue squares to a metal. Laskowski, R. A. (2001). *Nucleic Acids Res* **29**, 221-222.



**Figure S3** Structural alignment of several Class II FBPases. Structural alignment for *Mycobacterium tuberculosis* T84S (6ayy), *Escherichia coli* Class II (3d1r), *Synechocystis* FBP/SBPase (3rpl) and *Thermosynechococcus elongatus* FBP/SBPase (5a5l). Strictly conserved residues have a red capital letter in the consensus line, conserved homologous residues are in lower case and variant residues or gaps are represented by dots. The conservation profile is higher when more species have the conserved residue(s). RMSD line represents the distance of C<sub>α</sub> pairs. Numeric details are given in Table 2 in terms of RMSD among the different proteins.



**Figure S4** Comparisons of chains of *MtFPBaseII* structures. (A) RMSD deviations among A chains from the variants and apo *MtFBPaseII* structures. Black box highlights the region of largest structural differences between the apo and the two variants, aside from the C-terminus. (B) B-factor values for the A and B chains of *MtFBPaseII* structures.  $\beta$ -sheets are bounded by double head arrows, emphasizing the most stable portions of the enzyme. Graphs were prepared with Prism.