

S1 Table

Protein (#ch, #res)	PDB ID (ligands)	Ligated Site (A/I/S)	$\Delta g_A(\mathcal{P} \rightarrow A\mathcal{P})$ ($\Delta g_{mer}(\mathcal{P} \rightarrow A\mathcal{P})$) kcal/mol	Regulated Site	$\Delta g_F(\mathcal{P} \rightarrow A\mathcal{P})$ ($\Delta g_{mer}(\mathcal{P} \rightarrow A\mathcal{P})$) kcal/mol
ATCase (2x3+3x2, 2736)	3d7s (apo)	6 x ATP/CTP (A/I)	-3.35 (-2.02) ^(*)	PAL	1.98 (1.47) ^(**)
	1rac (CTP)	6 x ATP/CTP (A/I)	-3.27 (-1.61) ^(*)	PAL	1.94 (1.83) ^(**)
	7ati (PAL, ATP)	6 x ATP/CTP (A/I)	-2.80 (-1.55) ^(*)	PAL	1.88 (1.73) ^(**)
	1d09 (PAL)	6 x ATP/CTP (A/I)	-2.32 (-1.35) ^(*)	PAL	1.28 (1.18) ^(**)
AnthS (2+2, 1426)	1i7q (BEZ, PYR, GLU)	2 x TRP (I)	-2.87 (-0.42) ^(*)	BEZ+PYR GLU	-0.60 (-0.42) ^(*) 2.13 (2.29) ^(**)
	1i7s (TRP)	2 x TRP (I)	-2.14 (-0.28) ^(*)	BEZ+PYR GLU	-0.11 (-0.28) ^(*) 1.63 (1.90) ^(**)
BGDH (6, 2976)	1nr7 (apo)	6 x ADP (A)	-1.51 (-0.16)	NDP GLU	0.11 -0.88 (-0.16)
		6 x GTP (I)	-0.32 (0.61)	NDP GLU	0.14 0.47 (0.61)
		6 x ADP (A) GTP (I)	-0.64 -0.40 (0.60)	NDP GLU	0.32 -0.01 (0.60)
	1hwz (NDP, GLU, GTP)	6 x ADP (A)	-1.41 (-0.41)	NDP GLU	-0.55 -0.83 (-0.41)
		6 x GTP (I)	-1.61 (-0.11)	NDP GLU	-0.94 -0.19 (-0.11)
		6 x ADP (A) GTP (I)	-1.06 -2.18 (-0.32)	NDP GLU	-1.18 -0.62 (-0.32)
	1nqt (ADP)	6 x ADP (A)	-1.32 (0.02)	NDP GLU	0.26 -0.66 (0.02)
		6 x GTP (I)	-0.26 (0.65)	NDP GLU	0.23 0.49 (0.65)
		6 x ADP (A) GTP (I)	-0.52 -0.31 (0.77)	NDP GLU	0.52 0.16 (0.77)
		CAP (2, 418)	2wc2	1 x cAMP (A)	-1.49 (-0.13) ^(#)
(apo)	2 x cAMP (A)		-2.37 (-0.30)	DNA	0.85 (-0.30)
1run	1 x cAMP (A)		-2.07 (-0.64) ^(#)	DNA cAMP	-0.41 -0.55 (-0.08) ^(##)
(cAMP)	2 x cAMP (A)		-3.32 (-0.49)	DNA	0.44 (-0.49)
1o3q	1 x cAMP (A)		-1.80 (-0.47) ^(#)	DNA cAMP	-0.09 0.10 (0.67) ^(##)
(cAMP, DNA)	2 x cAMP (A)		-1.53 (-0.52)	DNA	-0.26 (-0.52)
DAHPS (4, 1401)	1gg1 (PGA)	4 x PHE (I)	-2.33 (0.25)	PGA	0.33 (0.25)
	1kfl (PGA, PHE)	4 x PHE (I)	-1.36 (0.40)	PGA	0.31 (0.40)
DAK (2, 735)	3ju5 (apo)	1 x ADP (S) ARG (S)	-1.93 -0.76 (-0.72)	ADP ARG	0.49 1.03 (0.74)
		2 x ADP (S) ARG (S)	-0.85 -0.11 (-0.05)	ADP ARG	-0.85 -0.11 (-0.05)
	3ju6 (ANP, ARG)	1 x ADP (S) ARG (S)	-1.49 -0.69 (-0.60)	ADP ARG	1.32 0.95 (1.01)
		2 x ADP (S) ARG (S)	-0.91 -0.33 (0.24)	ADP ARG	-0.91 -0.33 (0.24)

S1 TABLE. Results on allosteric causality and energetics obtained for proteins analyzed in this work. Complete data obtained for all available forms of proteins. For designation of columns see Table 1 in the main text.

Protein (#ch, #res)	PDB ID (ligands)	Ligated Site (A/I/S)	$\Delta g_A(\mathcal{P} \rightarrow A\mathcal{P})$ ($\Delta g_{mer}(\mathcal{P} \rightarrow A\mathcal{P})$) kcal/mol	Regulated Site	$\Delta g_F(\mathcal{P} \rightarrow A\mathcal{P})$ ($\Delta g_{mer}(\mathcal{P} \rightarrow A\mathcal{P})$) kcal/mol
G6PD (6, 1596)	1cd5 (apo)	6 x 16G (A)	-0.04 (0.31)	AGP	0.37 (0.31)
	1hor (AGP)	6 x 16G (A)	-0.37 (0.17)	AGP	0.25 (0.17)
	1hot (16G)	6 x 16G (A)	-0.36 (0.10)	AGP	0.16 (0.10)
NADME (4, 2232)	1gz3 (FUM, ATP)	4 x FUM (A)	-0.85 (-0.32)	NAD	-0.40 (-0.32)
		4 x ATP (S/I)	-1.23 (0.19)	NAD	0.78 (0.19)
	1efk (NAD)	4 x FUM (A)	-0.53 (-0.14)	NAD	-0.14 (-0.14)
		4 x ATP (S/I)	-1.42 (-0.25)	NAD	0.11 (-0.25)
PFK (4, 1284)	3pfk (apo)	4 x PEP/ADPa (I/A)	-0.78 (0.16)	F6P ADP _f	0.71 -0.11 (0.16)
		4 x ADP _f (S/A)	-0.74 (0.50)	F6P	1.74 (0.50)
		4 x PEP/ADPa (I/A)	0.35 (0.68)	F6P	2.22 (0.68)
		4 x ADP _f (S/A)	-1.08		
	4pfk (F6P, ADP)	4 x PEP/ADPa (I/A)	-0.71 (0.11)	F6P ADP _f	0.76 0.19 (0.11)
		4 x ADP _f (S/A)	-0.79 (0.40)	F6P	1.64 (0.40)
		4 x PEP/ADPa (I/A)	-0.10 (0.55)	F6P	2.06 (0.55)
		4 x ADP _f (S/A)	-0.74		
	6pfk (PEP)	4 x PEP/ADPa (I/A)	-1.55 (0.08)	F6P ADP _f	0.64 0.60 (0.08)
		4 x ADP _f (S/A)	-0.64 (0.64)	F6P	1.78 (0.64)
		4 x PEP/ADPa (I/A)	-0.34 (0.71)	F6P	2.39 (0.71)
		4 x ADP _f (S/A)	-0.78		
PGDH (4, 1624)	1psd (SER ,NAD)	8 x SER (I)	-0.58 (0.03)	AKG NAD	0.08 0.38 (0.03)
		8 x SER (I)	0.23 (0.09)	AKG NAD	0.05 0.33 (0.09)
PKA (1, 336)	1atp (ATP)	1 xATP (I)	-4.28 (-0.10)	MPD	1.97 (-0.10)
	1j3h (MPD)	1 xATP (I)	-3.54 (0.18)	MPD	1.55 (0.18)
PTP1B (1, 278)	2hnp (apo)	1 x 892 (I)	-3.63 (-0.05)	BPM	0.36 (-0.05)
	1aax (BPM)	1 x 892 (I)	-1.37 (0.07)	BPM	0.30 (0.07)
	1t49 (892)	1 x 892 (I)	-3.52 (-0.20)	BPM	0.55 (-0.20)
SSUPRT (4, 868)	1xtu (U5P, CTP)	4 x CTP (I)	-2.89 (-0.53)	U5P	0.14 (-0.53)
	1xtt (U5P)	4 x CTP (I)	-2.62 (-0.01)	U5P	0.65 (-0.01)
ThrS (2, 884)	1e5x (apo)	1 x SAM (A)	-1.31 (0.02)	TRS PLP	-0.31 0.35 (0.02)
		2 x SAM (A)	-3.67 (-0.24)	TRS PLP	-0.54 0.52 (-0.24)
	2c2g (PLP)	1 x SAM (A)	-2.17 (0.01)	TRS PLP	-0.15 0.15 (0.01)
		2 x SAM (A)	-4.48 (-0.20)	TRS PLP	-0.45 0.09 (-0.20)
	2c2b (TRS, SAM, PLP)	1 x SAM (A)	-1.89 (-0.67)	TRS PLP	-0.50 -0.42 (-0.67)
		2 x SAM (A)	-2.69 (-0.41)	TRS PLP	-1.02 0.01 (-0.41)

S1 TABLE (continued)