Table S1
Crystal structures of allosterically activated PDCs mentioned in this paper

Species	**Mutation**	**Ligand**	**Binding at regulatory site**	**Dimer orientation within tetramer**	**Loop flexibility (always for both)**	**pdb id**	**R-free**	**Resol. (Å)**	**Reference**
*Sc*PDC	D28A	Pyruvate	cov. at C221	planar, open	ordered (all su)				this paper
*Sc*PDC	E477Q	Pyruvate	cov. at C221	planar, open	ordered (all su)				this paper
*Kl*PDC	wt	Methyl acetylphosphonate	cov. at C221	planar, open	ordered (all su)				this paper
*Sc*PDC	wt	Pyruvamide	non-cov. 10 Å away from C221	tilted, half site open	ordered at closed site	1QBP	.287	2.4	Lu et al., 2000
*Sc*PDC	wt	Ketomalonate	n. d.	tilted, half site open	n. d.	no entry	no entry	3.7	Furey et al., 1998
*Kl*PDC	wt	/	/	tilted, half site open	disordered (all su)	2G1I	.214	2.3	Kutter et al., 2006
*Sc*PDC	wt	/	/	planar, open	disordered (all su)	1PVD	n. a.	2.3	Arjunan et al., 1996

Table S2
Interaction distances of atoms of the loop regions 104-113 and 288-304 within the functional dimer. Interactions between loop atoms are shown in italic, those between atoms of different loops in bold.

Subunit	**Atom 1**	**Atom 2**	**Distance (Å)**
A-A	I104-N	N170-OD1	3.08
	I104-O	*Q107-N*	*3.42*
		A108-N	*2.90*
	S105-N	*S103-O*	*3.20*
	S105-O	*A108-N*	*3.16*
		L109-N	*3.13*
	A106-N	S103-O	3.13
	A106-O	*Q110-N*	*3.08*
		L111-N	*3.19*
	Q107-N	S103-O	3.00
	Q107-NE2	P102-O	2.86
	Q107-O	*Q110-NE2*	*2.50*
		Q110-N	*2.91*
		K109-N	*3.19*
	A108-O	*Q110-N*	*3.47*
	K109(LYS)-O	*L111-N*	*3.12*
	Q110-NE2	G120-O	3.47
	Q110-O	*L112-N*	*3.42*
	L111-O	*L113-N*	*2.85*
	L113-O	T116-N	3.46
		T116-OG1	2.71
	H114-O	T116-N	3.34
	L288-N	*D219-OD2*	*2.86*
	L288-O	*S290-N*	*2.92*
		N293-ND2	*2.87*
	S290-OG	*N293-N*	*3.34*
	S290-O	*T294-N*	*3.27*
		T294-OG1	*3.39*
		F292-N	*3.35*
		N293-N	*3.15*
	D291-OD2	*F292-N*	*2.74*
	D291-O	*T294-N*	*3.30*
		G295-N	*3.21*
		S296-N	*2.75*
		Q552-OE1	3.41
		N293-N	*3.41*
	F292-O	*T294-N*	*3.30*
	N293-OD1	P246-N	3.48
		M247-N	2.88
	N293-ND2	D219-OD2	3.31
		D219-OD1	2.88
	T294-O	*S298-N*	*3.20*
		S298-OG	*2.89*
	G295-O	*S298-OG*	*3.26*
	S296-N	Q552-OE1	3.41
	S296-OG	Q552-NE2	2.78
	S296-O	*S298-N*	*3.51*
	S298-O	*S300-N*	*3.35*
	S300-N	E277-OE2	2.97
	S300-OG	*K302-NZ*	*3.08*
	S300-O	*K302-NZ*	*2.58*
		K302-N	*3.37*

		E277-OE1	3.41
	K302-N	E277-O	3.21
	K302-NZ	E277-OE1	3.43
	T303-OG1	A279-O	3.47
	K304-O	K306-N	2.87
A-B	K109-NZ	K562-NZ	2.85
	L112-O	***D291-N***	***3.01***
	H114-N	***D291-OD1***	***3.05***
		D291-OD2	***3.17***
	H114-ND1	***D291-OD1***	***2.97***
	H115-N	W412-O	3.45
		L411-O	2.94
	H115-ND1	W412-O	2.64
	H115-NE2	PYG602-O3	3.12
		PYG602-O1	2.86

Figure S1
Crystal structures of the loop regions 104-113 and 288-304. Orientation of the structure according to the amino acid sequence given in line 2 of the table. The Cα-line is illustrated as tube (white, without pronounced secondary structure, green, β-turn, red, α-helix), amino acid side chains are presented in ball-and-stick mode (grey, carbon, red, oxygen, blue, nitrogen).

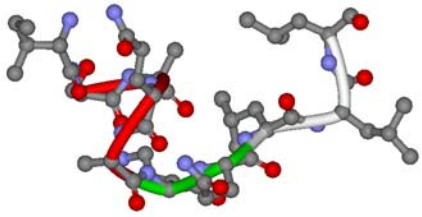
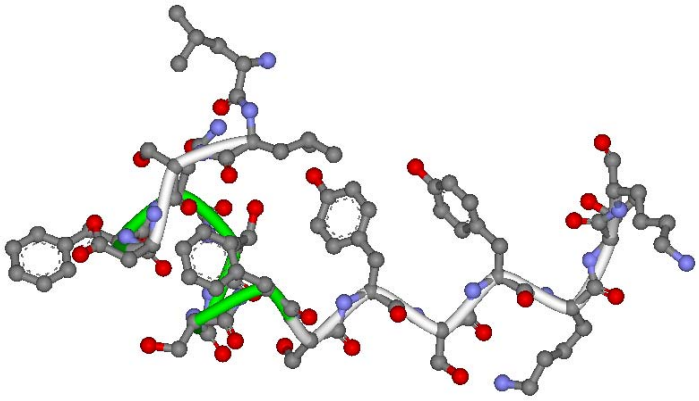
Loop 104-113	Loop 288-304
I104-S105-A106-Q107-A108- K109-Q110-L111-L112-L113	L288-L289-S290-D291-F292-N293-T294-G295-S296- F297-S298-T299-S300-T301-K302-T303-K304
	

Figure S2
Distances between location of Cα-atoms of one subunit in native *Kl*PDC and MAP activated *Kl*PDC. Loop regions 104-113 and 288-304 are highlighted in grey.