

Table S1: Families containing Dx[DN]xDG calcium-binding loops including those described in Rigden & Galperin (2004) The Dx[D]xDG motif for calcium binding: Multiple structural contexts and implications for evolution. J Mol Biol 343(4): 971-984.

	Representative ^a	SCOP class; fold of domain containing Dx[DN]xDG loop	PDB code, reference; position(s) of the first D of Dx[DN]xDG	Distribution of proteins containing Dx[DN]xDG loop	Frequency of Dx[DN]xDG loop in homologous proteins ^b	R.m.s. fit of Dx[DN]xDG to the first calmodulin motif	Distance between Dx[DN]xDG and later Ca ²⁺ ligands (residues)	Function of bound calcium
Novel structural contexts								
	<i>Thermococcus kodakaraensis</i> subtilisin	α + β ; Subtilisin-like ^b	2z2x [92]; 212	Some thermophilic archaea	<1% (Pfam PF00082)	0.12 Å	4/7	Folding, in the context of a 25 residues insertion [23]
	<i>Bifidobacterium longum</i> endo- α -N-acetylglactosaminidase	All β ; Supersandwich ^b	2zxq [21]; 601	Bifidobacteria	Approx 7%	0.15 Å	5	Possibly structural [21]
	<i>Escherichia coli</i> YgjK from glycoside hydrolase family GH65	All α ; α/α toroid ^b	3c68 [20]; 431	Some γ -proteobacteria	Approx 7% (Pfam PF01204)	0.12 Å	2/112	Not known
	<i>Porphyromonas gingivalis</i> gingipain adhesin domain	All β ; Galactose-binding domain-like ^c	3km5 [22]; 1179	<i>Porphyromonas gingivalis</i> , <i>Flavobacterium bacterium</i>	Approx 90% (Pfam PF07675)	0.35 Å	36	Possibly structural [22]
Calcium blades								
	Human integrin α V β 3	All β ; 7-bladed β -propeller	1jv2 [93]; 284; 349; 413	Eukaryotic	100% of 3 sites (Pfam PF01839)	0.61-1.07 Å	2	Potentially regulatory [93]
	<i>Bacillus subtilis</i> rhamnogalacturonan lyase	All β ; 8-bladed β -propeller ^c	2z8r [24]; 158; 222; 369	[†]	[†]	0.22-0.36 Å	2	Not known (further calcium-binding site required for activity) [24]
	<i>Pseudomonas aeruginosa</i> pilus-biogenesis factor PilY1	All β ; 7-bladed β -propeller ^c	3hx6 [25]; 851	Bacterial	Approx 75% (Pfam PF05567)	0.37 Å	2	Regulation of pilus biogenesis and motility [25]
	<i>Psathyrella velutina</i> lectin	All β ; 7-bladed β -propeller ^c	2bwr [26]; 177; 233; 343 ^e	[†]	[†]	0.48-0.55 Å	2	Possibly structural [26]
From Rigden and Galperin, 2004								
	<i>Paramecium tetraurelia</i> calmodulin	All α ; EF Hand-like	1exr; 20; 56; 93; 129	Mainly eukaryotic, few bacterial, very few archaeal	Almost 100% of variable number of sites (4 in representative)	0.00 - 0.42 Å	5 (when present)	Regulation or structural or buffering/transport

<i>Salmonella typhimurium</i> periplasmic galactose-binding protein	α/β ; Periplasmic binding protein-like I	1gcg; 134	Bacterial	Approx. 3%	0.27 Å	3/65	Structural
<i>Sphingomonas</i> sp. periplasmic alginate-binding protein	α/β ; Periplasmic binding protein-like II	1kwh; 171	Bacterial	Approx 1%	0.36 Å	2/3	Potentially sensor
<i>Clostridium thermocellum</i> dockerin	All α ; Type I dockerin domain	1daq; 8; 40	Bacterial, very few archaeal	100% of 2 sites	0.98-1.12 Å	5	Structural
<i>Escherichia coli</i> soluble lytic transglycosylase Slt35	$\alpha+\beta$; Lysozyme-like	1qut; 237	Bacterial	100%	0.42 Å	8	Not known
<i>Bacillus anthracis</i> protective antigen	Membrane and cell-surface; Anthrax protective antigen	1acc; 177	Bacterial	100%	0.31 Å	2 ^d /5	Structural
<i>Thermotoga maritima</i> 4- α -glucanotransferase	α/β ; TIM β/α -barrel	1lwj; 13	Eukaryotic and bacterial	Approx. 35%	0.71 Å	2	Not known
<i>Pseudomonas</i> 'Tac II 18' alkaline protease	$\alpha+\beta$; Zincin-like	1h71; 49	<i>Pseudomonas</i> , <i>Serratia</i>	Approx. 35%	0.18 Å	2/59	Not known
<i>Pseudomonas aeruginosa</i> alkaline protease	All β ; β -roll	1kap; 446	<i>Pseudomonas aeruginosa</i>	Approx. 15%	0.37 Å	2	Not known
Human thrombospondin-1	Small proteins; TSP type-3 repeats	1ux6; 828; 843; 866; 879; 915; 902	Metazoan	100% of 5 binuclear sites 100% of 1 mononuclear site	0.18-0.26 Å 0.24 Å	2 ^e /5 2 ^c	Regulation of binding
Human transglutaminase 3	$\alpha+\beta$; Cysteine proteinases	1vjj; 301	Eukaryotic	Approx 20%	0.42 Å	18	Regulation of catalytic activity
<i>Thermoascus aurantiacus</i> cellulase	α/β ; TIM β/α -barrel	1gzj; 287	Bacterial and yeast	Approx. 10%	0.72 Å	No later D or E predicted to bind calcium	Not known

^a With the exception of the *Thermoascus aurantiacus* cellulase (last line of the Table), all proteins have been demonstrated to bind calcium ions, see Rigden & Galperin (2004) for additional references

^b As defined by Pfam, SMART or by full-length matches in PSI-BLAST (E-value of 0.0001) run until convergence.

^c Based on the entry for a homologous protein or from authors' description

^d Through water interaction with calcium

^e The motif commencing from residue 233 is not bound to Ca²⁺ in the deposited structure but crystal soak data show that it is capable of doing so [26]

^f A distinct group could not be defined with PSI-BLAST