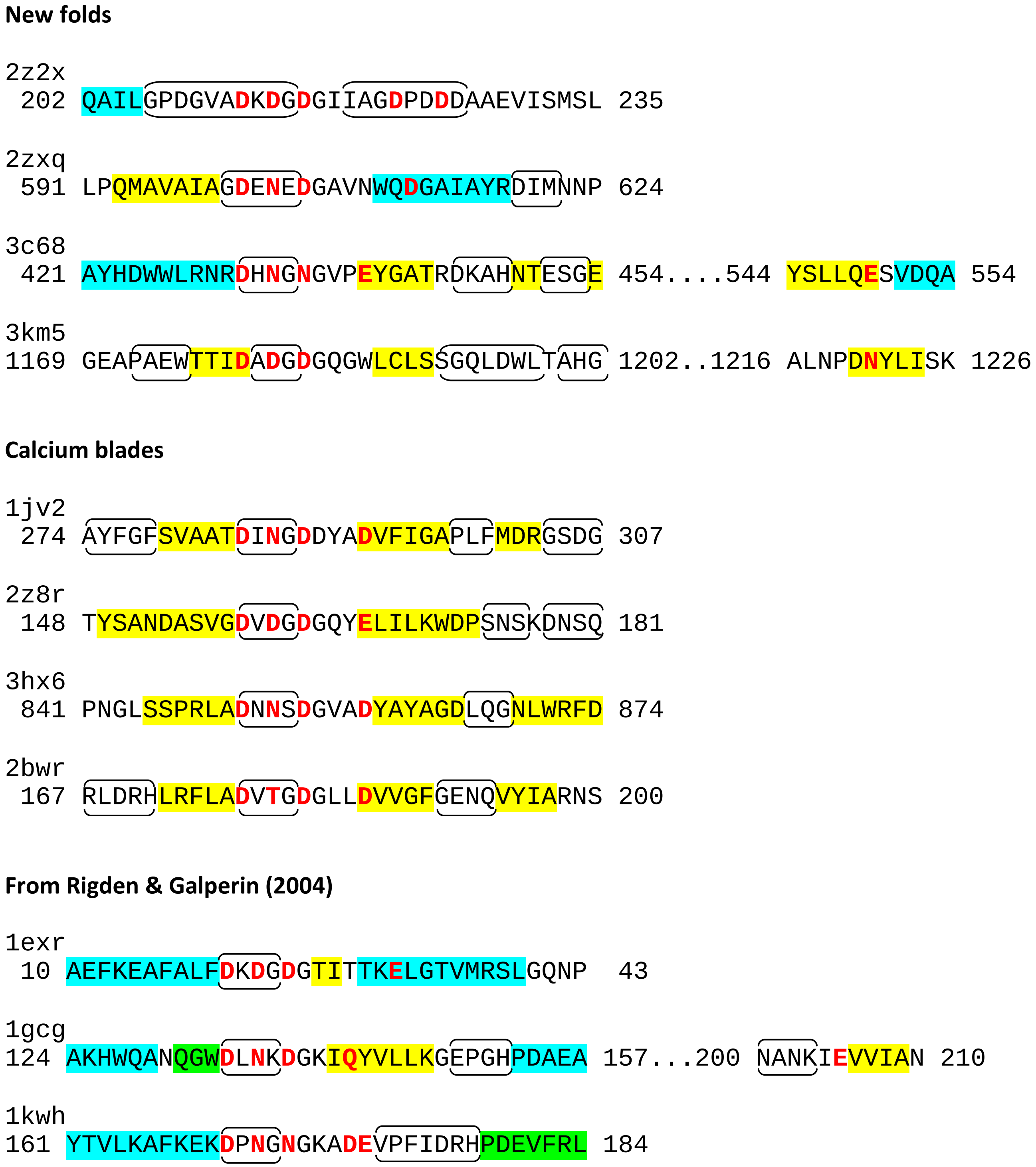
Figure S1. Secondary structure context of the Dx[DN]xDG motifs, highlighting additional metal-binding residues (Table 1). The figure includes those motifs described in ref. [15], Rigden & Galperin (2004) The DxDxDG motif for calcium binding: Multiple structural contexts and implications for evolution. J Mol Biol 343(4): 971-984. Residues binding to metal using side chains are in red (direct interaction with calcium) or purple (through-water interaction). Secondary structure as defined by STRIDE [74] is indicated as follows: α-helices, blue shading; β-strands, yellow shading; 3_{10} helices, green shading; turns, brackets.



New folds

2z2x
202 QAILGPDGVADKDGDGIIAGDPDDDAAEVISMSL 235

2zxq
591 LPQMAVAIAGDENEDGAVNWQDGAIAYRDIMNNP 624

3c68
421 AYHDWWLRNRDHNGNGVPEYGATRDKAHNTESGE 454....544 YSLLQESVDQA 554

3km5
1169 GEAPAEWTTIDADGDGQGWLCLSSGQLDWLTAHG 1202..1216 ALNPDNYLISK 1226

Calcium blades

1jv2
274 AYFGFSVAATDINGDDYADVFIGAPLFMDRGSDG 307

2z8r
148 TYSANDASVGDVDGDGQYELILKWDPSNSKDNSQ 181

3hx6
841 PNGLSSPRLADNNSDGVADYAYAGDLQGNLWRFD 874

2bwr
167 RLDRHLRFLADVTGDGLLDVVGFGENQVYIARNS 200

From Rigden & Galperin (2004)

1exr
10 AEFKEAFALFDKDGDGTITTKELGTVMRSLGQNP 43

1gcg
124 AKHWQANQGWDLNKDGKIQYVLLKGEPGHPDAEA 157...200 NANKIEVVIAN 210

1kwh
161 YTVLKAFKEKDPNGNGKADEVPFIDRHPDEVFRL 184

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1daq
  1 ___MSTKLYGDVNDDGKVNSTDAVALKRYVLRSG  21

1qut
227 MPSSYKQYAVDFSGDGHINLWDPVDAIGSVANYF 260

1acc
167 PELKQKSSVPDRDNDGIPDSLEVEGYTVDVKNKR 200

1lwj
  3 GYQIYVRSFRDGNLDGVGDFRGLKNAVSYLKELG  36

1h71
 39 QLTRSGASWHDLNNDGVINLTYTFLTAPPVGYAS  72...109 AARGDDGHQTF 119

1kap
436 AASKAGSLAIDFSGDAHADFAINLIGQATQADIV 469

1ux6 binuclear
833 RIGDTCDNNQDIDEDGHQNNLDNCPYVPNANQAD 866

1ux6 mononuclear
892 CRLVPNPDQKDSDGDGRGDACKDDFDHDSVPDID 925

1vjj
291 RVITNFNSAHDTDRNLSVDVYYDPMGNPLDKGSD 324
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