

Figure S3. Examples of protein-DNA interfaces captured in protein data bank (PDB) structures of MYB transcription factors. Numbers inside nitrogen bases indicate the number of contacts with proteinside chains within 4.5 Å. Dashed bases correspond to the core GTT motif, which is recognized by conserved amino acid side-chains in entries 1MSE (Ogata et al., 1994) and 2KDZ (Lou et al., 2009). Upstream bases are also specifically recognized but the involved side-chains are not conserved. Filled bases display DNA geometry alterations typical of indirect readout mechanisms. The horizontal double head arrows below delimitate the segments where recognition helices make direct contacts with DNA nitrogen bases as seen in these and on another PDB entries. Numbers refers to the amino acid positions from the start codon (Met) which correspond to the following positions in Figure 5A: Glu<sup>132</sup> (1MSE) and Glu<sup>41</sup> (2KDZ) = Glu<sup>44</sup>/Leu<sup>44</sup> (A. thaliana R2 helix 3), Asn<sup>179</sup> (1MSE) and Asn<sup>88</sup> (2KDZ) = Asn<sup>40</sup> (A. thaliana R3 helix 3), and Asn<sup>183</sup> (1MSE) and Asn<sup>92</sup> (2KDZ) = Asn<sup>44</sup> (A. thaliana R2 helix 3). These structures show that when comparing the DBD/DNA interface of two MYB proteins that interact with two different types of MYB-core motif (i.e. type I in the top part vs type II in the bottom part) it can be observed that indeed some amino acids are conserved. This is for instance the case for two residues that recognized the GTT DNA motif, namely the Glu<sup>44</sup> and the Asn<sup>40</sup> from the R2 and R3 helices 3, respectively. It is noteworthy that the Glu<sup>44</sup> residue is generally replaced in plants by a Leu<sup>44</sup>. However, it can also be observed that the number of amino acid residues (and as a consequence the type) that directly interact with each of the nucleotides surrounding the GTT core is highly variable.