Supporting Information

Molecular Dynamics Simulations Reveal Differentiated Context –Dependent Conformational Dynamics of Two Proteins of the Same Family

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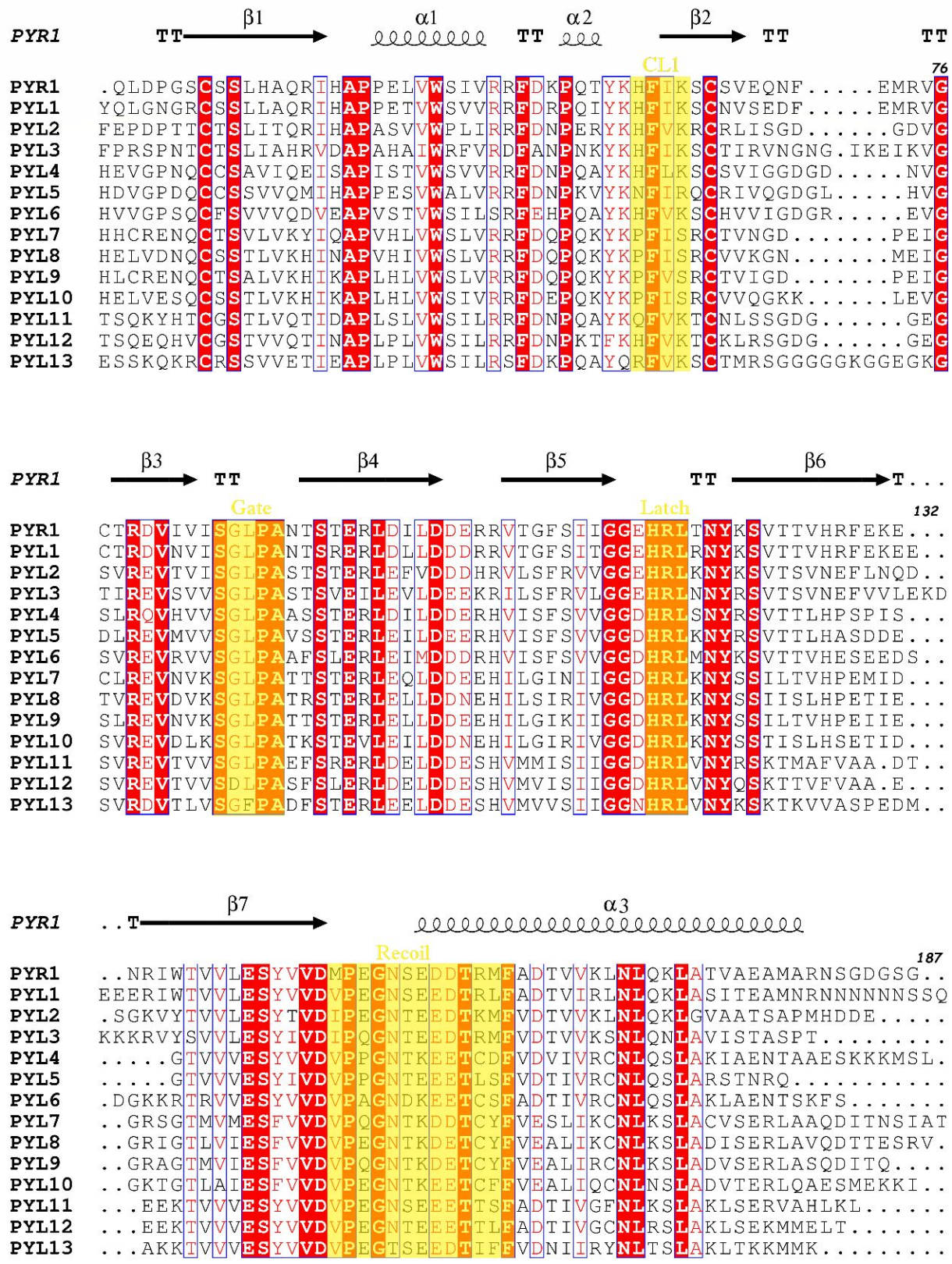

Figure S1. Aligned sequences of PYL members. Annotations of secondary structures are based on the closed conformation of PYR1 in 3K3K. Highly conserved positions are colored in red. Regions of interest are highlighted in yellow.

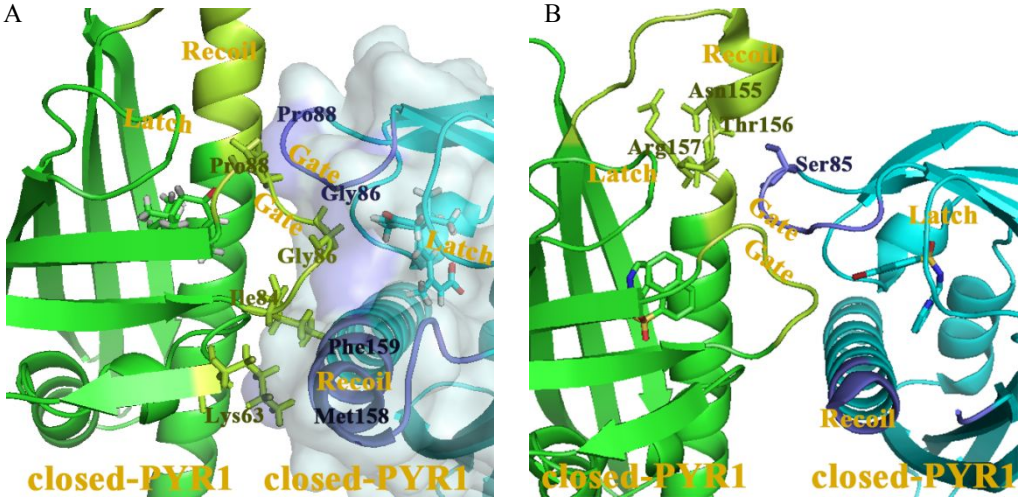

Figure S2. (A) Inter-subunit steric clashes in a homodimer structure modeled by replacing PYR1-open with PYR1-closed in the asymmetric homodimer. (B) The structure of closed form PYR1 homodimers bound with two ABA analogs, the recoil helix has been partially disrupted around Thr156.

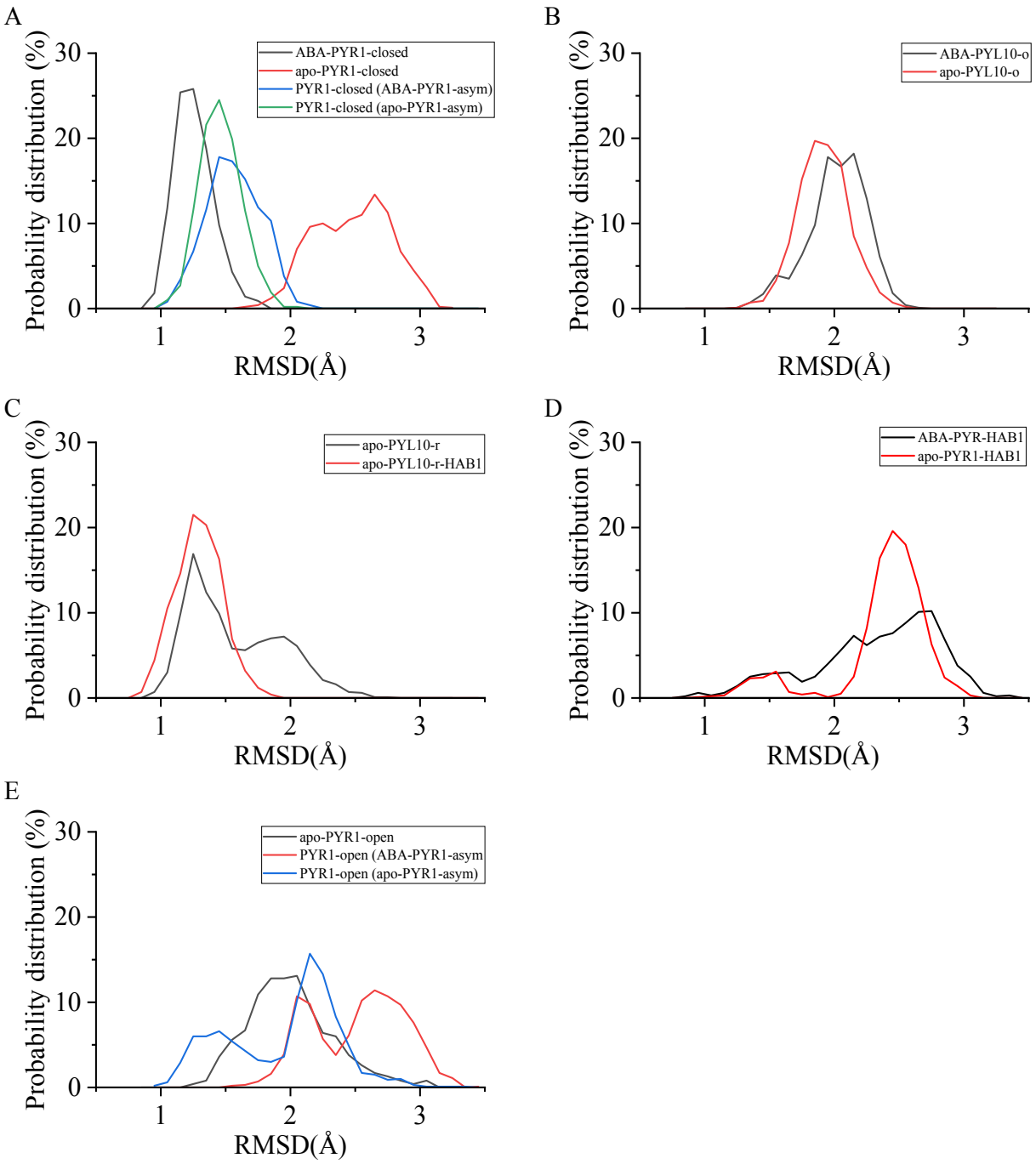

Figure S3. RMSD distributions from the MD simulations. (A) RMSDs from the PYR1-closed reference structure (the closed subunit in PDB 3K3K); (B) RMSDs from the PYL10-o reference structure (PDB 3R6P); (C) RMSDs from the PYL10-r reference structure (the PYL-10 subunit in PDB 3RT0); (D) RMSDs from the PYR1-closed reference structure in the PYR1-HAB1 complex (the PYR1 subunit in PDB 3QN1); (E) RMSDs from the PYR1-open reference structure (the open subunit in PDB 3K3K). The legends indicate the simulated systems.

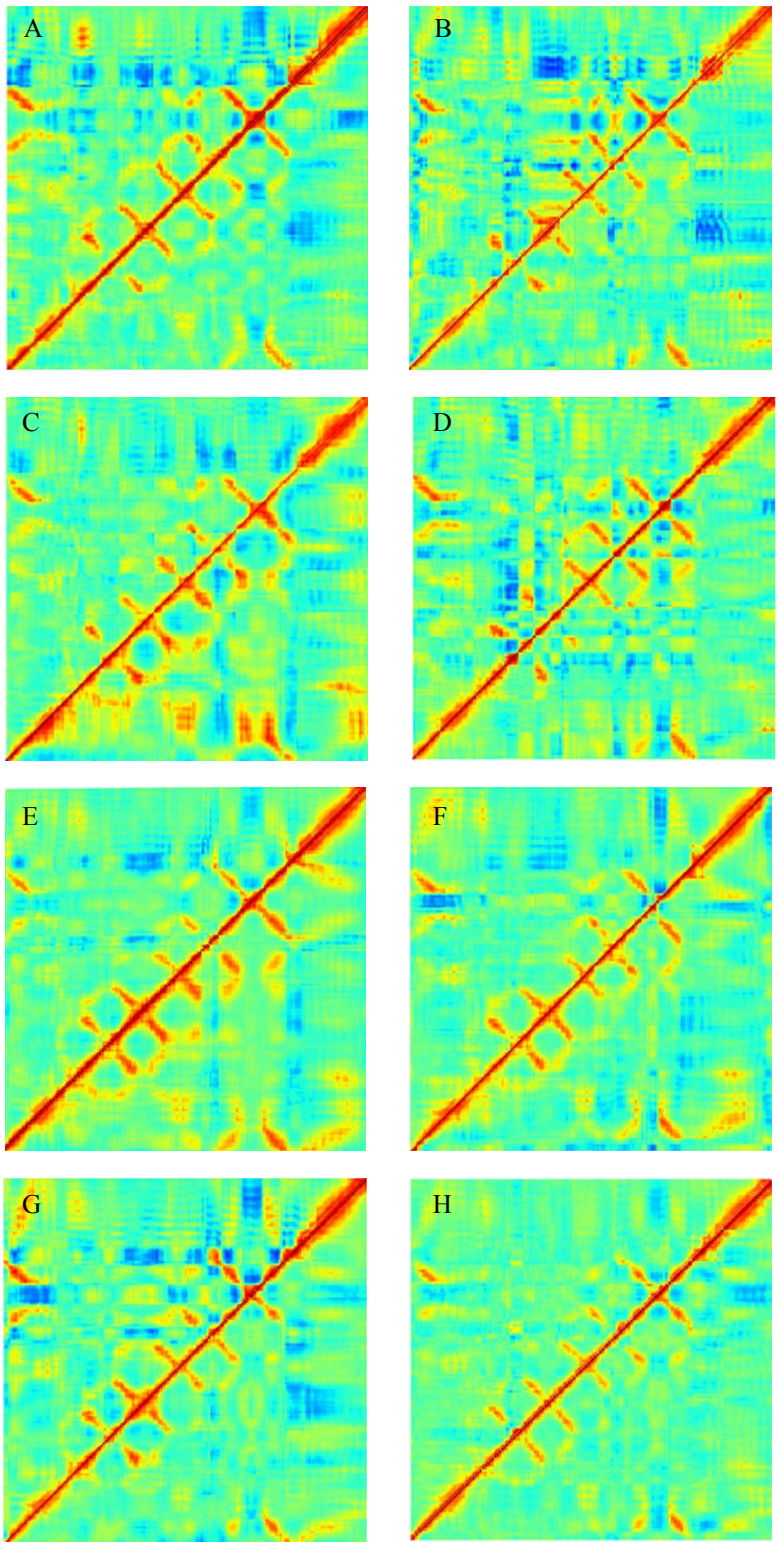

Figure S4. Comparisons of cross-correlations computed from different 100 ns simulations of the same system. (A) apo-PYR1-open; (B) apo-PYR1-closed; (C) ABA-PYR1-closed; (D) apo-PYR1-closed in apo-PYR1-HAB1; (E) apo-PYL10-o; (F) ABA-PYL10-o; (G) apo-PYL10-r; (H) apo-PYL10-r in apo-PYL10-HAB1.

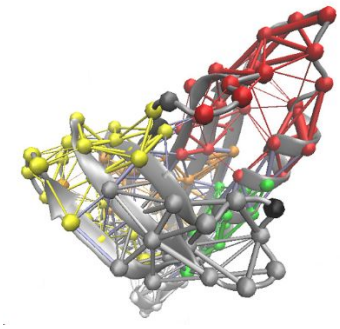

Figure S5. Community structure of apo-PYL10-r.