Figure S7

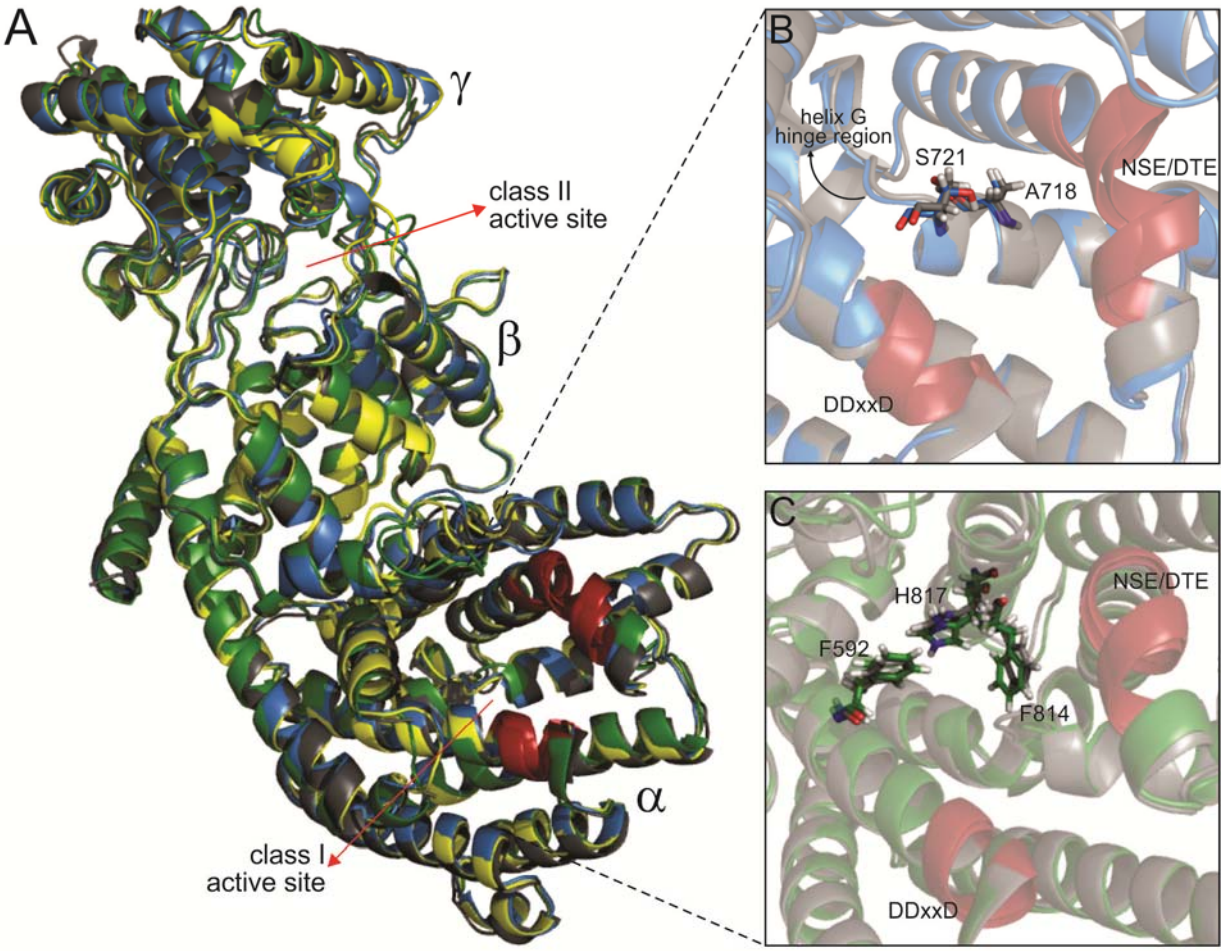

Figure S7. Homology modeling of pine monofunctional diterpene synthases. The structural models of *Pb*mPIM1, *Pbm*ISO1 and *Pb*mdiTPS1 with the template *Taxus brevifolia* taxadiene synthase (Köksal et al., 2010; PDB-ID 3P5R, chain A) are shown as representatives for all of the modeled monofunctional diTPS from lodgepole pine and jack pine. [**A**] Superimposed homology models of *Pb*mPIM1 (blue), *Pb*mISO1 (yellow) and *Pb*mdiTPS1 (green), possess the characteristic α-helical tri-domain structure. Each model is comprised of the N-terminal βγ-domain, which harbors the class I active site and C-terminal α-domain that contains the class I active site. [**B**] Class I active site cavity of *Pb*mPIM1 (blue) and *Pc*mPIM1 (grey), illustrating Ala718 and Ser721 as putative catalytic residues that impact product specificity. [**C**] Class I active site cavity of *Pb*mdiTPS1 (green) and *Pc*mdiTPS1 (grey), highlighting Phe592, Phe814 and His817 as possible residues that contribute to the enzyme's loss of function. The class I signature motifs DDxxD and NSE/DTE are depicted in red.