



**Figure S1. The ML-87 and the ML-91 models fitted to WAG.** Each element  $\log-O(\langle S \rangle(\hat{\tau}, \hat{\sigma}))_{ab}$  of the log-odds matrices of (A) the ML-87 and (B) the ML-91 models fitted to the 1-PAM WAG matrix is plotted against the log-odds  $\log-O(S^{\text{WAG}}(1 \text{ PAM}))_{ab}$  calculated from WAG. Plus, circle, and cross marks show the log-odds values for one-, two-, and three-step amino acid pairs, respectively. The dotted line in each figure shows the line of equal values between the ordinate and the abscissa.