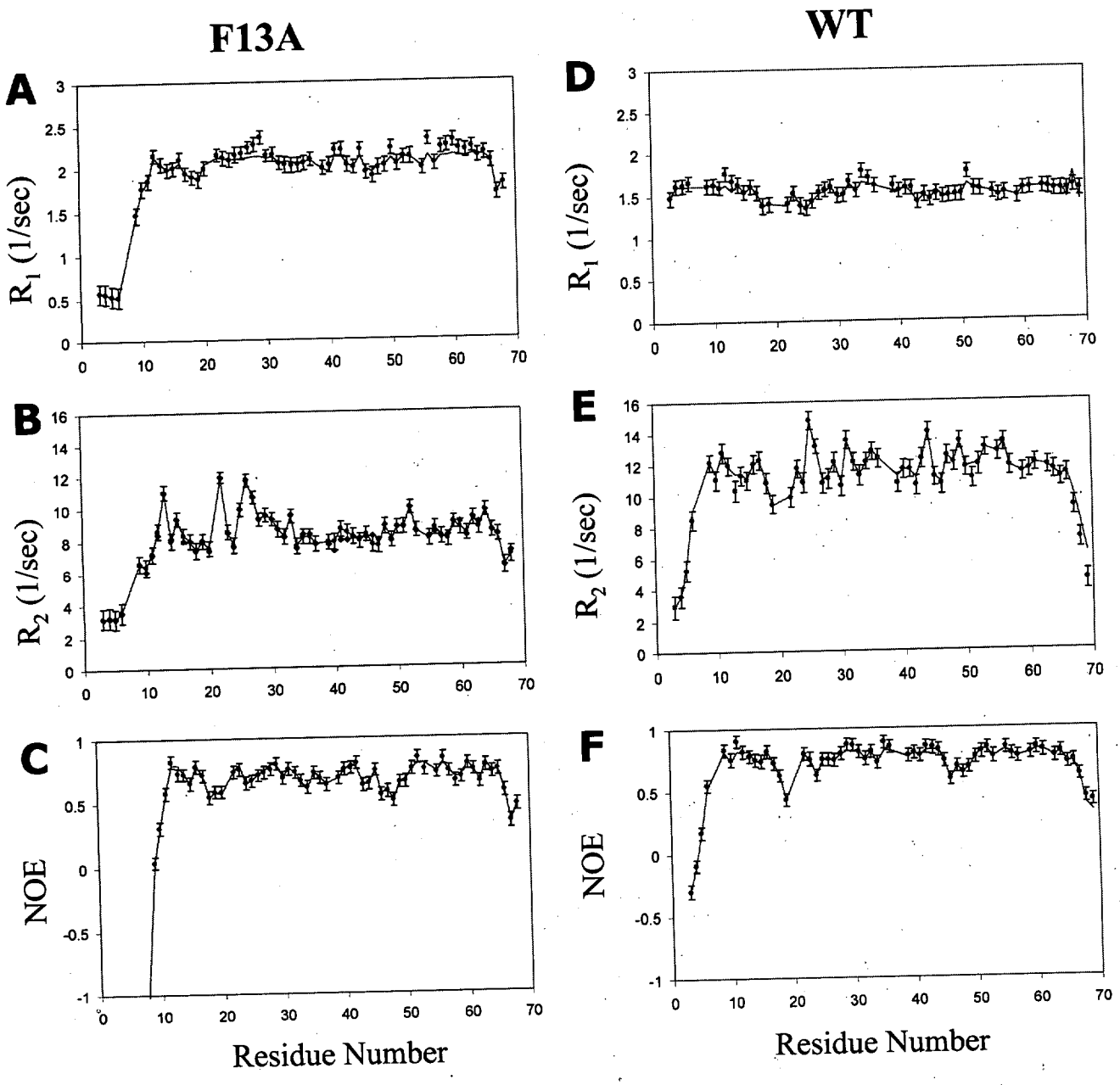
Supporting Information for World Wide Web Edition

Figure S1. ^{15}N R_1, R_2, and NOE NMR relaxation data of MIP-1β F13A (A, B, C) and WT (D, E, F). Relaxation data are plotted with error bars as a function of residue. Solid lines are back calculated R_1, R_2, and NOE values from the dynamics parameter values in Figure S3 to show the goodness of fit.

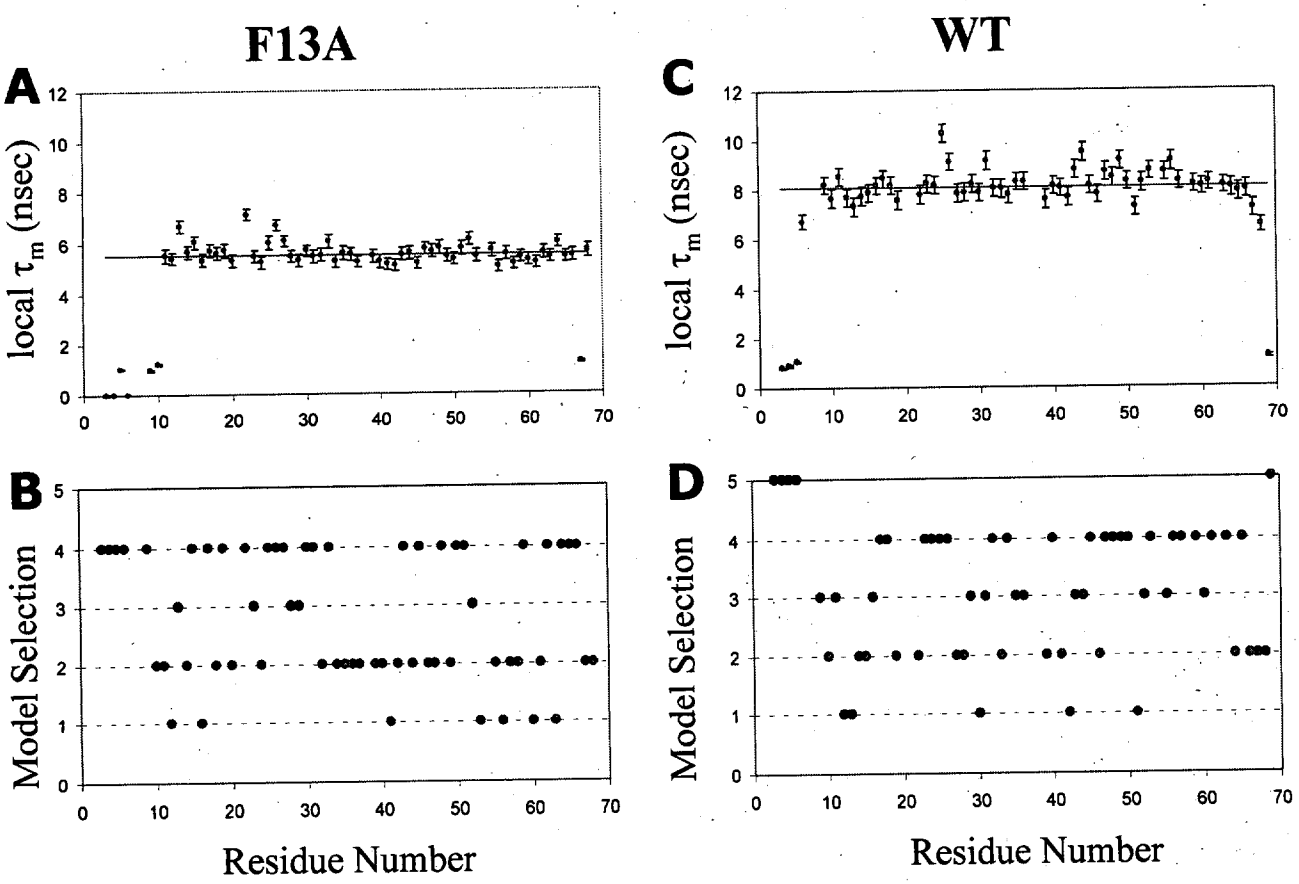
Figure S2. τ_m and model selection in dynamics analyses of MIP-1β F13A (A, B) and WT (C, D). Local τ_m (closed circle) was calculated residue by residue from the relaxation data in Figure S1. The solid straight lines show global τ_m values: 5.52 nsec for F13A and 8.07 nsec for WT. With fixed global τ_m, five different internal models in isotropic model free analysis were applied to fit the relaxation data. Model 1 includes only S_s^2, model 2 includes S_s^2 and τ_e, model 3 includes S_s^2 and R_{ex}, model 4 includes S_s^2, τ_e, and R_{ex}, and model 5 includes S_s^2, τ_e, and S_f^2. The best model was selected residue by residue based on F-test of SSE's (sum of squared errors) with 80% confidence limit or direct comparison of SSE or parameter errors when the degree of freedom becomes zero. SSE is an error function to be minimized in modeling and defined as $(R_1 - R_1')^2/\sigma_{R1}^2 + (R_2 - R_2')^2/\sigma_{R2}^2 + (NOE - NOE')^2/\sigma_{NOE}^2$ where R_1', R_2', and NOE' are back calculated values of R_1, R_2, and NOE and σ_{R1}, σ_{R2}, and σ_{NOE} are experimental uncertainties in R_1, R_2, and NOE.

Figure S3. Dynamics parameter values of MIP-1β F13A (A, B, C, D) and WT (E, F, G, H). Based on the best model in model selection in Figure S2, the parameter values describing the internal motion were plotted by residue.

Kim et al., Fig. S1



Kim et al., Fig. S2



Kim et al., Fig. S3