

WT <sup>547–935</sup>		MU <sup>547–935</sup>	
conformation	rms	conformation	rms
4217	0.65	2531	0.68
34238	0.68	19157	0.67
42356	0.64	30180	0.65
49260	0.58	36987	0.73

**Table S2.** RMS deviations (in Å) upon energy minimization calculated on C- $\alpha$  atoms for every MD conformation used for NMA. The value obtained for the structure 1T45 is 1.55 Å.