Supplementary Information

Mutated Form (G52E) of Inactive Diphtheria Toxin CRM197: Molecular Dynamics Simulations Clearly Display Effect of this Mutation to NAD Binding

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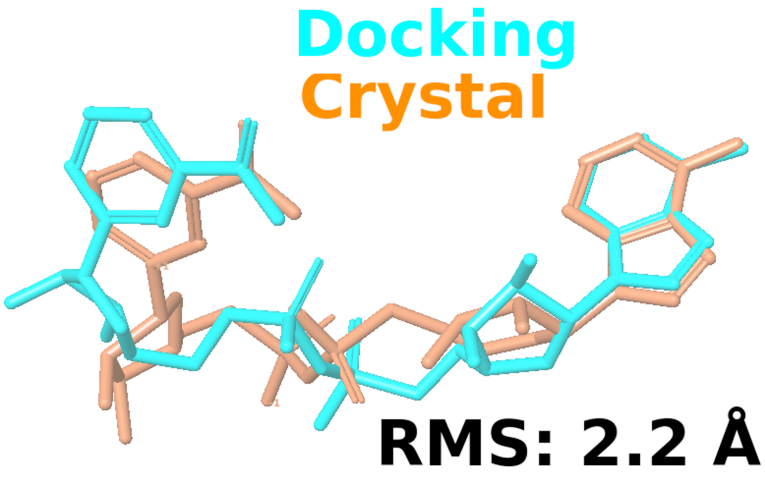

Figure S1. Superimposition of co-crystallized and docked NAD into CRM197.

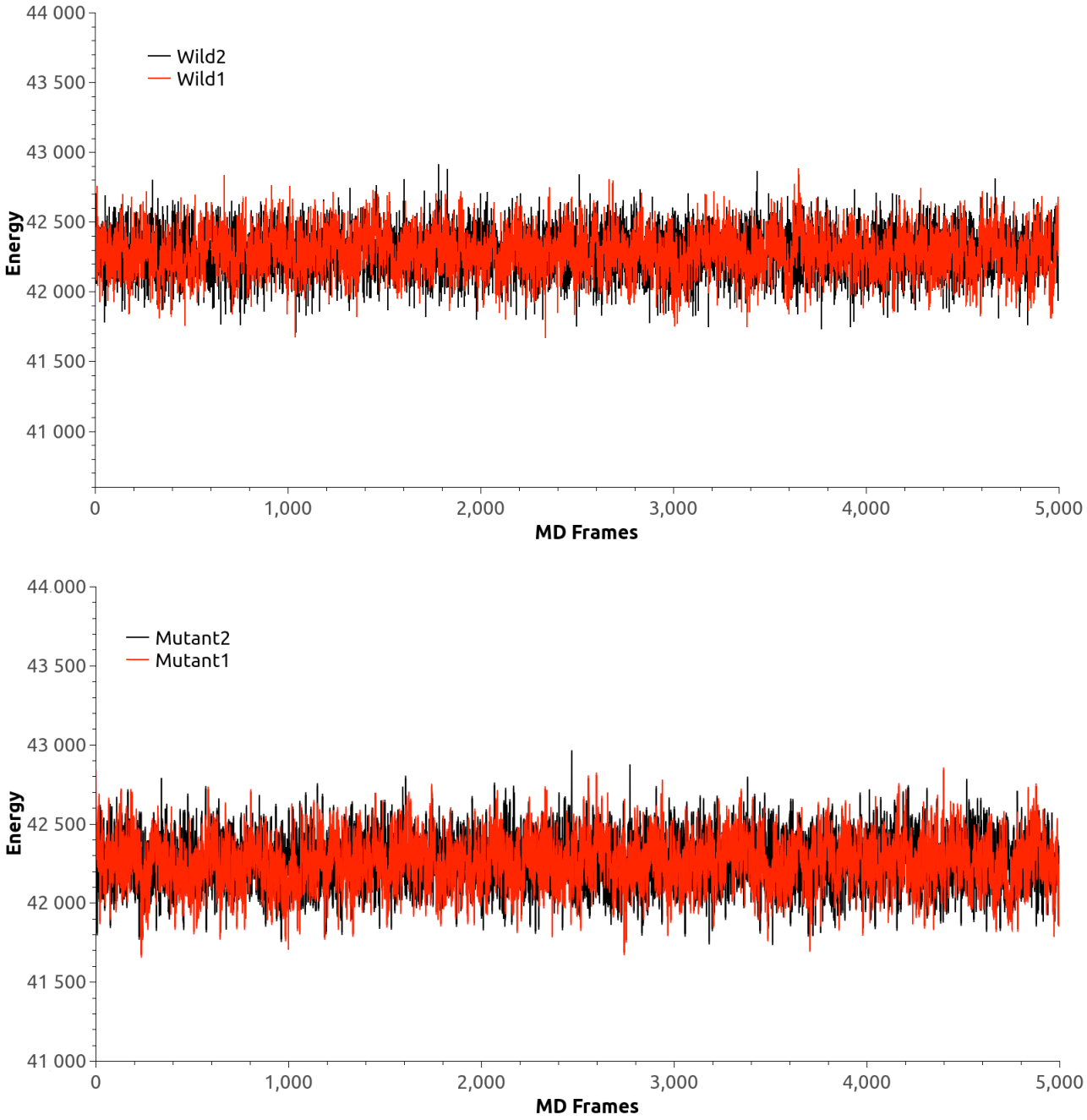

Figure S2. Kinetic energies of the studied systems simulated with different initial velocities. Energy values were calculated in kcal/mol.

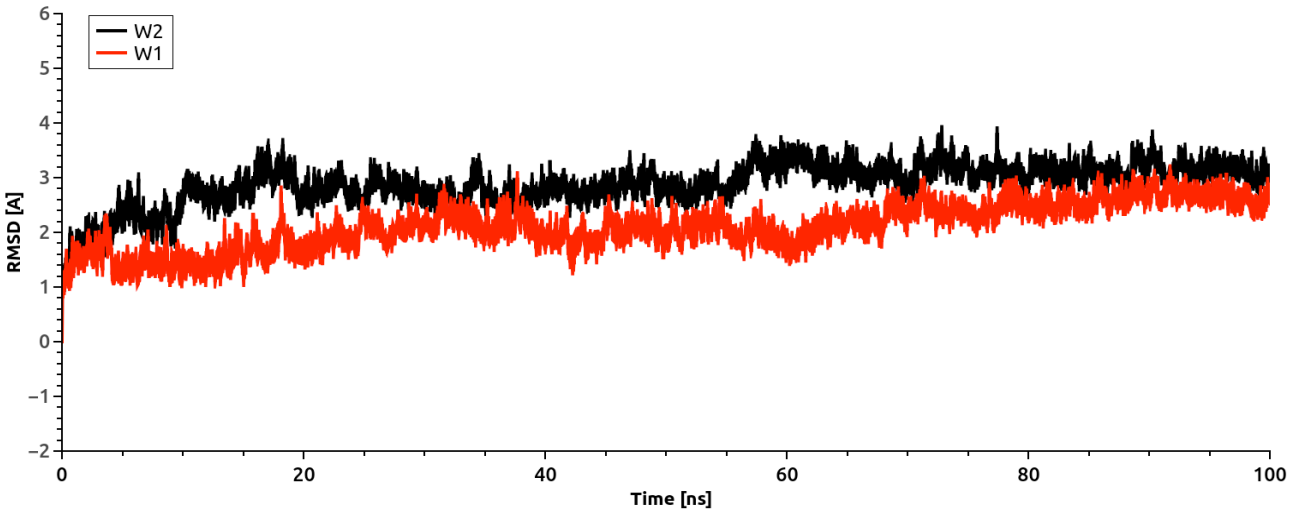

Figure S3. Evolution of RMSD of wild proteins based on Ca atoms along 2 MD simulations with different random seeds.

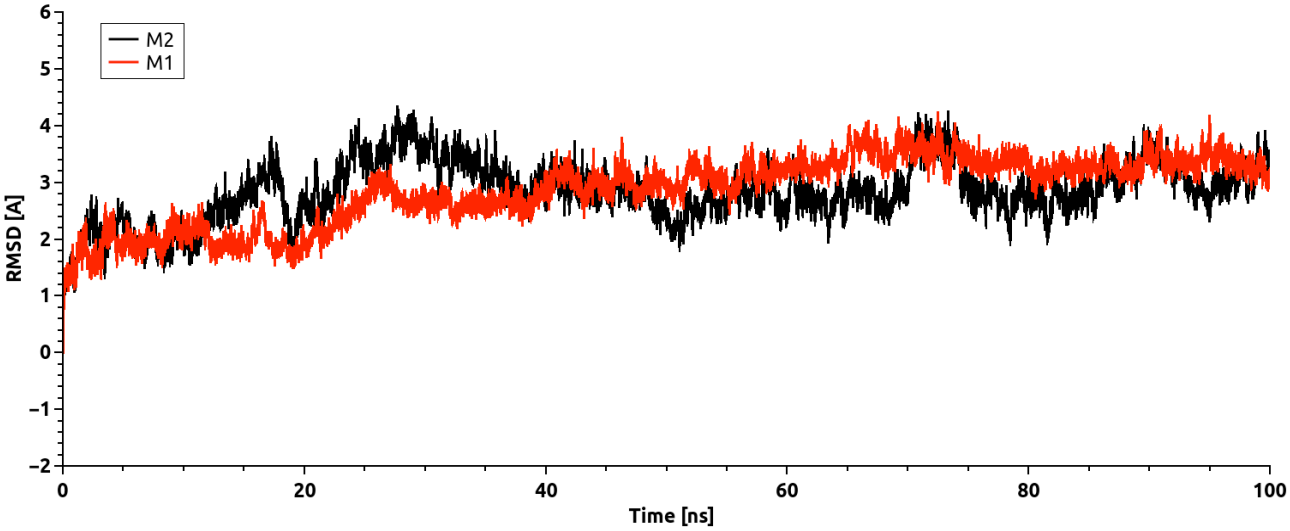

Figure S4. Evolution of RMSD of mutant proteins based on Ca atoms along 2 MD simulations with different random seeds.

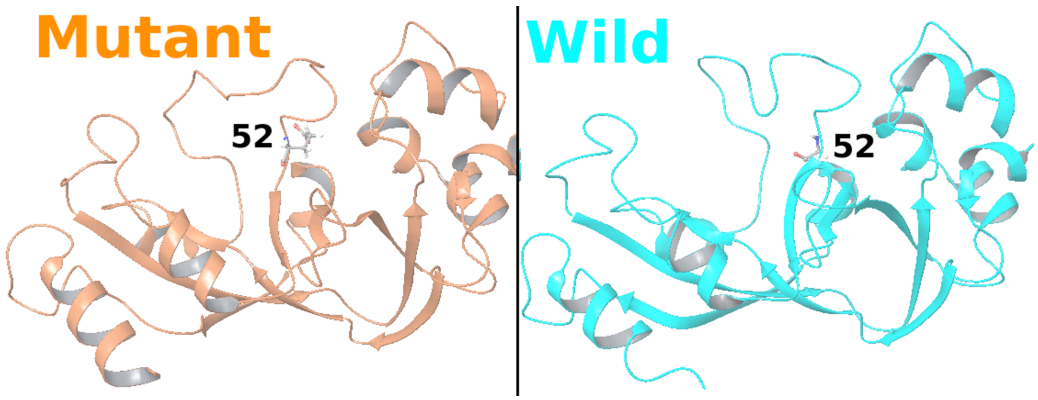

Figure S5. A stereo view of representative structures derived from simulations in wild and mutant forms.

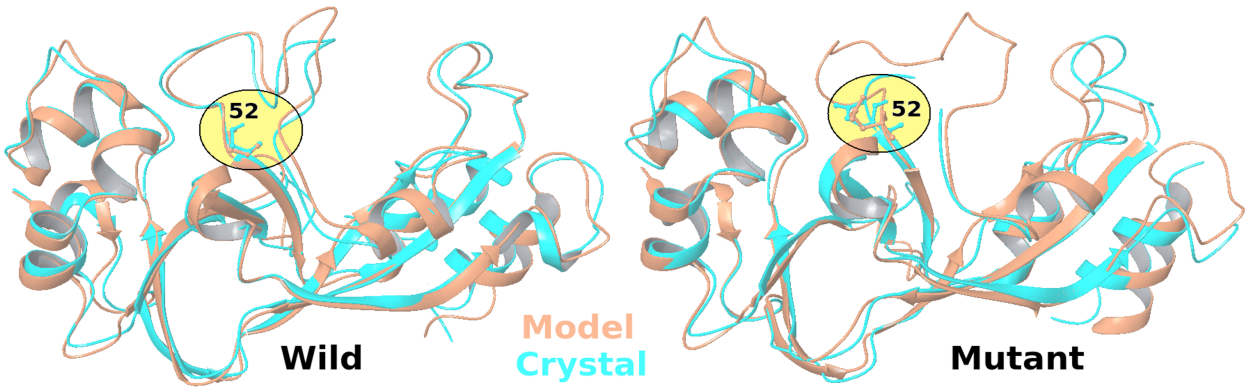

Figure S6. Representation of Wild and mutant forms of model and crystal structures, superimposed based on their backbone atoms.

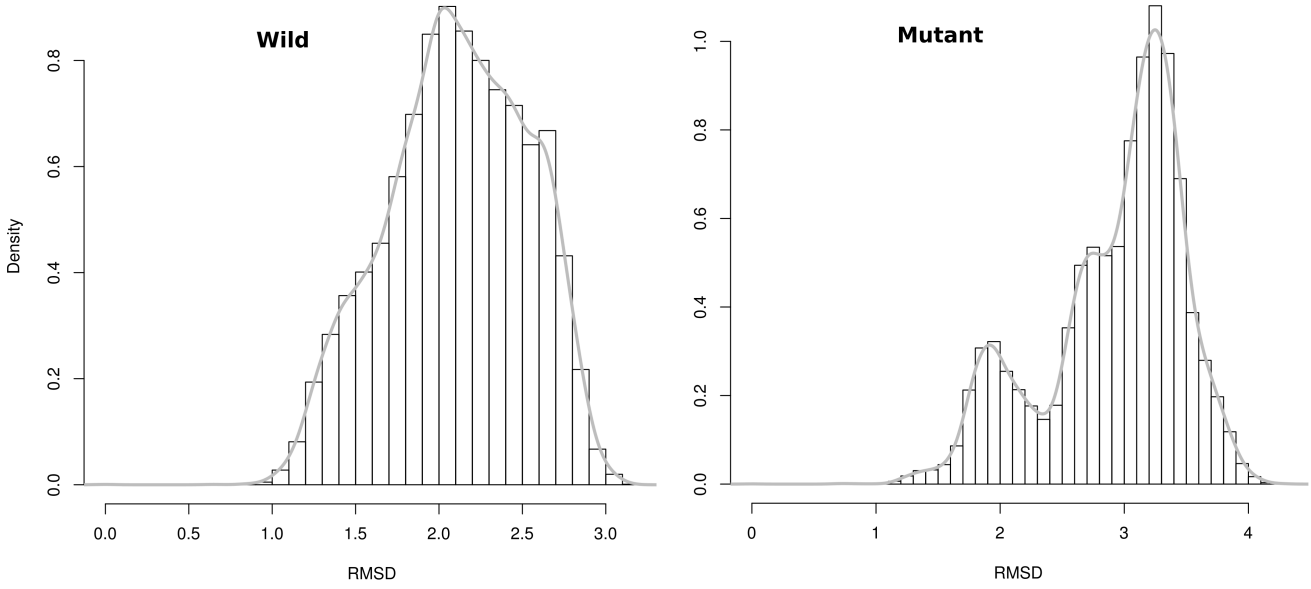

Figure S7. RMSD histograms for wild (left) and G52E mutated CRM197 (right). RMSD histograms show that mutant form is less stable than wild type. While populated RMSD value is observed ~2.2 Å at the wild form, corresponding value is observed at ~3.2 Å at mutant CRM197.

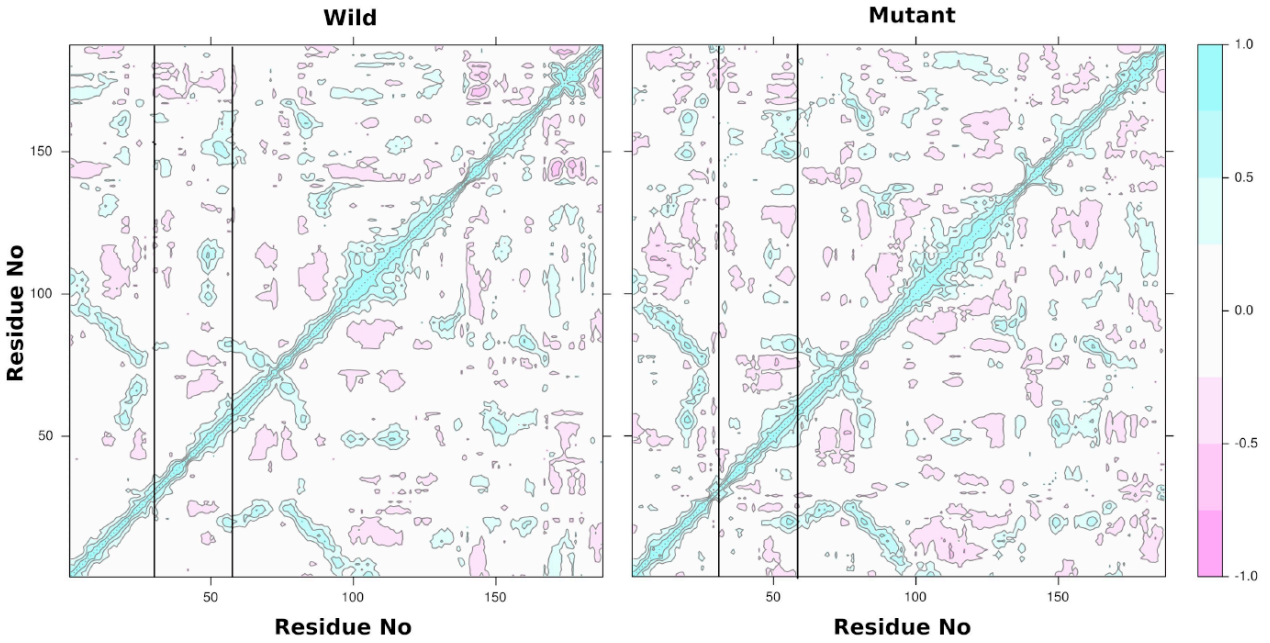

Figure S8. Dynamic cross-correlation maps (DCCMs) of the CRM197 for (a) wild and (b) mutant subunits using different alignment criteria. Black lines indicates the active-site loop domains for each systems.

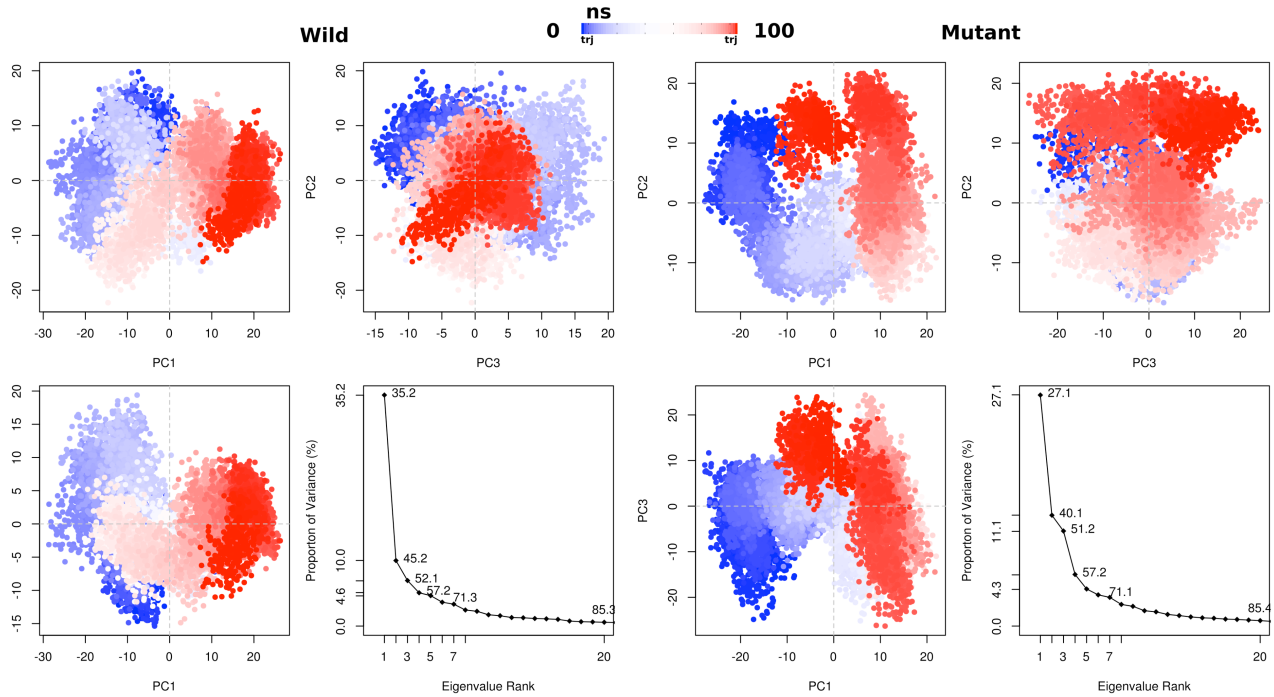

Figure S9. Clustering analysis results of average-linkage algorithm on different subspace dimensions projected on 2D plane formed by first three PCs. Clustering was performed on the entire MD trajectory data for (a) wild type and (b) mutant type.