Direct Observation of β-barrel Intermediates in the Self-assembly of Toxic SOD1$_{28-38}$ and Absence in Non-toxic Glycine Mutants

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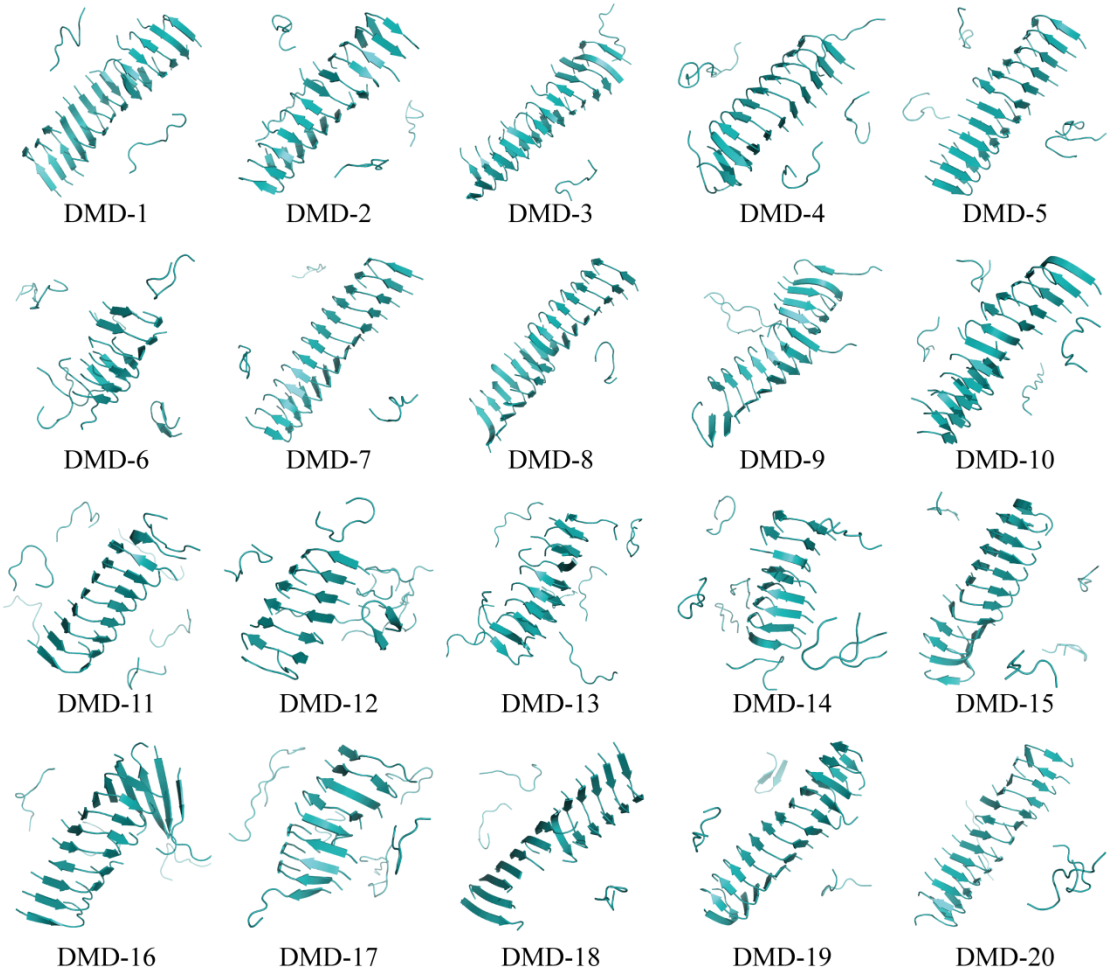

Fig. S1. The final assembled structures of SOD1$_{28-38}$ in each of the 20 independent DMD simulations for the 16-peptide system.

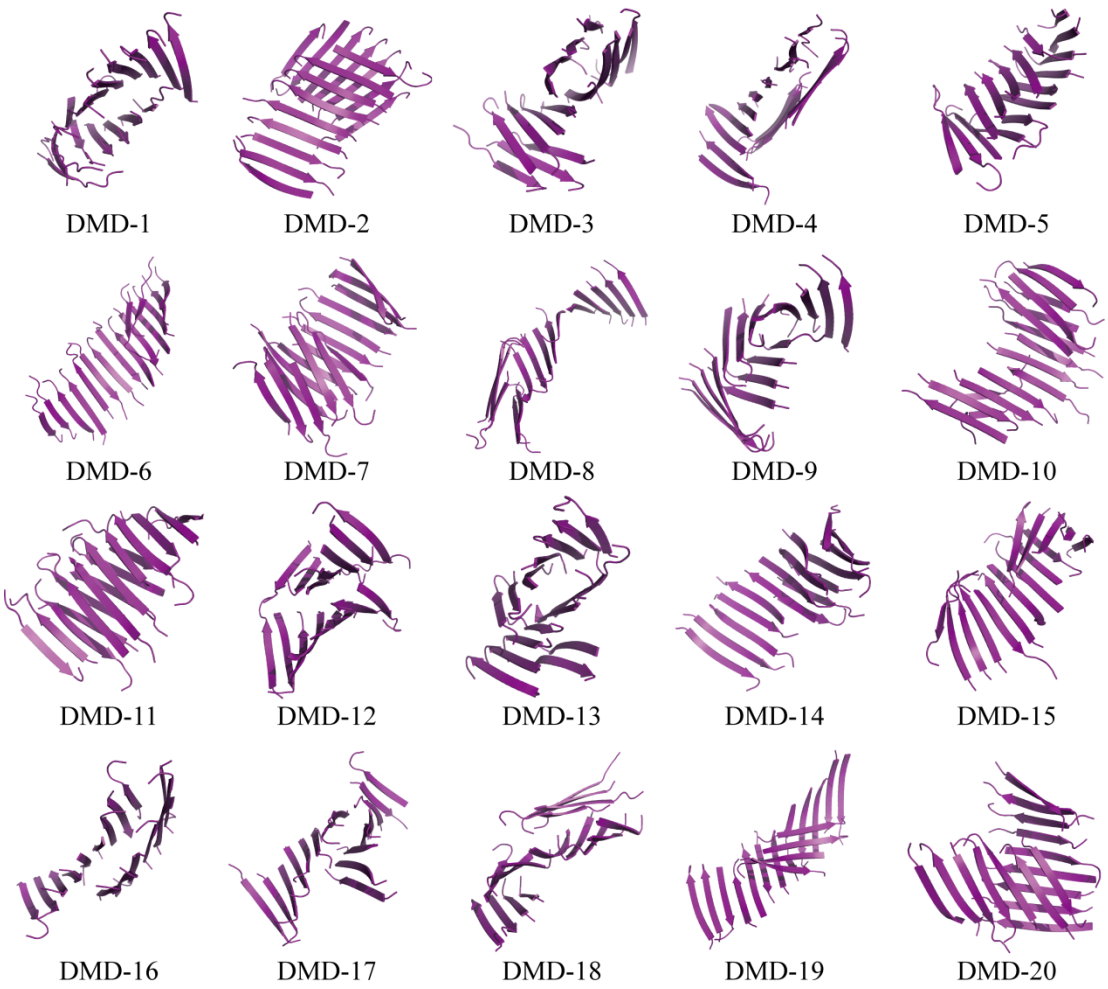

Fig. S2. The final assembled structures of $SOD1_{28\text{-}38}^{G33V}$ in each of the 20 independent DMD simulations for the 16-peptide system.

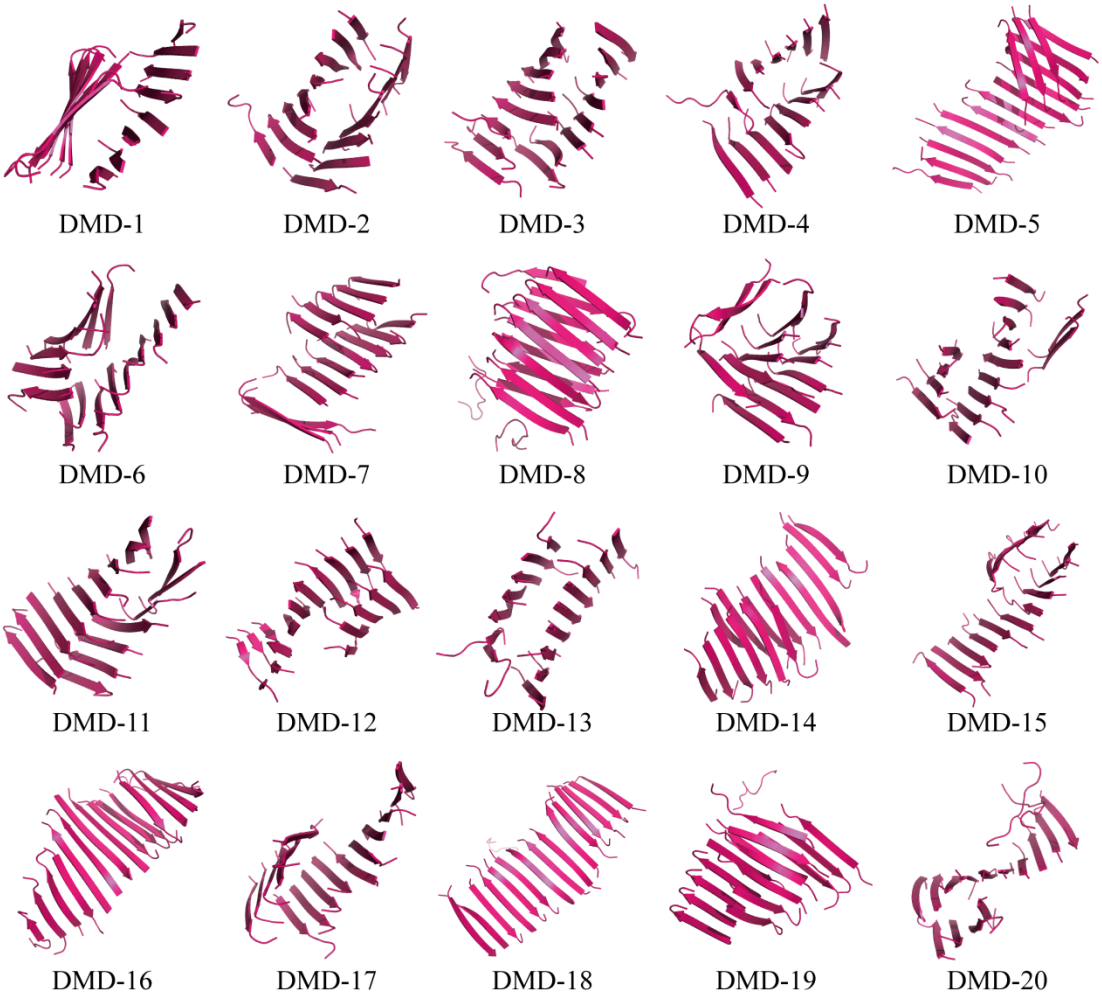

Fig. S3. The final assembled structures of $SOD1_{28\text{-}38}^{G33W}$ in each of the 20 independent DMD simulations for the 16-peptide system.

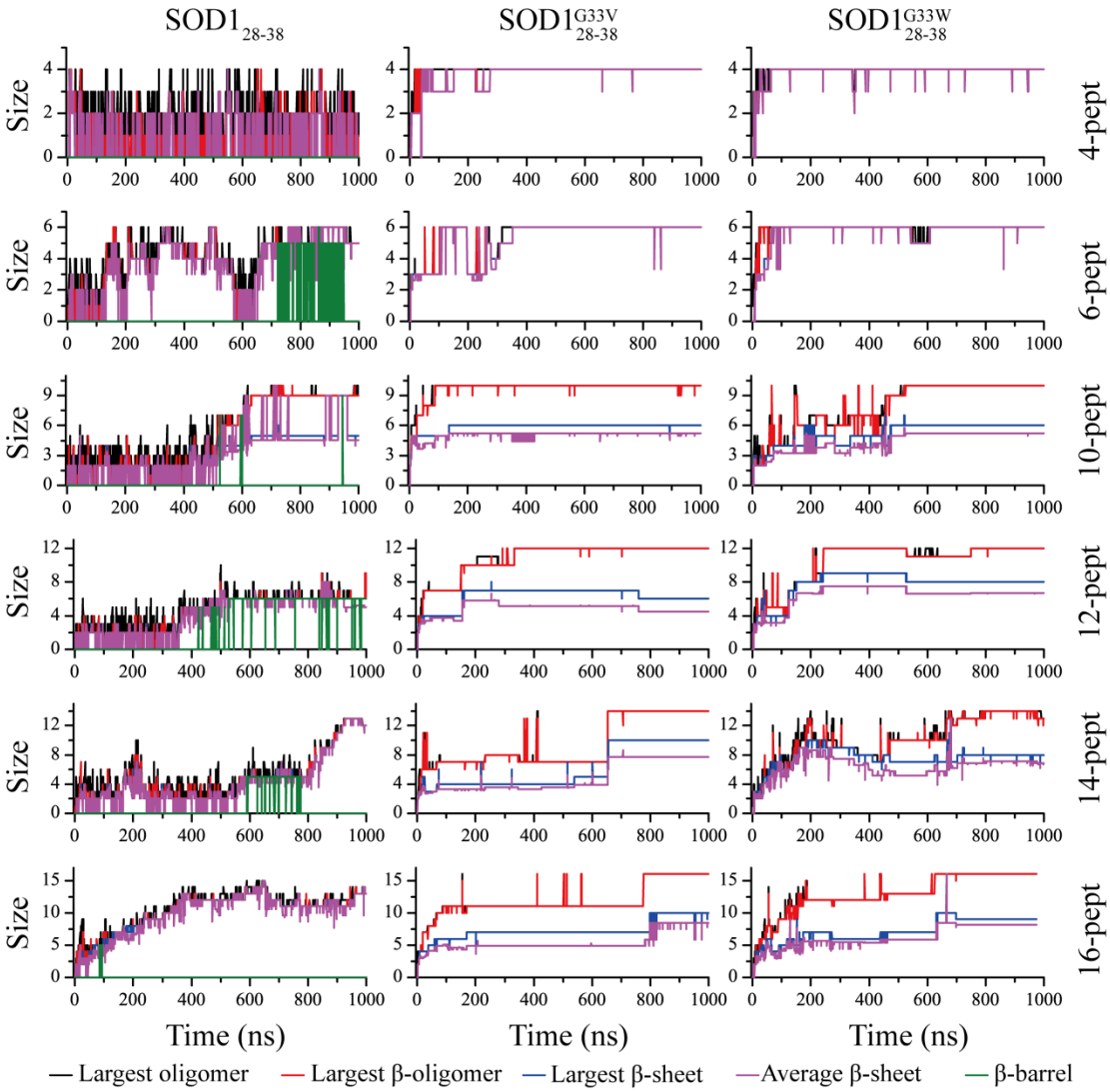

Fig. S4. The self-assembly dynamics of different molecular systems. The self-assembly dynamics of $SOD1_{28\text{-}38}$ (left panel), $SOD1_{28\text{-}38}^{G33V}$ (middle panel), and $SOD1_{28\text{-}38}^{G33W}$ (right panel) peptides were monitored by the time evolution of the largest oligomer size (black), largest β-sheet oligomer size (red), largest β-sheet size (blue), averaged β-sheet layer size (purple) and β-barrel size (green). For each molecular system (the number of simulated peptides, labeled to the right), one representative trajectory was selected.

Table S1. The probability of β-barrel formation observed in each molecular system with different number of simulated peptides for each type of peptides. All independent simulation trajectories were included for the probability calculation.

system	$SOD1_{28\text{-}38}$	$SOD1_{28\text{-}38}^{G33V}$	$SOD1_{28\text{-}38}^{G33w}$
4	0	0	0
6	0.00849	0	0
8	0.00335	0	0
10	6.8E-4	0	0
12	0.02509	0	0
14	0.01536	0	0
16	0.01205	0	0