Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supporting Information

Table S1: C_α-atom numbers of semi-rigid domains within TCR/pMHC/CD8. Results of spatio temporal clustering for k = 9 and Δ_{th} = 0.

Table S1 gives quantitative results for definition of semi rigid domains for use in fitting of MD trajectories and display in Fig. 11. For each C_α (column A) find (in column B) the number of domain members (C_α-atoms) and find in column C the domain label. Domains are sorted according to decreasing size with increasing numeric labels. The number of domains to be considered further (e.g. plotted in color) was set to 8, yielding labels 1,2,…,8 (eight largest domains). Domain 9 and all other smaller domains were given the same label (1054). The choice of eight domains to be labelled is arbitrary in principle. In our case eight was selected since eight colors suffice to discriminate between those domains actually found and reasonably can be used (for fitting MD trajectories).

Protein structure:

A structure description in pdb-format for the complex TCR/pMHC/CD8 together with a sample trajectory is available from http://www.meduniwien.ac.at/msi/biosim/multistageClusteringConsolidation/B4405SampleData.zip