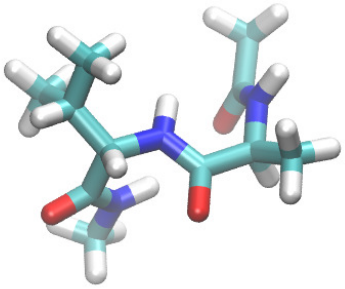

Project: MSM comparison of Ac-AV-NHMe and Ac-VA-NHMe dimer

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The relevant coordinates for the two dimers are given in terms of the Alanine dihedral angles, (ϕ_A, ψ_A) and the Valine dihedral angles (ϕ_V, ψ_V). We want to build MSMs to compare the dynamics of the two dimer-molecules.

For the Ac-AV-NHMe molecule

- Use the provided file `dihedral_AV.npy` containing the dihedral angle trajectory $(\phi_A, \psi_A, \phi_V, \psi_V)$ with a time-step of $1ps$.
- Plot (ϕ_A, ψ_A) and (ϕ_V, ψ_V) trajectories seperately and compare your plots to the stationary distribution for Alanine-Dipeptide from the tutorial. What do you observe?
- Define a coarse discretization for the system. It might be helpful to first obtain a discretized trajectory for each monomer and to combine them in a second step.
- Build a reversible MSM and compute time-scales.

Repeat the above for the Ac-VA-NHMe molecule using the dihedral angles in `dihedral_VA.npy`. Compare the computed time-scales for both dimers. What do you find? Visualize the dominant right eigenvectors. What can you say about the slowest processes in the system?