

# Resource Summary Report

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## Molecular Simulation Trajectories Archive of a Villin Variant

RRID:SCR\_002704

Type: Tool

### Proper Citation

Molecular Simulation Trajectories Archive of a Villin Variant (RRID:SCR\_002704)

### Resource Information

**URL:** <https://simtk.org/home/foldvillin>

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**Description:** An archive of hundreds of all-atom, explicit solvent molecular dynamics simulations that were performed on a set of nine unfolded conformations of a variant of the villin headpiece subdomain (HP-35 NleNle). It includes scripts for accessing the archive of villin trajectories as well as a VMD plug-in for viewing the trajectories. In addition, all starting structures used in the trajectories are also provided. The simulations were generated using a distributed computing method utilizing the symmetric multiprocessing paradigm for individual nodes of the Folding\_at\_home distributed computing network. The villin trajectories in the archive are divided into two projects: PROJ3036 and PROJ3037. PROJ3036 contains trajectories starting from nine non-folded configurations. PROJ3037 contains trajectories starting from the native (folded) state. Runs 0 through 8 (in PROJ3036) correspond to starting configurations 0 through 8 discussed in the paper in J. Mol. Biol. (2007) 374(3):806-816 (see the publications tab for a full reference), whereas RUN9 uses the same starting configuration as RUN8. Each run contains 100 trajectories (named clone 0-99), each with the same starting configuration but different random velocities. Trajectories vary in their length of time and are subdivided into frames, also known as a generation. Each frame contains around 400 configurational snapshots, or timepoints, of the trajectory, with the last configurational snapshot of frame *i* corresponding to the first configurational snapshot of generation *i*+1. The goal is to allow researchers to analyze and benefit from the many trajectories produced through the simulations.

**Abbreviations:** Molecular Simulation Trajectories Archive of a Villin Variant

**Resource Type:** data or information resource, d spatial image, data set

**Defining Citation:** [PMID:17950314](#)

**Keywords:** dynamic, atom, headpiece, molecular, simulation, solvent, protein folding, villin, molecule, trajectory, simulation, molecular dynamics trajectory

**Funding:** Stanford University; California; USA ;  
Graduate Fellowship ;  
NIH ;  
NIGMS R01-GM062868;  
NSF MCB-0317072

**Availability:** Acknowledgement requested, Available in Gromacs and PDB formats.

**Resource Name:** Molecular Simulation Trajectories Archive of a Villin Variant

**Resource ID:** SCR\_002704

**Alternate IDs:** nif-0000-23331

**License:** MIT License

**Record Creation Time:** 20220129T080214+0000

**Record Last Update:** 20260808T185753+0000

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## Ratings and Alerts

No rating or validation information has been found for Molecular Simulation Trajectories Archive of a Villin Variant.

No alerts have been found for Molecular Simulation Trajectories Archive of a Villin Variant.

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## Data and Source Information

**Source:** [SciCrunch Registry](#)

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## Usage and Citation Metrics

We have not found any literature mentions for this resource.