

# Resource Summary Report

Generated by [NIF](#) on Aug 23, 2026

## NAMD

RRID:SCR\_014894

Type: Tool

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### Proper Citation

NAMD (RRID:SCR\_014894)

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### Resource Information

**URL:** <http://www.ks.uiuc.edu/Research/namd/>

**Proper Citation:** NAMD (RRID:SCR\_014894)

**Description:** Parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. NAMD uses the popular molecular graphics program VMD for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR.

**Resource Type:** simulation software, software application, software resource, source code

**Defining Citation:** [PMID:16222654](#)

**Keywords:** simulation, molecules, biomolecular systems, visualization

**Availability:** Open source

**Resource Name:** NAMD

**Resource ID:** SCR\_014894

**Record Creation Time:** 20220129T080322+0000

**Record Last Update:** 20260821T194029+0000

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### Ratings and Alerts

No rating or validation information has been found for NAMD.

No alerts have been found for NAMD.

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### Data and Source Information

## Usage and Citation Metrics

We found 2754 mentions in open access literature.

**Listed below are recent publications.** The full list is available at [NIF](#) .

Wiley B, et al. (2026) Atomistic Insights into Anomeric and Stereochemical Effects on Glucose Transport by GLUTs. *Journal of the American Chemical Society*, 148(5), 5189.

Ralph D, et al. (2026) Molecular Interactions of Fluoroquinolone Antibiotics with Lipid Membranes. *Langmuir : the ACS journal of surfaces and colloids*, 42(6), 4386.

Rossi Sebastiano M, et al. (2026) MK4 Repositioning for IAHSF: Overcoming In Vivo Data Gaps through In Silico Refinement and In Vitro Validation. *ACS chemical neuroscience*, 17(6), 1115.

Ajmera P, et al. (2026) Molecular Mechanism of Mitochondrial Complex I Disruption by m.14484T>C Underlying Leber Hereditary Optic Neuropathy. *bioRxiv : the preprint server for biology*.

Zdorevskiy O, et al. (2026) Catalytic relevance of a quinol anion in biological energy conversion by respiratory complex I. *Chemical science*, 17(13), 6688.

Roth R, et al. (2026) PUFA modulation of ASIC3 involves both specific and lipid solvent-like interactions. *bioRxiv : the preprint server for biology*.

Bhattacharya S, et al. (2026) Development of a highly active engineered PETase enzyme for polyester degradation. *The FEBS journal*, 293(2), 443.

Peña-Vilches N, et al. (2026) Identification of 14-3-3 Proteins as Binding Partners of TRP Channels. *Journal of chemical information and modeling*, 66(7), 3987.

Pan L, et al. (2026) Dual ubiquitin signalling by SLOMO controls AUX1 activity and turnover during root gravitropism. *The EMBO journal*, 45(8), 2739.

de Oliveira Filho JA, et al. (2026) Virtual screening of compounds for the development of thyroid hormone analogues for potential application in cardiac regeneration. *Journal of computer-aided molecular design*, 40(1).

Trujillo-González F, et al. (2026) RNase A is inhibited by the cysteine-rich protein thionein but not by the metal-containing form metallothionein. *Molecular and cellular biochemistry*, 481(5), 1989.

Brownd M, et al. (2026) An Investigation of the Conformational Dynamics of ABC Exporter PCAT1 using Microsecond-Level MD Simulations. *bioRxiv : the preprint server for biology*.

Ricaña CL, et al. (2026) Lenacapavir prevents production of infectious HIV-1 by abrogating immature virus assembly. *bioRxiv : the preprint server for biology*.

Biswas KH, et al. (2026) E50A Mutation Increases the Bioluminescence Activity of picALuc. *Biosensors*, 16(3).

Callahan TJ, et al. (2026) Interpretable machine learning uncovers structural determinants of Wnt-Wntless binding specificity from atomistic simulations. *Communications chemistry*, 9(1).

Tefft NM, et al. (2026) Encapsulation in a Bacterial Microcompartment Shell Improves Thermal Stability of a Glycolytic Enzyme. *ACS synthetic biology*, 15(5), 1980.

Haspel N, et al. (2026) How Functional Variants Reconfigure the Rac2 Conformational Landscape. *bioRxiv : the preprint server for biology*.

Penfield J, et al. (2026) Molecular Behavior of Human  $\alpha$ -Defensin Type 3 Embedded in Different Model Lipid Membranes. *Journal of chemical information and modeling*, 66(9), 5357.

Pang YT, et al. (2026) DeepPath: overcoming data scarcity for protein transition pathway prediction using physics-based deep learning. *Chemical science*, 17(24), 12055.

Tellería F, et al. (2026) PSG6: A mitochondrially-targeted gentisic acid derivative exerts antiplatelet action via mitochondrial complex I inhibition. *Redox biology*, 94, 104200.