

Resource Summary Report

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

bio3d

RRID:SCR_024266

Type: Tool

Proper Citation

bio3d (RRID:SCR_024266)

Resource Information

URL: <https://cran.r-project.org/web/packages/bio3d/index.html>

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Description: Softwar R package for comparative analysis of protein structures. Used to process, organize and explore protein structure, sequence and dynamics data. Used to read and write structure, sequence and dynamic trajectory data, perform sequence and structure database searches, data summaries, atom selection, alignment, superposition, rigid core identification, clustering, torsion analysis, distance matrix analysis, structure and sequence conservation analysis, normal mode analysis, principal component analysis of heterogeneous structure data, and correlation network analysis from normal mode and molecular dynamics data. Enables statistical and graphical power of R environment to work with biological sequence and structural data.

Synonyms: r-cran-bio3d, bio3d: Biological Structure Analysis

Resource Type: software resource, software toolkit

Defining Citation: [PMID:16940322](#)

Keywords: comparative analysis of protein structures, process protein structure, organize and explore protein structure, sequence and dynamics data,

Availability: Free, Available for download, Freely available,

Resource Name: bio3d

Resource ID: SCR_024266

Alternate IDs: OMICS_12577

Alternate URLs: <https://sources.debian.org/src/r-cran-bio3d/>

License: GPL-2 | GPL-3 [expanded from: GPL (? 2)]

Record Creation Time: 20230830T050217+0000

Record Last Update: 20260821T194258+0000

Ratings and Alerts

No rating or validation information has been found for bio3d.

No alerts have been found for bio3d.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 341 mentions in open access literature.

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

Bouricha EM, et al. (2026) The impact of PD-1 mutations on pembrolizumab binding: insights from molecular dynamics and MM-GBSA analysis. Scientific reports, 16(1).

Tang G, et al. (2026) Bioinformatics and computational exploration of novel inhibitors targeting KRAS G12C mutant protein in lung adenocarcinoma. Discover oncology, 17(1).

Versiani AF, et al. (2026) Integrated reiterative pipeline for rapid epitope-based pan-alphavirus vaccines. Science advances, 12(11), eaeb2066.

Soheilypour M, et al. (2026) Intrinsically disordered regions facilitate Mlp1-Nab2 recognition in mRNA quality control. Nucleus (Austin, Tex.), 17(1), 2680376.

Ali A, et al. (2026) TZ1391: a computationally designed circular mRNA multi-epitope vaccine candidate against Mycobacterium tuberculosis via TLR3 immunomodulation. BMC immunology, 27(1).

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.

Tariq SS, et al. (2026) Computational elucidation of stomidazolone mediated inhibition of stomatal differentiation and its implication in plant developmental regulation. PloS one, 21(2), e0329401.

Khan MU, et al. (2026) Molecular docking and dynamics reveal novel CDK6 inhibitors for targeted glioblastoma therapy. Scientific reports, 16(1).

Kumutima J, et al. (2026) Alanine Rewires the Communication Pathways Established During the Allosteric Activation of Liver Pyruvate Kinase by Fructose Bisphosphate. Journal of chemical information and modeling, 66(11), 6637.

Prihanti GS, et al. (2026) Computational discovery of fenugreek-paitan-turmeric (FPT) bioactive compounds targeting SGLT2 and DPP-4 for glucose homeostasis regulation. *Journal of Taibah University Medical Sciences*, 21(4), 639.

Cavalcanti IDL, et al. (2026) Activation of the Complement System: Morphological Differences in the Surface of PIBCA Nanoparticles Coated with Polysaccharides. *ACS nanoscience Au*, 6(3), 457.

Sahoo RK, et al. (2026) Genome assembly and protein structure modeling reveal key molecular features of divergent wmk homologs in *Wolbachia*. *Microbiology spectrum*, 14(2), e0289325.

Hu G, et al. (2026) Selective binding of divalent cations reshapes nucleosome mechanics and unlocks histone tail dynamics. *Communications biology*, 9(1).

Wang Y, et al. (2026) Hotspot Interactions between Two Fab Molecules in Molecular Dynamics Simulations Improve Predictive Models of Aggregation Kinetics. *Molecular pharmaceutics*, 23(3), 1722.

Khan SA, et al. (2026) Integrative computational approaches, molecular docking, and dynamic simulations reveal the antimycobacterial activity of fisetin as a potential inhibitor of *Mycobacterium tuberculosis*. *Journal of computer-aided molecular design*, 40(1).

Alzahrani AR, et al. (2026) Human Metapneumovirus Nucleocapsid Inhibitors Discovery for Targeting Viral Replication and Genome Encapsidation: An In Silico Approach. *Journal of tropical medicine*, 2026, 3511825.

Elabed S, et al. (2026) Doxorubicin-driven reconfiguration of BSA-cushioned DPPC liposomes an integrated molecular-dynamics and AFM roadmap for next-generation drug-delivery platforms. *Nanoscale advances*, 8(13), 3769.

Nanna V, et al. (2026) MD Simulations of Human Sigma-1 Receptor Trimer Uncover Cholesterol-Dependent Stabilization and Ligand-Specific Dynamics. *Journal of chemical information and modeling*, 66(12), 7296.

Bhatt JS, et al. (2026) Atomistic scattering modeling of the solution structure of human dimeric IgA1 reveals a structural and mechanistic basis for IgA nephropathy. *The Journal of biological chemistry*, 302(7), 113156.

Gani R, et al. (2026) Evaluation of free radical scavenging and anxiolytic activities of *Bunium persicum* (Boiss.) B. Fedtsch. bioactive metabolites through multi-method experimental and computational approaches. *Frontiers in pharmacology*, 17, 1805095.