

Resource Summary Report

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PDB-REDO

RRID:SCR_018936

Type: Tool

Proper Citation

PDB-REDO (RRID:SCR_018936)

Resource Information

URL: <https://pdb-redo.eu/>

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Description: Web server for macromolecular structure model optimisation and databank of optimised structure models. Focuses on automating final steps of crystallographic process: optimisation of structure model through refinement, rebuilding, and validation. Can automatically optimise most of crystallographic structure models based on input model and diffraction data. Web server works on user provided data, databank has updated versions of Protein Data Bank entries based on original experimental data that were deposited with atomic coordinates in PDB.

Synonyms: PDB_REDO

Resource Type: data access protocol, data processing software, data repository, service resource, software application, software resource, storage service resource, web service

Defining Citation: [DOI:10.1107/S2052252514009324](https://doi.org/10.1107/S2052252514009324)

Keywords: Macromolecular structure, model optimization, crystallographic process, final step automating, structure model optimization, structure refinement, structure rebuilding, atomic coordinate, PDB

Funding: Netherlands Organization for Scientific Research

Availability: Free, Freely available

Resource Name: PDB-REDO

Resource ID: SCR_018936

License URLs: <https://pdb-redo.eu/license.txt>

Record Creation Time: 20220129T080342+0000

Ratings and Alerts

No rating or validation information has been found for PDB-REDO.

No alerts have been found for PDB-REDO.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 35 mentions in open access literature.

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

Foster SP, et al. (2026) It started off as a Cys, how did it end up like this? Identifying the extent of unmodelled oxidatively modified cysteines within the Protein Data Bank. Acta crystallographica. Section D, Structural biology, 82(Pt 7), 700.

Romano A, et al. (2026) In Silico Drug Repositioning Identifies SYK Kinase Inhibitors as Potential Neuroprotective Agents for Ataxia-Telangiectasia. Chemical biology & drug design, 108(1), e70354.

Wang CY, et al. (2026) Heart failure pleural fluid impairs endothelial barrier through miR 501-3p mediated ZO 1 remodeling. iScience, 29(5), 115549.

Petrides AC, et al. (2025) Reconstructing biological molecules with help from video gamers. Acta crystallographica. Section D, Structural biology, 81(Pt 11), 598.

Wlodawer A, et al. (2025) A Critical Look at the Crystal Structures of cAMP-Dependent Protein Kinases. Kinases and phosphatases, 3(3).

Sarrau C, et al. (2025) Exploration of questionable backbone conformations in crystallographic structure models using a structural alphabet. Acta crystallographica. Section D, Structural biology, 81(Pt 12), 734.

Buccheri R, et al. (2025) High-Throughput, High-Quality: Benchmarking GNINA and AutoDock Vina for Precision Virtual Screening Workflow. Molecules (Basel, Switzerland), 30(16).

Costanzo G, et al. (2024) Design, Synthesis, and Evaluation of Novel (-)-cis-N-Normetazocine Derivatives: In Vitro and Molecular Modeling Insights. Chemical biology & drug design, 104(6), e70037.

Lushchekina S, et al. (2024) Why is binding of a divalent metal cation to a structural motif containing four carboxylate residues not accompanied by a conformational change? Protein science : a publication of the Protein Society, 33(12), e5206.

Zhang R, et al. (2024) Analysis of Tumor-Associated AXIN1 Missense Mutations Identifies Variants That Activate β -Catenin Signaling. *Cancer research*, 84(9), 1443.

Barbhuiya TK, et al. (2024) Targeting the hSSB1-INTS3 Interface: A Computational Screening Driven Approach to Identify Potential Modulators. *ACS omega*, 9(7), 8362.

Hekkelman ML, et al. (2023) AlphaFill: enriching AlphaFold models with ligands and cofactors. *Nature methods*, 20(2), 205.

Ou J, et al. (2023) A yeast-based system to study SARS-CoV-2 Mpro structure and to identify nirmatrelvir resistant mutations. *PLoS pathogens*, 19(8), e1011592.

Jernigan RJ, et al. (2023) Room-temperature structural studies of SARS-CoV-2 protein NendoU with an X-ray free-electron laser. *Structure (London, England : 1993)*, 31(2), 138.

Gres AT, et al. (2023) Multidisciplinary studies with mutated HIV-1 capsid proteins reveal structural mechanisms of lattice stabilization. *Nature communications*, 14(1), 5614.

van Alderwerelt van Rosenburgh IK, et al. (2022) Biochemical and structural basis for differential inhibitor sensitivity of EGFR with distinct exon 19 mutations. *Nature communications*, 13(1), 6791.

Qin J, et al. (2022) Structures of PKA-phospholamban complexes reveal a mechanism of familial dilated cardiomyopathy. *eLife*, 11.

Zacharchenko T, et al. (2022) Structural basis of Apt48 inhibition of the BCL6 BTB domain. *Structure (London, England : 1993)*, 30(3), 396.

Hassani Nia F, et al. (2022) Structural deficits in key domains of Shank2 lead to alterations in postsynaptic nanoclusters and to a neurodevelopmental disorder in humans. *Molecular psychiatry*.

Thomson EC, et al. (2021) Circulating SARS-CoV-2 spike N439K variants maintain fitness while evading antibody-mediated immunity. *Cell*, 184(5), 1171.