

PDB-assistant: an integrated web tools for analyzing and editing PDBs

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Problems & Ideas

- The three-dimensional (3D) structure of proteins is a crucial resource for elucidating molecular biological functions and facilitating protein engineering endeavors. Nonetheless, the existing computational tools designed for manipulating protein 3D structure files have yet to adequately meet the pressing demands of the research community.
- **Ideas:** Developing a comprehensive web server that integrates various analysis and editing functions with unique features.

Main Contributions

- Contributions:

- We have developed an intuitive online platform for the editing and analysis of Protein Data Bank (PDB) files.
- Our platform integrates a total of 10 specialized tools, comprising three for PDB analysis and seven for PDB editing.
- The majority of these tools have been uniquely developed in-house, offering distinctive features tailored to the needs of our users.

Category	Tool Name	Description
PDB-Analysis	StructureAlign	Superposing two proteins to evaluate their structural similarity with customized- region alignment
	BreakCheck	Checking whether the input protein PDB file has main chain breaks
	PDB2FAS	Extracting protein sequences from a PDB file
PDB-Editing	AA-Mutate	Replacing residues of a given protein with the customized residues
	PE-Minimize	Generating the energy minimized conformation of the given protein
	PDB-Repair	Fixing missing atoms or residues of the given input
	PDB-Split	Splitting a protein complex into individual chains
	PDB-Assemble	Assembling multiple subunits to complex by referring to the template structure
	PDB-ReNumber	Modifying the residue indexes of a PDB file
	PDB-AddH	Adding hydrogen atoms on a given protein (CHARMM22 defined hydrogen atoms)

