

Automated Protein Structure Determination with *BnP*

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*BnP*¹ is a protein structure determination package with a graphical user interface suitable for both manual and automated operation. *BnP*'s main function is to couple the direct-methods program *SnB*, used to determine heavy atom/anomalous scatterer substructures, with the protein-phasing package *PHASES*, used for heavy atom refinement, protein phasing, density modification, and skeletonization. It also creates data and scripts for external programs required for automated chain tracing, graphical visualization, and refinement. In addition to seamlessly interfacing the various packages, near total automation is implemented such that one needs only to specify a few parameters, and the entire phasing process starting with diffraction data and resulting in interpretable electron-density maps is carried out by clicking a single button. With a couple of additional button clicks external programs for automated chain tracing or chain tracing/refinement can then be launched. The overall strategies and methodology employed will be described, with emphasis on those aspects required to facilitate automation and recent developments simplifying user input. Extensive test results verify the package's effectiveness. This work was supported by NIH grant EB002057.

[1] C. M. Weeks et. al., *Z. Kristallogr.*, 2002, **217**, 686-693.

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