

# BALL (Biochemical Algorithms Library) and BALLView – a multiplatform molecular viewer and modeling tool

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We present the Biochemical Algorithms Library (BALL) [1, 2], an object oriented framework for rapid application development in molecular modeling and structural bioinformatics. Among other things BALL provides an extensive set of data structures as well as classes for molecular mechanics, like energy minimizations and molecular dynamics simulations. With BALL it is also possible to calculate electrostatic potentials using a native implementation of a Finite Difference Poisson Boltzmann (FDPB) solver. The potentials can be visualized by coloring solvent accessible/excluded surfaces and isocontour surfaces similar to GRASP. Furthermore the library provides data structures and algorithms for advanced solvation methods, comparison and analysis of protein structures, file import/export, NMR shift prediction, and 3D interactive visualization.

BALL has been carefully designed to be robust, easy to use, and open to extensions. Especially its extensibility resulting from an object-oriented and generic programming approach distinguishes it from other software packages.

To reduce turn-over times for developing new methods, we added Python bindings for the majority of the BALL classes. This scripting language allows for easier inspection of the data structures and the code can be modified at runtime without time-consuming compile or link stages. Once the Python code works as desired, it is very simple to port it to C++.

Using the functionality of BALL, we have developed BALLView, a stand-alone molecular visualization tool featuring molecular modeling capabilities. The graphical user interface gives the user easy access to common functions employed in molecular modelling. BALLView provides state-of-the-art graphics and visualization: for high performance hardware accelerated 3D graphics, BALLView uses the OpenGL or Mesa libraries available on almost all platforms and graphics cards. The level of detail for each representation can be adjusted to the machine's graphics performance thus enabling the visualization of large structures even on laptops with low-end graphic accelerator cards. BALLView also provides support for stereo 3D viewing, both for shutter glasses and side by side stereo. Publication quality images can be generated by using the POVray export feature. Employing the comprehensive API, users can expand BALLView to fit their specific requirements.

BALL and BALLView are freely available as source code and as binary packages/installer for Linux, Windows and MacOS. These files can be downloaded from the BALL project website [3].

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[1] N. Boghossian, O.Kohlbacher, and H. Lenhof, *J. Exp. Algorithmics* p. 5:16 (2000).

[2] O. Kohlbacher and H. Lenhof, *Bioinformatics* **16(9)**, 815824 (2000).

[3] <http://www.ball-project.org>.

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