Visualization of Structural Information with xPSSS

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A new molecular graphics viewer, jV [1], has been extended to display structural volume data, like electron densities. Display of these data is possible either as contour line grids or as isosurfaces. xPSSS, found at http://www.pdbj.org/xpsss/, uses an applet version of the viewer to display such volume information. Electron density maps are available for about 15,000 structures of the PDB and were calculated from deposited X-ray structures refined against deposited structure factor data. The visualization capabilities have been further extended to display other grid-based information such as molecular orbital data generated by the program AMOSS, stored in XML-format.

The software for most of the calculations is written in Python and Fortran-95 modules for computationally intensive operations. These modules are used as Python extensions. The volume data are stored in a binary byte-map format. Contour and isosurface data are stored as XML files.

[1] Kinoshita K., Nakamura H., *Bioinformatics*, 2004, **20**, 1329.

Keywords: databases, data representation, visualization