Location: http://www.avatar.se/molscript/. Operating system: UNIX. Type: source code and binary. Language: C. Distribution: free academic.

An enhanced variant of *MOLSCRIPT*, called *BOBSCRIPT*, has been developed by Robert Esnouf (http://orval.rega.kuleuven.ac.be/~robert/Bobscript/). In addition to the functions provided by *MOLSCRIPT*, *BOBSCRIPT* can generate an input file automatically and allows for the display of electron density.

25.1.9.4. *NUCPLOT*

NUCPLOT (Luscombe *et al.*, 1997) is a program which generates schematic diagrams of protein–nucleic acid interactions. The program automatically identifies these interactions from the 3D atomic coordinates of the complex from a PDB file and generates a plot that shows them in a clear and simple manner.

Location: http://www.biochem.ucl.ac.uk/~nick/nucplot.html. Operating systems: UNIX, IRIX, LINUX and Windows. Type: source code. Language: C. Distribution: free academic.

25.1.9.5. *ORTEP*

The Oak Ridge Thermal Ellipsoid Plot (*ORTEP*, version III) program (Burnett & Johnson, 1996) is a computer program for drawing crystal-structure illustrations. Ball-and-stick type illustrations of a quality suitable for publication are generated with either spheres or thermal-motion probability ellipsoids, derived from anisotropic temperature-factor parameters, on the atomic sites. The program also produces stereoscopic pairs of illustrations that aid in the visualization of complex arrangements of atoms and their correlated thermal-motion patterns.

Location: http://www.ornl.gov/ortep/ortep.html. Operating systems: UNIX, LINUX, DOS, MacOS and Windows. Type: source code and binary. Language: Fortran77. Distribution: free.

25.1.9.6. *RasMol*

RasMol is a molecular-graphics program intended for the visualization of proteins, nucleic acids and small molecules. The program is aimed at display, teaching and generation of high-quality images for publication. It is easy to use and produces beautiful space-filling three-dimensional colour images. *RasMol* reads in molecular coordinate files in a number of formats and interactively displays the molecule on the screen in a variety of colour schemes and representations. The X Windows version of *RasMol* provides optional support for a hardware dials box and accelerated shared memory rendering (*via* the XInput and MIT-SHM extensions) if available.

Location: http://www.umass.edu/microbio/rasmol/. Operating systems: UNIX, VAX/VMS, Windows and MacOS. Type: source code. Distribution: free.

25.1.9.7. *Raster3D*

Raster3D (Bacon & Anderson, 1988; Merritt & Murphy, 1994; Merritt & Bacon, 1997) is a set of tools for generating high-quality raster images of proteins or other molecules. The core program renders spheres, triangles and cylinders with special highlighting, Phong shading and shadowing. It uses an efficient software Z-buffer algorithm that is independent of any graphics hardware. Ancillary programs process atomic coordinates from PDB files into rendering descriptions for pictures composed of ribbons, space-filling atoms, bonds, ball-and-stick *etc.* *Raster3D* can also be used to render pictures composed in Per Kraulis' program *MOLSCRIPT* (Section 25.1.9.3) in glorious 3D with highlights, shadowing *etc.* Output is pixel image files with 24 bits of colour information per pixel.

Location: http://www.bmsc.washington.edu/raster3d/raster3d.html. Operating systems: DEC, SGI, ESV, SUN, IBM, HP and LINUX. Type: source code and binary. Distribution: free.

25.1.9.8. *Ribbons*

Ribbons software (Carson & Bugg, 1986; Carson, 1997) interactively displays molecular models, analyses crystallographic results and creates publication-quality images. Space-filling and ball-and-stick representations, dot and triangular surfaces, electron-density-map contours, and text are also supported. Input atomic coordinates are in Protein Data Bank (PDB) format. Output may be produced in the Inventor/VRML format.

Location: http://www.cmc.uab.edu/ribbons/. Operating systems: UNIX, LINUX and PC. Type: source code and binary. Distribution: commercial.

25.1.9.9. *SETOR*

SETOR (S. V. Evans, 1993) is designed to render high-quality raster images of macromolecules that can undergo rotation and translation interactively. *SETOR* can render standard all-atom and backbone models of proteins or nucleic acids, but focuses on displaying protein molecules by highlighting elements of secondary structure. The program has a very friendly user interface that minimizes the number of input files by allowing the user to interactively edit parameters such as colours, lighting coefficients and descriptions of secondary structure *via* mouse-activated dialogue boxes. The choice of polymer-chain representation can be varied from standard vector models and van der Waals models, to a beta-spline fit of polymer backbones that yields a smooth ribbon, and to strict Cardinal splines that interpolate the smoothest curve possible that will precisely follow the polymer chain. The program provides a photograph mode, save/restore facilities, and efficient generation of symmetry-related molecules and packing diagrams. Additionally, *SETOR* is designed to accept commands and model coordinates from standard output. Ancillary programs provide a method to edit interactively hardcopy plots of all vectors and many solid models generated by *SETOR*, and to produce standard HPGL or PostScript files.

Location: http://flint.biochm.uottawa.ca/~setor_docs/. Operating system: SGI. Type: binary. Distribution: commercial.

25.1.9.10. *VMD*

VMD (Visual Molecular Dynamics) is designed for the visualization and analysis of biological systems such as proteins, nucleic acids, lipid bilayer assemblies *etc*. It may be used to view more general molecules, as *VMD* can read standard PDB files and display the structure contained in them. *VMD* provides a wide variety of methods for rendering and colouring a molecule: simple points and lines, CPK spheres and cylinders, licorice bonds, backbone tubes and ribbons, cartoon drawings, and others. *VMD* can be used to animate and analyse the trajectory of a molecular-dynamics (MD) simulation. In particular, *VMD* can act as a graphical front end for an external MD program by displaying and animating a molecule undergoing simulation on a remote computer.

Location: http://www.ks.uiuc.edu/Research/vmd/allversions. Operating systems: SGI, SUN, DEC Alpha, IBM AIX, HP-UX and LINUX. Type: binary. Distribution: free.

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references