will output an r.m.s. deviation and, optionally, the fitted coordinates. R.m.s. deviations may also be calculated without actually performing a fit. Zones for calculating the r.m.s. deviation can be different from those used for fitting.

Location: http://www.biochem.ucl.ac.uk/~martin/programs/index.html. Operating system: SGI. Type: binary. Language: C. Distribution: free.

25.1.8.10. *PROSA*

The *PROSA* (PROtein Structure Analysis) program is a useful tool in protein structure research. *PROSA* supports and guides your studies aimed at the determination of a protein's native fold. It is helpful for experimental structure determinations and modelling studies.

Locations: http://www.iucr.org/sincris-top/logiciel/prg-prosa.html, ftp://Gundi.came.sbg.ac.at/pub/Prosa/. Operating systems: SGI and DEC Alpha. Type: binary. Distribution: free academic.

25.1.8.11. *SARF*

SARF (Spatial ARangement of backbone Fragments; Alexandrov, 1996) can perform a search for similar structural motifs in a list of structures or analyse a new structure that is not in the PDB. Comparison of the protein backbone can provide more information than classification of protein structures, because it can reveal unexpected local similarities important for protein function.

Location: http://www-lmmb.ncifcrf.gov/~nicka/prerun.html. Operating systems: SGI and DEC. Type: binary. Distribution: free.

25.1.8.12. *SQUID*

The program *SQUID* (Oldfield, 1992) was developed for the graphical display of information and the analysis of data. Major applications of the program are the analysis of protein structures and molecular-dynamics simulations.

Location: http://www.ysbl.york.ac.uk/~oldfield/squid/. Operating systems: UNIX, SGI, SUN, VAX, DEC and DOS. Type: source code and binary. Language: Fortran. Distribution: free.

25.1.8.13. *STAMP*

The *STAMP* program package comprises 15 programs for alignment and analysis of three-dimensional structures of protein molecules. The program package has the following applications: (1) fast alignment and superimposition of two or more protein structures; (2) generation and display of superimposed 3D structures of protein molecules, as well as sequence alignments; (3) comparison of a protein 3D structure to a database of other protein structures; (4) direct interface to *MOLSCRIPT* (Section 25.1.9.3) and *ALSCRIPT* drawing programs; and (5) a clear method for assigning which regions within a family of proteins are structurally equivalent, without the need for graphical intervention.

Location: http://www.iucr.org/sincris-top/logiciel/prg-stamp.html or e-mail gjb@bioch.ox.ac.uk. Operating system: UNIX. Type: binary. Distribution: free academic.

25.1.8.14. *SURFNET*

SURFNET (Laskowski, 1995) is a program that generates molecular surfaces, cavities and intermolecular interactions from coordinate data files in PDB format. These molecular surfaces and void regions can be visualized graphically.

Location: http://www.biochem.ucl.ac.uk/~roman/surfnet/surfnet.html; ftp://ftp.biochem.ucl.ac.uk. Operating system: UNIX. Type: source code and binary. Distribution: free academic.

25.1.8.15. *WHAT CHECK*

WHAT CHECK (Rodriguez *et al.*, 1998) is a free subset of protein verification programs from the *WHAT IF* package (Section 25.1.8.16).

Location: http://www.sander.embl-heidelberg.de/whatcheck/. Operating systems: SGI and OSF1. Type: source code. Distribution: free.

25.1.8.16. *WHAT IF*

WHAT IF (Vriend, 1990) is a versatile protein structure analysis program that can be used for mutant prediction, structure verification, molecular graphics *etc*. The program makes extensive use of structural databases, permitting diverse query possibilities in structural analysis.

Location: http://www.cmbi.kun.nl/whatif/index.html. Operating systems: UNIX and Windows. Type: binary. Distribution: minor licence fee for academic users.

25.1.9. Structure presentation

25.1.9.1. *GRASP*

GRASP (Nicholls *et al.*, 1991) is a molecular visualization and analysis program. It is particularly useful for the display and manipulation of the surfaces of molecules and their electrostatic properties. Its particular strength compared to other such programs is its facility for surfaces and electrostatics. The program contains extremely rapid algorithms for the construction of rendered molecular surfaces and for solving the Poisson–Boltzmann equation. *GRASP*'s surface can be molecular or accessible and can be colour-coded by electrostatic potential derived from its internal Poisson–Boltzmann solver or external programs such as *DelPhi*. This representation has become a standard tool in assessing electrostatic character of large, typically protein, molecules. Surfaces can also be coloured by other properties, such as any of those of the underlying atoms (*e.g.* hydrophobicity) or by its own intrinsic properties, such as local curvature. The program also contains several other unique data-representation forms in addition to standard ones such as ball-and-stick for atoms and bonds, and backbone splines, or 'worms', to indicate secondary structure. See Chapter 22.3 for more details.

Location: http://honiglab.cpmc.columbia.edu/grasp/. Operating system: IRIX. Type: binary. Distribution: commercial.

25.1.9.2. *LIGPLOT*

The *LIGPLOT* program (Wallace *et al.*, 1995) automatically generates schematic diagrams of protein–ligand interactions for a given PDB file. The interactions shown are those mediated by hydrogen bonds and by hydrophobic contacts.

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

25.1.9.3. *MOLSCRIPT*

MOLSCRIPT (Kraulis, 1991) is a program for creating schematic or detailed molecular-graphics images in the form of PostScript plot files from molecular 3D coordinates, usually, but not exclusively, of protein structures. Possible representations are simple wire models, CPK spheres, ball-and-stick models, text labels and Jane Richardson-type schematic drawings of proteins, based on atomic coordinates in various formats. Colour, greyscale, shading and depth cueing can be applied to the various graphical objects. See Section 25.2.7 for a detailed description.

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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