Improved ribbon-drawing programs

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We describe significant improvements to RIBBON (a program system that produces schematic pictures of proteins) that extend its capabilities and simplify its use. Enhanced features include the drawing of ligands as an integral part of the picture and in a variety of styles, greater control of the displayed image, and a much improved user-interface.

Keywords: protein structure, ribbon drawing program, stylized protein picture, computer graphics

INTRODUCTION

The wealth of information implicit within a protein structure defies complete representation in a simple or lucid manner. One common simplification is the use of highly schematic diagrams to show the overall structural pattern or 'fold.' These so-called "ribbon drawings" depict β-strands as arrows, α-helices as spiral ribbons or cylinders, and other structure as a coiling rope. From relatively crude early attempts,[1,2] the development of this approach has culminated in the much admired drawings of Jane Richardson.[3,4] The considerable time, patience, and artistic skill required to produce such pictures has led to the development of computer programs capable of generating these illustrations automatically;[5–9] the programs that most nearly capture the considerable aesthetic appeal of Richardson's work are those of Priestle.[10] Lacking many of the approximations of other programs, Priestle's RIBBON suite produces schematic pictures of proteins that are a compromise: while very easy to produce, they manage to retain the highly pleasing appearance of hand-drawn diagrams and to represent accurately the character of the protein secondary structure. Thus RIBBON is fast becoming the method of choice for producing such illustrations. Despite this it lacks many desirable features, motivating our efforts to improve the program. This note details significant enhancements to the system that extend its capabilities and simplify its use; these improvements include the incorporation of the drawing of ligands as an integral part of the picture, greater control of the displayed image, and a much improved user interface.

OVERVIEW

In contrast to the modifications announced by others,[11] we have retained the modular, device-independent character of the suite while revising the programs and introducing new features. Figure 1 shows a flow diagram of this program system. Creating the picture proceeds in two stages: first, a set of α-carbon coordinates is transformed into stylized picture elements (arrows, ribbon spirals, and rope coils). This is achieved by the program RIBBON. Second, these elements are made into a complete picture through hidden-line removal, the addition of shading lines, the detailed drawing of ligands, and the automatic generation of stereo images (if required). This is done by the POSTPLOT program. The final drawing can then be displayed using a range of flexible device-driving programs.

RIBBON

Priestle's original program has been extensively modified to remove errors and inconsistencies and to introduce keyworded, free format intput of instructions. RIBBON requires a list of secondary structure elements given as residue

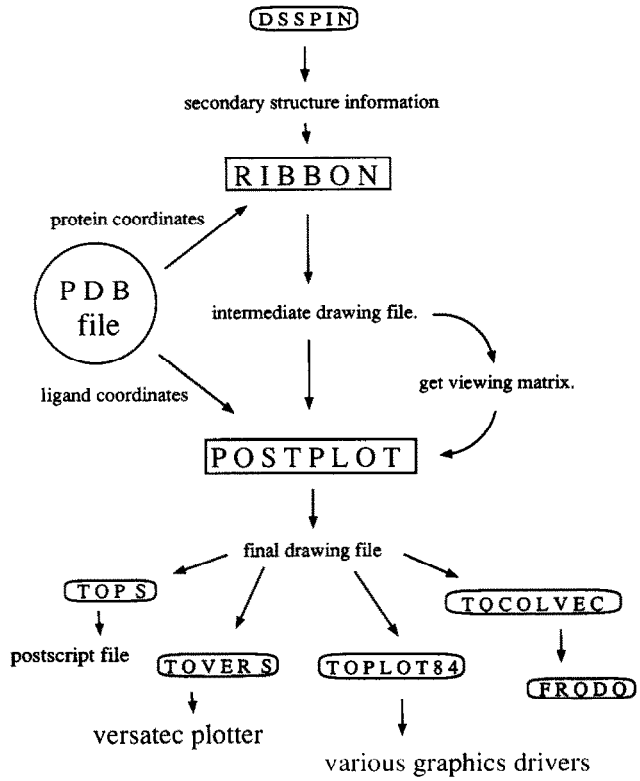

Figure 1. A flow chart for the revised RIBBON suite

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ranges via Helix or Strand keywords. These can be extracted directly from the output of the program DSSP[12] using our program DSSPIN. The output from RIBBON can be displayed in FRODO and then reorientated to its best view. The resulting viewing matrix can be applied directly by the program POSTPLOT, eliminating the need for the RIBROT program, which fulfills this function in Priestle's original system.

POSTPLOT

The final drawing is produced by the program POSTPLOT, which has been revised thoroughly and now accepts free format control input via keywords. This new version has options for displaying ligands in wire-frame, ball-and-stick (with open or filled bonds), or space-filling representations. We feel this new feature rectifies the major inadequacy of Priestle's original implementation compared to rival programs, such as that of Lesk.[5,6] Examples of drawings with ligands are given in Figure 2 (space filling) and in the color plates (ball and stick).

VIEWING THE FINAL DRAWING

The final drawing file can be displayed using specific device-driving programs: thus overall device independence is maintained. We have developed several such drivers: TOPLOT84, which produces a PLOT84 file that dovetails into several display programs; TOCOLVEC, which produces files read by the COLVEC option in FRODO; TOPS, which produces a postscript file encoding a gray-scale shaded picture (as a monotone approximation to a color image); and TOVERS, which drives a Versatec plotter for color plots up to A2 size. These display drivers are written to allow for considerable user control of differences in regional shading or coloring of the final image, enabling sections of the ribbon or separate ligands to be displayed differently. This is often used in distinguishing or highlighting features of particular interest. Figure 2 is an example of such a postscript gray-scale picture.

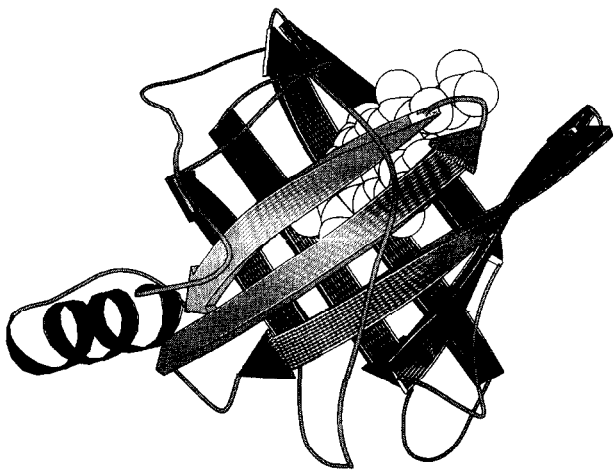

Figure 2. A gray-scale RIBBON picture of Apo-lipoprotein D with a space-fill bound bilin ligand (Brookhaven Protein Databank entry 1APD)

SUMMARY

We feel these enhancements to the programs of the RIBBON suite greatly facilitate their use and the introduction of ligand drawing and other features extends the capacities of the system significantly. The programs will be made available via CCP4 at the SERC Daresbury laboratory. The author is grateful for a Wellcome Prize Studentship.

REFERENCES

1 Holbrook, J.J., Liljas, A., Steindel, S.J. and Rossmann, M.G. In: *The Enzymes* (P.D. Boyer, Ed.) Academic Press, New York, 1975, **11**, 191–292
2 Branden, C.I., Jornvall, H., Eklund, H. and Furugren, B. In: *The Enzymes* (P.D. Boyer, Ed.) Academic Press, New York, 1975, **11**, 103–190
3 Richardson, J.S. *Adv. Prot. Chem.* (1981) **34**, 167–339
4 Richardson, J.S. *Methods Enzymol.* (1985) **115**, 359–380
5 Lesk, A.M. and Hardman, K.D. *Science* (1982) **216**, 539–540
6 Lesk, A.M. and Hardman, K.D. *Methods Enzymol.* (1985) **115**, 381–390
7 Billeter, M., Engeli, M. and Wuthrich, K. *J. Mol. Graphics* (1985) **3**, 79–83
8 Carson, M. and Bugg, C. *J. Mol. Graphics* (1986) **4**, 121–122
9 Burridge, M.J. and Todd, S.P.J. *J. Mol. Graphics* (1986) **4**, 220–221
10 Priestle, J.P. *J. Appl. Crystallogr.* (1988) **21**, 572–576
11 Callahan, T., Gleason, W.B. and Lybrand, T.P. *J. Appl. Crystallogr.* (1990) **23**, 434–436
12 Kabsch, W. and Sander, C. *Biopolymers* (1983) **22**, 2577–2637