DRAWNA: A program for drawing schematic views of nucleic acids

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A program for drawing automatically exact and schematic views of nucleic acids is described. The program is written in C ANSI and uses the Silicon Graphics GL and Xirisw libraries within the X11/Motif environment. Through menus, the user can choose, specify, and manipulate in real time the three-dimensional views to be displayed. Drawing options include partitioning of structures into differently colored or shaped fragments, representation of backbones as flat or with conic-section ribbons, display of paired or free bases as rods, and display of surfaces as filled or outlined and stereo or depth-cued views.

Keywords: nucleic acids, three-dimensional representation, GL, Motif, B-spline

INTRODUCTION

Nucleic acids are characterized by the sequence of bases attached on the polynucleotide sugar–phosphate backbone (normally numbered in the 5′ to 3′ direction). In DNA, the main structure is the antiparallel double-stranded helix maintained via hydrogen bonds involving atoms of Watson–Crick complementary bases (A . . . T and G . . . C). Except in some viruses where it serves as genetic material, RNA is generally single-stranded, and folding of the polynucleotide sugar–phosphate backbone allows the bases to interact and form hydrogen-bonded double-stranded helices separated by single-stranded regions. The formed elements of secondary structure (helices, loops, or bulges) interact with each other to stabilize the tertiary structure, which can be as intricate and complex as in proteins.[1,2]

For understanding the function as well as evolutionary and mutational data of biological macromolecules, it is necessary to visualize and study three-dimensional (3D) folding, i.e., the relative spatial organization of molecular components. To do so, molecular biologists need to have at their disposal computer graphics programs able to give rapid and exact schematic views of 3D structures within a reasonable time and without extensive computer know-how. Such programs, displaying 3D representations of biological macromolecules are now available, e.g., RIBBONS,[3,4] MOLSCRIPT,[5] and SETOR,[6] among others. These programs are convenient for drawing proteins and sometimes may also be applied to nucleic acids. This is usually done by renaming phosphorus atoms as C_α in the input coordinate file. However, their schematic representations of structural subunits (cylinders, β-sheets, etc.) are inadequate for drawing base pairs in the case of nucleic acids. The program RIBBONS[4] produces beautiful drawings of nucleic acids, but requires a cumbersome number of separate files preventing an automation of the drawing process.

We wish to present a new program, DRAWNA, specifically devoted to fast and automatic drawing of 3D structures of ribonucleic (RNA) or deoxyribonucleic (DNA) acid structures with the possibility of displaying at the same time biological or chemical data. Besides atomic and detailed molecular representations, schematic drawings constitute important mnemotechnic and heuristic tools. Indeed, like the sketches of humorists, schematic drawings outline the relevant and salient features compared with the contingent appearances. However, the usefulness of a schematic drawing is directly correlated with its accuracy; i.e., the detailed and schematic representations should be congruent. This twofold requirement (''objective drawings of subjective representations'') leads to potential ambiguities since the usefulness proceeds from the partiality in the choice of the emerging characteristics.[7] The choices made should therefore be explicitly stated, along with their limits and bias. In this way, iconography can reach a status other than merely that of being supplementary material.

Nowadays, RNA folding is viewed as resulting from the compaction of preformed two-dimensional (2D) components in 3D space.[8] According to this hierarchical view, helices and hairpin loops form first. Helices then interact locally end-to-end through stacking or by forming pseudoknots or triple helices. Finally, these autonomously folded subdomains associate cooperatively by loop–loop

Color Plates for this article are on page 196.

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base pairings and by numerous contacts involving loops, bulges, and helices. Our modeling approach follows this hierarchy,[9] and consists of assembling on a graphics system the overall architecture from preconstructed 3D motifs. Consequently, the drawing program should be able to represent substructures as a whole or independently in the overall architecture. This implies that a single RNA might be split into several strands, the length of which might vary during the modeling process. Also, the program should be able to represent the successive steps of a self-splicing reaction and to highlight the various components (5′-exon, 3′-exon, and intron). Further, important ribonucleoprotein particles, like the spliceosome, contain several RNA molecules, and the user might wish to treat them separately or as a complex.

Modeling of nucleic acids uses extensively data coming either from chemical attack at specific atomic locations on the bases or the sugar–phosphate backbone or from enzymatic action specific for single or double-stranded regions.[10] In complexes with other molecules (proteins, RNAs, or drugs), footprinting or cross-linking data are also of great use in modeling. It is therefore necessary to visualize the protected or attacked regions according to the level of reactivity or to the type of reactant.

PROGRAM DESCRIPTION

Overview

The advantages of using pencil (or stick) models for representing nucleic acids has been previously discussed.[11] We have chosen to represent tertiary 3D structures with the following simplifications:

(1) For each strand, the backbone is represented as a two-tone ribbon.
(2) Unpaired bases are shown as rods extended from the C4′ atoms (which are roughly between two successive phosphates) perpendicular to the ribbon. Alternatively, these rods may join atoms that link bases to sugars.
(3) Paired bases are shown as a single rod between the two corresponding C4′ atoms.
(4) Purine bases are shown longer than pyrimidine bases.

DRAWNA has been written in C ANSI on a SGI Irix workstation. It includes the GL and the Xirisw libraries for 3D drawing and the Motif library for its surrounding. This makes it especially easy to use, even for nonspecialists. More precisely, the widget surrounding makes command files useless, as the user can specify in real time the way 3D structures should be displayed.

DRAWNA presents the traditional aspect of a X11/Motif application and therefore needs only the mouse to run (see Color Plate 1). The main window is subdivided into three areas: the menu bar, the 3D display area, and a command area. The command area is divided into five parts. As redrawing time can take up to twenty seconds, according to the number of activated time-consuming options, redrawing is not done after each option activation but only when desired after clicking one of both push buttons located in the first part. The second one allows the user to take pictures, as only the 3D area is displayed. In parts 2 and 3 are grouped the toggle button widgets used for the selection of the drawing options. The three scale widgets in the fourth part are used to rotate the molecule along the screen axis (values are given in degrees). In the last part are located the x and y translation scale widgets (values in angstroms) and the zoom scale widget. For the latter, values are given on a logarithmic scale: increasing the value of 10 units will cause the structure to be drawn twice bigger. In the view part, the catalytic core of group I intron is displayed as outlined ribbons[1] against a blue background. Loading a new structure is done by selecting the appropriate item in the file menu, whereas the other menu panels allow the user to modify various parameters concerning the ribbon geometry, to modify the partition into multicolored segments, or to modify the PostScript™ rendering interface. The command area groups all toggle buttons related to the available drawing options, as well as rotation and translation scales. This widget hierarchy is resumed in Figure 1. The program allows the user to take high-quality pictures of the displayed structure, or to create a PostScript™ file to obtain a black-and-white copy.

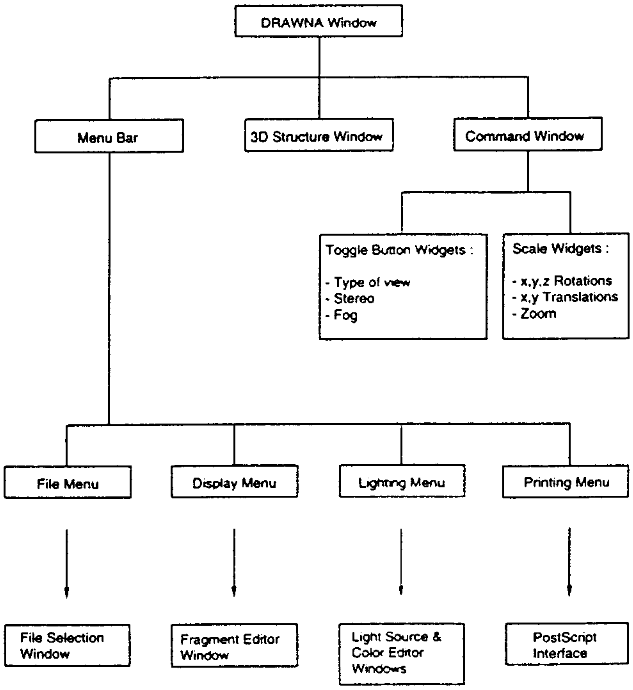


Figure 1. The main widget hierarchy in the program DRAWNA. All widgets connected by a continuous line are always activable. The four arrows indicate main transient windows that will appear after selection of the corresponding menu item.

File configuration

The number of requested or generated files for each molecule has been reduced as much as possible. For an RNA molecule, an rna.p file would be needed in order to draw the backbone. Such files contain coordinates of phosphorus atoms (P), and possibly N9 or N1 nitrogen atoms from purine or pyrimidine bases, respectively. The syntax of such files is the same as that used in the NUCLIN and NUCLSQ[12] programs, which generates refined 3D coordinates of all atoms from a studied structure. The line format is as below (with the FORTRAN notation: I for integer, A for ASCII, F for floating number):

atom number (I5), two blanks, residue name (A1), residue
number (I3), atom name (A4), atom identification (I3),
X, Y and Z coordinates (3 F10.4)

A routine exits for file conversion with other formats, like that of the Protein Data Bank. When available, a rna.hb file is automatically read after the rna.p file. This file is needed to represent paired bases, as it contains, line by line, the numbers of the paired nucleotides for the RNA molecule.

Finally, all data concerning orientation and drawing options that should be activated may be read from a rna.prm file. This file contains a variable number of lines, each beginning with a character indicating the kind of information that follows: rotation matrices, *x* and *y* translations, zoom factors, drawing option flags, color definitions, data related to each segmented strand, stereo parameters, and so on. Although these files are normally written by the program while running, they might be modified by the user with a text editor.

The program may in turn generate a rna.ps file, which is in fact the PostScript™ code needed to draw the structure on a laser printer. Ribbons will appear as two curves, following the edges of the ribbons, and linked one to the other with straight lines at the phosphate positions. Far more sophisticated black-and-white or color prints may in fact be rendered using the snapshot utility. The resulting image file is then converted into a PostScript™ file through the Silicon Graphics Showcase utility.

Available drawing options

Several general drawing modes may be activated or disabled at any time using toggle button widgets located in the general command area:

(1) Drawing backbones as flat or tubular ribbons. Flat ribbons are shown outlined in black to improve rendering of surimpressed ribbons.
(2) Drawing of base pairs or free bases as rods.
(3) Drawing of two-tone ribbons. When set, bases are colored the same way as the internal side of the ribbon they stem from. Elsewhere, bases are colored according to their type by a user-defined code.
(4) Drawing of filled or outlined surfaces. Outlined surfaces are drawn much faster than filled ones, so this option is rather useful when seeking for the correct orientation (see Color Plate 1).
(5) Stereo view. Both angle and distance between the two stereoscopic view may be modified by using the suited scale widget in a transient window (see Color Plate 2).
(6) Depth-cued view. The depth of the displayed structure may be highlighted by watching it through a fog, the density of which may be modified.

The following options may be defined for only parts of the structure:

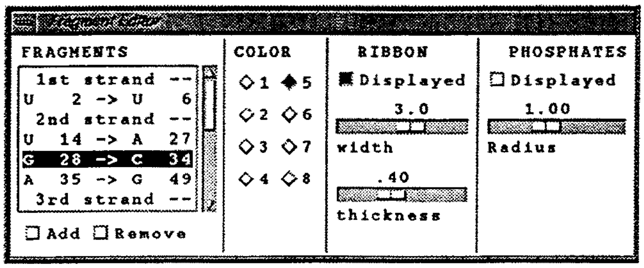
(7) Show fragments as differently shaped or colored ribbons.
(8) Show phosphorus atoms as spheres (see Color Plate 3).

DRAWING OF THE SUGAR–PHOSPHATE BACKBONE

Backbone partition

As seen above, coordinate files contain no information about the number of single strands in the structure of the corresponding nucleic acid. In fact, phosphates coordinates are listed one after the other for each strand, without specification of the strand to which they belong. However, this is easily recognized by the program by calculating the distance between two successives phosphates. As this distance is usually in the range 5–7 Å, a value greater than 8 Å will ensure that the concerned phosphates belong to different single strands. In this way, the whole primary sequence is cut into as many smaller independent sequences as there are single strands in the structure. This partition is made only once by the program after reading the coordinates file.

Furthermore, the user has the ability to divide each single strand into several segments. A new segment is defined as soon as its first phosphate is specified; it will extend until the 3′ end of the segment, or until another one is defined in the same way. The number of user-defined segments is limited only by the number of nucleotides in the displayed nucleic



```
 1st strand --
U   2 -> U   6
 2nd strand --
U  14 -> A  27
G  28 -> C  34
A  35 -> G  49
 3rd strand --
```

■ Displayed
3.0 width
.40 thickness

□ Displayed
1.00 Radius

Figure 2. The fragment editor window. In the scrolled list, widget type and identification number of first and last nucleotide of each fragment appear line by line. Adding a new fragment is done in two steps. First, one activates the adding mode by clicking the Add *button. This makes a base list widget appear. Second, one selects in this list the nucleotide that should be the first one in the new fragment. This new fragment inherits data from the previous one, that will be shortened to the selected position. Removing fragments is done in a similar way. First, one clicks the* Remove *button and then selects the useless fragment. For safety, the removing mode is then automatically disabled. The previous fragment will now extend to the end of the removed fragment. Other parts of the window indicate data related to the selected fragment. In the RIBBON part, the toggle button widget specifies if this fragment should be displayed or not. The width scale widget shows a width value (Å) for whatever ribbons are drawn flat or with a conic section. In the latter case, the thickness scale widget will indicate the ratio* thickness/width *for the selected fragment. The activated color index toggle button widget specifies, among the 8 couples of front and back color, which one is used to fill external and internal sides of the ribbon. Finally, in the PHOSPHATES part, the user has the ability to choose if spheres centered at phosphate positions must be drawn or not, with a radius determined by the scale widget value. The sphere color may be modified in the atom color selection window.*

acid. New partitions may be added, deleted or modified at any time through mouse-activated dialog boxes (Figure 2). Segment geometry, drawing options and colors may be as well edited by the user. It becomes possible in this way to focus on or highlight parts of the structure.

Drawing of ribbons

B-spline functions The Silicon Graphics GL library provides powerful ready-to-use instructions for high-quality rendering of lighted or shaded surfaces. In particular, the use of B-splines in drawing procedures allows the display of a wide variety of curves and surfaces.

A nth order B-spline curve is a parametric curve following harmoniously a set of at least n control points M_i. There is a basis function, corresponding to each control point, indicating how much the related control point attracts the curve. These functions are actually (n-1)th degree polynomial functions, and have nonzero values only near the control point they represent. This implies that control points have only a local influence upon the curve. Another consequence is that at most n basis functions have nonzero values at the same place, these values adding up to exactly 1. This is the reason why B-splines do not necessarily pass through any control point, but only through the first and the last one. The smoothness of such a curve is strongly related to its order n, assuming that an order equal to n will ensure (n-2)th derivation continuity. In practice, fourth-order B-splines are usually used to render smooth curves with second derivation continuity.

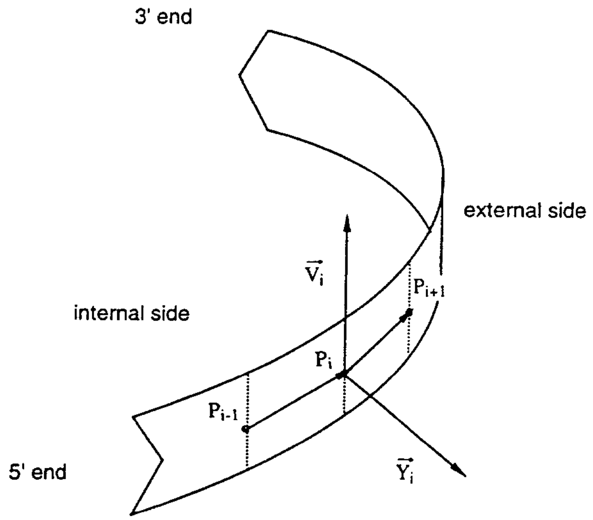


Figure 3. For each phosphate P_i, *the unit-length* V_i *vector is determined by calculating the normalized cross product of the* $P_{i-1}P_i$ *and* P_iP_{i+1} *vectors. Vectors* V_i *corresponding to first and last phosphates of a given strand are taken equal to the second and the next to last, respectively. The* M_{1i} *and* M_{2i} *points are placed below and above the* P_i *position, according to the* V_i *direction, and at a distance depending on the current fragment. The* Y_i *vector, perpendicular to the* V_i *vector, is used while setting control points on a circle or on a ellipse centered on the* P_i *position to draw ribbons with a conic section.*

Backbones as flat ribbons B-spline functions are also heavily used while drawing parametric surfaces. Each point of a 2D net of control points will be associated with two basis functions, that will represent the weight of this point in both directions. These basis functions do not have to be of equal order. This property will be useful while drawing flat ribbons. When representing an n-nucleotide long fragment, a net of $n \times 2$ control points has to be defined. This allows the drawing of a surface of order 4 along its length, while an order equal to only 2 along its width is enough to join both edges of the ribbon. The way two control points are placed around each phosphorus atom is detailed in Figure 3.

Flat two-sided ribbons are drawn using, for each fragment, the related front-face and back-face color indexes (for external and internal sides, respectively). Partitioning the backbone into several subsegments has no effect upon the ribbon smoothness, which would remain the same if each strand was made of only one segment.

Backbones with conic section DRAWNA allows also the user to draw nucleic acid backbones as tubes with either circular or elliptical sections. This is done by setting 9 control points (one every $\pi/4$ rad) along the circumference for a given phosphorus atom (the first and the ninth points being identical in order to close the surface along this direction). A B-spline order equal to 3 along the circumference is enough in this case. Moreover, the points placed at $\pi/4$, $3\pi/4$, $5\pi/4$ and $7\pi/4$ must have their weight reduced from 1 to $2^{-1/2}$.

Both wide and small axis values may be set by the user using scale widgets. The front- and back-face colors are used the same way as with flat ribbons.

Determination of control points coordinates If phosphates coordinates are directly used as control points, the resulting ribbons would not necessarily contain these points. Most of the time, the slight displacement does not distort ribbons and has no influence upon the general aspect of a schematic view. Color Plates 4 and 5 illustrate for a tRNA how the ribbon is affected when phosphates are used directly as control points or not. However, for strongly curved parts of the backbone, the displacement may be too important to be neglected any longer. The answer consists in treating mathematically phosphate coordinates P_i in order to produce a set of control points M_{0i}, that would force ribbons going through phosphate positions. These control points are determined in the following way:

$$\begin{bmatrix} P_1 \\ P_2 \\ \vdots \\ P_n \end{bmatrix} = \begin{bmatrix} M_{01} \\ M_{02} \\ \vdots \\ M_{0n} \end{bmatrix} * \mathbf{M}_n^{-1}$$

where the $\mathbf{M}_n^{-1}$ matrix has for a fourth-order B-spline the form below:

$$\mathbf{M}_n^{-1} = \frac{1}{6}\begin{bmatrix} 6 & & & & & 0 \\ 1 & 4 & 1 & & \cdot^{\cdot^{\cdot}} & \\ & 1 & 4 & 1 & & \\ & & & \ddots & & \\ & & & 1 & 4 & 1 \\ & & \cdot^{\cdot^{\cdot}} & 1 & 4 & 1 \\ 0 & & & & & 6 \end{bmatrix}$$

Inverting the $\mathbf{M}_n^{-1}$ matrices would be necessary in order to obtain exact control points coordinates. These $\mathbf{M}_n$ matrices have a rather complicated form, but may be obtained recursively. Below are represented the three first $\mathbf{M}_n$ matrices:

$$\mathbf{M}_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{M}_3 = \frac{1}{-4}\begin{bmatrix} -4 & 0 & 0 \\ 1 & -6 & 1 \\ 0 & 0 & -4 \end{bmatrix}$$

$$\mathbf{M}_4 = \frac{1}{15}\begin{bmatrix} 15 & 0 & 0 & 0 \\ -4 & 24 & -6 & 1 \\ 1 & -6 & 24 & -4 \\ 0 & 0 & 0 & 15 \end{bmatrix}$$

Each n-nucleotide long strand would involve the calculation of a square $\mathbf{M}_n$ matrix, as well as its fraction denominator N_n. However, these matrices are quickly determined by observing these rules:

$$\begin{array}{lll}
N_1 & = 0 & \\
N_2 & = 1 & \\
N_n & = -4N_{n-1} - N_{n-2} & \text{with } n \geq 3 \\
\mathbf{M}_n[1][j] & = \mathbf{M}_n[n][n+1-j] = N_{n+1-j} & \text{with } 1 \leq j \leq n \\
\mathbf{M}_n[i][1] & = \mathbf{M}_n[i][n] = 0 & \text{with } 2 \leq i \leq n-1 \\
\mathbf{M}_n[2][j] & = \mathbf{M}_n[n-1][n+1-j] = -\mathbf{M}_n[1][j] * 6 & \text{with } 2 \leq j \leq n-1 \\
\mathbf{M}_n[i][j] & = -\mathbf{M}_n[i-1][j] * N_i/N_{i-1} & \text{with } 3 \leq i \leq n-2 \text{ and } i \leq j \leq n-1 \\
\mathbf{M}_n[i][j] & = -\mathbf{M}_n[i+1][j] * N_{n+1-i}/N_{n-i} & \text{with } 3 \leq i \leq n-2 \text{ and } 2 \leq j \leq i
\end{array}$$

As one can see, the position of a control point associated to a given phosphate P_j depends on the position of all phosphates P_i, but less and less as the distance between P_i and P_j increases. In fact, the weight of P_i might be neglected as soon as $|i - j| > 5$. This implies that only 11 nonzero values per matrix line are enough. Moreover, the weight of P_i decreases by a factor N_{i+1}/N_i as P_i is one position farther from P_j. As this factor quickly converges to the value $2 + 3^{1/2}$, it makes useless the calculation of the values of N_n with $n > 10$. Except near ribbons end, control points coordinates are thus determined by this 11-long phosphate coordinates weighted average.

Backbone extremities: 3'- and 5'-end arrows As mentioned above, a B-spline curve or surface passes only through its end control points. This means that the partition of a single strand into several segments should modify ribbons geometry at junction points between these internal fragments. To avoid this, each segment is drawn 4 bases longer at both ends. Thus, the end ribbon displacement has no influence upon the ribbon position at the level of the phosphate which starts this fragment. For the first or the last segment of a given strand, the extra phosphate positions are interpolated from the two first or last phosphate coordinates. By using the trimming facilities of the GL library, only the interesting part of the ribbon will be actually drawn. Moreover, the trimming allows the user to distinguish between ribbon ends. Whatever the choice (flat or conic sections), their 3'- and 5'-ends are symbolized with salient and reentrant arrows, respectively. These arrows are also reported along the ribbons, between successive differently colored sequences.

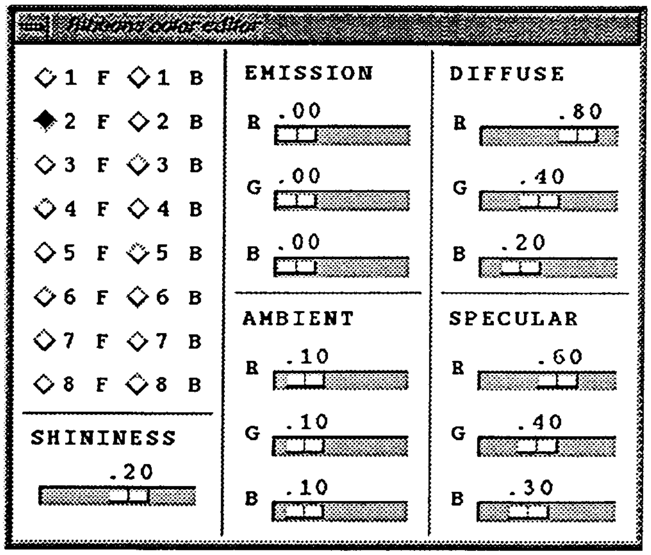
Drawing of rods

Rods are drawn almost the same way as a cylindrical tube. The only difference consists in the use of a first-degree B-spline function along the length, as only two sets of control points are needed. The first points are placed around the C4' atoms that lie between two successive phosphates, while the second points depend on the desired drawing option. If unpaired bases are shown, rods will join the N1 or N9 position; if paired bases are shown, two corresponding rods will meet exactly between the C4' atoms. In the present version, there is no provision for drawing base triplets or quadruplets. However, these can be drawn by using a mixture of rods corresponding to paired and unpaired bases. Usually, rods are colored the same way as the internal side of the ribbon they stem from. Alternatively, rods may also be colored by a user-defined code, according to the type of base they represent.

3D Viewing

DRAWNA has been written in order to exploit the hardware capabilities of SGI workstations, that perform real-time, ray-traced representations of solid 3D structures. Z-Buffer, in combination with backfacing elimination, allows hidden surfaces removal. Three-dimensional rendering may be further improved by the use of a stereographic view, with redefinable distance and angle, or in mono by activating the fog mode. In this mode, object colors are blended with the background color, according to the distance to the nearest clipping plane.

Displayed structures are usually lighted by a single infinite light source, placed behind the viewer. This is generally enough to render a realistic 3D view. If desired, more infinite or point light sources may be turned on to improve shaded surfaces representation. As written above, 16 redefinable colors are available for drawing two-tone ribbons. It has been preferred to assign to each segment a color index rather than a complete color definition, as it will be generally useful to represent different segments in the same way. Eight other colors are reserved for atoms (C, O, N and P) and base planes (A, C, G, T or U) while displaying ball-and-stick structures. Each of these 24 materials has its own red, green, and blue components for emission and diffuse, ambient or specular reflectance. These components may be



SHININESS .20

EMISSION R .00 G .00 B .00

AMBIENT R .10 G .10 B .10

DIFFUSE R .80 G .40 B .20

SPECULAR R .60 G .40 B .30

Figure 4. The ribbon color editor window. Each toggle button widget in the upper left corner of the window is associated with one of the 8 available front or back color. Selecting one of these toggle button widgets will reactualize each scale widget values. Each ribbon color is in fact the result of five sets of parameters. (1) The diffuse reflectance specifies how much red, green, and blue light is reflected in all directions. This kind of reflectance characterizes mat surfaces. (2) The specular reflectance indicates red, green, and blue components of the light reflected perpendicular to the ribbon. This reflectance renders the ribbon brightness. (3) The shininess parameter indicates how important the specular reflectance is in the final aspect. A value of 0 actually disables shiny effects. (4) The ambient reflectance: as the previous parameters are related to the light directly reflected from the light source, these parameters characterize the importance of the ambient light. They are generally useless while using a white light source. (5) The emission parameters indicate how much red, green, and blue the ribbons emit in all directions. Their use is limited, as it disables shading effects. They may be useful however, to highlight hidden parts of a structure.

modified one after the other using scale widgets in a transient dialog box (Figure 4).

HARDWARE REQUIREMENTS

DRAWNA has been developed on a Silicon Graphics Indigo Entry 4000 workstation, and should run on other IRIS-4D workstations without changes. It requires full *Z*-buffer capacities and at least a 16-Mb memory. The Indigo series workstations are in fact not powerful enough to exploit complete graphics capabilities of the program, assuming that the available 8 color bitplanes allow only dithered shading. Twenty-four color bitplanes are in fact required to obtain a smoother shading. Moreover, an 8-bit overlay buffer would be useful when managing transient windows, by limiting redrawing time. However, as can be judged from Color Plates 4 and 5, the use of entry-level graphics is quite satisfying. Color Plates 2, 3, and 6 were made on more sophisticated equipment. The software is freely available and can be obtained by sending an e-mail message to *westhof@ibmc.u-strasbg.fr* or by writing.

REFERENCES

1 Michel, F. and Westhof, E., Modeling of the three-dimensional architecture of group I catalytic introns based on comparative sequence analysis. *J. Mol. Biol.* 1990, **216,** 585–610

2 Jaeger, L., Westhof, E., and Michel, F., Monitoring of the cooperative unfolding of the *sunY* group I intron of bacteriophage T4. *J. Mol. Biol.* 1993, **234,** 331–346

3 Carson, M. and Brugg, C.E., Algorithm for ribbon models of proteins. *J. Mol. Graphics* 1986, **4,** 121–122

4 Carson, M., Ribbon models of macromolecules. *J. Mol. Graphics* 1987, **5,** 103–106

5 Kraulis, P.J., MOLSCRIPT: A program to produce both detailed and schematic plots of protein structures. *J. Appl. Cryst.* 1991, **24,** 946–950

6 Evans, S.V., SETOR: Hardware-lighted three-dimensional solid model representations of macromolecules. *J. Mol. Graphics* 1993, **11,** 134–138

7 Wood, D., The power of maps. *Scientific Amer.* 1993, **268,** 43–53

8 Westhof, E. and Michel, F., Some tertiary motifs of RNA foldings. In *Structural Tools for the Analysis of Protein-Nucleic Acid Complexes* (D.M.J. Lilley, H. Heumann, and D. Suck, Eds.) Birkhäuser Verlag, Basel, 1992, pp. 255–267

9 Westhof, E., Modeling the three-dimensional structure of ribonucleic acids. *J. Mol. Struct. (Theochem)* 1993, **286,** 203–210

10 Westhof, E., Romby, P., Ehresmann, C., and Ehresmann, B., Computer-Aided Structural Biochemistry of Ribonucleic Acids. In *Theoretical Biochemistry & Molecular Biophysics* (D.L. Beveridge and R. Lavery, Eds.) Adenine Press, New York, 1990, pp. 399–409

11 Brown, J.W., A toolkit for creating three-dimensional RNA pencil models. *CABIOS* 1993, **9,** 465–467

12 Westhof, E., Dumas, P., and Moras, D., Crystallographic Refinement of Yeast Aspartic Acid transfer RNA. *J. Mol. Biol.* 1985, **184,** 119–145

13 Felden, B., Florentz, C., Giegé, R., and Westhof, E., Solution Structure of the 3′-end of Brome Mosaic Virus Genomic RNAs. Conformational Mimicry with Canonical tRNAs. *J. Mol. Biol.* 1994, **235,** 508–531