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Further additions to *MolScript* version 1.4, including reading and contouring of electron-density maps

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MolScript is one of the most popular programs for the generation of publication-quality figures and the recent re-working of the program should ensure its continued popularity. However, some functionality of particular interest to crystallographers is not part of the standard program. A modified *MolScript* version 1.4 has been described previously, with more flexible colouring schemes among its new features. This report describes further enhancements to *MolScript* version 1.4, including facilities for drawing rods for helices and ribbons for oligonucleotides and allowing several formats of electron-density maps to be read and contoured using either lines or smoothed triangulated surfaces.

1. Introduction

MolScript (Kraulis, 1991) is one of the most widely used programs for generating figures for publication. It can be used for detailed pictures at the atomic level, such as CPK representations of atoms and ball-and-stick representations of molecules. It is also equally useful for drawing schematic representations of macromolecules (especially proteins), such as traces through the Cα-atom positions, smoothed coils through the protein backbone, helices for α structure and arrows for β structure. All these features can be freely combined owing to the flexibility of the *MolScript* syntax. Output from *MolScript* version 1.4 can be either a PostScript (Adobe Systems, Inc.) 'cartoon' or an input file for the *Raster3D* rendering program (Bacon & Anderson, 1988; Merritt & Murphy, 1994) for a more photo-realistic effect. Recently released, *MolScript* version 2.0 adds increased functionality (such as split-bond atom-coloured ball-and-stick models, cylinders to represent helices and ribbons to represent double-stranded oligonucleotides) and support for a wide variety of new output formats (such as VRML, OpenGL, SGI RGB, JPEG and PNG).

Several output features of particular interest to crystallographers were not provided by *MolScript* version 1.4, and an enhanced version of this program was developed (Esnouf, 1997) which included the ability to colour models according to properties of individual atoms (such as position in the primary sequence or atomic *B* factor). However, the most important omission from a crystallographic standpoint was the lack of support for electron-density maps. Some programs, such as *MINIMAGE* (Arnez, 1994), provide support in a separate program which describes a contour of an electron-density map as a 'pseudo-PDB' file and a series of *MolScript* statements to connect these 'atoms' with suitable lines. Although effective, these methods are relatively slow and cumbersome to use.

This report describes further major additions to the modified version (Esnouf, 1997) of *MolScript* version 1.4, including the ability to read several formats of electron-density maps directly and to contour them either with lines or with triangulated surfaces. Other enhancements include facilities for representing helices as solid rods which may be smoothly fitted to the Cα-atom positions to show bent helices, a method for representing oligonucleotide backbones by ribbons or tubes and improvements to the PostScript representation of CPK objects to account for the intersections between spheres. Additionally, a program is described for the conversion of *Raster3D* input files into *POV-Ray* input files (Persistence of Vision Ray-Tracer Development Team, http://www.povray.org/). These converted files can be edited to utilize the extra features offered by the *POV-Ray* rendering program.

This modified *MolScript* version 1.4 ('*BobScript*' version 2.4, but see http://biop.ox.ac.uk/bobscript/ for current information) can be obtained from the author by institutions already having a licence for *MolScript*. Such licences can be obtained from Per Kraulis (e-mail: pjk@avatar.se).

2. Electron-density maps

Several formats of electron-density map are readable, including *CCP*4 ASCII and binary maps, DSN6 maps, brix maps, *X-PLOR* ASCII maps, *GRID* maps and bricked maps from the

Rice University version of *FRODO* (but not binary maps created by machines which use different numeric representations). The program is able to read parts of maps surrounding arbitrary atom selections, saving internal working space and speeding up contouring. Maps are associated with an origin vector and vectors along the map axes. These vectors have to be transformed along with the atoms in order to draw correct pictures, requiring an alteration to the *MolScript* '*transform*' command. Contours can be produced with either PostScript output or *Raster3D* input files and they can be represented using either lines or triangulated surfaces.

Fig. 1(*a*) shows PostScript output of an $F_{\rm obs} - F_{\rm calc}$ omit map. The modified program facilitates the drawing of such stereo pairs, the extra commands '*leftstereo*' and '*rightstereo*' handling the required transformations while ensuring that exactly the same graphical objects are drawn in each figure. Contouring can be limited to a volume surrounding a specified set of atoms ('atom covering'), although care should be taken to avoid misleading the reader about the quality of the electron density. It is also possible to show a map section (slab) of different thickness to the slab used for other graphical objects, allowing a thin slab of map to be drawn while showing a larger section of the surrounding model to provide a clearer context.

Maps can be represented as triangulated surfaces, which are particularly striking when the surfaces are rendered semi-transparently in *Raster3D* figures. Whilst it is not common to show electron density by isopycnic surfaces, other properties which can be represented in maps (such as molecular envelopes and cavities) may be clearly represented by surfaces. For example, Fig. 1(*b*) shows an inhibitor binding to a protein in a pocket connected to the bulk solvent by a narrow channel. Three further features increase the effectiveness of this figure. Firstly, the molecular surface is relatively smooth, owing to the algorithm used to calculate it (*VOLUMES*; R. M. Esnouf, unpublished program). Grid points in the map hold the value zero if they can be at the centre of a water molecule in the bulk solvent, and the other grid points are set to contain the distance from the nearest 'zero' grid point. Contouring at a value equivalent to the radius of a water molecule gives a smooth surface. Secondly, the program calculates averaged normals for each shared triangle vertex, which *Raster3D* then uses to smooth the shading of the surface. Finally, different colours are specified for the 'lower density' and 'higher density' surfaces of the contour, allowing the eye to follow the convolutions of the complex surface more easily.

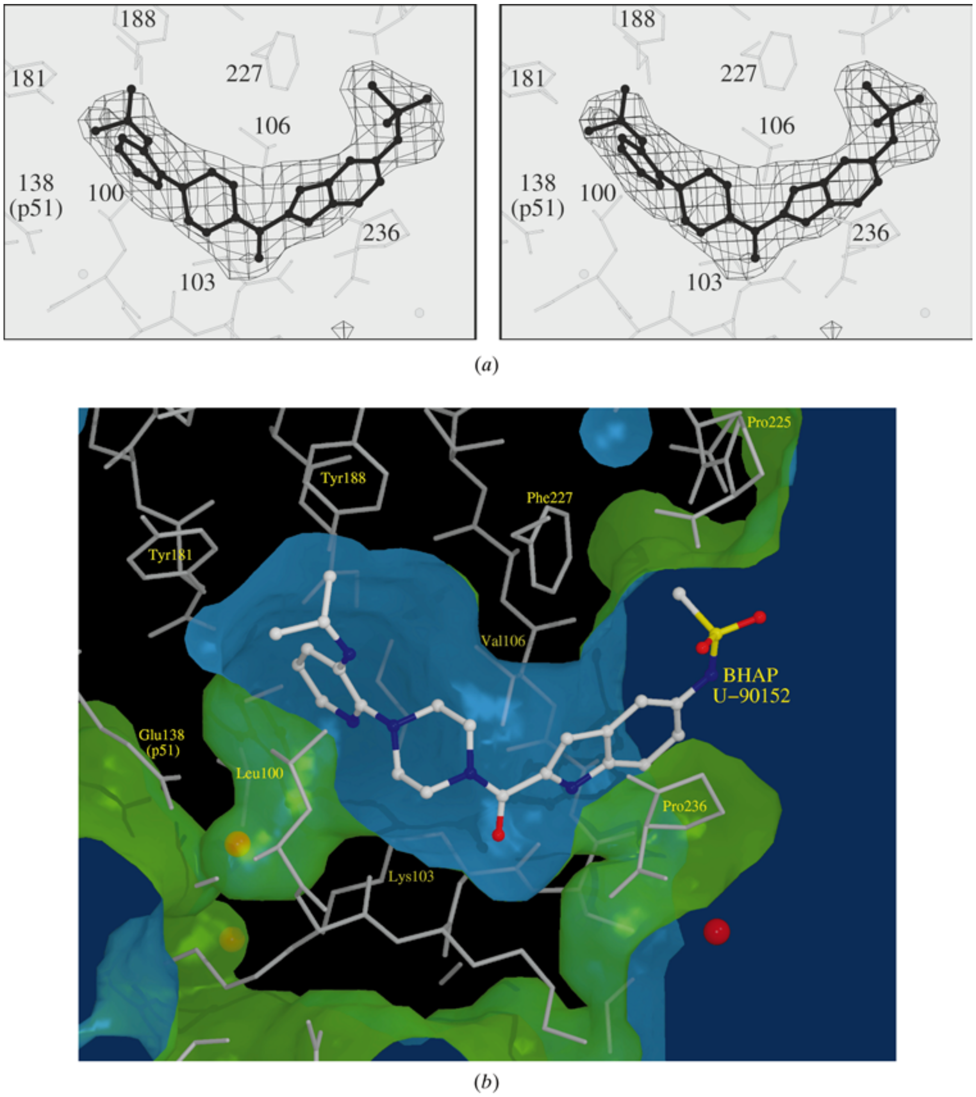

Figure 1
Examples of map contouring using this modified version of *MolScript*. (*a*) A PostScript stereo diagram showing $F_{\rm obs} - F_{\rm calc}$ omit electron density contoured at 3σ for the inhibitor delavirdine (shown by the ball-and-stick model) bound to HIV-1 reverse transcriptase (shown by thin sticks). (*b*) A figure rendered with *Raster3D* showing the non-nucleoside-inhibitor-binding pocket in HIV-1 reverse transcriptase as a semi-transparent surface with the green face pointing towards the protein and the blue face towards the solvent. The inhibitor, delavirdine, is shown as an atom-coloured ball-and-stick model, the surrounding protein structure is shown by thin grey sticks and water molecules are indicated by red spheres. Figures reprinted, with permission, from Esnouf *et al.* (1997).

3. New graphics features

Although PostScript support is currently limited, helices can be represented as solid rods for *Raster3D*. Straight helices are characterized by their axis vector, pitch, number of residues per turn and radius of the enclosing cylinder. These parameters are optimized by minimizing the residual root-mean-square error in positions between idealized helices and the Cα-atom positions using the *MATFIT* subroutine (Remington, unpublished work) based on the algorithms of McLachlan (1972) and Kabsch (1976, 1978). By fitting idealized α-helical fragments to small overlapping sections of bent helices, it is possible to represent these by smoothly bending rods, with the degree of smoothing depending on the length of the helical fragments. Coil sections leading into and out of helical rods can either be forced to hit the centres of the plane faces or be allowed to join at the edges.

Ribbons (like β-sheet arrows) or tubes (like coil segments) can be drawn to represent sugar–phosphate backbones of oligonucleotide strands (or any other repeating units) using an algorithm based on that used to draw arrows. Ribbons can have user-specified widths, thicknesses and, optionally, tapers towards their ends. Both solid rods representing helices and ribbons or tubes representing oligonucleotide strands can have colour ramps applied to them (*i.e.* coloration depending on the position in the primary sequence, on the atomic *B* factor or on the colours defined for individual atoms) in the manner described previously (Esnouf, 1997).

For PostScript output, *MolScript* represents spheres by simply shaded circles. However, for CPK representations the intersections between atom spheres affects their appearance very significantly. The previous enhancements to *MolScript* (Esnouf, 1997) allowed spheres to be represented by more realistically shaded circles, and now these further enhancements allow the intersections between spheres to be calculated so that convincing CPK representations can be drawn in PostScript. Equivalent intersection calculations can also be applied to ball-and-stick representations.

4. Creating input for *POV-Ray*

The quest for increased photo-realism has led to interest in *POV-Ray* rendering (Persistence of Vision Ray-Tracer Development Team, http://www.povray.org/). Supported features include metallic surfaces, refractive glass objects, reflections between surfaces, radiosity (inter-diffuse reflections), texture mapping, multiple coloured lights and atmospheric effects. Although modifying *MolScript* to provide full *POV-Ray* support would be a major task (*PovScript* goes some of the way, see http://www.rose.brandeis.edu/users/peisach/povscript/info.html), it is relatively simple to convert a *Raster3D* input file into a *POV-Ray* version 3.0 input file, and a conversion program is distributed with this version of *MolScript*. However, the translation does not implement any of the extra features of *POV-Ray* automatically, and manual editing of the *POV-Ray* input file is required to create special effects.

The changes to *MolScript* version 1.4 outlined here and previously have resulted in the program almost doubling in size, yet it is still merely a version of *MolScript*. Without the clear code and comments of Per Kraulis these changes would not have been feasible and I thank him for his efforts and for allowing distribution of the modified version. I also thank John Tate and Pam Williams (now at the Scripps Institute) for finally persuading me to write support for electron-density maps, Dave Stuart (Oxford University) for continuing encouragement and Rick Lewis (now at York University) for christening the modified program. RME is supported by the Foundation for Scientific Research, Vlaanderen.

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