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# PBM: a software package to create, display and manipulate interactively models of small molecules and proteins on IBM-compatible PCs

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**Abstract**

*The PBM package was developed to create, display and conveniently manipulate protein and small molecule structures on IBM-compatible microcomputers. It consists of four modules: CREATE, SPHERE, RIBBON and CONVERT. CREATE includes commands to create or alter ('mutate') the primary and subsequently the tertiary structure of a given peptide or protein by defining $\phi$ and $\psi$ angles of residues at will, options to add, delete or alter atoms in a structure, utilities to choose easily between the most common rotamers of amino acid residue sidechains and options to analyse in various ways a protein conformation. SPHERE provides for an interactive manipulation of structures containing up to 2700 atoms which can belong up to six different molecules. All manipulations can be made with the use of an ordinary mouse, by choosing from a variety of pull-down menus. Three types of models can be implemented to display molecules on the computer screen or the plotter: skeletal, solid space-filling and wireframe space-filling models. RIBBON creates ribbon models of proteins and allows for a limited variety of interactive manipulations. CONVERT is a file converter, which is capable of converting files of atom coordinates of literally any format to Brookhaven Data Bank format files. The package produces very good results for protein molecules of reasonable sizes, both in terms of graphics quality and speed of operations, on an 80486 IBM PC-compatible machine equipped with a 1 MByte VGA display card and a colour VGA monitor, which is a recommended configuration.*

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The PBM package, which consists of four modules CREATE, SPHERE, RIBBON and CONVERT, can easily be installed on any DOS-based IBM-compatible microcomputer with a VGA graphics board, at least 640 Kbytes of RAM and a hard disk. The package occupies ~1 Mbyte of disk space. Programs can take full advantage of a maths coprocessor if present. Because of the use of large data arrays in the main memory, it is recommended to have a minimum amount of memory-resident programs, which should not exceed a total of 128 Kbytes.

All programs were written using Turbo Pascal version 5.5 (Borland International, Twyford, Berkshire, UK). The mouse driver is the Genius mouse driver (Kun Ying Enterprise Co. Ltd). All necessary libraries to provide routines for operating the mouse, the plotter and pull-down menus were also written and compiled using Turbo Pascal 5.5.

CREATE uses the following algorithms:

1. The Create algorithm. This produces the structure of a user-defined amino acid sequence in an extended conformation ($\phi = \psi = 180°$).
2. The Tetra algorithm. This algorithm adds, deletes or alters atoms at will in a given structure, in any geometry specified by the user. It can easily be used to build from scratch small molecule structures of any geometry, or modify existing small or large structures.
3. The Change algorithm. This can be used to change ('mutate') types of residues in a structure.
4. The Side algorithm. This allows the user to place a sidechain in any conformation, or to put a sidechain in a preferred g+, t or g– conformation (McGregor *et al.*, 1987; Maigret *et al.*, 1978).
5. CREATE also uses algorithms for rotations, parallel projections and angle modifications employing rotation matrices according to Harrison (1982). Calculation of bond lengths, angles and torsion angles can be performed using simple routines based on analytical geometry formulae.

SPHERE uses the following algorithms:

1. A hidden line elimination algorithm to draw wireframe space-filling models.

**Table I.** Overview of the command summary of PBM

| | | |
|---|---|---|
| **CREATE** | | |
| CREATE | #Residue name | adds a specific residue in a sequence |
| | **LINE** | adds a sequence given in one-letter code |
| | Del last | deletes the last residue of the sequence |
| TETRA | Choose triplet | chooses a triplet of atoms |
| | Enter rotation variables | defines desired bond length and angles for a new atom |
| | Change new atom data | specifies type of new atom |
| | Next Triplet | uses the next triplet of atoms |
| | Add atom(s) at end of file | appends new atom(s) in the data file |
| | Insert atom(s) | inserts new atom(s) in the data file |
| | Change Side Chain | changes the sidechain of a residue |
| CHECK | Bond length | calculates a bond length |
| | Angle | calculates a bond angle |
| | Torsion angle | calculates a torsion angle |
| | Phi,Psi | calculates $\phi$,$\psi$ angles of a residue |
| | Range of Phi,Psi | calculates a range of $\phi$,$\psi$ angles |
| | Phi,psi of residue | calculates $\phi$,$\psi$ for a type of residue |
| | Print all phi,psi | prints all $\phi$,$\psi$ angles |
| | Print all torsion angles | prints all torsion angles |
| | Print analysis | prints a complete analysis |
| ROTATE | Around X,Y,Z | rotates molecule around $x$,$y$,$z$ axes |
| | Around Vector | rotates around a vector |
| | Around Bond | changes a torsion angle |
| | Bond project | projects along a bond |
| | Phi,psi rotations | changes $\phi$,$\psi$ angles |
| | Sequential phi,psi | changes a range of $\phi$,$\psi$ angles |
| | Common phi,psi | changes $\phi$,$\psi$ angles of specific residues |
| | Prolines | sets $\phi$ angle of prolines to $-60°$ |
| LOAD | | loads a PDB format file |
| SAVE | | saves molecule in PDB format |
| PRINT | | prints a PDB file |
| SIDE CHAIN | One | changes side chain for one residue |
| | X1...X4 | chooses torsion angles to change |
| | g+,g−,t | chooses preferred conformation |
| | User defined | |
| | Range | as for One but for a range of residues |
| | Sequence | as for One but for a sequence of residues |
| | All | as for One but for all residues |
| | Residue | as for One but for all residues of a certain type |
| CRYSTAL | converts fractional crystallographic coordinates to orthogonal coordinates in Å | |
| ORTEPPC | utility to prepare an ORTEP format command file from a SHELXL-93 format file | |
| **RIBBON** | | |
| File | Load | loads a Ribbon format file |
| | Make | makes a Ribbon format file from a PDB file (Warning!! use before loading Ribbon format file!) |
| | Delete | deletes any file |
| | Change Dir | changes current directory |
| | Data Dir | lists PDB data files in current directory |
| | Directory | lists all files in current directory |
| | QUIT | quits Ribbon program |
| Settings | Length | sets number of residues to be displayed |
| | Width | Changes the width of the Ribbon |
| | Threads | sets the number of threads for the ribbon |
| | Line seg | sets lines to approximate a curve section |
| | Translation | sets translation away from helix axis |
| Rotation | same as for SPHERE | |
| | Real Time | enter mode for interactive rotations |
| Utilities | Adj.screen | moves and magnifies the picture |
| | Circle Heta | turns on/off circle display of heteroatoms |

| | | |
|---|---|---|
| | Fill Heta | turns on/off filling for circle heteroatoms |
| | Linear Heta | turns on/off heteroatoms and side chains |
| | Colour | turns on/off colour display of Ribbon |
| View | | view the molecule with current settings |
| Stereo | | view in stereo mode |
| **SPHERE** | | |
| File | Load | loads a PDB file |
| | Merge | loads up to six PDB files together |
| | Delete | deletes any file |
| | Change Dir | changes current directory |
| | Data Dir | lists PDB format data files in current directory |
| | Directory | lists all files in current directory |
| | Save | saves the active molecule(s) in a PDB file |
| | QUIT | quit SPHERE program |
| Settings | *Set Active Molecule | sets the active and background molecules |
| | Delete Molecule | deletes a molecule from memory |
| | Add Molecule | loads a PDB file, without erasing old ones |
| | Set Length | sets the number of atoms to be displayed |
| | Maximum Bond | Length sets maximum distance to be taken as a bond |
| | Environment | sets maximum distance for environment calculations |
| | Wireframe Resolution | sets analysis for wireframe models |
| | Set Solid Shading | sets position of light source for shading |
| | Set types of labels | sets types of atoms that will be labelled |
| | Colour by residue | turns colouring by residue on and off |
| | *Torsion Angle Atoms | defines four atoms that form a torsion angle |
| | *Calculate Torsion | calculates a torsion angle |
| Rotation | *Around X,Y,Z | rotation around $x,y,z$ axes |
| | Ar.Atom | rotation around an atom |
| | Ar.Vector | rotation around a vector |
| | *Ar.Bond | changes torsion angle |
| | Bond proj | projects a molecule on a plane perpendicular to a bond |
| | Phi,Psi | changes $\phi,\psi$ angles for a residue |
| | Sequential | changes a range of $\phi,\psi$ angles |
| Interactive | | enter the 'Interactive Graphics' screen |
| | (Commands marked with an asterisk are also available) | |
| | Move X,Y,Z | moves active molecule(s) |
| | Zoom in/out | zooming |
| | Environment | calculates distances of neighbouring atoms |
| Utilities | Solid fill | turns solid space-filling model on/off |
| | Wireframe | turns wireframe space-filling model on/off |
| | Skeletal | turns skeletal model on/off |
| | Superimpose | superimposes skeletal model of active molecule |
| | Plot Skeletal | outputs a skeletal model to the plotter |
| | Labelling | turns labelling option on/off |
| View | | enter the 'Graphics' screen |
| Stereo | | enter the 'Graphics' screen in stereo mode |

**CONVERT**

CONVERT reads a data file of virtually any format and creates a coordinate data file with a PDB format. The user suitably predefines the format of the input data file

2. A $z$-buffer algorithm as described by Watt (1989), with some alterations in order to fit in the memory of the computer. This algorithm is used to create space-filling models of molecules. The main problem with a $z$-buffer algorithm is that it uses a lot of memory (in order to draw on a screen with $800 \times 600$ pixels resolution, a 960 Kbyte matrix is needed). The trick implemented to overcome this problem is simply to run the $z$-buffer algorithm more than once, each time for a different part of the screen, small enough to store its data in 400 Kbytes.
3. An algorithm for drawing skeletal models. This is rather simple, and not so flexible and efficient for reasons of computer speed. It interconnects atoms further apart closer than a user-defined distance.
4. A shading algorithm used for solid space-filling models.

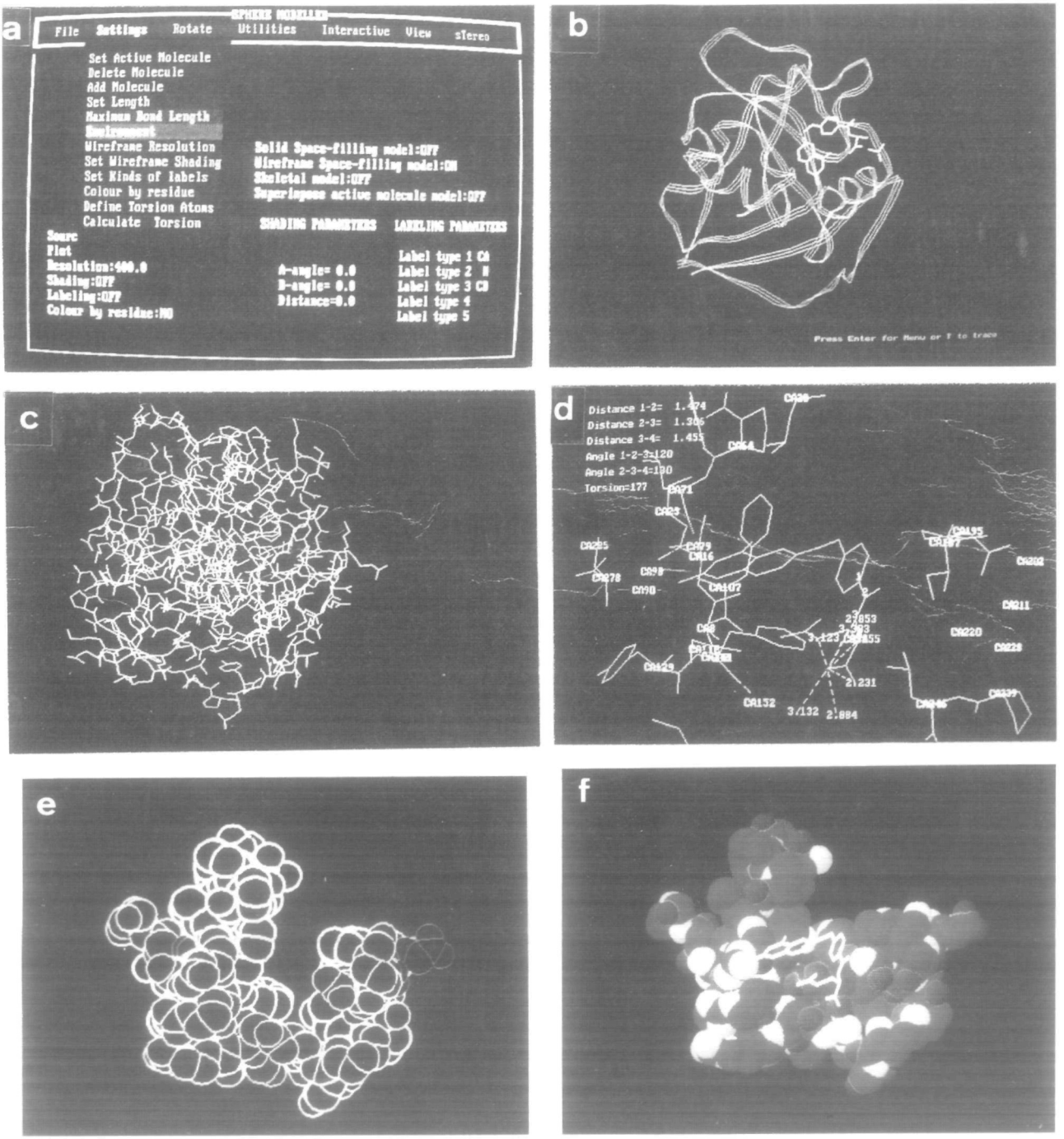


**Fig. 1.** (a) The control screen of SPHERE demonstrating the use of pull-down menus. (b) A ribbon model of human dihydrofolate reductase (DHFR) complexed with dihydrofolate, which is drawn as a skeletal model. (c) A skeletal model of human dihydrofolate reductase (DHFR) in the same orientation as in (b). (d) A close-up view of DHFR's active site Four atoms, suitably selected, are numbered in the centre of the screen as 1, 2, 3, 4 and distances and angles between them are displayed in the top left corner. The 'environment' command is used to calculate and display distances from one atom of the complexed dihydrofolate molecule to all neighbouring atoms. All $C_\alpha$s are labelled. (e) A 'wireframe space-filling' model showing atoms of residues comprising the active site of human DHFR, in the same orientation as in (d). (f) A 'space-filling model' of the active site of human DHFR in the same orientation as in (e). A skeletal model of dihydrofolate is superimposed.

This is a dithering algorithm as described by Rogers (1985) which was modified to run depending on the number of colours available from the graphics board.

RIBBON can be used for drawing ribbon models of proteins, following a simplification of the algorithm described by Carson and Bugg (1987). This was based on an algorithm for $\beta$-spline fitting (Harrison, 1982).

For a summary of the module commands is given in Table I.

The main characteristic of the package is user friendliness. For the non-graphics programs (CREATE and CONVERT) this is achieved with the use of pull-down menus for input and output. These menus can easily be operated using the mouse or the numeric keypad. For the graphics programs (SPHERE and RIBBON) there exist three modes of operation: the command mode, which is a text screen displaying values of several program variable, which can easily be altered using pull-down menus or even directly by selecting a variable with the mouse; the interactive mode, implemented to handle the molecule(s) in real time as skeletal models; and the view mode, which has been designed to view the molecule(s) as space-filling or ribbon models, to produce output to the plotter or even combine various kinds of representations in one screen (e.g. to have a skeletal and a space-filling model at the same time). For all kinds of representations, except for solid space-filling models, the program is capable of creating stereo-pairs which can be viewed with the use of special glasses (green–red) and to give a three-dimensional perspective. The program can also create stereo-plots via a plotter for publication purposes. Figure 1 is a composite figure illustrating, in black and white, some different display features of the package.

The package is available on request from Professor S.J.Hamodrakas, at a cost of approximately US$25 to academic users, to cover diskette cost, postage and handling.

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