Garlic - Version 1.3

Free Molecular Viewer and Editor

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This is the home of garlic - free, open source molecular viewer and editor. Garlic is the most portable molecular viewer in the unix world. Follow the links below to find more about garlic. Don't forget to visit the screenshot gallery !

Garlic is supported by the Ministry of Science and Technology, Republic of Croatia, as Project #0219031.

What is garlic? **Screenshot gallery** **Download garlic** **Installation guide**

Documentation **Similar programs** **License (GNU GPL)** **Author**

Release date: April 01, 2003. All versions are listed here .

Garlic home: [Croatia]

Auto-mirrors: [Australia] [Canada] [United Kingdom] [United States]

Linux distributions with precompiled garlic: [Debian] [Mandrake] [SuSE]

HPUX archives (check the program version!): [Canada] [France] [Germany] [Italy] [Japan] [Netherlands] [South Africa] [United Kingdom] [USA (Utah)]

AIX archive (check the program version!): [The Henry Samueli School, UCLA]

2003/04/01: Version 1.3 released.

Questions, Bug Reports, Comments and Suggestions

Send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) .

Garlic

The Most Portable Molecular Viewer and Editor in Unix World

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

The statement that garlic is the most portable molecular viewer/editor in unix world might look quite bold at the first sight, but it is based on serious arguments. Garlic requires only three libraries to run: the standard C library (libc), the standard math library (libm), and the standard X11 library (libX11). These libraries are available on every serious unix or unix compatible system. All other programs, (except one: mdxvu) require some additional binary libraries.

Compiling and/or installing a program which requires numerous libraries may turn into nightmare. Not only that all these libraries must be present on your system: a version number is important too! And if you manage to compile and/or install the program, it may behave strange when you try to use it: there is a chance that one or more libraries were not tested enough before shipping, causing core dumps and other runtime problems.

Check the list of freely available molecular visualization programs for unix and unix clones. This page lists also the libraries required to run each of these programs.

Free Molecular Visualization Programs for Unix and/or Linux

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free molecular visualization programs, free molecular viewers, list of molecular visualization programs, list of molecular viewers, molecular rendering, protein visualization tools, molecular visualization resources, download page, download source, download executable, download binary, AMMP, B, BRAGI, Cn3D, Deep View Swiss-PDBViever, DINO, Flex, garlic, gdpc, Ghemical, gOpenMol, Grasp, ICMlite, Jmol, Kinemage, mdxvu, Mercury, MOIL-View, MOLDEN, MOLEKEL, MOLMOL, MolScript, Moviemol, NAMOT, QMOL, PREPI, PyMOL, RasMol, Raster3D, spock, VEGA, Viewmol, WinMGM, VMD, XMakemol, XmMol, XMol, Ymol, biological macromolecule, protein structure, DNA structure, PDB, unix, linux, free software download, open source software, Damir Zucic.

This page contains the list of free molecular visualization programs, complete with links. Only freely available programs which run on unix or unix compatible platform are listed. Some of these programs are available only as binary code for some specific platform(s).

Most programs were found using AltaVista, Lycos and Google, while some others were suggested by readers of this list. Thanks to all of them!

Some of the programs listed below have a very limited license. Be sure to read the license before using such program!

The time-limited trial versions of commercial programs were omitted from the list.

The programs listed here were not evaluated and no comparison was made.

If you have your own free molecular visualization program for unix or linux, or if you know for such program which is not included in the list below, please send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) . Please send corrections and changes to the same address.

Last updated: March 20, 2003.

The information contained here was valid before that day. As developing is going on, it is likely that some additional libraries may become necessary for some of the programs listed here. However, it is almost certain that libraries listed here will be required in future versions too.

PROGRAM	LIBRARIES REQUIRED	PROGRAM TYPE / LICENSE
AMMP	libc, libm, libX11, libXt, libXext, libXmu, libXm, libSM, libICE, libNoVersion	Stand alone program, modified GNU GPL license.
B (where is it now?)	Java based package.	Your browser should support Java Virtual Machine.

BRAGI	It seems that this program is still under development.	The license has to be negotiated.
Chimera	Needs Python, Tcl/Tk, Tix, Togl, PIL, Numeric, Grail, Pmw, msms, VRML, JPEG, Info-ZIP, TR, ScientificPython; still under development.	Stand alone program, online registration required. Requires many libraries.
Cn3D	libc, libm, libX11, libXt, libXext, libXmu, libXp	Both browser plug-in and stand alone program.
Deep View Swiss-PdbViewer	libc, libm, libX11, libXt, libXext, libXmu, libXi, libXp, libMesaGL, libMesaGLU, libpthread, libz	Stand alone program, IRIX or linux required.
DINO	libc, libm, libX11, libXt, libXext, libXmu, libXi, libgdbm, libGL, libGLU	Stand alone program.
Flex	libc, libm, libX11, libxview, libolgx, xlibflexdraw	Stand alone, binaries for DEC/alpha, DEC/MIPS, IBM RS, SGI, Sun.
garlic	libc, libm, libX11	Stand alone program, GNU GPL license.
Ghemical	requires g++ compiler, f2c compiler, glut, GNOME, gtkglarea, mpich, MPQC ...	Stand alone program, GNU GPL license.
gdpc	libc, libm, libX11, libXext, libXi, libgtk, libgdk, libgmodule, libglib, libdl, libpthread	Stand alone program.
gOpenMol	libc, libm, libX11, libXt, libXext, libXmu, libXi, libdl, libXaw, Tcl/Tk, + Mesa or Open GL libraries	Graphics interface to the OpenMol set of programs; GNU GPL license.
Grasp	This program has been written for Silicon Graphics computers.	Under special circumstances, the $500 fee will be waived.
ICMlite	Binaries: SGI, DEC Alpha, SUN, Linux; libc, libm, libX11, libXt, libXext, libXmu, libSM, libICE, libpthread	Stand alone program, free for academic use.
Jmol	Java-based application.	Stand alone program (Java-based application).
Kinemage	libc, libm, libX11, libXt, libXm	Stand alone program.
mdxvu	libc, libm, libX11, precompiled for some systems	Stand alone program.

Mercury	libc, libm, libX11, libXt, libXext, libXmu, libXi, libXft, libXRender, libMesaGLU, libMesaGL, libSM, libICE, libjpeg, libpng, libmng, libdialogs, libwidgets, libqt, libqtspecific, libguiindep, libtoolkit, libcsd, libCif, libKCC-eh, libz, libfreetype, liblcms	Stand alone program, read conditions of use carefully.
MOIL-View	FORTRAN program, binaries available for Silicon Graphics workstations.	Stand alone program, registration expected.
MOLDEN	FORTRAN 77, libc, libm, libX11	Stand alone, free for academic use.
MOLEKEL	libc, libm, libX11, libXext, libXmu, libXi, libMesaGL, libMesaGLU, libtiff, libjpeg	Precompiled for SGI IRIX, linux PC and SunOS, registration required.
MOLMOL	libc, libm, libX11, libXt, libXext, libXm, libGL, libGLU, libGLcore, libC, libgen, libgen, libpng, libz	Stand alone, binaries for DEC/MIPS, DEC/alpha, SGI, SPARC and RS/6000.
MolScript	libc, libm, libX11, libXt, libXext, libXmu, libGL, libGLU, libGLcore, libmedia, libC, libgen, libvice, libjpeg, libpng, libz	Stand alone, online registration required.
Moviemol	libc, libm, libX11, libXext, libYgl or OpenGL	Stand alone program.
NAMOT	libc, libm, libX11, libxview, libolgx	Stand alone program.
QMOL	libc, libm, libX11, libXt, libXext, libXm, libGLw, libMesaGL, libMesaGLU, libstdc++, libSM, libICE	Stand alone program.
PREPI	Precompiled binary for Silicon Graphics IRIX.	Stand alone, registration required (written agreement).
PyMOL	libc, X libs, libpng, zlib, python, Mesa	Requires Python, an intepreted programming language.
RasMol	libc, libm, libX11 libXext, libXi	Stand alone program.
Raster3D	Mixed FORTRAN 77 and C code, requires both compilers.	Stand alone program.
spock	libc, libm, libX11, libXt, libXext, libXmu, libXm, libXi, libXpm, libMesaGL, libMesaGLU, libSM, libICE, libjpeg, libtiff, libcrypt, libz, libNoVersion	Stand alone program, free for some users, registration required.

VEGA	libc, libm, libz, liblocale	No OpenGL support for linux version.
Viewmol	libc, libm, libX11, libXt, libXext, libXm, libXi, libXp, libGL, libGLU, libtiff, libtiff, libpthread, libdb, libdl, libutil	Graphical front end for comp. chemistry programs, GNU GPL license.
WinMGM	libc, libm, libMesaGL, libsubplex, libchelpers, libmgmcalctools, libmolecules, libmolenergy	Stand alone, some custom libraries required.
VMD	Statically linked binaries for AIX, HPUX, IRIX, linux, Solaris and TRU64.	Stand alone, online registration required.
XMakemol	libc, libm, libX11, libXt, libXm, libXpm, libGL, libGLU	Stand alone program, GNU GPL license.
XmMol	libc, libm, libX11, libXt, libXext, libXm, libXp, libSM, libICE; Motif or openMotif required.	Free for academic use, registration required (written agreement).
XMol	Precompiled binaries for SGI, Sun-3, Sun-4 and RS/6000.	Some other binaries may be found in some other archives; development seems to be halted.
Ymol	libc, libm, libX11, libXext	Stand alone program.

Garlic Screenshot Gallery

Version 1.3

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains twelve garlic screenshots reduced to a size suitable for fast downloading. Click the selected image to load the full-sized version. All images are stored in PNG format. The true-color display is recommended for viewing this page.

What is Garlic?

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic is a free molecular viewer and editor written for unix and unix clones.

Garlic was born September 30, 1998. At that time I needed a good molecular visualization program and almost the only thing at hand was RasMol. I had some hard time with RasMol so I tryed to adapt it to my needs. However, I realized that it is very hard to read and change RasMol source code, so I decided to write my own molecular visualization program.

Further, I decided to learn programming for the X window system, and this is my first serious program written for X11.

Since 1997 I use GNU/Linux software, so I concluded that it would be fair to add something useful and modern to the existing collection of free software because this software significantly improved my working conditions.

Garlic was forgotten few times, for months, as I had some other things to do, but now it is finaly operative.

Though the version number of the current version (1.3) is not very high, the program is very stable and robust, at least on systems which were available for testing here at University of Osijek, Croatia.

The name garlic was choosen because my original intention was to write a modular program, which will be capable to call a number of modules via system calls. In fact, I did the opposite thing: garlic now consists of a single unit which integrates all functions. Anyway, back in 1998 I thought that this program will be similar to garlic - a small core with a number of units packed around this core. I also like garlic.

Later, I reallized that program name may be reinterpreted as follows:
G stands for GNU (license),
AR for analysis and rendering,
LI for linux,
C for C (the computer language).

Who might be interested to use this program?

Students
As garlic is free and open, students may find it interesting as a learning tool. Garlic may be installed on a cheap, no-name PC (running a free linux distribution) or even on a laptop (very handy!).

University assistents and professors
It is somewhat delicate to use commercial software for lectures and seminars (assignments). In their later carrier students may be boosted toward the software which they used during their study just because they have some experience with it. Universities should not influence the software market by choosing certain commercial product just because it is cheap or for some other reason suitable for university assignments.

Professionals
Many professionals would like to use some molecular visualization program at home or on a portable computer. Some others may be interested to adapt the program to their own needs. Software makers are unwilling to give the source code and to allow modification of their product. They also try to drain as much money as possible for additional (home) copies. Anyone wishing to cut the rope is invited to use and modify garlic, but the final product has to remain free and open, in agreement with the GNU General Public License .

Others
Anyone interested to learn something about proteins, DNA and some other molecules may find garlic useful.

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Version 2, June 1991

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If your browser failes to recognize what should be done with the choosen file, please try the following:

(1) Click the right mouse button while pointing at the choosen file.

(2) Select the option "Save Link As ..." (from the pop-up menu).

(3) A dialog box will be opened - change directory and file name if necessary.

HTTP DOWNLOAD

Croatia: http://garlic.mefos.hr/sources/garlic-1.3

DEBIAN PACKAGES

Program: http://packages.debian.org/stable/science/garlic.html

Documentation: http://packages.debian.org/stable/doc/garlic-doc.html

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RPM PACKAGES

The RPM package may be found at at.rpmfind.net . Use the search engine (at this site) to find the appropriate RPM package.

At least two RPM-based linux distributions contain garlic:

[Mandrake] [SuSE]

Garlic Installation

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic is the most portable molecular viewer/editor in the unix world, because the only libraries required by this program are the standard C library (libc), the standard math library (libm) and the standard X library (libX11). All other molecular visualization programs require some additional libraries.

Before starting the installation, you might be interested to check the technical requirements . Most contemporary unix and unix-like systems (like linux) meet these requirements without need to change the configuration, so you can skip this text if you are impatient.

If you have Apple McIntosh running Xtools from Tenon, please read these hints , contributed by Chris from Macinchem.

To compile and install garlic, follow these instructions:

(1)	Put garlic package (garlic-1.3.tar.gz) into some empty directory.
(2)	Uncompress and unpack the package: gzip -d garlic-1.3.tar.gz tar xf garlic-1.3.tar
(3)	Change your working directory: cd garlic-1.3
(4)	Check which C compiler is available on your system. If you don't know how to find this information, try this: man -k compiler to obtain the list of available compilers.
(5)	If gcc (GNU C) compiler is not available on your system, use your favorite editor to edit Makefile. Replace gcc in: CC = gcc line with the name of your compiler (this may be cc, for example). If gcc is available on your system, do not change the CC line.

(6)	Find a directory which contains the Xlib library. Try this: cd / find . -name libX11* Check where is the file libX11.so (sharable library - prefered) or libX11.a (static library - reserve option). If your directory is different from /usr/X11R6/lib, modify the line: LIBPATH = -L/usr/X11R6/lib in Makefile. For example, if libX11.so is stored in /usr/shlib directory on your system, the LIBPATH should be changed to: LIBPATH = -L/usr/shlib
(7)	Compile the package - just type: make and wait, it will take some time.
(8)	If everything worked fine, copy the executable to a choosen directory. /usr/local/bin may be a good choice. This job should be done by root (system administrator): cp garlic /usr/local/bin If you don't have root privileges, ask your local administrator to install garlic, or just leave it in one of your directories.
(9)	Now the .garlicrc configuration file and the file which contains the template residues should be copied to a directory where these files will be accessible to everyone. If this is not done, garlic will work anyway, using hard-coded default configuration, but you will be unable to replace residues and to create peptides. The recommended directory is /usr/local/lib/garlic but if directory /usr/local/lib does not exist on your system, /usr/lib/garlic may be may be used. This should be done by root (system administrator): mkdir /usr/local/lib/garlic cp .garlicrc /usr/local/lib/garlic cp residues.pdb /usr/local/lib/garlic
(10)	It may be good idea to copy the configuration file to your home directory or to the subdirectory garlic of your home directory. The same may be done with the file residues.pdb. If you do this, you will be able to personalize your garlic sessions, because your private files will override the system-wide defaults. Of course, you don't need root privileges to do this: cp .garlicrc $HOME cp residues.pdb $HOME or: mkdir $HOME/garlic cp .garlicrc $HOME/garlic cp residues.pdb $HOME/garlic

(11)	It is recommended to set the environment variable MOL_PATH, so garlic will search all directories listed in this variable to find the specified file. Click here for detailed instructions.
(12)	Clean up the mess (sources and .o files). Be sure to leave all .pdb files for later practice. Leave also the files with the extension .script, these are some garlic tutorial scripts.

If garlic refuses to work because it fails to get the TrueColor visual, try to execute xdpyinfo and xwininfo (click into the root window); check the list of supported visuals and the current color depth. Choose the color depth for which the TrueColor visual is available. If you have the SGI Octane workstation, please read this text , contributed by Randal R. Ketchem. If you have IBM RS6000 with AIX, read this hint, contributed by Nicolas Ferre.

The list of sites with proteins, nucleic acids and hetero compounds is here .

If you can't compile, install or run garlic, write to me (Damir Zucic), my address is zucic@garlic.mefos.hr .

Technical Requirements

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic tends to be POSIX compliant. It is also ANSI C compliant, to the maximum possible extent. Xlib functions are the only non-ANSI functions used by this program.

OPERATING SYSTEM
Unix or unix clone and the X window system. Linux and XFree86 recommended.

SUPPORTED HARDWARE PLATFORMS
Desktop PC, laptop, notebook, unix workstation equipped with a color monitor with a color depth of at least 8 bits per pixel. Garlic may also be used on Apple MacIntosh running Xtools from Tenon . Click here for instructions if you have such system. No dials are required. Some X servers do not support TrueColor visual at 8 bits per pixel: try to switch to higher color depth (12, 15, 24, ...)! If you have the SGI Octane workstation, you might be interested to read this text. If you have IBM RS6000 with AIX, read this hint.

CPU
Intel, Digital Alpha, HP, SUN MIPS, SGI and some others. This program has no special hardware requirements.

GRAPHICS INTERFACE
Garlic requires the X window system. The recommended version is X11R6, but older versions may work too.
THE X SERVER SHOULD BE CAPABLE TO SUPPORT THE TrueColor VISUAL!
Some older servers may be unable to support the TrueColor visual; if you have such X server, garlic will refuse to work. Some modern X servers do not support the TrueColor visual at 8 bits per pixel, but these are usually running on a hardware which may offer 12 or more bits per pixel.

COMPILER
GNU C compiler is recommended, but other compilers compliant with ANSI C standard should work too.

REQUIRED LIBRARIES
The only required libraries are libc (C), libm (mathematical) and libX11 (the standard X11 library).

KEYBOARD
The standard PC 101/102 keyboard should work fine. The laptop keyboard may be used too. If you have some kind of unix workstation with terminal keyboard, this may work too.

MOUSE

Any mouse should serve well.

THE LIST OF COMPATIBLE SYSTEMS

Up to now, it is confirmed that garlic may be compiled and used on these systems:
Intel and compatible processors;
Digital Alpha;
Sun Solaris;
SGI (Silicon Graphics);
HPUX (Hewlett-Packard);
MacOSX (Apple).

Please inform me (zucic@garlic.mefos.hr) if you successfully compiled and used garlic on a system which is not listed here.

Compiling Garlic on Apple McIntosh

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Here you can read how to compile garlic for Apple MacIntosh running Xtools from Tenon . I would like to thank Chris from Macinchem for this contribution. Chris is also porting other chemistry related programs to Apple MaxIntosh. Please visit his Macinchem site: http://www.macinchem.fsnet.co.uk/macosx.htm

---

If you don't have access to Chris site, here is the important part:

```
... This was my first port, it requires X-Tools from Tenon.
Minor modifications of the Makefile allow compilation ...

        CC = gcc

        CCOPT = -O -I/usr/X11R6/include

        #CCOPT = -O3

        #CCOPT = -ansi -pedantic -O -Wall -Wstrict-prototypes -g3

        HEADERS = defines.h typedefs.h

        LIBPATH = -L/usr/X11R6/lib

        LINKOPT = -lX11 -lm
```

Setting the Color Depth on SGI Octane

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Some people are using SGI Octane in 8 bits per pixel mode. The TrueColor visual is not available at this color depth on this system. If you have such system, think of using it at its full power. I have no access to SGI Octane, so I had no idea how to change the color depth. I would like to thank Mr. Randal R. Ketchem for contributing the answer to this question.

Edit /usr/lib/X11/xdm/Xservers and change the argument list passed to /usr/bin/X11/X.

e.g.
To change the default configuration from the 8-bit pseudomap visual to the 24-bit TrueColor visual, change the single line:
:0 secure /usr/bin/X11/X -bs -nobitscale -c -pseudomap 4sight -solidroot sgilightblue -cursorFG red -cursorBG white

to a single line with:
:0 secure /usr/bin/X11/X -bs -nobitscale -c -class TrueColor -depth 24 -solidroot sgilightblue -cursorFG red -cursorBG white

---

Setting the Color Depth on IBM RS6000 with AIX4.3

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

To use the X window system with 24 bits per pixel, run the following command:

xinit -- -x dbe -x abx -layer 0 -d 24 -cc TrueColor

I would like to thank Mr. Nicolas Ferre (Nancy, France) for this hint.

Environment Variable MOL_PATH

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

The environment varible MOL_PATH may be used to define the list of directories which should be searched when you are trying to load certain PDB file. It is not mandatory to define this environment variable, but it is very practical.

MOL_PATH is not the only environment variable recognized by garlic. There is also MOL_DIR, but it is capable to specify only one directory, so it is not recommended.

The exact procedure which should be used to define the environment variable MOL_PATH depends on the shell you use. The procedure is described here for some commonly used shells.

If you don't know what is you shell, execute these commands:

```
echo $shell
echo $SHELL
```

Bourne Shell

If you are using the Bourne shell (sh) or the GNU clone called Bourne-again shell (bash), use the example bellow to create your own MOL_PATH variable. Use colon (:) to separate directories. It is important to export the variable! You should define this variable through your .bash_profile or .bashrc resource file in your home directory. Don't forget to replace the user name and directories.

```
MOL_PATH="/home/zucic/pdb:/home/zucic/glob:/home/zucic/memb"
export MOL_PATH
```

C Shell

If you are using the C shell (csh) or it's clone tcsh, use the command setenv to define the environment variable MOL_PATH. Use colon (:) to separate directories. You should define this variable through your .cshrc, .tcshrc or .login resource file in your home directory. The user name and directories should be replaced, of course.

```
setenv MOL_PATH /home/zucic/pdb:/home/zucic/glob:/home/zucic/memb
```

Other Shells

For other shells, read the manual page to learn how to define the environment variable MOL_PATH. In most cases, the method is similar to one of the methods described above.

Molecular Structures

PDB files, proteins, nucleic acids, vitamins, sugars, lipids, small organic compounds, flavors, garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains the list of sites with molecular structures. This list contains only the sites which contain data in PDB format. Note that links are subject to changes. If this happens, use Google or some other search engine to find the site. Use the words (or even entire titles) from the middle column as search terms.

DATA	LINK	REFERENCE
Proteins and Nucleic Acids	The Protein Data Bank, http://www.rcsb.org/pdb/	H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov, P.E.Bourne, The Protein Data Bank, Nucleic Acids Research 28, pp. 235-242 (2000).
Hetero Compounds	Hetero-compound Information Centre - Uppsala, http://xray.bmc.uu.se/hicup/	Kleywegt, G.J. and Jones, T.A. (1998). Databases in protein crystallography. Acta Cryst D54, 1119-1131 (CCP4 Proceedings).
Many Small Molecules	Molecular Models from Chemistry at Okanagan University College, http://people.ouc.bc.ca/woodcock/molecule/molecule.html	Prepared by Dr. Dave Woodcock.
Smells Database	Smells Database, ChemConnections Project, College of Chemistry, University of California, Berkeley, http://mc2.cchem.berkeley.edu/Smells/index.html	ChemConnections Project.

Pedagogical PDB's, Vitamins	Computer Based Resources for Chemistry and Biochemistry Students, Department of Chemistry, Georgia State University, http://chemistry.gsu.edu/glactone/	Glactone Project, University System of Georgia.
Small Organic Compounds	Klotho: Biochemical Compounds Declarative Database, biocheminfo.org, http://www.biocheminfo.org/klotho Compound List: http://www.biocheminfo.org/klotho/compound_list.html	Klotho: Biochemical Compounds Declarative Database, Brian H. Dunford-Shore, Waheeda Sulaman, Brian Feng, Francis Fabrizio, Jason Holcomb, William Wise and Toni Kazic.
Vitamins	PDB Files of the Vitamins and Their Cofactor Derivatives, Glactone's CD-ROM of PDB Files, Department of Chemistry, Georgia State University, http://chemistry.gsu.edu/cwcs/MM-CD/workshop02/docs/vitamins.htm	Glactone's CD-ROM of PDB Files.
Sugars	PDB Files of Some Sugars, Glactone's CD-ROM of PDB Files, Department of Chemistry, Georgia State University, http://chemistry.gsu.edu/cwcs/MM-CD/workshop02/docs/sugars.htm	Glactone's CD-ROM of PDB Files.
Lipids	PDB Files of Some Lipids, Glactone's CD-ROM of PDB Files, Department of Chemistry, Georgia State University, http://chemistry.gsu.edu/cwcs/MM-CD/workshop02/docs/lipids.htm	Glactone's CD-ROM of PDB Files.
Flavors	PDB Files of Some Flavors, Glactone's CD-ROM of PDB Files, Department of Chemistry, Georgia State University, http://chemistry.gsu.edu/cwcs/MM-CD/workshop02/docs/flavors.htm	Glactone's CD-ROM of PDB Files.

Garlic Documentation

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic documentation is written in HTML format. The sections are listed below, with a brief description. Newbies are recommended to read at least parts of each section. The most important (and the most extensive) section is the one with garlic commands.

Garlic Features	An overview of garlic features.
Controls	Reserved keys: rotations, translations, slab and color.
Commands	Detailed descriptions of garlic commands.
Mouse Usage	Mouse tricks specific for garlic.
Reference Card	A quick reminder, both for newbies and experienced users.
Tutorial	A collection of lessons and demonstration scripts.
Options	Command line options.
Configuration File	Configuration file for garlic, called .garlicrc (for experts).
Environment Variables	Environment variables recognized by garlic.
Molecular Structures	Proteins, nucleic acids and hetero compounds.

Garlic Features

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page describes the most important features of garlic, free molecular visualization program.

Garlic is free. The source code is available to everyone.
With garlic, you will be able to replace residues, to create new structures and to adjust bond angles.
Atoms may be drawn as spheres of different sizes. Bonds may be drawn as cylindrical sticks, conical sticks or as curved surfaces.
Five types of slab are available: planar, spherical, semi-spherical, cylindrical and semi-cylindrical.
The slab position and thickness are visible in a small window.
Atomic bonds as well as atoms are treated as independent drawable objects.
The atomic and bond colors depend on position. Five mapping modes are available (as for slab).
Garlic is capable to display stereo image.
Garlic is capable to display other geometric objects, like membrane, for example.
In addition to standard chemical elements, garlic allows the usage of two imaginary elements, called "jellium" (J) and "quarkonium" (Q). These elements may be used to draw some special objects. Jellium never forms any bonds, while quarkonium binds to neighboring atoms in the list (so it forms no bond, one bond or two bonds at most). Imaginary atoms may be used to adapt garlic for medical imaging, for example.
Atomic information is available for atom covered by the mouse pointer. No click required, just move the mouse pointer over the structure!
Garlic is capable to load more than one structure.
It will be possible to color the residues according to hydrophobicity and other properties.
Garlic is capable to draw Ramachandran plot, helical wheel, Venn diagram, averaged hydrophobicity, hydrophobic moment plot and sequence comparison plot.
The command prompt is available at the bottom of the main window. It is capable to display one error message and one command string.

Garlic Controls

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

The image in the main window is controled by CONTROLS and by COMMANDS . This page contains description of garlic controls.

Garlic controls are reserved keys, which may be used to rotate and translate the structure, to rotate bonds, to shift selected atoms and to change the position of slab surfaces and to change the way color depends on distance from the observer. At present, the reserved keys are numeric keypad keys and four function keys (F1, F2, F3 and F4).

Some desktop environments are reserving function keys for some special purposes. This means that some function keys will fail to work properly with garlic. To avoid this problem, you can use mouse to click on dummy buttons in control window. Another solution will be to change your desktop environment settings.

Numeric keypad	Function keys

For each control, five steps are available: normal, large, very large, small and very small. If you press the control without holding a modifier key (shift, alt or control), the normal step will be used.

Modifier keys may be used in combination with reserved keys to select large, very large, small or very small step. Here is the table of modifier keys:

MODIFIER KEYS	STEP	EXAMPLE
none	Normal	
shift	Large	
alt_shift	Very large	
control	Small	

shift_control	Very small	

Be sure to avoid ctrl_alt combinations, because some of these combinations may have a very interesting effect (try, for example, ctrl_alt_del or ctrl_alt_F1).

The table below contains the list of controls and the corresponding default actions upon the structure which is currently handled (held, catched). These default actions will be active in default editing mode (no editing at all, just viewing the structure). If editing atoms or bonds some of the controls will have different role. The table refers to PC (101/102) keyboard. There are slight differences between PC and terminal keyboard; three terminal keys are listed in the table (KP_F2, KP_F3, KP_Separator). If you have some exotic keyboard, use the program xshowkey to check the mapping of keys and send this list to the author: zucic@garlic.mefos.hr

KEY	LOCATION	ACTION
0	Numeric keypad	Translate structure along z in negative direction.
1	Numeric keypad	Move back (distant) slab surface along z in positive direction.
2	Numeric keypad	Rotate structure clockwise around x.
3	Numeric keypad	Move back (distant) slab surface along z in negative direction.
4	Numeric keypad	Rotate structure clockwise around y.
5	Numeric keypad	Translate structure along z in positive direction.
6	Numeric keypad	Rotate structure counterclockwise around y.
7	Numeric keypad	Rotate structure counterclockwise around z.
8	Numeric keypad	Rotate structure counterclockwise around x.
9	Numeric keypad	Rotate structure clockwise around z.
delete	Numeric keypad	Move front (close) slab surface along z in positive direction.
enter	Numeric keypad	Move front (close) slab surface along z in negative direction.
/ (slash) KP_F2	Numeric keypad	Translate structure left.
* (asterisk) KP_F3	Numeric keypad	Translate structure right.
- (minus)	Numeric keypad	Translate structure up.

+ (plus) KP_Separator	Numeric keypad	Translate structure down.
F1	Function keys	Move back (distant) color surface along z in positive direction.
F2	Function keys	Move back (distant) color surface along z in negative direction.
F3	Function keys	Move front (close) color surface along z in positive direction.
F4	Function keys	Move front (close) color surface along z in negative direction.
Num Lock	Numeric keypad	Unused key.
Escape	Top left corner	Return to the main drawing mode (display structure).

Here are the illustrations:

PC keyboard	**Terminal keyboard**

Garlic Commands

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

The image in the main window is controled by CONTROLS and by COMMANDS. This page contains the list of garlic commands.

Garlic commands are strings, consisting of one or more words. A command is executed when you press the RETURN key (this key is labeled ENTER on some keyboards). Note that ENTER key on the numeric keypad (the one in the bottom right corner of your keyboard) is NOT the right key! Commands will be displayed in the area called the input window.

The input window is placed at the bottom of the main garlic window, left justified. You don't have to the click into this area to enter the command string - just type it. The input window is capable to display a single error message (top) and a single command (bottom).

You can access previously executed commands by using arrow keys on your keyboard (the UP arrow scans the history buffer backwards and DOWN arrow in the opposite direction).

This page contains the alphabetic list of garlic commands with a short description and with link to detailed description.

Commands are generally case insensitive, but file names are case sensitive because unix (linux) is case sensitive.

SHORT FORM	LONG FORM	SHORT DESCRIPTION
ADD	ADD	Expand current selection.
ANG	ANGLE	Define angle.
ATO	ATOMS	Change atom drawing style.
BAC	BACKBONE	Draw backbone.
BACKG	BACKGROUND	The same as BG.
BAL	BALLS	Set the ball radius.
BG	BACKGROUND	Change main window background color.
BLU	BLUR	Blur (soften) the image in the main window.
BON	BONDS	Change bond drawing style.

CAT	CATCH	Catch the specified structure.
CEN	CENTER	Change the internal coordinate system origin.
COL	COLOR	Set color.
COM	COMPARE	Compare two sequences.
CRE	CREATE	Create structure.
DIS	DISCARD	Discard structure.
DOC	DOCK	Prepare two structures for docking.
EDI	EDIT	Edit structure.
EXE	EXECUTE	Execute garlic script.
EXI	EXIT	Quit garlic session.
EXP	EXPAND	The same as ADD.
FAD	FADING	Change color fading style or parameter(s).
FG	FOREGROUND	Change main window foreground color.
FON	FONT	Change font.
FOREG	FOREGROUND	The same as FG.
GRO	GROUP	Group (catch simultaneously) the specified structures.
HID	HIDE	Hide selected atoms.
HYB	HYBONDS	Generate hydrogen bonds.
IGN	IGNORE	Ignore (this command does nothing).
LAB	LABELS	Show labels.
LOA	LOAD	Load the specified file.
LOG	LOG	Write commands to log file.
MEM	MEMBRANE	Membrane manipulation.
MON	MONO	Switch to mono mode.
MOV	MOVE	Define which object should be moved.
NEI	NEIGHBORHOOD	Show or hide the sequence neighborhood.
PAU	PAUSE	Pause execution (useful in scripts).
PLA	PLANE	Plane manipulation.
PLO	PLOT	Plot averaged hydrophob. and/or hydrophobic moment.
POS	POSITION	Move structure to specified position.

PRO	PROBE	Set the bond probe radius (used to draw nice bonds).
QUI	QUIT	The same as exit.
RAD	RADIUS	Define sphere radius (used for selection).
RAM	RAMACHANDRAN	Draw Ramachandran plot.
REA	READ	The same as LOAD.
REF	REFRESH	Switch graphics refreshing on or off.
REG	REGISTER	Register garlic.
REP	REPLACE	Replace selected residues.
RES	RESTRICT	Restrict current selection.
ROT	ROTATE	Rotate structure.
SAV	SAVE	Save atomic data to file.
SCA	SCALE	Select hydrophobicity scale.
SEL	SELECT	Select atoms.
SEQ	SEQUENCE	Sequence buffer manipulation.
SET	SET	Set the specified dihedral angle.
SHO	SHOW	Show selected atoms.
SLA	SLAB	Change slab style or parameter(s).
SSB	SSB	Change drawing style for disulfide bonds.
STE	STEREO	Switch to stereo mode.
STI	STICKS	Set the stick radius.
STR	STRUCTURE	Secondary structure manipulation.
TAG	TAG	Assign tag (short text) to structure.
TAK	TAKE	The same as CATCH.
TBG	TEXT_BACKGROUND	Change text background color.
TFG	TEXT_FOREGROUND	Check text foreground color.
TIT	TITLE	Add title to the main window.
TRA	TRANSLATE	Translate structure.
VEN	VENN	Draw Venn diagram.
WHE	WHEEL	Draw helical wheel.
WIN	WINDOW	Set sliding window width.

ADD, EXP, EXPAND

NAME
ADD, EXP, EXPAND - add specified atoms to current selection.

SYNOPSIS
ADD chain_identifiers/residue_serials/residue_names/atom_names
ADD residue_ranges
ADD residue_names
ADD ATO atomic_ranges
ADD ATOMS atomic_ranges
ADD keyword
ADD ELE chemical_symbol
ADD ELEMENT chemical_symbol

DESCRIPTION
Add specified atoms to current selection. Atoms are added according to the specified cryteria. The command EXPAND does exactly the same job as ADD. The essential difference between ADD and SELECT is that ADD does not overwrite the previous selection. Four types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword);
(5) selection by chemical symbol;
(6) selection by atom serial number.

DETAILED SELECTION
In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain_identifiers/residue_serials/residue_names/atom_names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

add a/*/*/*	Add all atoms from chain A to current selection.
add * exc m/*/*/ca	Add CA atoms from all chains except chain M.
add */*/*/* exc ca,c,n,o	Add all atoms except CA, C, N and O.
add a/* exc 72-112/*/ca	Add CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

add 1-100	Add residues from 1 to 100 to current selection.
add 1-100 exc 20-40	Add residues 1-100 but exclude 20-40.
add 1, 4, 8, 11-48 exc 20-32	Add residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY ATOMIC SERIAL NUMBERS

To add a single atom by the atomic serial number, combine the command ADD and the keyword ATO (ATOMS). For example, to add the atom number 102 to the current selection type:

add ato 102

The same keyword may be used to add a range of atoms or to add two or more ranges. Examples:

add ato 1-100	Add atoms which have serial numbers in the range between 1 and 100.
add 1-20 40-50	Add atoms which have serial numbers between 1 and 20 and between 40 and 50.

Do not combine the keywords EXC (EXCLUDE) and ATO (ATOMS).

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

add phe,tyr,trp	Add PHE, TYR and TRP to current selection.

SPECIAL SELECTION KEYWORDS

Some special keywords may be combined with ADD to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

add * add all	Add all atoms to current selection, i.e. select all.
add abo add above	Add atoms above the plane.
add aci add acidic	Add acidic amino acids (GLU and ASP).
add ali add aliphatic	Add aliphatic amino acids (ILE, LEU and VAL).
add alt	Add atoms at alternate positions.
add bad	Add bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
add bas add basic	Add basic amino acids (ARG, LYS and HIS).
add bel add below	Add atoms below the plane.
add cha add charged	Add charged amino acids (ARG, LYS, HIS, GLU and ASP).
add cis	Add cis residues.
add com add complement	Add atoms which were not select previously.
add het add hetero	Add hetero atoms (heme groups, water etc.).
add pho add hydrophobic	Add hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
add mai add main_chain	Add main chain atoms (CA, C, N and O).

add mod serial_number add model serial_number	Add model specified by serial_number. NMR structure is a set of models. Example: add mod 1
add neg add negative	Add negatively charged amino acids (GLU and ASP).
add pol add polar	Add polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
add pos add positive	Add positively charged amino acids (ARG, LYS and HIS).
add seq add sequence	Add sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
add sid add side_chains	Add atoms which belong to side chains (all except CA, C, N and O).
add sma add small	Add small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
add sph add sphere	Add atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
add tin add tiny	Add tiny amino acids (GLY,ALA and SER).
add tra add trans	Add trans residues.
sel tri sel triplet	If there are three (or more) positively charged residues in a fragment of up to five protein residues, add these residues to the current set of selected atoms. Detailed explanation may found in the article: D. Juretic, L. Zoranic and D. Zucic, Basic charge clusters and predictions of membrane protein topology, Journal of Chemical Information and Computer Sciences 42, No. 3, 620-632 (2002).

EXPANDING SELECTION WITH THE SPECIFIED CHEMICAL ELEMENT

To add certain chemical element to the selection, use the keyword ELEMENT (short form: ELE) and the standard chemical symbol. To expand your selection with iron atoms, for example, you should type the following command:

add ele fe

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and "quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1.

The interatomic distance is not important! Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. Note that symbols J and Q are not used in the periodic table of elements.

NOTES

(1) The command ADD resets the editing mode to default (no editing).

RELATED COMMANDS

EXPAND does exactly the same job as ADD. SELECT overwrites the previous selection. RESTRICT restrics the previous selection.

RAD, RADIUS

NAME
RAD, RADIUS - set sphere radius.

SYNOPSIS
RAD value
RADIUS value

DESCRIPTION
Set the sphere radius for selection. The value should be given in angstroms. The command SELECT SPHERE may be used to select only the atoms which fit into the sphere of a given radius around the current geometric center.

EXAMPLES

COMMAND	DESCRIPTION
rad 4.5	Set radius value to 4.5 angstroms.
sel 210-212 cen rad 10 sel sphere sel com hide	Select residues from 210 to 212, redefine the geometric center, set sphere radius to 10 angstroms and select atoms in a given sphere. Select all atoms outside the given sphere and hide them.

RELATED COMMANDS
SELECT SPHERE is used to select atoms in a sphere around the current geometric center. CENTER is used to redefine the position of the geometric center.

ANG, ANGLE

NAME
ANG, ANGLE - set angle.

SYNOPSIS
ANG value
ANGLE value

DESCRIPTION
Set the rotation angle between adjacent residues. This angle is stored as an internal variable and used to draw helical wheel or hydrophobic moment plot. The value should be specified in degrees. Default value is 100 degrees, which corresponds to alpha helix rotation angle. To prepare helical wheel or hydrophobic moment plot you have to make the assumption about the secondary structure. The assumption is made by setting the rotation angle for adjacent residues. The table below lists the common structural motifs and the corresponding angles.

STRUCTURAL MOTIF	RESIDUES PER TURN	ANGLE (DEGREES)
alpha helix	3.6	100
3-10 helix	3	120
beta strand	2.3	160

3-10 helices are usually short, but if you assume that more than three residues fold into 3-10 helix, modify the angle used to draw the helical wheel. If you use the realistic angle (120 degrees), some residues will be obscured (hidden behind the residues which are drawn later). Use 115 or 125 instead of 120 degrees, to avoid overlapping of residues.

RELATED COMMANDS
WHEEL draws the helical wheel. PLOT draws the hydrophobic moment plot.

ATO, ATOMS

NAME
ATO, ATOMS - change drawing style for atoms.

SYNOPSIS
ATO style
ATOMS style

DESCRIPTION
Change drawing style for atoms. Atom style is defined separately from bond style. For BALLS, BA2, BIG, BI2, COVALENT, CO2, SMALL, SM2, SPACEFILL and SP2 style, atomic radii are read from .garlicrc file. If this file is not available, hard-coded defaults are used. The styles listed above may be used to produce nice output but require more CPU time than other styles. The list of realistic, nice styles, sorted by size, from the smallest to the largest:
(1) SMALL and SM2;
(2) COVALENT and CO2;
(3) SPACEFILL and SP2;
(4) BIG and BI2.

Note that BALLS and BA2 style are not included in this list. All atoms drawn using this style will have the same physical size.

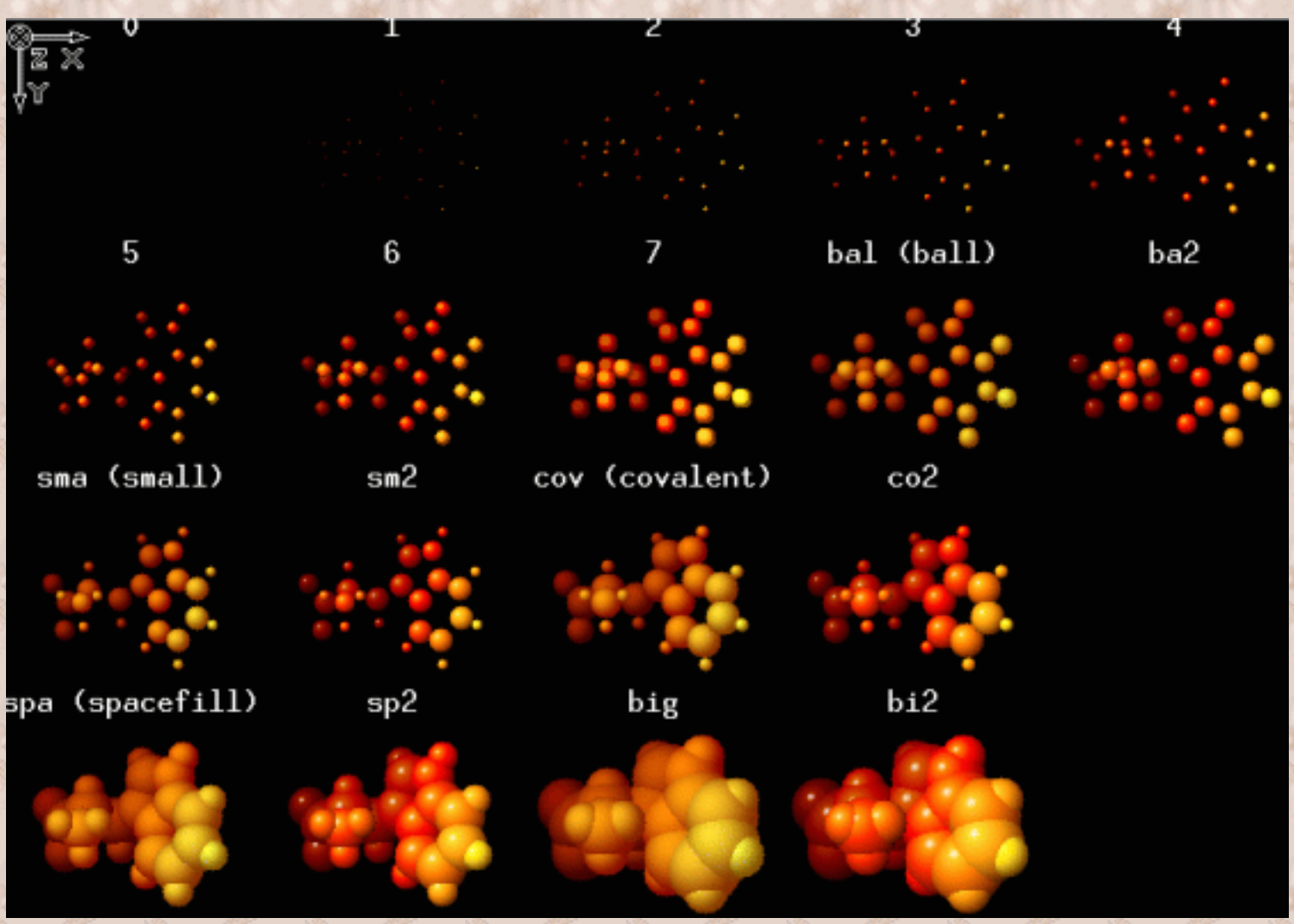
The second version of a given style has more enhanced contrast and more specular look than the first version (BA2 vs. BALL, BI2 vs. BIG etc). See the image at the bottom of this page to understand this difference.

STYLE	DESCRIPTION	SIZE
0	Unvisible atoms.	Fixed size.
1	A single pixel.	Fixed size.
2	3x3 cross (5 pixels).	Fixed size.
3	3x3 square (9 pixels).	Fixed size.
4	5x5 circle (21 pixel).	Fixed size.
5	7x7 square (37 pixels).	Fixed size.
6	9x9 circle (61 pixel).	Fixed size.
7	11x11 circle (109 pixels).	Fixed size.
bal balls	Balls (suitable to draw balls and sticks).	Proportional.
ba2	Balls with enhanced contrast.	Proportional.

sma small	Small style (default: 70% of covalent radius).	Proportional.
sm2	Small style, enhanced contrast.	Proportional.
cov covalent	Covalent style (default: covalent radius).	Proportional.
co2	Covalent style, enhanced contrast.	Proportional.
spa spacefill	Spacefill style (default: 70% of van der Waals radius).	Proportional.
sp2	Spacefill style, enhanced contrast.	Proportional.
big	Big style (default: van der Waals radius).	Proportional.
bi2	Big style, enhanced contrast.	Proportional.

EXAMPLES

The image below shows all drawing styles for atoms. To reproduce this image, execute the script atoms.script; the file trp.pdb (tryptophan) is required as input.



NOTES

(1) Unvisible atoms (style 0) are not treated as hidden - they are just invisible.

(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

(3) The ATOM keywords SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2 may be combined with the command BONDS NICE to produce very nice images. All other atomic styles (0 - 7, BALL, BA2) will not work with BONDS NICE.

RELATED COMMANDS

The command BAL (BALLS) is used to change the ball radius. BON (BONDS) is used to change drawing style for bonds. PRO (PROBE) is used to change the bond probe radius (this probe is used to draw nice bonds).

BAC, BACKBONE

NAME
BAC, BACKBONE - draw backbone.

SYNOPSIS
BAC
BAC OFF
BAC bond_style

DESCRIPTION
Draw polypeptide (protein) backbone, by connecting neighbouring CA (C alpha) atoms. All other atoms in the selected portion of the structure will be hidden. At present, five bond styles are available, all of them fixed in size.

If this command is specified without any arguments, default bond style (5) will be used.

The command BAC OFF hides the backbone and shows atoms and bonds which were visible before.

STYLE	THICKNESS	TYPE
0	Unvisible bonds	Fixed width.
1	single, thin line	Fixed width.
2	Three lines	Fixed width.
3	Five lines	Fixed width.
4	Seven lines	Fixed width.
5	Nine lines	Fixed width.

NOTES
(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.

RELATED COMMANDS
BON (BONDS) changes drawing style for bonds, but does not affect the backbone. ATO (ATOMS) command may be used to add atoms to the backbone. It is recommended to show only CA atoms, using BALL or SPACEFILL style.

BG, BACKG, BACKGROUND

NAME
BG, BACKG, BACKGROUND - change the main window background color.

SYNOPSIS
BG color
BACKG color
BACKGROUND color

DESCRIPTION
Change the main window background color. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted.

This command does not affect the main window in the sequence comparison mode. Check the command COMPARE .

EXAMPLES

COMMAND	DESCRIPTION
bg white	White
bg DarkSlateGray	Dark dark slate gray
bg #3000a0007000	Kind of green
bg rgb:0/0/8	Dark blue
bg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
FG (FOREG, FOREGROUND) changes the main window foreground (text) color.

COM, COMPARE

NAME
COM, COMPARE - compare two sequences.

SYNOPSIS
COM
COM minimal_score segment_width
COM OFF
COM COR serial1 serial2
COM ZOO zoom_factor
COMPARE
COMPARE minimal_score segment_width
COMPARE OFF
COMPARE CORNER serial1 serial2
COMPARE ZOOM zoom_factor

DESCRIPTION
Compare two sequences. Garlic mantains two sequence buffers: the main sequence buffer and the reference sequence buffer. After initializing both buffers, the command COMPARE may be used to prepare the plot with comparison of these two sequences. Matching residues will be marked by dots or squares, depending on the zoom factor. Dots or squares which represent residue pairs which match exactly will be colored yellow, while residues which are different but have similar properties will be colored red. The reference sequence will be assigned to the horizontal (x) axis, while another (investigated) sequence will be assigned to the vertical (y) axis.

The plot will contain only residues which belong to the segments for which the score of matching residues is equal to or larger than minimal score. The minimal score (the number of matching pairs) and the width of the segment used for comparison may be specified by the user. Hard-coded defaults are SEGMENT_WIDTH and MINIMAL_SCORE, defined in defines.h file. The values used in the original garlic package: SEGMENT_WIDTH=5, MINIMAL_SCORE=5.

SCORING
Two sequences are compared using fixed width segments. The matrix shown below is used to identify matching residues. It was inspired by Dayhoff PAM250 matrix. However, while PAM250 matrix contains a range of values, both positive and negative, the only values used in the substitution matrix below are zero and one. One is used to identify matching residue pairs and zero for pairs which do not match.

		A	B	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	Z	X
ALA	A	1	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0
ASX	B	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	0	0	0	0	0	0	1	0
CYS	C	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	D	0	1	0	1	1	0	1	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
GLU	E	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
PHE	F	0	0	0	0	0	1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0	0
GLY	G	1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
HIS	H	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	1	0	0	0	0	0	1	0
ILE	I	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
LYS	K	0	1	0	0	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	0
LEU	L	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
MET	M	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
ASN	N	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	0	1	0	0	0	0	1	0
PRO	P	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0
GLN	Q	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	1	0	0	0	0	0	1	0
ARG	R	0	0	0	0	0	0	0	1	0	1	0	0	0	0	1	1	0	0	0	1	0	0	0
SER	S	1	0	0	0	0	0	1	0	0	0	0	0	1	1	0	0	1	1	0	0	0	0	0
THR	T	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
VAL	V	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
TRP	W	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0
TYR	Y	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
GLX	Z	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
UNK	X	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

The scoring scheme used in garlic is much simpler than the elaborate schemes used in advanced programs for sequence alignments. However, this scheme is still quite useful and I believe that many users will like to play with the various segment widths and scores.

KEYWORDS AND PARAMETERS

All keywords and associated parameters are explained in the table below. Note that the minimal score may not exceed the segment width.

KEYWORD AND/OR PARAMETERS	DESCRIPTION
None	Draw sequence comparison, using default segment width and default minimal score.

OFF	Return to the main drawing mode. The same may be achieved by hiting the ESCAPE key.
minimal_score segment_width	Draw sequence comparison, using the specified segment width and the specified minimal score. Both parameters should be positive.
CORNER ref_offset main_offset	Draw sequence comparison, but skip some leading residues. Skip (ref_offset - 1) residues of the reference sequence and (main_offset - 1) residues of the main sequence.

MOUSE USAGE

The pointing device (mouse) may be used to find the residue serial numbers and names for matching pairs and residues which follow after them. After a chosen pair is reached with the pointer, the information about this pair and residues which follow them will be available in the output window (the bottom right corner). Color codes: yellow is used for residues which are equal, magenta for acceptable substitutions and red for mismatching residues.

HORIZ.	VERT.
23GLY	GLY27
24SER	SER28
25CYS	CYS29
26TRP	TRP30
27ALA	ALA31
28PHE	PHE32
29SER	GLY33
30ALA	ALA34
31VAL	VAL35
32VAL	GLU36
33THR	ALA37

EXAMPLES

COMMAND	DESCRIPTION

load 9PAP.pdb sel het sel com seq from 1 seq copy load 1HUC.pdb sel a,b/*/*/* seq from 2 compare 8 10	Load the structure of papain, select all hetero atoms and then select the complement of this selection. The purpose of this trick is to exclude all hetero atoms from selection. Extract the sequence and copy it to the reference buffer. After that, load the structure of human cathepsin B, select chains A and B (one molecules consists of two chains), extract the sequence and compare it with the content of the reference buffer. The minimal score is 8 and the segment width is 10.
load 9PAP.pdb sel het sel com seq from 1 seq copy seq load sample.fasta compare 6 7	Load the structure of papain and copy the sequence to the reference buffer using the same method as in the previous example. Read the second sequence from the specified FASTA file (one letter codes). Compare two sequences, using the specified minimal score and segment width (5/7). This is the typical usage of sequence comparison: compare a fresh sequence with the sequence of a solved structure.
com zoom 4	Change zoom factor to 4.
com cor 100 100	Skip the first hundred residues of both sequences.

NOTES

(1) You don't need protein 3D structures to compare two sequences. The minimal information required for protein comparison is the primary structure, i.e. the protein sequence.

RELATED COMMANDS

The command SEQ (SEQUENCE) is used to manipulate the content of the main sequence buffer and of the reference sequence buffer. LOAD is used to load the PDB file. SELECT, ADD and RESTRICT are used for selection.

BAL, BALLS

NAME
BAL, BALLS - set the ball radius.

SYNOPSIS
BAL value
BALLS value

DESCRIPTION
Set the ball radius (in angstroms). The ball radius is used to draw the selected atoms as balls. To draw atom as balls, execute the command ATOMS BA2 (specular balls) or ATOMS BALLS (balls with lower contrast). Short forms: ATO BA2, ATO BAL. Default ball radius is 0.40 angstroms, but this may be changed in the configuration file .garlicrc .

The ball radius may be set individually for each atom. Just select a single atom or more atoms and execute the command BAL with a single parameter (a new ball radius). The command BALLS affects the selected atom of the structure which is currently "caught" (see the command CATCH) .

RELATED COMMANDS
BONDS is used to define drawing style for bonds. SSB is used to define drawing style for disulfide bonds. ATOMS is used to define drawing style for atoms. STICKS is used to define the sticks radius (many people like to draw structures as balls and sticks).

Garlic Configuration File - Version 1.3

.garlicrc

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains the sample configuration file for garlic. When started, garlic will try to find the configuration file called .garlicrc (or garlicrc, in one case!) in up to six directories, in the following order:

(1) in the current working directory (file .garlicrc);
(2) in user's home directory ($HOME/.garlicrc);
(3) in garlic subdirectory of user's home directory ($HOME/garlic/.garlicrc);
(4) in /etc directory (Debian GNU/Linux style, /etc/garlicrc, without dot!);
(5) in /usr/local/lib/garlic directory (file /usr/local/lib/garlic/.garlicrc);
(6) in /usr/lib/garlic directory (file /usr/lib/garlic/.garlicrc).

The recommended pathnames:

/usr/local/lib/garlic/.garlicrc (system-wide configuration file),
$HOME/.garlicrc (private configuration file).

If all attempts fail, the hard-coded defaults will be used. The configuration file .garlicrc should be included in the original garlic package. Most parameters are explained below (read the comments). Anyway, if you have some questions, send an e-mail to me:
zucic@garlic.mefos.hr

```
# Personal initialization file for garlic, free molecular viewer and editor.
# Version 1.3.
# Last modification: January 15, 2003.


# Geometry of the main window. Use the keyword default, or specify the
# geometry string (for example 780x560+10+10).

main window geometry: default


# Margins; used only if geometry string is not given. Geometry string may be
# given through command line arguments.

main window left margin: 50 pixels
main window right margin: 50 pixels
main window top margin: 50 pixels
main window bottom margin: 70 pixels
```

```
# Main font:

main font: 10x20


# Main window cursor. If you don't like default cursor, replace it; read
# the file /usr/include/X11/cursorfont.h ; remove the XC_ prefix to obtain
# the cursor name.

main window cursor: default


# A small coordinate system may be displayed in the top left corner (yes/no):

show coordinate system: yes


# Control window (top right corner) may be visible or hidden (yes/no):

show control window: yes


# Sequence neighborhood of the residue under
# the pointer may be visible or hidden (yes/no):

show sequence neighborhood: yes


# Stereo flag (yes/no):

display stereo image: no


# Parameters for stereo image:

stereo internal margin (screen units): 10 pixels
stereo angle: 5.0 degrees


# Light source theta and phi angle (theta is defined with respect to z axis,
# phi with respect to x axis:

light source theta angle: 150 degrees
light source phi angle:   225 degrees


# Default slab mode (possible modes are off, planar, sphere, half-sphere,
# cylinder and half-cylinder):

default slab mode: planar
```

```
# Default color fading mode (off, planar, sphere, half-sphere, cylinder and
# half-cylinder):

default color fading mode: planar


# Default drawing style for atoms (0, 1, 2, 3, 4, 5, 6 or 7):

default atom drawing style: 2


# Default drawing style for bonds (0, 1, 2, 3, 4 or 5):

default bond drawing style: 3


# Default drawing style for backbone:

default backbone drawing style: 5


# Window colors:

main window background color: black
main window foreground color: white
text background color: black
text foreground color: white


# The number of color fading surfaces:

number of color fading surfaces: 3


# Default colors for atoms and bonds. For each fading surface, three colors
# should be specified. The surface index is a small integer following the
# word color. The largest surface index is equal to:
# (number of color fading surfaces) - 1,
# which is in this case 2. Color may be changed at runtime, of course.
# This choice of colors is equivalent to the scheme called hot.

left   color 0: RGB:FFFF/FFFF/4444
middle color 0: RGB:FFFF/DDDD/0000
right  color 0: RGB:8888/5555/0000

left   color 1: RGB:FFFF/8888/0000
middle color 1: RGB:FFFF/0000/0000
right  color 1: RGB:8888/0000/0000

left   color 2: RGB:8888/0000/0000
```

```
middle color 2: RGB:4444/0000/0000
right  color 2: RGB:2222/0000/0000


# Default color schemes for molecular surfaces. Choose from this list:
# red, green, blue, cyan, magenta, yellow, white, orange,
# cyan-blue, cyan-green, yellow-green, magenta-blue, magenta-red,
# orange-yellow, orange-red. Do not use the following color schemes:
# hot, cold, monochrome, cpk, zebra, chain, hyphob and model.

surface outer color scheme: magenta
surface inner color scheme: blue


# Rotation steps. Normal steps is used if numeric key is pressed without
# any modifier. Large step is selected by holding [shift] while pressing
# the key, and very large step is selected by using both [alt] and [shift].
# Small step is selected by holding [control] while pressing the key, and
# very small step by using both [alt] and [control].

rotations steps: 0.2 1.0 5.0 30.0 90.0


# Five translation steps (very small, small, normal, large and very large).
# Use angstrom units.

translation steps: 0.2 1.0 5.0 25.0 100.0


# Five slab steps (very small, small, normal, large and very large).
# Use angstrom units.

slab steps: 0.2 1.0 5.0 20.0 80.0


# Five fading steps (very small, small, normal, large and very large).
# Use angstrom units.

fading steps: 0.2 1.0 5.0 20.0 80.0


# Window size limits: used only if screen width and/or height are larger
# than values specified here. By default, screen width and height are used.

maximal main window width: 3000 pixels
maximal main window height: 2500 pixels


# The nearest line (bond) thickness; used only if drawing bonds as lines
# and line thickness is used for perspective.
```

```
the nearest line thickness: 5 pixels


# Screen dimensions and position of garlic user in real world. Use realistic
# values. Do not change units (mm). Strange values may cause image distortions.

screen width in real world: 270 millimeters
screen height in real world: 195 millimeters
distance between user and screen in real world: 500 millimeters


# Scaling information: used to scale user and screen down to atomic scale.
# Only screen width is required, in angstrom units.

screen width in atomic world: 1.0 angstroms


# User z coordinate in atomic coordinate system. It must be negative
# and absolute value should be quite large. The x axis points to the right,
# y axis downward and z axis in direction opposite to observers direction.

user position in atomic coordinate system: -150.0 angstroms


# Maximal bond length is used to check which atoms and bonds are invisible.
# It is assumed that there are no atoms with radius larger than this length.

maximal bond length: 2.3 angstroms


# Crude limits for bond lengths. No distinction between N-CA and C-N is made.
# Use angstrom units. Be tolerant, there are many bad structures around.
# Generic bond length is used for atomic pairs which are not recognized.

approximate C-C bond length: from 1.3 to 1.8 angstroms
approximate C-N bond length: from 1.0 to 1.7 angstroms
approximate C-O bond length: from 1.0 to 1.5 angstroms
approximate C-S bond length: from 1.4 to 2.1 angstroms
approximate C-H bond length: from 0.8 to 1.2 angstroms
approximate N-O bond length: from 1.2 to 1.7 angstroms
approximate N-H bond length: from 0.9 to 1.3 angstroms
approximate O-H bond length: from 0.7 to 1.3 angstroms
approximate S-H bond length: from 0.9 to 1.6 angstroms
approximate O-P bond length: from 1.2 to 1.8 angstroms
approximate S-S bond length: from 1.8 to 2.3 angstroms
generic bond length:         from 0.8 to 2.0 angstroms
hydrogen bond length:        from 2.0 to 5.0 angstroms


# Hydrogen bond C-O...N angle range (obsolete since version 1.3!):
```

```
hydrogen bond C-O...N angle: from 125 to 180 degrees


# The upper limit for CA-CA distance for neighbouring residues. Used to
# draw backbone, connection neighbouring CA atoms.

maximal CA-CA distance: 4.1 angstroms


# Atomic radii, used for spacefill style. 70% of van der Waals radius may be
# a good choice.

hydrogen radius:   0.70 angstroms
carbon radius:     1.20 angstroms
nitrogen radius:   1.05 angstroms
oxygen radius:     1.00 angstroms
sulfur radius:     1.25 angstroms
phosphorus radius: 1.25 angstroms
generic radius:    1.40 angstroms


# Covalent atomic radii, used for covalent style.

hydrogen covalent radius:   0.30 angstroms
carbon covalent radius:     0.77 angstroms
nitrogen covalent radius:   0.70 angstroms
oxygen covalent radius:     0.66 angstroms
sulfur covalent radius:     1.04 angstroms
phosphorus covalent radius: 1.10 angstroms
generic covalent radius:    1.20 angstroms


# Small atomic radii. 70% of covalent radius may be a good choice.

hydrogen small radius:   0.21 angstroms
carbon small radius:     0.54 angstroms
nitrogen small radius:   0.49 angstroms
oxygen small radius:     0.46 angstroms
sulfur small radius:     0.73 angstroms
phosphorus small radius: 0.77 angstroms
generic small radius:    0.84 angstroms


# Van der Waals radii.

hydrogen van der Waals radius:   1.00 angstroms
carbon van der Waals radius:     1.70 angstroms
nitrogen van der Waals radius:   1.50 angstroms
oxygen van der Waals radius:     1.40 angstroms
sulfur van der Waals radius:     1.80 angstroms
phosphorus van der Waals radius: 1.80 angstroms
```

```
generic van der Waals radius:    2.00 angstroms


# Default ball radius (used to draw atoms as balls of equal size):

default ball radius: 0.40 angstroms


# Default bond probe radius, used to draw nice bonds with curved surfaces:

default bond probe radius: 0.80 angstroms


# Default stick radius, used to draw bonds as sticks:

default stick radius: 0.15 angstroms


# For a given atom, the chemical bonds are identified by inspecting
# distances to the neighboring atoms. The array with atomic data should
# be scanned in forward and backward direction (with respect to the given atom)
# to find which atoms are bound to the given atom. The following parameters
# define how many neighboring atoms should be checked in each direction.

number of bond candidates: 50 before and 50 after the given atom


# Blur rectangle width and height (default values). Bluring is used to reduce
# the contrast. The color of the pixel in the center of the rectangle is
# calculated by averaging the colors of all pixels in the rectangle. Both
# values should be positive integers.

blur rectangle width:  3
blur rectangle height: 3
```

CAT, CATCH

NAME
CAT, CATCH - catch the specified macromolecular complex.

SYNOPSIS
CAT identifier
CATCH identifier

DESCRIPTION
Catch the specified structure (macromolecular complex). The structure is a set of atoms read from a single file. Thus, every file is treated as a separate structure. The structure identifier is positive integer. The value zero is not used; structures are numbered 1, 2, 3, etc. When you catch a single structure, all transformations (rotations, translations etc.) are applied to this structure, leaving other structures intact. Selection (commands SELECT, ADD, RESTRICT) are also applied only to this structure. The command CATCH is used when working with more than one structure - for example, when docking an inhibitor to a substrate. When only one structure (file) is loaded, this command has no purpose. Examples:

COMMAND	DESCRIPTION
cat 1	Catch the structure number 1.
cat 7	Catch the structure number 7.

NOTES
(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure you want to catch. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
PHE 192
CE2  1433  C
t.f.: 64.06
trans
phi:-120.71
psi:  72.93
phob:  1.19
selected
x:    -3.276
y:   -18.665
z:   -13.754
```

(2) The command CATCH resets the editing mode to default (no editing).

RELATED COMMANDS

TAK (TAKE) does exactly the same job as CATCH. DIS (DISCARD) is used to discard the macromolecular complex (structure). GRO (GROUP) is used to catch more than one structure simultaneously.

BLU, BLUR

NAME
BLU, BLUR - blur (soften) the image in the main window.

SYNOPSIS
BLU width height
BLU OFF
BLUR width height
BLUR OFF

DESCRIPTION
The command BLUR (short form: BLU) will blur (soften) the image in the main window. The color of each pixel in the main window will be replaced with the averaged color of

width x height

pixels surrounding this pixel. The original color of this pixel will be used too, weighted equally as all other pixels. The contrast will be reduced. Larger blur rectangle will result in softer image. The textual content of the main window (titles, labels) will remain unchanged. Default blur rectangle width and height: 3x3 pixels (see the configuration file, .garlicrc).

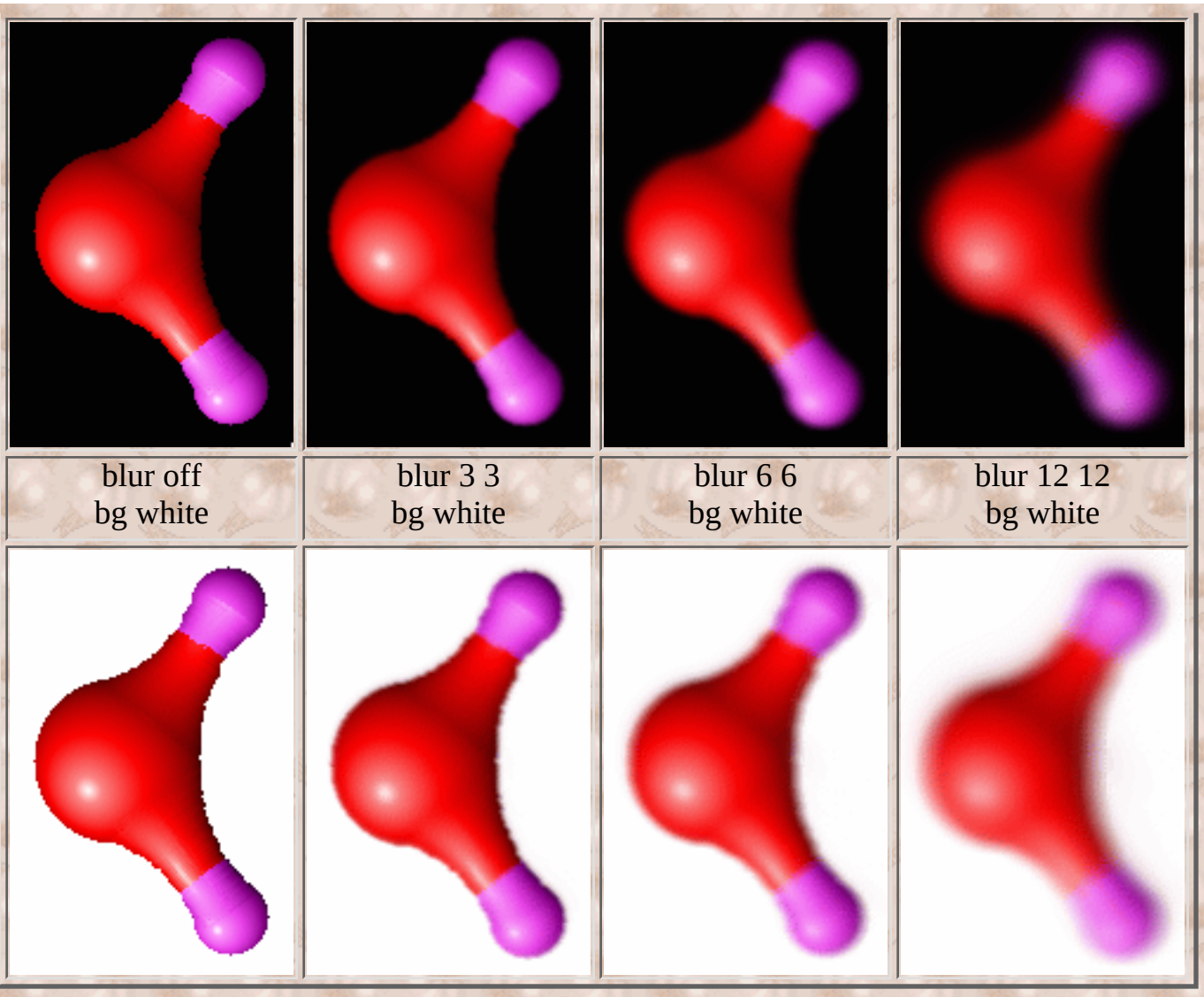
Use the command BLUR OFF (short form: BLU OFF) to switch blur off.

EXAMPLES

COMMAND	DESCRIPTION
blur	Soften the image in the main window, using default blur rectangle.
blur 4 4	Soften the image in the main window, using 16 pixels to calculate color of the central pixel.
blur off	Switch blur off.

The following eight images show the water molecule on two different backgrounds, white and black. No blur was applied on two images in the leftmost column.

blur off bg black	blur 3 3 bg black	blur 6 6 bg black	blur 12 12 bg black



RELATED COMMANDS

BG changes the background color.

BON, BONDS

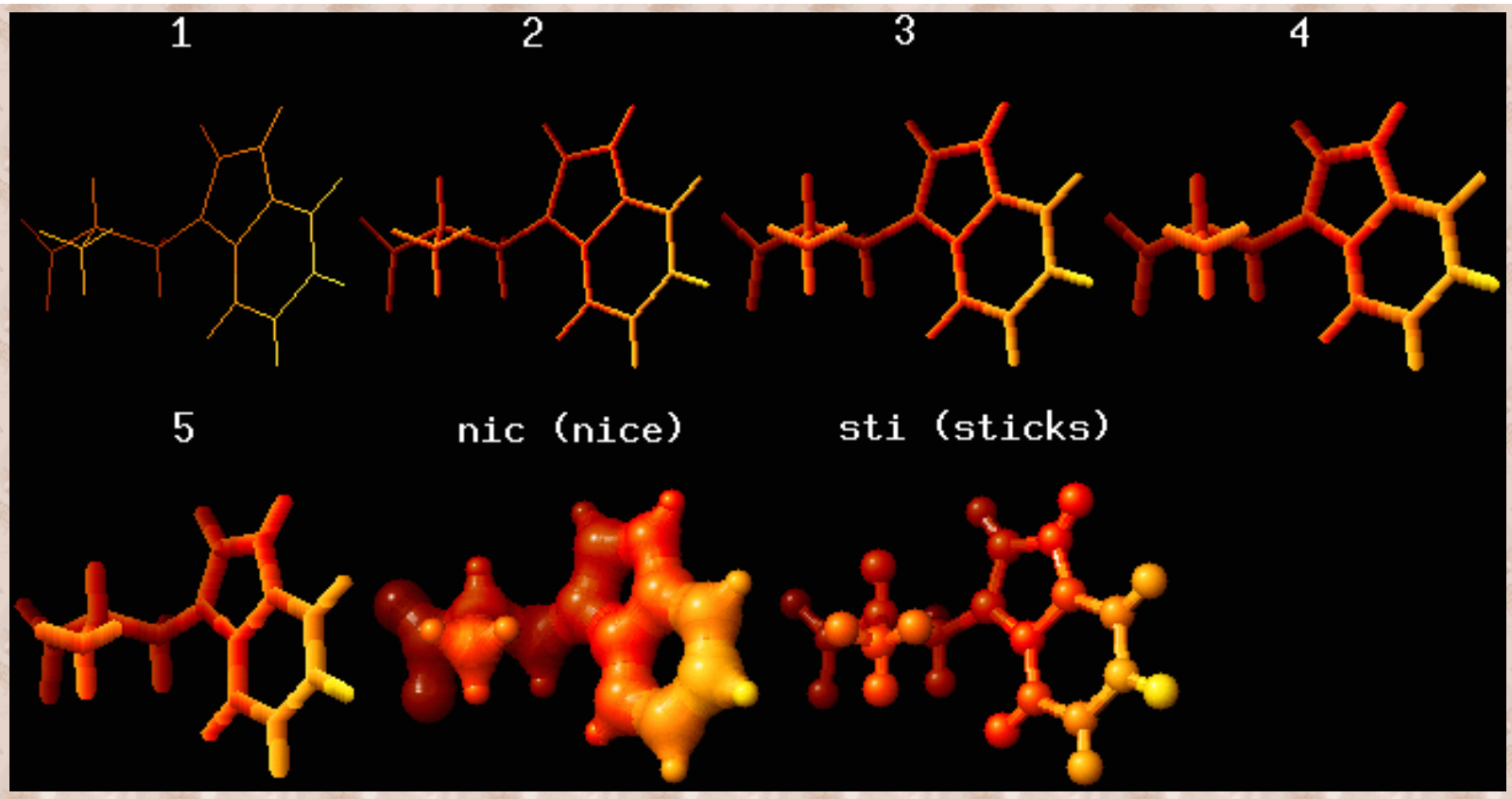
NAME
BON, BONDS - change drawing style for bonds.

SYNOPSIS
BON style
BONDS style

DESCRIPTION
Change drawing style for bonds. Bond style is defined separately from atom style. This command does not affect disulfide bonds: the command SSB should be used for that purpose. Note that there is no separate keyword for curved bonds and sticks (nice style): the bond curvature is defined by the command PROBE .

STYLE	THICKNESS	TYPE
0	Unvisible bonds.	Fixed width.
1	A single line.	Fixed width.
2	Three lines.	Fixed width.
3	Five lines.	Fixed width.
4	Seven lines.	Fixed width.
5	Nine lines.	Fixed width.
nic nice	Curved bonds, conical sticks or cylindrical sticks, depending both on the bond probe radius and the atomic radii. This bond style is available for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2. Do not combine the nice bond style with atomic styles 0, 1, 2, 3, 4, 5, 6, 7, BALL and BA2.	Proportional.
sti sticks	Cylindrical sticks. The command BONDS STICKS (short form: BON STI) is the most convenient way to draw bonds as sticks. Default stick radius may be changed by using the command STICKS (short form: STI).	Proportional.

The image below shows all drawing styles for bonds. To reproduce this image, execute the script bonds.script; the file trp.pdb (tryptophan) is required as input.

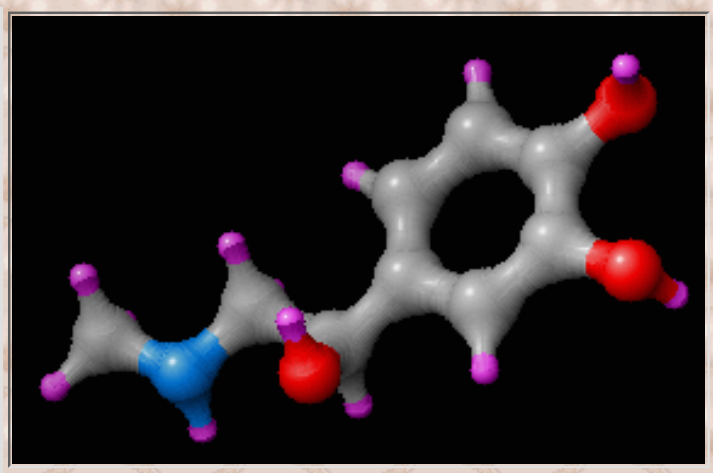


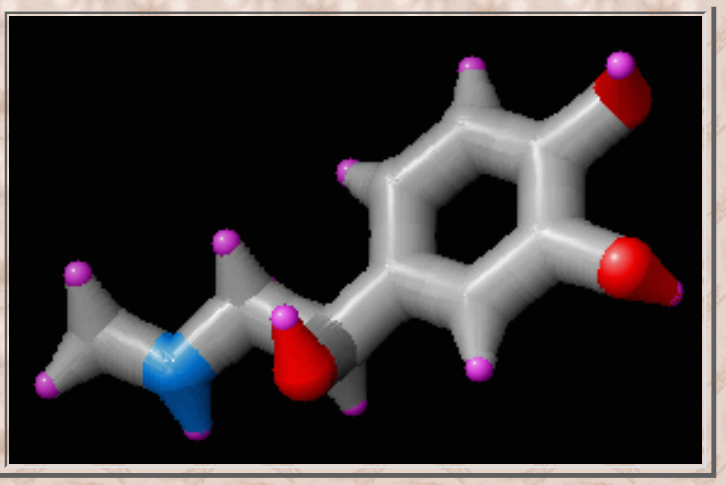
NICE BONDS

Nice bonds may be curved or straight, cylindrical or conical, depending on the bond probe radius. If this radius is small (like 0.8 angstroms), the bonds will be curved. Probe radius of 10 angstroms will give the straight bonds. If you want to draw the chemical bonds as cylindrical sticks, use the same atomic radius for all atoms and a relatively large probe. It is, however, more convenient to use the command BONDS STICKS (short form: BON STI) to draw cylindrical sticks. The command BONDS STICKS may be combined with the command STICKS, which is used to adjust the stick radius. If your atoms are drawn using different radii (and this is true for most atomic styles), the bonds will appear conical. This is one of the things which make garlic different from most other programs: in garlic, conical sticks are just the special case of nice bonds. Most other programs are capable to draw just simple cylindrical sticks.

The images below shows the same structure (adrenalin) drawn using two different bond probes: 0.8 angstroms (curved bonds, the left image) and 10 angstroms (conical sticks, the right image). In both cases all atoms were drawn using the small atomic style with enhanced contrast (ATOMS SM2).

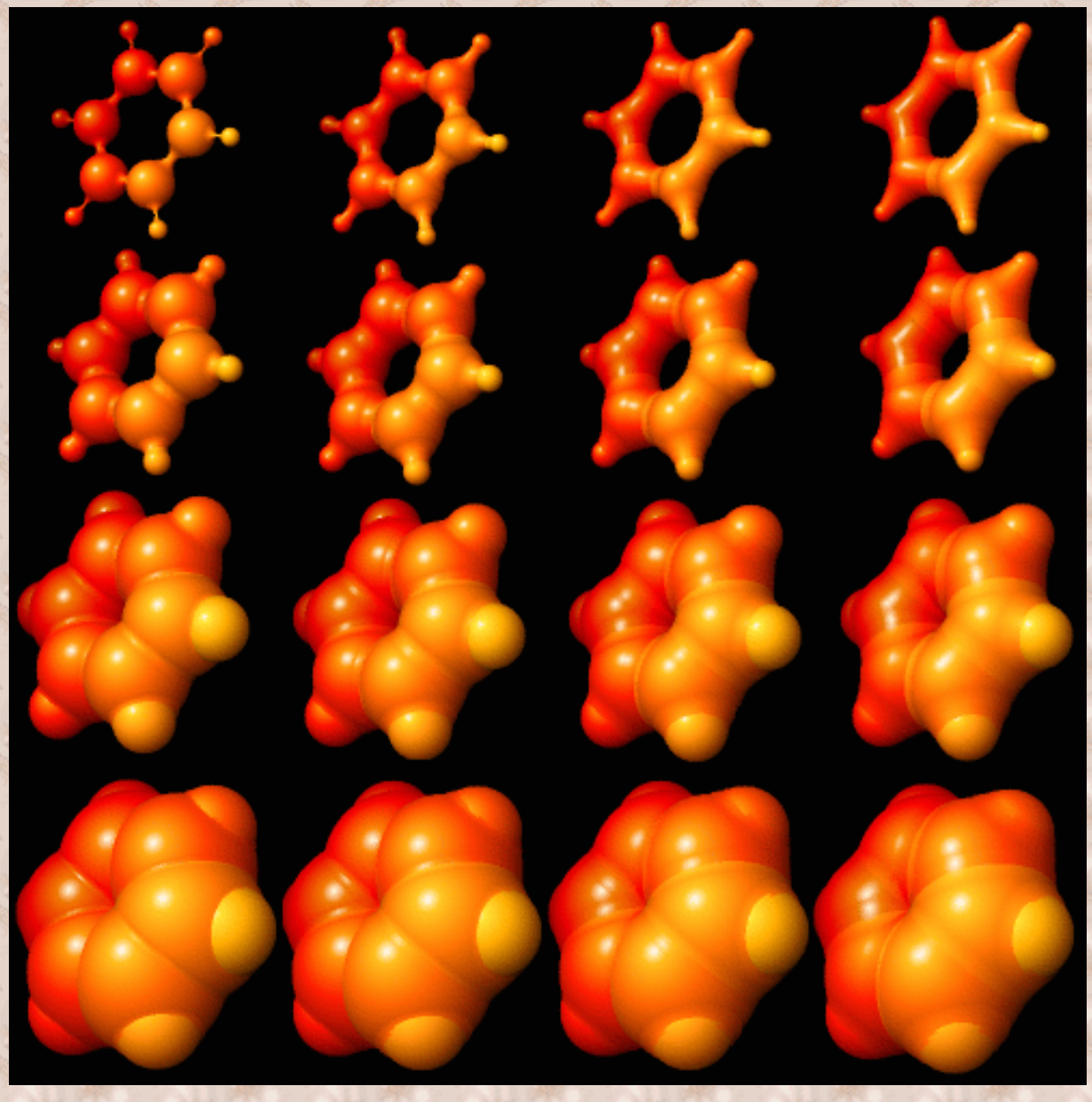
probe 0.8	probe 10





EXAMPLES

In this example, four drawing styles for atoms were combined with nice bonds, drawn with four different probe radii. The following drawing styles were used (vertical, from top to bottom): sm2, co2, sp2 and bi2. Probe radii (angstroms, from left to right): 0.25, 0.50, 1.00 and 2.00. A single benzene molecule was used to prepare this image.



NOTES

(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.

(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

(3) The nice bond style is allowed for ordinary covalent bonds and for disulfide bonds, but not for hydrogen bonds.

(4) Remember that the nice bond style works only for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2.

RELATED COMMANDS

PRO (PROBE) is used to set the probe radius. ATO (ATOMS) is used to change the drawing style for atoms. SSB is used to change the bond drawing style for disulfide bonds. STI (STICKS) is used to change the stick radius. BALLS is used to set the ball radius.

PRO, PROBE

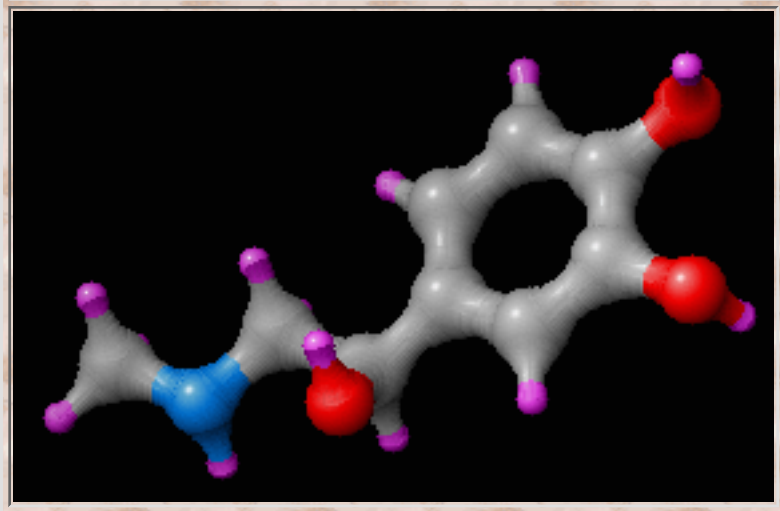
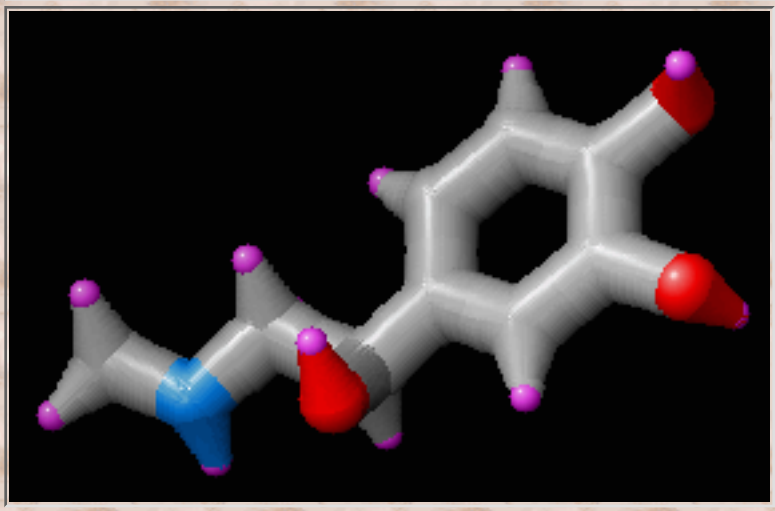
NAME
PRO, PROBE - set the bond probe radius.

SYNOPSIS
PRO value
PROBE value

DESCRIPTION
Set the bond probe radius. The bond probe is used to draw nice bonds (cones and sticks, curved or straight). Small probe (about 0.8 angstroms) is used to obtain curved bond shapes, while large probe (about 10 angstroms) may be used to draw cones or sticks. Be sure to read the text about the command BONDS to learn how to create nice images, playing with commands PROBE, ATOMS and BONDS. Default probe radius is 0.8 angstroms, but this may be changed in the configuration file .garlicrc .

One and only one bond probe radius is assigned to each loaded structure. The bond probe radius may be changed separately for each structure. The command PROBE affects only the structure which is currently "caught" (see the command CATCH) .

EXAMPLES
The images below show the same structure (adrenalin) drawn using two different probes: 0.8 angstroms (curved bonds, the left image) and 10 angstroms (conical sticks, the right image). In both cases all atoms were drawn using the small atomic style with enhanced contrast (ATOMS SM2). Bonds were drawn using the nice bond style (BONDS NICE).

probe 0.8	probe 10
	

NOTES
(1) Do not confuse the bond probe with the surface probe. The bond probe is used to draw bonds, while

the surface probe is used to generate surface points. Read the text about the command SURFACE to learn more about the surface probe.

(2) To draw sticks, it is more convenient to use the commands BONDS STICKS and STICKS. The keyword STICKS (short form STI) of the command BONDS is used to draw bonds as sticks, while the separate command STICKS is used to define the stick radius. (3) To draw balls and sticks, it is convenient to use commands BALLS, STICKS, BONDS STICKS and ATOMS BALLS.

RELATED COMMANDS

BONDS is used to define drawing style for bonds. SSB is used to define drawing style for disulfide bonds. ATOMS is used to define drawing style for atoms. STICKS is used to define the radius of sticks. BALLS is used to define the radius of balls.

CEN, CENTER

NAME
CEN, CENTER - change the origin of the internal coordinate system.

SYNOPSIS
CEN
CENTER

DESCRIPTION
An internal coordinate system is assigned to each structure. The command CEN (CENTER) redefines the position of this origin. A new origin will be equal to the geometric center position calculated for selected atoms. This may be quite useful if working with a large structure. By selecting a small portion of the structure, or even a single atom, the internal system origin may be set to a place which contains the most interesting part of the structure. Rotations, slab changes and color changes will be done with respect to new origin. This will keep the interesting part in the same part of the screen. It is recommended to hide the uninteresting part of the structure, to make rotations and other transformations faster. When you load the structure the geometric center of the whole structure is used as the internal system origin. If you displaced the origin but now you want to move it back to the original position, just execute the following commands:

```
sel all
cen
```

This command is applied to the structure which is currently hangled, i.e. the one to which the command CATCH was applied last.

NOTES
(1) The command CEN (CENTER) does not move the structure to the screen center. To do this, use the command POS (POSITION).

RELATED COMMANDS
POS sets the origin of the internal system to the specified position in the main (global) coordinate system.

COL, COLOR

NAME
COL, COLOR - change the color of selected atoms and their corresponding bonds.

SYNOPSIS
COL color_scheme_name
COL left_1 middle_1 right_1 ... ... left_N, middle_N, right_N

DESCRIPTION
Change the color used to draw selected atoms and their corresponding bonds. Half of each bond belongs to one atom, while half of the same bond belongs to another atom. The easy way to specify color is to use the predefined color scheme. The powerfull (but more complicated) way to specify color is to issue detailed color specification.

COLOR USAGE
In garlic, colors are used to create 3D illusions. In most color schemes, the atoms close to the observer have bright colors, while distant atoms have dark colors. Atoms and bonds look like three-dimensional objects because one side is brighter than the other. Here are some technical details about color usage:

At least one and at most eight surfaces are assigned to each structure. These surfaces are equidistant planes, spheres or cylinders. The surface which is nearest to the observer is called "front surface", while the most distant surface is called "back surface". To each surface, three colors are assigned: left, middle and right color. In most color schemes, left color is bright and right color is dark. Atoms may be divided in three groups:

(1) Atoms which are in front of the front surface;
(2) Atoms which are behind the back surface;
(3) All other atoms, positioned in the sandwich between two surfaces.

All atoms which are in front of the front surface are drawn using the same set of three colors which assigned to front surface. Atoms behind the back surface are colored using three colors assigned to back surface. Colors for atoms laying between two surfaces are prepared by linear interpolation of colors assigned to these two surfaces. This is what I call color fading (this term was not the best choice I could make, sorry).

In a special case, when only one surface is used, color does not depend on distance.

Almost all predefined color schemes typically define two surfaces, i.e. a total of six colors. There are some exceptions: color schemes HOT and COLD use three surfaces, while MONOCHROME uses only one.

Planes, spheres and cylinders
For most proteins and other molecules, planar fading is the best choice. In this case, a set of planes,

perpendicular to z axis is used. Concentric spheres may be used when working with large globular proteins, while cylinders may be used for beta-barrel proteins, like porins. The axis of concentric cylinders is parallel to y.

USING PREDEFINED COLOR SCHEMES

Twenty predefined color schemes are available:

SCHEME NAME	DESCRIPTION
RED	Red color scheme; distant atoms are dark
GREEN	Green, distant atoms are dark
BLUE	BLUE (deep sea), distant atoms are dark
YELLOW	Yellow, distant atoms are dark
CYAN	Cyan (cloudless sky), distant atoms are dark
MAGENTA	Magenta, distant atoms are dark
WHITE	Shades of gray, distant atoms almost black
YELLOW-GREEN	Somewhere between yellow and green, distant atoms dark
CYAN-GREEN	Somewhere between green and blue-green, distant atoms dark
CYAN-BLUE	Somewhere between blue and blue-green, distant atoms dark
MAGENTA-BLUE	Somewhere between blue and magenta, distant atoms are dark
MAGENTA-RED	Somewhere between red and magenta, distant atoms are dark
ORANGE	Orange, distant atoms are dark
HOT	The nearest atoms are yellow, atoms in the middle are orange and distant atoms are dark red
COLD	The nearest atoms are cyan, atoms in the middle are cyan-blue and distant atoms are dark blue
MODEL	Use different colors for different NMR models
MONOCHROME	Edge black, central region white, distance independent
CPK	Modified Corey-Pauling-Kultun color scheme, distant atoms are dark
ZEBRA	Residues with even serial number are red, odd residues cyan-blue, distant atoms are dark

CHAIN	Use color to distinguish chains; distant atoms are should be dark
HYPHOB	Assign color according to hydrophobicity; distant atoms are dark

Do not abbreviate the color scheme name! Case is not important. Some selected schemes are shown below.

DETAILED COLOR SPECIFICATION

Most users should be satisfied with predefined color schemes. Anyway, it is fairly easy to use colors which are not available through predefined schemes. To define N color planes (up to eight), you have to define 3 * N colors. The keyword OLD may be used to leave the previous value unchanged. Here are some examples:

col yellow orange red red DarkRed black	Define two color surfaces with six colors.
col rgb:ffff/ffff/4444 rgb:ffff/dddd/0000 DarkRed	One color surface, three colors.
col old old old black black black	Leave the front colors unchanged, set all back colors to black.

Be careful with the keyword OLD - it may be used only if the currently used color scheme has at least as many colors as a new one.

RELATED COMMANDS

FADING may be used to change the position of outer color surfaces and to switch color fading on and off.

CRE, CREATE

NAME
CRE, CREATE - create structure

SYNOPSIS
CRE
CREATE

DESCRIPTION
Create structure, using the sequence from the main sequence buffer and the secondary structure from the main secondary structure buffer. At present (version 1.3), garlic is capable to create polypeptides only. Do not use this command to create DNA or RNA structure.

Both buffers have to be initialized before issuing the command CREATE. A typical use will be to create a short peptide, which will be tryed as an inhibitor for a larger, experimentally determined structure.

The present version (garlic 2.1) will correctly interpret the secondary structure codes for alpha helix (H), 3-10 helix (G) and beta strand (E), while coil (C) and turn (T) will be treated the same way as beta strand.

TEMPLATE RESIDUES
The new structure will be created using the residues from the template file. The template file contains 20 standard residues. This file should be named residues.pdb and stored to at least one of the following directories (listed in the search order):
(1) The current working directory.
(2) $HOME/garlic (garlic subdirectory of user's home directory).
(3) /usr/local/lib/garlic (the system-wide template).

If you want to add some extra residues (like modified amino-acids) to the template file, make your own copy of the file residues.pdb and keep it either in $HOME/garlic subdirectory or in your favorite working directory. It is very easy to add residues to the template file: just copy and paste the chosen exotic residue from the PDB file where you have it to the end of garlic template file. Be sure to include hydrogen atoms! There is one more thing: be sure that your residue does not have the same residue serial number as the preceding residue. You don't have to worry about the position and the orientation of your residue.

If you don't have the file residues.pdb, click here for HTML version. It is very easy to convert this version to the plain PDB, just save it as the plain text.

EXAMPLE

seq = asp ala phe tyr trp asn str = eeeeee cre	Define a short sequence (six residues), use extended structure for all residues and create the short peptide.

NOTES

(1) The command CREATE resets the editing mode to default (no editing).

RELATED COMMANDS

Use SEQUENCE to prepare the protein sequence and STRUCTURE to prepare the secondary structure.

Garlic Template File

residues.pdb

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains the template file for garlic. This file contains the template residues, which are used as basic building blocks required to create a new polypeptide. If you don't have the template file, save this HTML file as text and remove all lines which do not contain the string ATOM at the beginning. Don't forget to check the bottom lines.

Recommended locations (listed in search order):

Special template file	residues.pdb in the current working directory
User's private template file	$HOME/garlic/residues.pdb
System-wide template file	/usr/local/lib/garlic/residues.pdb

Garlic uses only one template file. The program first looks in the current working directory, then in $HOME/garlic, and last in /usr/local/lib/garlic.

```
ATOM      1  N    ALA     1      -20.307  17.277  25.298  1.00  0.18
ATOM      2  CA   ALA     1      -20.293  16.365  24.112  1.00  0.19
ATOM      3  C    ALA     1      -18.873  16.278  23.541  1.00  0.20
ATOM      4  O    ALA     1      -18.190  17.275  23.428  1.00  0.25
ATOM      5  CB   ALA     1      -21.238  16.916  23.045  1.00  0.24
ATOM      6  H    ALA     1      -19.804  18.120  25.278  1.00  0.19
ATOM      7  HA   ALA     1      -20.622  15.383  24.409  1.00  0.18
ATOM      8  HB   ALA     1      -21.767  17.771  23.437  1.00  1.03
ATOM      9  HB   ALA     1      -20.670  17.215  22.176  1.00  1.00
ATOM     10  HB   ALA     1      -21.949  16.156  22.760  1.00  1.09
ATOM     11  N    ARG     2      -18.461  15.068  23.192  1.00  0.36
ATOM     12  CA   ARG     2      -17.108  14.831  22.625  1.00  0.36
ATOM     13  C    ARG     2      -17.200  13.824  21.484  1.00  0.30
ATOM     14  O    ARG     2      -17.868  12.814  21.598  1.00  0.30
ATOM     15  CB   ARG     2      -16.196  14.274  23.713  1.00  0.44
ATOM     16  CG   ARG     2      -15.991  15.334  24.791  1.00  0.76
ATOM     17  CD   ARG     2      -15.008  14.797  25.834  1.00  1.23
ATOM     18  NE   ARG     2      -15.444  15.244  27.185  1.00  1.90
ATOM     19  CZ   ARG     2      -14.847  14.759  28.240  1.00  2.72
ATOM     20  NH1  ARG     2      -13.673  14.207  28.102  1.00  3.38
ATOM     21  NH2  ARG     2      -15.449  14.840  29.395  1.00  3.41
ATOM     22  H    ARG     2      -19.080  14.321  23.320  1.00  0.39
ATOM     23  HA   ARG     2      -16.702  15.755  22.254  1.00  0.40
ATOM     24  HB   ARG     2      -16.648  13.394  24.149  1.00  0.54
ATOM     25  HB   ARG     2      -15.243  14.004  23.284  1.00  0.52
ATOM     26  HG   ARG     2      -15.593  16.232  24.346  1.00  1.17
```

ATOM	27	HG	ARG	2	-16.935	15.559	25.265	1.00	1.11
ATOM	28	HD	ARG	2	-14.990	13.717	25.799	1.00	1.78
ATOM	29	HD	ARG	2	-14.018	15.178	25.632	1.00	1.69
ATOM	30	HE	ARG	2	-16.171	15.891	27.280	1.00	2.34
ATOM	31	HH1	ARG	2	-13.244	14.162	27.199	1.00	3.40
ATOM	32	HH1	ARG	2	-13.202	13.832	28.898	1.00	4.14
ATOM	33	HH2	ARG	2	-16.349	15.268	29.460	1.00	3.47
ATOM	34	HH2	ARG	2	-15.007	14.474	30.213	1.00	4.18
ATOM	35	N	ASN	3	-16.516	14.122	20.389	1.00	0.23
ATOM	36	CA	ASN	3	-16.511	13.242	19.206	1.00	0.22
ATOM	37	C	ASN	3	-15.108	13.209	18.611	1.00	0.21
ATOM	38	O	ASN	3	-14.478	14.235	18.461	1.00	0.29
ATOM	39	CB	ASN	3	-17.499	13.783	18.172	1.00	0.25
ATOM	40	CG	ASN	3	-18.879	13.944	18.814	1.00	0.28
ATOM	41	OD1	ASN	3	-19.878	13.516	18.270	1.00	1.09
ATOM	42	ND2	ASN	3	-18.984	14.560	19.961	1.00	1.16
ATOM	43	H	ASN	3	-16.007	14.953	20.385	1.00	0.26
ATOM	44	HA	ASN	3	-16.802	12.256	19.501	1.00	0.22
ATOM	45	HB	ASN	3	-17.163	14.742	17.812	1.00	0.27
ATOM	46	HB	ASN	3	-17.571	13.097	17.340	1.00	0.29
ATOM	47	HD2	ASN	3	-19.865	14.666	20.382	1.00	1.18
ATOM	48	HD2	ASN	3	-18.188	14.915	20.404	1.00	1.98
ATOM	49	N	ASP	4	-14.646	12.011	18.281	1.00	0.22
ATOM	50	CA	ASP	4	-13.290	11.823	17.688	1.00	0.23
ATOM	51	C	ASP	4	-13.353	10.783	16.560	1.00	0.26
ATOM	52	O	ASP	4	-13.923	9.723	16.723	1.00	0.37
ATOM	53	CB	ASP	4	-12.317	11.360	18.770	1.00	0.24
ATOM	54	CG	ASP	4	-12.487	9.860	19.000	1.00	0.34
ATOM	55	OD1	ASP	4	-13.592	9.399	18.774	1.00	0.30
ATOM	56	OD2	ASP	4	-11.499	9.262	19.390	1.00	0.57
ATOM	57	H	ASP	4	-15.232	11.245	18.441	1.00	0.25
ATOM	58	HA	ASP	4	-12.947	12.761	17.282	1.00	0.25
ATOM	59	HB	ASP	4	-11.302	11.560	18.460	1.00	0.28
ATOM	60	HB	ASP	4	-12.519	11.886	19.691	1.00	0.29
ATOM	61	N	CYS	5	-12.755	11.118	15.426	1.00	0.19
ATOM	62	CA	CYS	5	-12.735	10.212	14.247	1.00	0.18
ATOM	63	C	CYS	5	-11.387	10.282	13.528	1.00	0.17
ATOM	64	O	CYS	5	-10.854	11.350	13.300	1.00	0.22
ATOM	65	CB	CYS	5	-13.830	10.645	13.279	1.00	0.21
ATOM	66	SG	CYS	5	-13.702	12.314	12.591	1.00	0.48
ATOM	67	H	CYS	5	-12.320	11.996	15.387	1.00	0.23
ATOM	68	HA	CYS	5	-12.923	9.205	14.564	1.00	0.20
ATOM	69	HB	CYS	5	-13.843	9.950	12.454	1.00	0.29
ATOM	70	HB	CYS	5	-14.779	10.571	13.783	1.00	0.36
ATOM	71	HG	CYS	5	-14.465	12.816	12.884	1.00	1.05
ATOM	72	N	GLN	6	-10.853	9.121	13.180	1.00	0.36
ATOM	73	CA	GLN	6	-9.537	9.034	12.469	1.00	0.44
ATOM	74	C	GLN	6	-9.597	7.976	11.351	1.00	0.45
ATOM	75	O	GLN	6	-10.108	6.893	11.547	1.00	0.58
ATOM	76	CB	GLN	6	-8.455	8.664	13.479	1.00	0.54
ATOM	77	CG	GLN	6	-7.073	8.995	12.898	1.00	0.74
ATOM	78	CD	GLN	6	-6.557	10.290	13.531	1.00	1.23

ATOM	79	OE1	GLN	6	-6.781	11.372	13.028	1.00	1.93
ATOM	80	NE2	GLN	6	-5.860	10.221	14.633	1.00	1.76
ATOM	81	H	GLN	6	-11.351	8.307	13.403	1.00	0.44
ATOM	82	HA	GLN	6	-9.303	9.992	12.038	1.00	0.52
ATOM	83	HB	GLN	6	-8.606	9.223	14.392	1.00	0.62
ATOM	84	HB	GLN	6	-8.513	7.615	13.699	1.00	0.53
ATOM	85	HG	GLN	6	-6.384	8.193	13.114	1.00	1.07
ATOM	86	HG	GLN	6	-7.145	9.127	11.830	1.00	0.95
ATOM	87	HE2	GLN	6	-5.521	11.040	15.049	1.00	2.25
ATOM	88	HE2	GLN	6	-5.674	9.349	15.042	1.00	2.11
ATOM	89	N	GLU	7	-9.064	8.328	10.190	1.00	0.29
ATOM	90	CA	GLU	7	-9.049	7.403	9.010	1.00	0.28
ATOM	91	C	GLU	7	-7.686	7.419	8.299	1.00	0.26
ATOM	92	O	GLU	7	-7.148	8.467	8.000	1.00	0.35
ATOM	93	CB	GLU	7	-10.129	7.836	8.034	1.00	0.35
ATOM	94	CG	GLU	7	-11.459	7.206	8.446	1.00	0.41
ATOM	95	CD	GLU	7	-12.574	7.746	7.549	1.00	0.87
ATOM	96	OE1	GLU	7	-12.323	8.763	6.924	1.00	1.57
ATOM	97	OE2	GLU	7	-13.617	7.109	7.538	1.00	1.56
ATOM	98	H	GLU	7	-8.674	9.224	10.127	1.00	0.32
ATOM	99	HA	GLU	7	-9.262	6.412	9.338	1.00	0.30
ATOM	100	HB	GLU	7	-10.214	8.903	8.055	1.00	0.38
ATOM	101	HB	GLU	7	-9.865	7.519	7.035	1.00	0.38
ATOM	102	HG	GLU	7	-11.405	6.132	8.340	1.00	0.61
ATOM	103	HG	GLU	7	-11.679	7.452	9.475	1.00	0.66
ATOM	104	N	GLY	8	-7.151	6.234	8.041	1.00	0.56
ATOM	105	CA	GLY	8	-5.835	6.094	7.357	1.00	0.58
ATOM	106	C	GLY	8	-5.892	4.945	6.343	1.00	0.54
ATOM	107	O	GLY	8	-6.415	3.885	6.628	1.00	0.51
ATOM	108	H	GLY	8	-7.651	5.435	8.316	1.00	0.81
ATOM	109	HA	GLY	8	-5.598	7.013	6.848	1.00	0.65
ATOM	110	HA	GLY	8	-5.077	5.885	8.095	1.00	0.56
ATOM	111	N	HIS	9	-5.343	5.186	5.162	1.00	0.28
ATOM	112	CA	HIS	9	-5.323	4.163	4.075	1.00	0.29
ATOM	113	C	HIS	9	-3.961	4.180	3.378	1.00	0.30
ATOM	114	O	HIS	9	-3.437	5.233	3.066	1.00	0.50
ATOM	115	CB	HIS	9	-6.415	4.486	3.051	1.00	0.34
ATOM	116	CG	HIS	9	-7.790	4.408	3.717	1.00	0.36
ATOM	117	ND1	HIS	9	-8.354	5.354	4.314	1.00	0.43
ATOM	118	CD2	HIS	9	-8.677	3.349	3.788	1.00	0.46
ATOM	119	CE1	HIS	9	-9.496	5.008	4.752	1.00	0.50
ATOM	120	NE2	HIS	9	-9.788	3.742	4.463	1.00	0.50
ATOM	121	H	HIS	9	-4.942	6.069	5.014	1.00	0.33
ATOM	122	HA	HIS	9	-5.501	3.186	4.494	1.00	0.30
ATOM	123	HB	HIS	9	-6.264	5.483	2.663	1.00	0.36
ATOM	124	HB	HIS	9	-6.371	3.778	2.237	1.00	0.41
ATOM	125	HD1	HIS	9	-7.966	6.246	4.430	1.00	0.51
ATOM	126	HD2	HIS	9	-8.513	2.366	3.373	1.00	0.57
ATOM	127	HE1	HIS	9	-10.157	5.667	5.297	1.00	0.62
ATOM	128	N	ILE	10	-3.412	2.996	3.147	1.00	0.20
ATOM	129	CA	ILE	10	-2.084	2.856	2.475	1.00	0.22
ATOM	130	C	ILE	10	-2.133	1.649	1.498	1.00	0.19

ATOM	131	O	ILE	10	-2.638	0.603	1.845	1.00	0.19
ATOM	132	CB	ILE	10	-1.018	2.598	3.544	1.00	0.28
ATOM	133	CG1	ILE	10	-0.940	3.822	4.469	1.00	0.30
ATOM	134	CG2	ILE	10	0.340	2.380	2.864	1.00	0.36
ATOM	135	CD1	ILE	10	0.029	3.539	5.629	1.00	1.04
ATOM	136	H	ILE	10	-3.906	2.196	3.434	1.00	0.26
ATOM	137	HA	ILE	10	-1.841	3.758	1.955	1.00	0.22
ATOM	138	HB	ILE	10	-1.282	1.724	4.112	1.00	0.32
ATOM	139	HG1	ILE	10	-0.589	4.677	3.909	1.00	0.80
ATOM	140	HG1	ILE	10	-1.920	4.039	4.864	1.00	0.74
ATOM	141	HG2	ILE	10	0.263	2.610	1.812	1.00	0.89
ATOM	142	HG2	ILE	10	1.082	3.022	3.313	1.00	0.97
ATOM	143	HG2	ILE	10	0.644	1.352	2.980	1.00	1.01
ATOM	144	HD1	ILE	10	0.183	2.476	5.731	1.00	1.68
ATOM	145	HD1	ILE	10	0.977	4.018	5.436	1.00	1.64
ATOM	146	HD1	ILE	10	-0.382	3.927	6.549	1.00	1.58
ATOM	147	N	LEU	11	-1.600	1.848	0.301	1.00	0.27
ATOM	148	CA	LEU	11	-1.575	0.787	-0.735	1.00	0.30
ATOM	149	C	LEU	11	-0.233	0.783	-1.459	1.00	0.24
ATOM	150	O	LEU	11	0.238	1.809	-1.905	1.00	0.24
ATOM	151	CB	LEU	11	-2.698	1.086	-1.726	1.00	0.39
ATOM	152	CG	LEU	11	-3.390	-0.197	-2.223	1.00	0.46
ATOM	153	CD1	LEU	11	-4.099	-0.917	-1.040	1.00	1.23
ATOM	154	CD2	LEU	11	-4.415	0.243	-3.301	1.00	1.19
ATOM	155	H	LEU	11	-1.216	2.733	0.120	1.00	0.31
ATOM	156	HA	LEU	11	-1.737	-0.165	-0.277	1.00	0.33
ATOM	157	HB	LEU	11	-3.430	1.722	-1.245	1.00	0.53
ATOM	158	HB	LEU	11	-2.289	1.611	-2.571	1.00	0.41
ATOM	159	HG	LEU	11	-2.660	-0.865	-2.671	1.00	0.73
ATOM	160	HD1	LEU	11	-4.377	-0.194	-0.287	1.00	1.69
ATOM	161	HD1	LEU	11	-4.981	-1.432	-1.378	1.00	1.82
ATOM	162	HD1	LEU	11	-3.429	-1.642	-0.603	1.00	1.73
ATOM	163	HD2	LEU	11	-4.595	1.304	-3.213	1.00	1.64
ATOM	164	HD2	LEU	11	-4.012	0.040	-4.277	1.00	1.87
ATOM	165	HD2	LEU	11	-5.348	-0.275	-3.188	1.00	1.68
ATOM	166	N	LYS	12	0.367	-0.394	-1.564	1.00	0.32
ATOM	167	CA	LYS	12	1.689	-0.552	-2.249	1.00	0.29
ATOM	168	C	LYS	12	1.677	-1.816	-3.107	1.00	0.25
ATOM	169	O	LYS	12	1.277	-2.870	-2.658	1.00	0.31
ATOM	170	CB	LYS	12	2.797	-0.640	-1.216	1.00	0.30
ATOM	171	CG	LYS	12	2.708	0.582	-0.296	1.00	0.47
ATOM	172	CD	LYS	12	3.897	0.594	0.672	1.00	0.53
ATOM	173	CE	LYS	12	3.927	-0.710	1.470	1.00	0.73
ATOM	174	NZ	LYS	12	4.644	-0.514	2.761	1.00	1.37
ATOM	175	H	LYS	12	-0.089	-1.166	-1.174	1.00	0.48
ATOM	176	HA	LYS	12	1.862	0.302	-2.883	1.00	0.31
ATOM	177	HB	LYS	12	2.681	-1.544	-0.648	1.00	0.37
ATOM	178	HB	LYS	12	3.755	-0.654	-1.711	1.00	0.35
ATOM	179	HG	LYS	12	2.722	1.481	-0.893	1.00	0.73
ATOM	180	HG	LYS	12	1.789	0.548	0.259	1.00	0.64
ATOM	181	HD	LYS	12	4.815	0.701	0.117	1.00	1.09
ATOM	182	HD	LYS	12	3.798	1.427	1.352	1.00	1.00

ATOM	183	HE	LYS	12	2.918	-1.036	1.670	1.00	1.30
ATOM	184	HE	LYS	12	4.437	-1.473	0.898	1.00	1.42
ATOM	185	HZ	LYS	12	4.882	0.493	2.876	1.00	1.79
ATOM	186	HZ	LYS	12	4.031	-0.815	3.547	1.00	1.83
ATOM	187	HZ	LYS	12	5.514	-1.079	2.765	1.00	2.00
ATOM	188	N	MET	13	2.125	-1.681	-4.347	1.00	0.26
ATOM	189	CA	MET	13	2.172	-2.830	-5.301	1.00	0.28
ATOM	190	C	MET	13	3.485	-2.804	-6.097	1.00	0.30
ATOM	191	O	MET	13	3.901	-1.774	-6.591	1.00	0.37
ATOM	192	CB	MET	13	0.978	-2.757	-6.255	1.00	0.35
ATOM	193	CG	MET	13	0.987	-1.419	-6.993	1.00	1.15
ATOM	194	SD	MET	13	1.240	-1.464	-8.785	1.00	2.09
ATOM	195	CE	MET	13	0.185	-0.054	-9.200	1.00	2.25
ATOM	196	H	MET	13	2.429	-0.788	-4.624	1.00	0.28
ATOM	197	HA	MET	13	2.121	-3.749	-4.747	1.00	0.28
ATOM	198	HB	MET	13	1.038	-3.564	-6.970	1.00	0.94
ATOM	199	HB	MET	13	0.061	-2.853	-5.692	1.00	0.92
ATOM	200	HG	MET	13	0.043	-0.929	-6.809	1.00	1.89
ATOM	201	HG	MET	13	1.765	-0.802	-6.569	1.00	1.80
ATOM	202	HE	MET	13	1.045	0.456	-8.787	1.00	2.50
ATOM	203	HE	MET	13	0.330	0.718	-9.941	1.00	2.60
ATOM	204	HE	MET	13	0.101	-0.633	-10.106	1.00	2.53
ATOM	205	N	PHE	14	4.121	-3.961	-6.207	1.00	0.19
ATOM	206	CA	PHE	14	5.407	-4.089	-6.950	1.00	0.20
ATOM	207	C	PHE	14	5.422	-5.373	-7.776	1.00	0.21
ATOM	208	O	PHE	14	4.987	-6.413	-7.322	1.00	0.35
ATOM	209	CB	PHE	14	6.569	-4.128	-5.957	1.00	0.22
ATOM	210	CG	PHE	14	6.335	-3.110	-4.845	1.00	0.20
ATOM	211	CD1	PHE	14	5.580	-3.441	-3.732	1.00	0.18
ATOM	212	CD2	PHE	14	6.878	-1.848	-4.937	1.00	0.23
ATOM	213	CE1	PHE	14	5.371	-2.516	-2.732	1.00	0.17
ATOM	214	CE2	PHE	14	6.668	-0.922	-3.937	1.00	0.22
ATOM	215	CZ	PHE	14	5.916	-1.255	-2.835	1.00	0.18
ATOM	216	H	PHE	14	3.718	-4.745	-5.779	1.00	0.25
ATOM	217	HA	PHE	14	5.527	-3.242	-7.606	1.00	0.21
ATOM	218	HB	PHE	14	6.646	-5.107	-5.524	1.00	0.24
ATOM	219	HB	PHE	14	7.493	-3.890	-6.465	1.00	0.26
ATOM	220	HD1	PHE	14	5.159	-4.431	-3.641	1.00	0.19
ATOM	221	HD2	PHE	14	7.479	-1.590	-5.792	1.00	0.27
ATOM	222	HE1	PHE	14	4.783	-2.782	-1.868	1.00	0.18
ATOM	223	HE2	PHE	14	7.096	0.067	-4.018	1.00	0.26
ATOM	224	HZ	PHE	14	5.753	-0.532	-2.052	1.00	0.19
ATOM	225	N	PRO	15	5.933	-5.274	-8.995	1.00	1.08
ATOM	226	CA	PRO	15	6.013	-6.426	-9.902	1.00	1.04
ATOM	227	C	PRO	15	7.369	-6.432	-10.606	1.00	0.87
ATOM	228	O	PRO	15	7.811	-5.433	-11.141	1.00	1.05
ATOM	229	CB	PRO	15	4.874	-6.214	-10.911	1.00	1.27
ATOM	230	CG	PRO	15	4.304	-4.781	-10.660	1.00	1.32
ATOM	231	CD	PRO	15	5.070	-4.187	-9.461	1.00	1.26
ATOM	232	HA	PRO	15	5.866	-7.336	-9.362	1.00	1.16
ATOM	233	HB	PRO	15	5.246	-6.289	-11.920	1.00	1.35
ATOM	234	HB	PRO	15	4.101	-6.951	-10.754	1.00	1.44

ATOM	235	HG	PRO	15	4.452	-4.166	-11.535	1.00	1.40
ATOM	236	HG	PRO	15	3.251	-4.839	-10.433	1.00	1.46
ATOM	237	HD	PRO	15	5.672	-3.346	-9.780	1.00	1.32
ATOM	238	HD	PRO	15	4.391	-3.889	-8.685	1.00	1.45
ATOM	239	N	SER	16	8.025	-7.583	-10.595	1.00	0.29
ATOM	240	CA	SER	16	9.351	-7.738	-11.238	1.00	0.25
ATOM	241	C	SER	16	9.398	-9.094	-11.925	1.00	0.26
ATOM	242	O	SER	16	8.952	-10.084	-11.375	1.00	0.35
ATOM	243	CB	SER	16	10.444	-7.648	-10.188	1.00	0.27
ATOM	244	OG	SER	16	9.952	-6.700	-9.252	1.00	0.40
ATOM	245	H	SER	16	7.599	-8.341	-10.141	1.00	0.33
ATOM	246	HA	SER	16	9.488	-6.965	-11.965	1.00	0.24
ATOM	247	HB	SER	16	10.589	-8.595	-9.717	1.00	0.39
ATOM	248	HB	SER	16	11.367	-7.297	-10.625	1.00	0.35
ATOM	249	HG	SER	16	9.508	-6.002	-9.741	1.00	0.91
ATOM	250	N	THR	17	9.946	-9.116	-13.132	1.00	0.19
ATOM	251	CA	THR	17	10.061	-10.373	-13.925	1.00	0.18
ATOM	252	C	THR	17	11.385	-10.357	-14.678	1.00	0.17
ATOM	253	O	THR	17	11.715	-9.370	-15.313	1.00	0.29
ATOM	254	CB	THR	17	8.903	-10.454	-14.925	1.00	0.20
ATOM	255	OG1	THR	17	8.956	-9.225	-15.643	1.00	0.28
ATOM	256	CG2	THR	17	7.548	-10.450	-14.220	1.00	0.31
ATOM	257	H	THR	17	10.280	-8.267	-13.498	1.00	0.23
ATOM	258	HA	THR	17	10.030	-11.227	-13.265	1.00	0.19
ATOM	259	HB	THR	17	8.997	-11.297	-15.585	1.00	0.28
ATOM	260	HG1	THR	17	8.383	-8.597	-15.200	1.00	0.90
ATOM	261	HG2	THR	17	7.694	-10.468	-13.151	1.00	1.06
ATOM	262	HG2	THR	17	7.002	-9.558	-14.491	1.00	1.00
ATOM	263	HG2	THR	17	6.981	-11.319	-14.517	1.00	1.09
ATOM	264	N	TRP	18	12.117	-11.458	-14.590	1.00	0.22
ATOM	265	CA	TRP	18	13.442	-11.587	-15.278	1.00	0.20
ATOM	266	C	TRP	18	13.562	-12.996	-15.852	1.00	0.19
ATOM	267	O	TRP	18	13.196	-13.958	-15.204	1.00	0.22
ATOM	268	CB	TRP	18	14.571	-11.352	-14.277	1.00	0.19
ATOM	269	CG	TRP	18	14.582	-9.877	-13.861	1.00	0.23
ATOM	270	CD1	TRP	18	13.809	-9.376	-12.906	1.00	0.27
ATOM	271	CD2	TRP	18	15.346	-8.932	-14.394	1.00	0.25
ATOM	272	NE1	TRP	18	14.132	-8.075	-12.880	1.00	0.30
ATOM	273	CE2	TRP	18	15.096	-7.710	-13.787	1.00	0.29
ATOM	274	CE3	TRP	18	16.298	-9.007	-15.404	1.00	0.27
ATOM	275	CZ2	TRP	18	15.785	-6.583	-14.183	1.00	0.33
ATOM	276	CZ3	TRP	18	16.983	-7.874	-15.795	1.00	0.32
ATOM	277	CH2	TRP	18	16.726	-6.665	-15.186	1.00	0.35
ATOM	278	H	TRP	18	11.763	-12.202	-14.052	1.00	0.23
ATOM	279	HA	TRP	18	13.512	-10.868	-16.075	1.00	0.21
ATOM	280	HB	TRP	18	14.418	-11.963	-13.407	1.00	0.20
ATOM	281	HB	TRP	18	15.515	-11.613	-14.724	1.00	0.18
ATOM	282	HD1	TRP	18	13.087	-9.894	-12.294	1.00	0.29
ATOM	283	HE1	TRP	18	13.720	-7.439	-12.260	1.00	0.33
ATOM	284	HE3	TRP	18	16.506	-9.945	-15.887	1.00	0.25
ATOM	285	HZ2	TRP	18	15.584	-5.634	-13.708	1.00	0.36
ATOM	286	HZ3	TRP	18	17.723	-7.937	-16.576	1.00	0.35

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ATOM    287  HH2 TRP    18      17.264  -5.781 -15.494  1.00  0.39
ATOM    288  N   TYR    19      14.078 -13.086 -17.069  1.00  0.41
ATOM    289  CA  TYR    19      14.257 -14.399 -17.759  1.00  0.33
ATOM    290  C   TYR    19      15.607 -14.436 -18.483  1.00  0.30
ATOM    291  O   TYR    19      15.983 -13.486 -19.139  1.00  0.32
ATOM    292  CB  TYR    19      13.133 -14.581 -18.781  1.00  0.36
ATOM    293  CG  TYR    19      11.787 -14.282 -18.118  1.00  0.38
ATOM    294  CD1 TYR    19      11.205 -15.200 -17.268  1.00  0.34
ATOM    295  CD2 TYR    19      11.135 -13.089 -18.359  1.00  0.47
ATOM    296  CE1 TYR    19       9.991 -14.931 -16.671  1.00  0.39
ATOM    297  CE2 TYR    19       9.922 -12.821 -17.761  1.00  0.51
ATOM    298  CZ  TYR    19       9.340 -13.739 -16.912  1.00  0.46
ATOM    299  OH  TYR    19       8.125 -13.470 -16.313  1.00  0.53
ATOM    300  H   TYR    19      14.344 -12.258 -17.512  1.00  0.45
ATOM    301  HA  TYR    19      14.215 -15.196 -17.040  1.00  0.33
ATOM    302  HB  TYR    19      13.280 -13.902 -19.610  1.00  0.43
ATOM    303  HB  TYR    19      13.133 -15.597 -19.148  1.00  0.36
ATOM    304  HD1 TYR    19      11.704 -16.139 -17.071  1.00  0.32
ATOM    305  HD2 TYR    19      11.580 -12.360 -19.021  1.00  0.54
ATOM    306  HE1 TYR    19       9.547 -15.660 -16.009  1.00  0.40
ATOM    307  HE2 TYR    19       9.423 -11.882 -17.958  1.00  0.60
ATOM    308  HH  TYR    19       7.495 -14.131 -16.609  1.00  1.09
ATOM    309  N   VAL    20      16.310 -15.550 -18.343  1.00  0.68
ATOM    310  CA  VAL    20      17.638 -15.729 -18.987  1.00  0.51
ATOM    311  C   VAL    20      17.763 -17.141 -19.547  1.00  0.46
ATOM    312  O   VAL    20      17.421 -18.106 -18.892  1.00  0.60
ATOM    313  CB  VAL    20      18.726 -15.508 -17.933  1.00  0.46
ATOM    314  CG1 VAL    20      19.513 -14.248 -18.276  1.00  1.11
ATOM    315  CG2 VAL    20      18.076 -15.336 -16.557  1.00  1.12
ATOM    316  H   VAL    20      15.933 -16.265 -17.799  1.00  0.81
ATOM    317  HA  VAL    20      17.760 -15.015 -19.781  1.00  0.57
ATOM    318  HB  VAL    20      19.388 -16.354 -17.912  1.00  0.67
ATOM    319  HG1 VAL    20      19.937 -14.338 -19.265  1.00  1.78
ATOM    320  HG1 VAL    20      18.857 -13.392 -18.246  1.00  1.49
ATOM    321  HG1 VAL    20      20.309 -14.115 -17.559  1.00  1.64
ATOM    322  HG2 VAL    20      17.459 -16.195 -16.333  1.00  1.59
ATOM    323  HG2 VAL    20      18.844 -15.246 -15.801  1.00  1.61
ATOM    324  HG2 VAL    20      17.465 -14.446 -16.548  1.00  1.71
```

DIS, DISCARD

NAME
DIS, DISCARD - discard the specified structure.

SYNOPSIS
DIS identifier
DIS ALL
DIS *
DISCARD identifier
DISCARD ALL
DISCARD *

DESCRIPTION
Discard the specified structure (macromolecular complex). The memory used to store the structure is freed. If keyword ALL is used (or asterisk, *), all structures will be discarded. Examples:

COMMAND	DESCRIPTION
dis 1	Discard the structure number 1.
dis 7	Discard the structure number 7.
dis *	Discard all. Nothing will be loaded after this command.

NOTES
(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure which should be discarded. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
PHE 192
CE2  1433  C
t.f.: 64.06
trans
phi:-120.71
psi:  72.93
phob:  1.19
selected
x:    -3.276
y:   -18.665
z:   -13.754
```

(2) If you discard everything, the indexing will be reset too. The first structure you load after discarding everything will be assigned index "1" (one).

(3) The command DISCARD resets the editing mode to default (no editing).

RELATED COMMANDS
LOAD (READ) loads the specified file.

DOC, DOCK

NAME
DOC, DOCK - prepare two structures for docking.

SYNOPSIS
DOC identifier_1 identifier_2
DOC OFF
DOCK identifier_1 identifier_2
DOCK OFF

DESCRIPTION
The command DOCK prepares two structures for docking. Before executing this command, two molecules (structures) have to be loaded. For each structure a region on the surface should be selected as a candidate region for interaction with another molecule. For example, if the first molecule is the substrate, the active site has to be identified as the region where the inhibitor should be placed. Assuming that another molecule is the inhibitor, the side which is expected to interact with the substrate should be identified.

When both molecules are ready for docking, the command DOCK should be executed. The identifiers of both molecules have to be issued as arguments. Both molecules will be translated and rotated to position and orientation suitable for docking. The first molecule will be moved to the bottom of the main window, with the selected region visible on the upper side. The second molecule will be placed atop the first molecule, with the selected region facing the first molecule.

Further, a special docking window will be opened, showing the orthogonal projections of polar side chains as symbols. The polar side chains of both molecules are projected to the plane associated with the first molecule. Cyan symbols belong to the bottom molecule (the first one) and red symbols belong to the top molecule. Hydrogen bond donors are shown as crosses, acceptors as circles, and side chains which are both hydrogen bond donors and acceptors are shown as crosses in circles.

The user might be able to combine two structures, using the information visible in both the main garlic window and in docking window. However, this routine is still quite naive, so don't expect too much. Docking is not an easy game. I hope that this command will be useful at least for educational purpose.

KEYWORDS
The keyword OFF is the only keyword which may be used with the command DOCK. DOCK OFF is used to hide docking window.

KEYWORD	DESCRIPTION
OFF	Hide docking window.

PARAMETERS

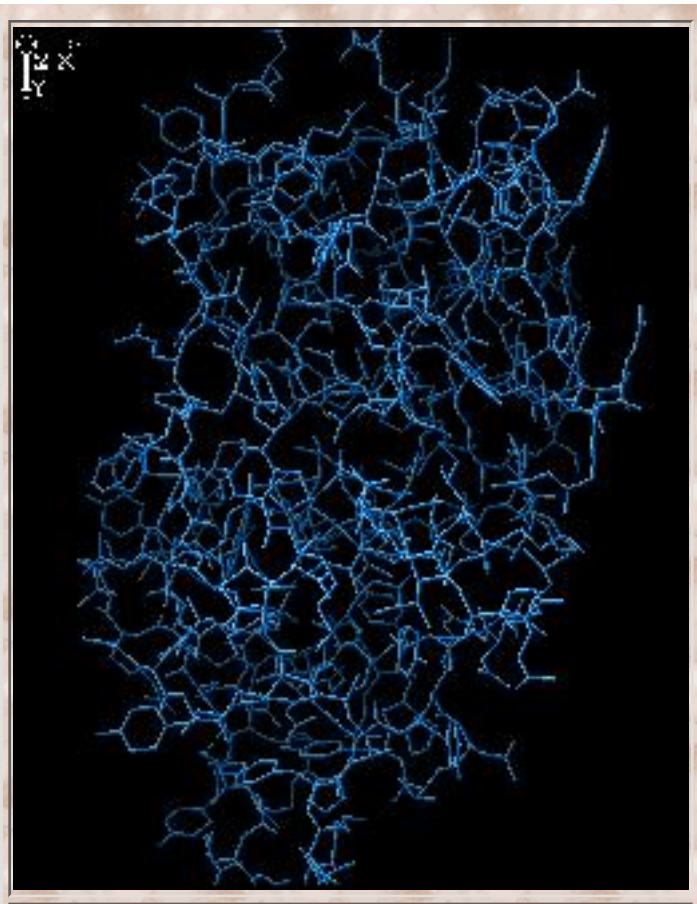
Except when used in combination with the keyword OFF, the command DOCK should be followed by two structure identifiers. If you have forgotten these numbers, just move the mouse pointer over the structure(s) and find the identifier(s) in the output window (the bottom right corner). The order is important: the first molecule will be placed to the bottom of the main window, while the second will be placed atop the first one.

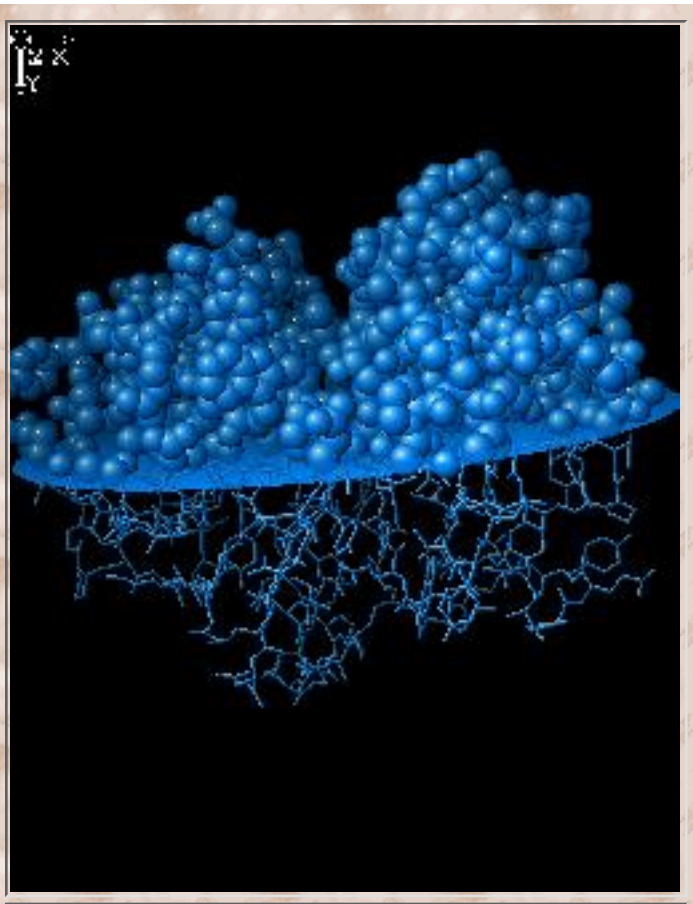
PARAMETER	DESCRIPTION
identifier_1	Identifier of the first molecule. (substrate, for example).
identifier_2	Identifier of the second molecule. (inhibitor, for example).

EXAMPLE

The example below shows how to prepare two structures for docking. In this example, the first structure is papain (reference 1) and the second structure is stefin (reference 2). The structure of the complex is known (PDB code 1STF).

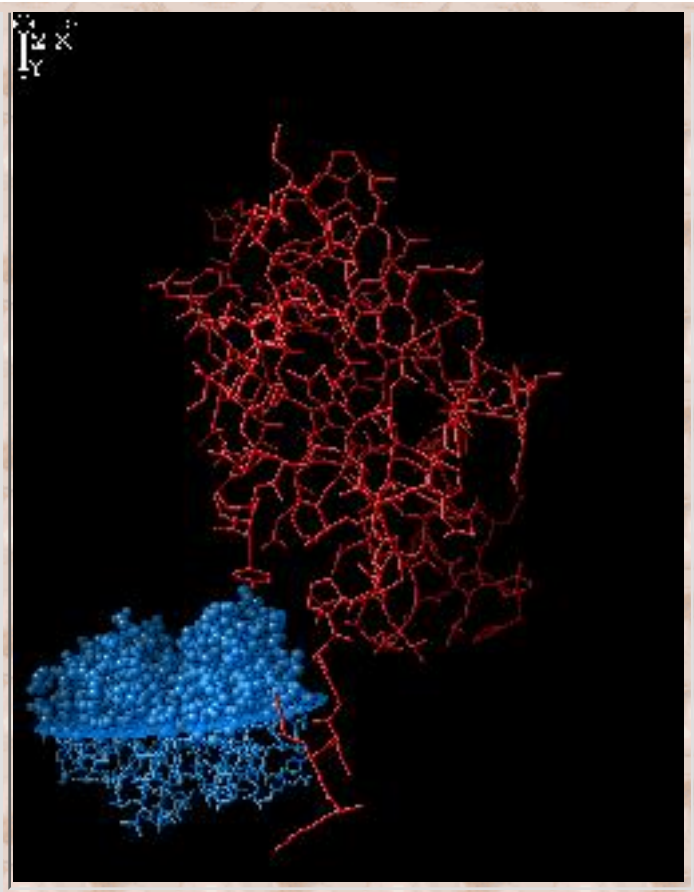
STEP1: Load the first structure: load file1.pdb Change the color. Cyan-blue might be a good choice: color cyan-blue	STEP 2: Make the plane visible: plane Prepare to move the plane: move plane Use plane to divide structure in two parts. The active site should be above the plane. Change drawing style for atoms or bonds. Here the spacefill style is used. This is bad idea if using slow machine. sel above atom sp2 Reset movement controls: move all

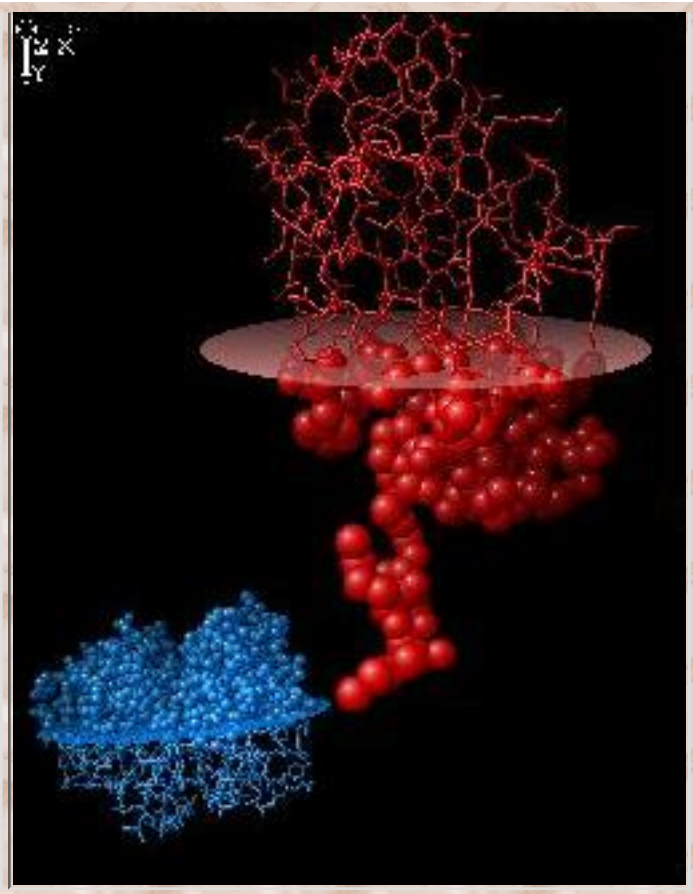




STEP 3:
Push the first structure to the corner.
Load the second structure:
load file2.pdb
Change color. Red is recommended here:
color red

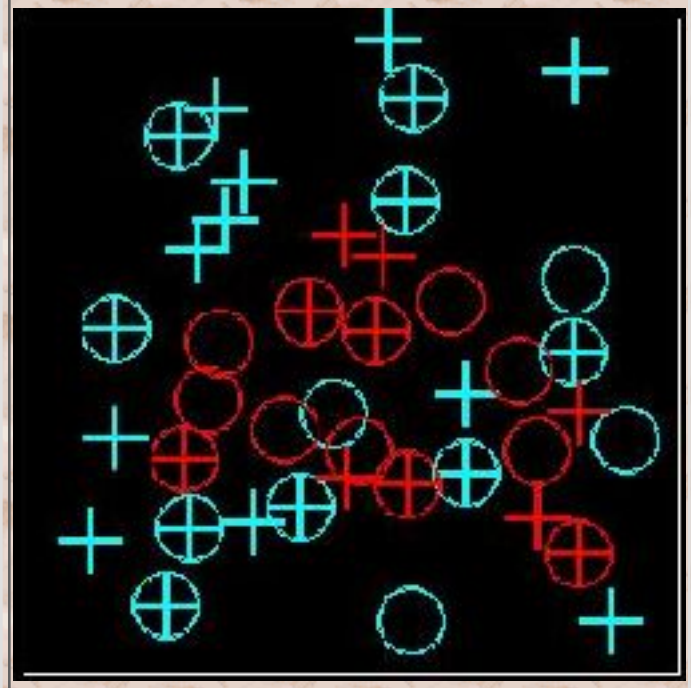
STEP 4:
Make the plane visible and divide the second structure in two parts. Change drawing style for atoms or bonds.
plane
move plane
(... now rotate and translate the plane)
sel above
atom sp2
Reset movement controls:
move all

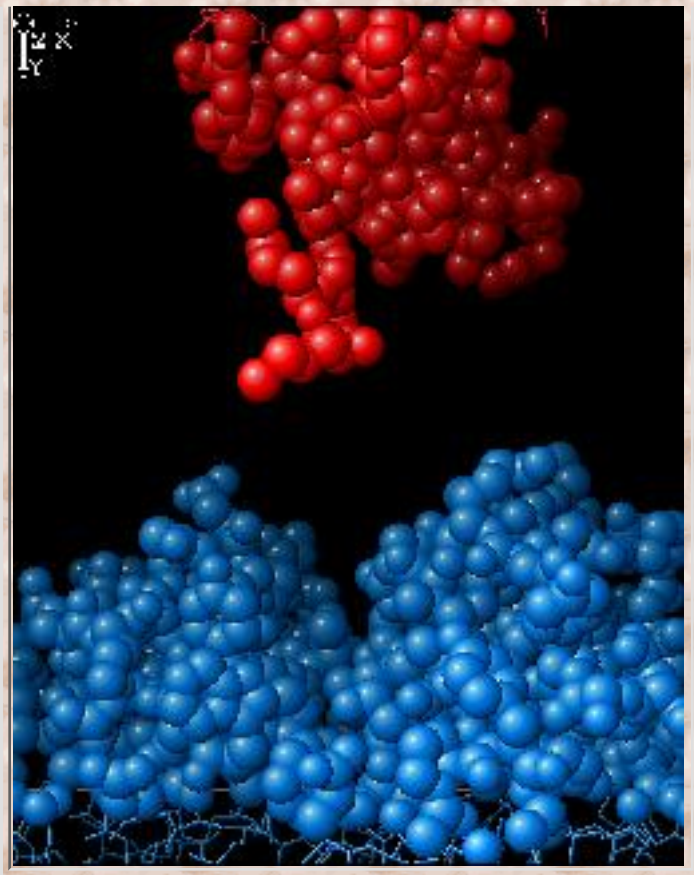




STEP 5:
Execute DOCK command:
dock 1 2

Rotate the second (top) structure. Check the relative arrangement of hydrogen bond donors and acceptors. The projections of these side chains are given in docking window.





NOTES

(1) If two structures are close, some important atoms might be unvisible (hidden by some closer atoms). Use slab to cut slices through structure(s).

(2) Don't forget to catch the right structure before applying some transformation. By default, after the command DOCK is executed, the movement controls are attached to the second (top) structure.

RELATED COMMANDS

LOAD is used to load the specified file (structure, molecule). MOVE is used to define which object should be moved (structure, plane or both). PLANE is used to manipulate the plane associated with the structure. CATCH is used to attach the movement controls to a chosen structure.

REFERENCES

(1) Kamphuis, I. G., Kalk, K. H., Swarte, M. B. A. and Drenth, J. (1984). J. Mol. Biol. 179, p. 233.

(2) Stubbs, M. T., Laber, B., Bode, W., Huber, R., Jerala, R., Lenarcic, B. and Turk, V. (1990). EMBO J. 9, p. 1939.

EDI, EDIT

NAME
EDI, EDIT - edit structure

SYNOPSIS

SHORT FORM	LONG FORM
EDI OFF	EDIT OFF
EDI ATO	EDIT ATOMS
EDI BON atom1 atom2	EDIT BOND atom1 atom2
EDI CLI	EDIT CLICK
EDI DIM	EDIT DIMENSIONS
EDI MAI	EDIT MAIN
EDI OME	EDIT OMEGA
EDI PHI	EDIT PHI
EDI PSI	EDIT PSI
EDI SID	EDIT SIDE

DESCRIPTION
The command EDI (EDIT), combined with one of associated keywords (except OFF), switches the program to editing mode. This will work for garlic version 1.2 or later. The keyword OFF may be used to switch the program to default mode (no editing). The command EDIT should always be combined with one of the keywords. The most comfortable keyword is CLI (CLICK): after executing the command EDI CLI (long form: EDIT CLICK), use the pointer (mouse) to pick one bond (torsion angle) for editing. Click the left mouse button.

The keywords ATO (ATOMS) and DIM (DIMENSIONS) are reserved for special purposes and should not be used to edit real molecular structures, unless you want to introduce (or to fix) some distortion. These keywords may be used to prepare some artificial structures, made from quarkonium and jellium atoms. An example of such structure is the model of the vascular system of human brain . Quarkonium and jellium are described here .

To avoid the accidental modification of the structure, a little sea creature will be visible at the position of the chosen bond or atom. If editing (moving) more than one bond (atom), the creature will be drawn at the position of the first bond (atom). If editing bonds (torsion angles), you will see a little seahorse. If editing atoms (keyword ATOMS) or dimensions (keyword DIMENSIONS) you will see a little squid. Why I have chosen these animals? Seahorse is a poor swimmer but has excellent maneuverability. Squid known hot to use jet propulsion for fast translation. These little creatures will warn you that you are working in editing mode. They will disappear after executing the command EDIT OFF.

The squid will be visible if using keywords DIMENSIONS or ATOMS and the seahorse will be visible if using keywords BOND, BOND, CLICK, MAIN, OMEGA, PHI, PSI or SIDE.

EDIT OFF
The keyword OFF may be used to switch the program to default mode (no editing, just viewing). The editing symbol (seahorse - if editing bonds or squid - if editing atoms) will disappear from the screen.

EDIT ATOMS
The command EDIT ATOMS (short form: EDI ATO) may be used to translate selected atoms. Normally, you will not use the keyword ATOMS if working with a real molecular structure. This keyword is intended for usage with artificial structures, consisting of polygonal lines. In rare cases, you may use this command to distort the molecular structure, for example to test your own molecular dynamics program. The model of the vascular system of human brain is an example of artificial structure, made from quarkonium and jellium atoms. Do not use this keyword unless you really know what you are doing!

The translation of atoms is done by using the keys /, *, +, -, 5 and 0 on numeric keypad.

EDIT BOND atom1 atom2
The command EDIT BOND (short form: EDI BON) should be followed by serial numbers of two atoms which form the bond. The keyword BOND may be used in scripts, to specify a single bond angle for editing. In interactive mode, the keyword CLICK is much more comfortable. Garlic will not allow the editing of the specified bond angle in two cases:
(1) If the specified two atoms do not form an ordinary covalent bond. Disulfide bonds are not counted as such.
(2) If these atoms form a covalent bond, but this bond in part of a closed structure (a ring).

The bond rotation may be done by using the keys 7 and 9 on numeric keypad. Garlic is capable to recognize the bond angle. For dihedral angles phi and psi, an auxiliary plot will be drawn to the bottom right corner of the main window. For dihedral angle omega, the auxiliary plot will be drawn to the bottom of the main window.

EDIT CLICK
The command EDIT CLICK (short form: EDI CLI) is the most comfortable way to chose a single bond angle for editing. Just execute this command and click a single bond. If this bond is as an ordinary covalent bond and if it is not part of some closed structure (a ring), the bond angle editing will be allowed. The seahorse will appear close to the place where the click occurred. Use the keys 7 and 9 on the numeric keypad to change the bond angle.

The keyword CLICK may be used to pick both the main chain bonds as well as side chain bonds. It may not replace the commands MAIN and SIDE, because these two keyword activate the simultaneous editing of two dihedral angles.

Be sure to select all atoms (residues) before using the command EDIT CLICK!

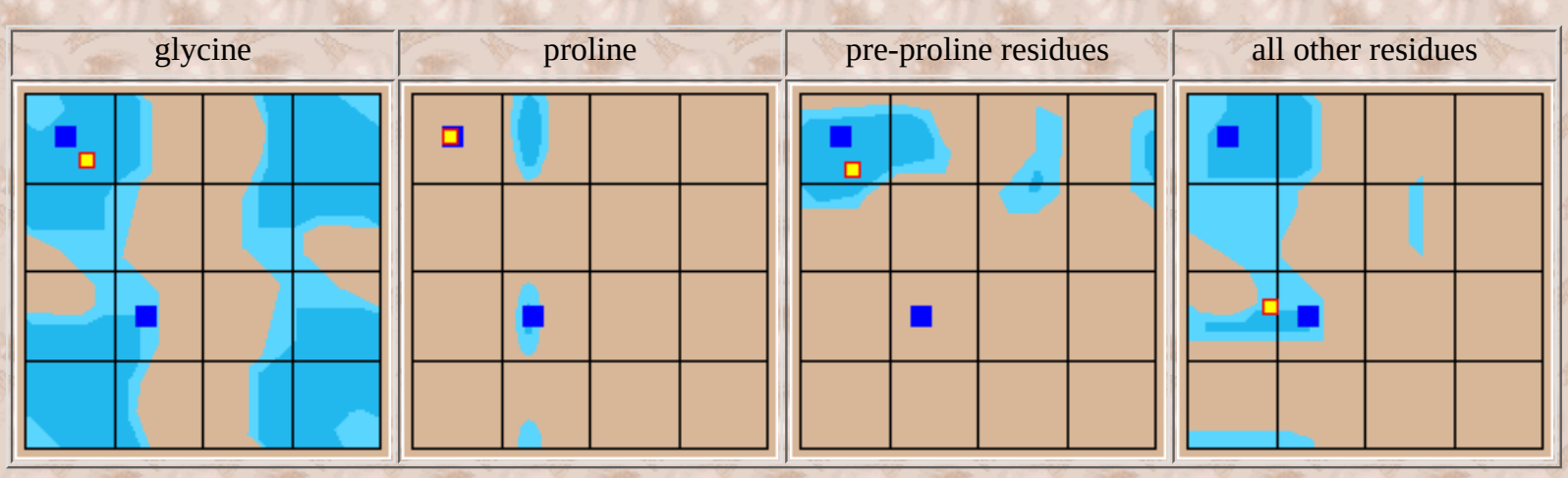
In some cases, a small auxiliary plot will appear in the main window. This means that you have chosen one of the main chain dihedral angles for editing. More details about these auxiliary plots may be found below (see EDIT MAIN).

EDIT DIMENSIONS
The command EDIT DIMENSIONS (short form: EDI DIM) may be used to resize the selected portion of the structure. Normally, you will not use the keyword DIMENSIONS if you are working with a real molecular structure. The translational controls should be used to change each of three dimensions independently: 0 and 5 may be used to change the depth of the structure, / and * to change the width and + and - to change the height of the structure. To resize the structure proportionally change all three dimensions consecutively. Be careful with the command EDIT DIMENSIONS!

EDIT MAIN

Change the main chain dihedral angles phi and psi, for all selected residues. A residue is treated as selected if the first atom of this residue is selected. Click here for detailed definitions of dihedral angles.

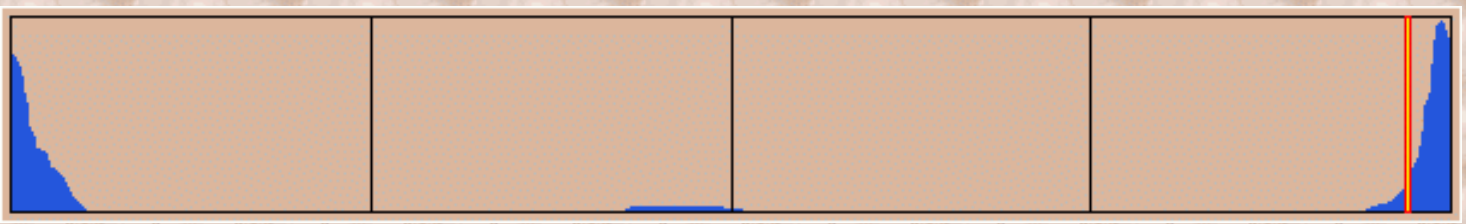
The current pair of values and the allowed regions for phi and psi will be visible in the auxiliary Ramachandran plot, in the bottom right corner of the main window. The current position in the Ramachandran plot may be recognized as the small, yellow square with red outline. The favorable regions are colored blue, with the more favorable regions colored dark blue. Two dark blue squares represent the positions of alpha helix and beta strand. Note that these conformations may be unfavorable in some cases (pre-proline in alpha helix, for example). There are four different types of auxiliary Ramachandran plot, describing residues with different steric constraints:



Be sure to read something about the revision of Ramachandran steric constrains:
http://xray.bmc.uu.se/~gerard/rama/ramarev.html

EDIT OMEGA

Change the angle omega. Click here for detailed definitions of dihedral angles. Most of residues in a protein are in trans conformation, with omega value of about 180 degrees. A small fraction of residues may be found in cis conformation, with omega value of about 0 degrees. The cis conformation is typical for proline. The auxiliary plot at the bottom of the main window shows the current omega value (yellow vertical line with red outline) and the statistical distribution of omega values, across the range between -180 degrees and +180 degrees. The blue peaks represent the most probable values. Note that -180 degrees is equivalent to +180 degrees; two prominent peaks in the auxiliary plot are actually two parts of the same (trans) peak. The central (cis) peak is almost invisible.



EDIT PHI

Change dihedral angle phi. Click here for detailed definitions of dihedral angles. The angle phi may be changed by using the keys 7 and 9 on numeric keypad. The operation will be done for every selected residue. A residue is treated as selected if the first atom of this residue is selected. An auxiliary Ramachandran plot (described above in EDIT MAIN section) will be visible in the bottom right corner.

EDIT PSI

Change dihedral angle psi. Click here for detailed definitions of dihedral angles. The angle psi may be changed by using the keys 7 and 9 on numeric keypad. The operation will be done for every selected residue. A residue is treated as selected if the first atom of this residue is selected. An auxiliary Ramachandran plot (described above in EDIT MAIN section) will be visible in the bottom right corner.

EDIT SIDE

Edit the side chain dihedral angles chi1 and chi2. Four numeric keys are used to change dihedral angles: 4 and 6 to change chi1 and 2 and 8 to change chi2. The command EDI SID (EDIT SIDE) is suitable for asparagine, aspartic acid, histidine, isoleucine, leucine, phenylalanine, proline, tyrosine and tryptophan.

NOTES

(1) The commands REPLACE, CREATE, LOAD, DISCARD, CATCH, SELECT, ADD and RESTRICT are switching program to default editing mode (no editing).

RELATED COMMANDS

The command SET may be used to set dihedral angles directly. It is more precise than the command EDIT. The commands ADD, RESTRICT and SELECT (short forms: ADD, RES and SEL) may be used to select one or more residues for editing. As it will be difficult to combine script execution and interactive rotational controls (numeric keys), the command ROTATE (short form: ROT) may be used to change dihedral angles in scripts, after executing the command EDIT.

Jellium (J) and Quarkonium (Q)

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and "quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1. The interatomic distance is not important! Quarkonium is capable to form at most two bonds. To break the polygonal line, skip one serial index. For example, if three consecutive Q atoms in PDB file have serial numbers i-1, i and i+2, the atoms i-1 and i will be bound, but there will be no bond between atoms i and i+2. The same trick may be used to force Q atom to form no bonds: use indices i-2, i and i+2.

Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. Click here for an example.

By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. The term jellium is used is solid state physics (jellium model for electrons in solid). Note that symbols J and Q are not used in the periodic table of elements. For that reason these two terms were abused in garlic. If I should be thrown through the window at the next meeting of Croatian Physical Society, please note that my colleague Dario Faj deserves the same treatment, he was also involved in this dirty job.

DIHEDRAL ANGLES

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dihedral angles, phi, psi, omega, chi1, chi2, chi3, chi4, chi5, rotamers, dihedral angle, definitions, garlic, Damir Zucic.

MAIN CHAIN DIHEDRAL ANGLES

The main chain dihedral angles are defined as follows:

(1) The phi angle is the angle of right-handed rotation around N-CA bond, the value being zero if CA-C bond is cis to C-N bond. Range: from -180 to 180 degrees.

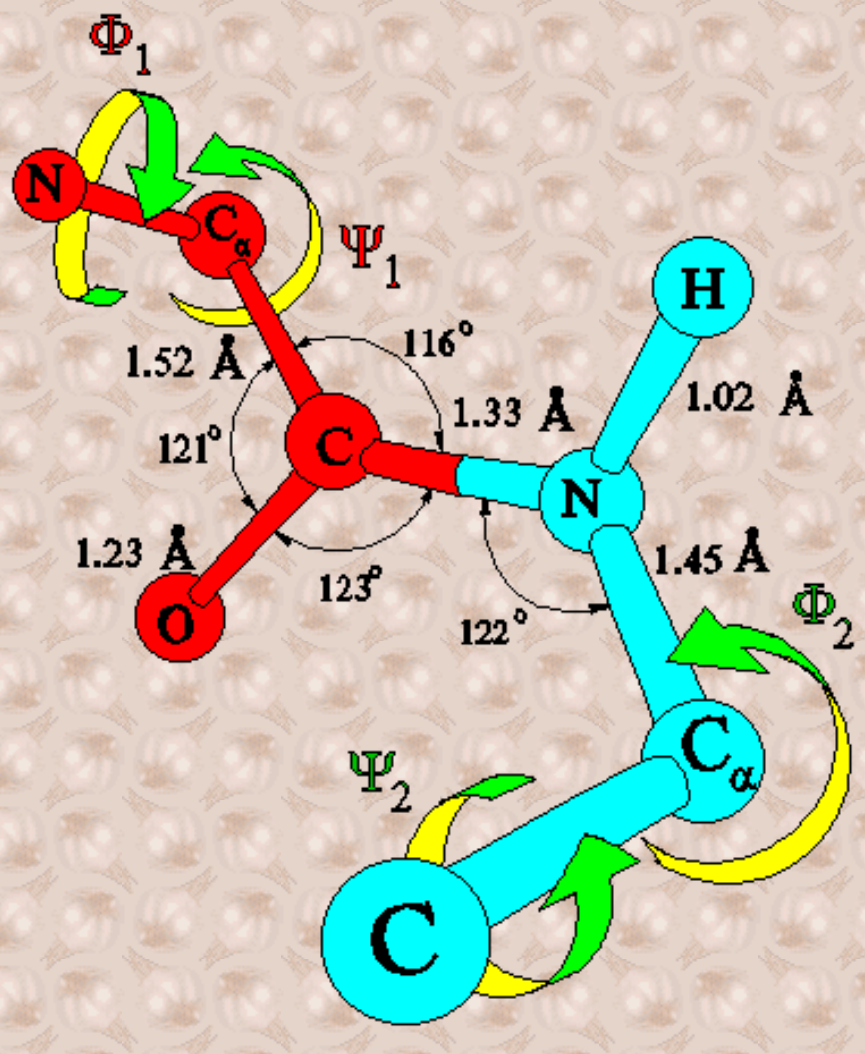
(2) The psi angle is the angle of right-handed rotation around CA-C bond, the value being zero if C-N bond is cis to N-CA bond. Range: from -180 to 180 degrees.

(3) The omega angle is the angle of right-handed rotation about C-N bond, the value being zero if CA-C bond of the preceding residue is cis to N-CA bond. Most residues in a typical protein are involved in the formation of two peptide bonds. The peptide bond formed by the residues I and I + 1 is assigned to the residue I + 1. The same applies to the omega angle. For that reason no omega angle is assigned to the first residue.

Since version 1.2, garlic uses the following procedure to calculate the main chain dihedral angles:

(1) In the first attempt, the coordinates of the main chain atoms are used to calculate the dihedral angles phi and psi. The phi angle will be missing for the first residue in each chain. The psi angle will be missing for the last residue in each chain.

(2) In the second attempt, the missing phi angles will be calculated using the coordinates of H (hydrogen) atoms, if available. The missing psi angles will be calculated using the coordinates of O (oxygen) atoms.

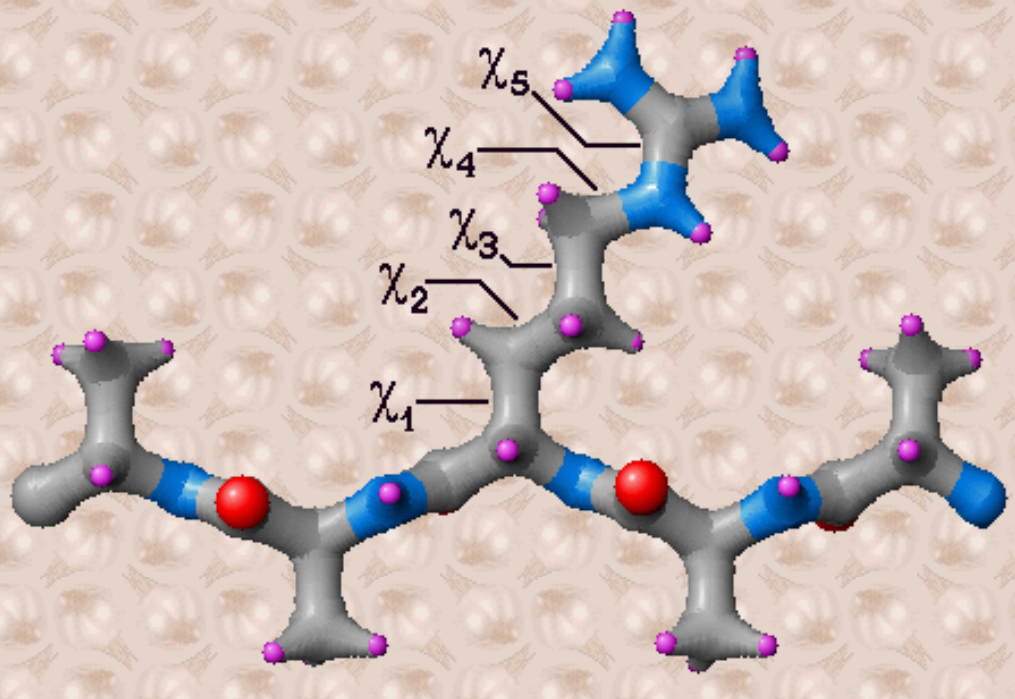


SIDE CHAIN DIHEDRAL ANGLES

For each side chain dihedral angle, the coordinates of four atoms are required. The table below contains the list of atoms and the range of values, for each side chain angle and for each residue. In garlic, the angle chi1 is not calculated for ALA and GLY. The angle chi2 is not calculated for ALA, CYS, GLY, SER, THR and VAL. The angle chi3 is calculated for ARG, GLN, GLU, LYS and MET, the angle chi4 is calculated for ARG and LYS and the angle CHI5 is calculated only for ARG.

CHI1				
SIDE CHAIN	AXIS	ATOMS USED TO DEFINE ANGLE	ZERO VALUE	FORMAL RANGE
ARG	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
ASN	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
ASP	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
CYS	CA-CB	N-CA-CB-SG	SG cis to N	from -180 to +180 deg
GLN	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
GLU	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
HIS	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
ILE	CA-CB	N-CA-CB-CG1	CG1 cis to N	from -180 to +180 deg

LEU	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
LYS	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
MET	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
PHE	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
PRO	CA-CB	N-CA-CB-CG	CG cis to N	CA-CB is part of ring
SER	CA-CB	N-CA-CB-OG	OG cis to N	from -180 to +180 deg
THR	CA-CB	N-CA-CB-OG1	OG1 cis to N	from -180 to +180 deg
TRP	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
TYR	CA-CB	N-CA-CB-CG	CG cis to N	from -180 to +180 deg
VAL	CA-CB	N-CA-CB-CG1	CG1 cis to N	from -180 to +180 deg
CHI2				
ARG	CB-CG	CA-CB-CG-CD	CD cis to CA	from -180 to +180 deg
ASN	CB-CG	CA-CB-CG-OD1	OD1 cis to CA	from -180 to +180 deg
ASP	CB-CG	CA-CB-CG-OD1	OD1 cis to CA	from -180 to +180 deg
GLN	CB-CG	CA-CB-CG-CD	CD cis to CA	from -180 to +180 deg
GLU	CB-CG	CA-CB-CG-CD	CD cis to CA	from -180 to +180 deg
HIS	CB-CG	CA-CB-CG-ND1	ND1 cis to CA	from -180 to +180 deg
ILE	CB-CG1	CA-CB-CG1-CD	CD cis to CA	from -180 to +180 deg
LEU	CB-CG	CA-CB-CG-CD1	CD1 cis to CA	from -180 to +180 deg
LYS	CB-CG	CA-CB-CG-CD	CD cis to CA	from -180 to +180 deg
MET	CB-CG	CA-CB-CG-SD	SD cis to CA	from -180 to +180 deg
PHE	CB-CG	CA-CB-CG-CD1	CD1 cis to CA	from -180 to +180 deg
PRO	CB-CG	CA-CB-CG-CD	CD cis to CA	CB-CG is part of ring
TRP	CB-CG	CA-CB-CG-CD1	CD1 cis to CA	from -180 to +180 deg
TYR	CB-CG	CA-CB-CG-CD1	CD1 cis to CA	from -180 to +180 deg
CHI3				
ARG	CG-CD	CB-CG-CD-NE	NE cis to CB	from -180 to +180 deg
GLN	CG-CD	CB-CG-CD-OE1	OE1 cis to CB	from -180 to +180 deg
GLU	CG-CD	CB-CG-CD-OE1	OE1 cis to CB	from -180 to +180 deg
LYS	CG-CD	CB-CG-CD-CE	CE cis to CB	from -180 to +180 deg
MET	CG-SD	CB-CG-SD-CE	CE cis to CB	from -180 to +180 deg
CHI4				
ARG	CD-NE	CG-CD-NE-CZ	CZ cis to CG	from -180 to +180 deg
LYS	CD-CE	CG-CD-CE-NZ	NZ cis to CG	from -180 to +180 deg
CHI5				
ARG	NE-CZ	CD-NE-CZ-NH1	NH1 cis to CD	from -180 to +180 deg


χ5
χ4
χ3
χ2
χ1

SET

NAME
SET - set dihedral angle

SYNOPSIS
SET PHI value
SET PSI value
SET OME value
SET OMEGA value
SET CHI1 value
SET CHI2 value
SET CHI3 value
SET CHI4 value
SET CHI5 value

DESCRIPTION
The command SET may be used to set the chosen dihedral angle. The value of the angle should always be given in degrees. The keyword OMEGA may be abbreviated to OME. Do not abbreviate the keywords CHI1, CHI2, CHI3, CHI4 and CHI5.

DIHEDRAL ANGLES
Click here for definitions of dihedral angles.

EXAMPLES
set phi -179.0
set ome 0
set chi1 62
set chi2 178.50

RELATED COMMANDS
The command EDIT may be used to change dihedral angles by using rotational controls.

EXE, EXECUTE

NAME
EXE, EXECUTE - load and execute garlic script.

SYNOPSIS
EXE file_name
EXECUTE file_name

DESCRIPTION
Load and execute the specified garlic script. The garlic script file should contain garlic commands. There is only one command which is not executed if added into garlic script: the EXE command. This is done to avoid endless loops; the script which executes itself will generate an endless loop. If you don't like it, change to source file execute_command1.c (use the source, Luke!). Examples:

COMMAND	DESCRIPTION
exe dance.script	Execute the script which loads trp.pdb and forces this molecule to play something similar to Argentinian tango.

RELATED COMMANDS
LOG may be used to store commands used during a garlic session. The log file may be used later as a script.

EXI, EXIT, QUI, QUIT

NAME

EXI, EXIT, QUI, QUIT - quit garlic session (exit from garlic).

SYNOPSIS

EXI
EXIT
QUI
QUIT

DESCRIPTION

Quit garlic session, i.e. exit from garlic. The main garlic window will be closed, memory freed etc. At present, garlic is not capable to save any data (this will be changed, of course), so there are no warning messages.

FAD, FADING

NAME
FAD, FADING - change the color dependence on a distance from the observer.

SYNOPSIS
FAD keyword
FAD FRONT shift
FAD BACK shift
FADING keyword
FADING FRONT shift
FADING BACK shift

DESCRIPTION
Change the way color depends on distance. Distance is measured from the atom to the observer. This command comes in three versions:

(1) FADING FRONT shift ----> move the front color surface;
(2) FADING BACK shift ----> move the back color surface;
(3) FADING keyword ----> switch fading off or change the type of the surfaces.

FADING FRONT shift
This command moves the front fading surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys F1 and F2). The shift value should be given in angstroms. Positive shift moves the front color surface away from the observer. With most color schemes, the front (closer) portion of the structure will be brighter after the positive shift. FRONT may be abbreviated to FRO.

FADING BACK shift
This command moves the back fading surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys F3 and F4). The shift value should be given in angstroms. Positive shift moves the back color surface away from the observer. With most color schemes, the contrast will be reduced after the positive shift. Negative shift results in better contrast, i.e. distant atoms will become darker. BACK may be abbreviated to BAC.

FADING keyword
Some keywords may be used to change the type of color surfaces and to switch color fading off. Here is the list of keywords:

SHORT FORM	LONG FORM	DESCRIPTION
OFF	OFF	Switch fading off: colors should become distance independent
PLA	PLANE	Use planes as color surfaces

SPH	SPHERE	Use spheres as color surfaces
CYL	CYLINDER	Use cylinders as color surfaces
HALF-SPH	HALF-SPHERE	Use spheres as color surfaces, but apply only to the front half of the structure.
HALF-CYL	HALF-CYLINDER	Use cylinders as color surfaces, but apply only to the front half of the structure.

For most structures, the planar fading is the best choice. Spherical and semi-spherical fading may be useful when working with large globular proteins, while cylindrical and semi-cylindrical fading is useful when working with beta-barrel proteins (like porins). The cylinder axis is parallel to y axis (vertical from users standpoint).

EXAMPLES

COMMAND	DESCRIPTION
fading off	Switch color fading off
fading front 4.5	Move the front color surface 4.5 angstroms away from the observer
fading back -2.8	Move the back color surface 2.8 angstroms closer to the observer
fading half-sph	Change fading to semi-spherical

RELATED COMMANDS

COLOR defines the color for selected atoms.

FG, FOREG, FOREGROUND

NAME
FG, FOREG, FOREGROUND - change the main window foreground color.

SYNOPSIS
FG color
FOREG color
FOREGROUND color

DESCRIPTION
Change the main window foreground color. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted. This color is used to draw labels and titles. Note that this color is not used to draw atoms and bonds.

This command does not affect the main window in the sequence comparison mode. Check the command COMPARE .

EXAMPLES

COMMAND	DESCRIPTION
fg white	White
fg DarkSlateGray	Dark dark slate gray
fg #3000a0007000	Kind of green
fg rgb:0/0/8	Dark blue
fg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
BG (BACKG, BACKGROUND) changes the main window background color.

FON, FONT

NAME
FON, FONT - change font.

SYNOPSIS
FON font_name
FONT font_name

DESCRIPTION
Change default font. At present, garlic uses only one font for input, output and main window. Try to execute xlsfonts on your system, to obtain a list of fonts. The initial font is set in .garlicrc file. Examples:

```
fon 10x20
fon olglyph-19
```

RELATED COMMANDS
FG changes the text color used to draw strings in the main window. TFG changes the text color used to draw strings in input and output window.

GRO, GROUP

NAME
GRO, GROUP - group structures: catch more than one structure.

SYNOPSIS
GRO identifier1 identifier2 ... identifierN
GRO ALL
GRO SAV filename
GRO SSC filename
GROUP identifier1 identifier2 ... identifierN
GROUP ALL
GROUP SAVE filename
GROUP SSC filename

DESCRIPTION
The command GROUP may be used to catch more than one structure. It is possible to group only one structure, but this doesn't make much sense. A typical usage will be to unite some inhibitor with a substrate.

The structures which form the group will be rotated about the common rotation axis and translated as a single object. Slab and color fading will be changed simultaneously for all structures. It is recommended to adjust slab and color fading before forming the group. Use much wider slab than usual!

Many other commands will be applied simultaneously for all structures (COLOR, BACKBONE etc.). The exceptions are SAVE , EDIT and REPLACE , which use only default structure (the one which was caught last or loaded as the last structure).

To break the group of structures, i.e. to cancel the command GROUP, execute the command CATCH with a single identifier as a command parameter, to catch only one structure. The command DISCARD may also be used to break the group of structures. Two other commands which cancel GROUP are CREATE and LOAD .

GROUP ALL
The keyword ALL may be used to group all structures into a single object. To break the group, use the command CATCH to catch only one structure.

GROUP SAVE filename
The keyword SAVE may be used to save the entire group as a single file. Each structure will be stored as a separate chain. If any of the structures contained more than one chain, it will be stored as a single chain. The first structure will be stored as the chain A, the second as the chain B etc. If there are more than 26 structures, some chain identifiers may be used more than once. The original chain identifiers will be lost. The original atomic serial numbers and residue serial numbers will be replaced by new serials.

These changes will affect only data stored to the output file. After breaking the group, each structure will remain intact. The file name is case sensitive.

GROUP SSC filename

The keyword SSC may be used to save the entire group into a single file. All structures will be stored as a single chain. The original chain identifiers will be lost. The original atomic serial numbers and residue serial numbers will be replaced by new serials. These changes will affect only data stored to the output file. After breaking the group, each structure will remain intact. The file name is case sensitive.

EXAMPLES

COMMAND	DESCRIPTION
gro 1 2 4	Group structures 1, 2 and 4.
gro all	Group all structures.
group 1 3 group save united.pdb	Group structures 1 and 3 and store as a single structure consisting of two chains to the output file united.pdb .
gro 2 5 gro ssc xyz.pdb	Group structures 2 and 5 and store as a single chain to the output file called xyz.pdb .

RELATED COMMANDS

CATCH is used to catch only one structure. The command CATCH breaks the group formed by the command GROUP.

SAV, SAVE

NAME
SAV, SAVE - save atomic data to the specified file.

SYNOPSIS
SAV file_name
SAV file_name SEL
SAVE file_name
SAVE file_name SEL

DESCRIPTION
Save atomic data to the specified file. By default, all atoms are saved. If keyword SEL is used, only selected atoms are saved. No header is written, just ATOM and HETATM records. You may copy and paste the header from the original (input) file. Coordinates will be expressed in the internal coordinate system (the geometric center used as the origin). Don't forget that unix (linux) file names are case sensitive. If the specified file exists already, it will be overwritten without warning!

RELATED COMMANDS
LOA (LOAD) loads the specified structure. DIS (DISCARD) discards the specified structure.

REP, REPLACE

NAME
REP, REPLACE - replace selected residues

SYNOPSIS
REP
REPLACE

DESCRIPTION
Replace the selected residues, using the sequence from the main sequence buffer. At present (version 1.3), garlic is capable to replace protein residues only. Do not use this command to replace nucleic bases or hetero residues. After the replacement, the structure will need some refinement.

A residue is treated as selected if the first atom which belongs to this residue is selected. For proteins, this is typically N (nitrogen).

The main sequence buffer has to be initialized before issuing the command REPLACE. The number of residues in the main sequence buffer should be equal to the number of selected residues.

SINGLE RESIDUE REPLACEMENT
To replace a single residue, use the following commands:
select residue_sequence_number
sequence = new_residue_name
replace

Example:
sel 29
seq = ser
rep

REPLACING THE ENTIRE SEQUENCE
The command REPLACE may be used to prepare the model of some protein using the experimentally solved structure of the related protein. To replace the entire protein sequence follow these general instructions:
(1) Prepare the file with the sequence of the unsolved protein (use FASTA format).
(2) Find the related, experimentally solved protein structure.
(3) Fix insertions and deletions in the sequence of the unsolved protein.
(4) Start garlic and load the known structure.
(5) Exclude hetero residues from selection (first SEL HET, than SEL COM).
(6) If there is more than one chain restrict selection (RES chain_id/*/*/*).
(7) Load the new sequence (use the command SEQ LOAD).
(8) Replace the old sequence.

Don't forget that the number of selected residues should match the number of residues in the sequence of the unsolved protein.

TEMPLATE RESIDUES

The selected residues will be replaced with the residues from the template file. Default template file contains 20 standard residues. This file should be named residues.pdb and stored to at least one of the following directories (listed in the search order):
(1) The current working directory.
(2) $HOME/garlic (garlic subdirectory of user's home directory).
(3) /usr/local/lib/garlic (the system-wide template).

If you want to add some extra residues (like modified amino-acids) to the template file, make your own copy of the file residues.pdb and keep it either in $HOME/garlic subdirectory or in your favorite working directory. It is very easy to add residues to the template file: just copy and paste the chosen exotic residue from the PDB file where you have it to the end of garlic template file. Be sure to include hydrogen atoms! There is one more thing: be sure that your residue does not have the same residue serial number as the preceding residue. You don't have to worry about the position and the orientation of your residue.

If you don't have the file residues.pdb, click here for HTML version. It is very easy to convert this version to the plain PDB, just save it as the plain text.

NOTES

(1) The command REPLACE resets the editing mode to default (no editing).

RELATED COMMANDS

Use the command SELECT to define the residues which should be replaced and SEQUENCE to define the residues which will be used as replacement.

LOA, LOAD, REA, READ

NAME
LOA, LOAD, REA, READ - load the specified file.

SYNOPSIS
LOA file_name
LOAD file_name
REA file_name
READ file_name

DESCRIPTION
Load and display the specified file. The file content will be treated as a separate structure. The unique structure identifier (positive integer) will be assigned to this structure. The structure will be placed in the middle of the screen.

You can load any file more than once. A total number of structures which may be simultaneously loaded depends on the available memory. The hard-coded maximum is 1000, which should be more than enough.

The command LOAD may be written in uppercase, lowercase or mixed case, but the file name should be specified in correct case - unix file names are case sensitive.

SEARCH PATH
One or more directories will be searched to find the specified file, in the following order:

(1) the current working directory;
(2) directory specified in the environment variable MOL_DIR;
(3) all directories specified in the environment variable MOL_PATH.

The recommended environment variable is MOL_PATH.

NOTES
(1) The command LOAD resets the editing mode to default (no editing).

RELATED COMMANDS
DIS (DISCARD) discards the specified structure. SAV (SAVE) saves the atomic data to a file.

HID, HIDE

NAME
HID, HIDE - hide selected atoms.

SYNOPSIS
HID
HIDE

DESCRIPTION
Hide selected atoms and associated bonds.

RELATED COMMANDS
SHOW shows selected atoms and associated bonds.

HYB, HYBONDS

NAME
HYB, HYBONDS - generate hydrogen bonds.

SYNOPSIS
HYB
HYB style
HYB OFF
HYBONDS
HYBONDS style
HYBONDS OFF

DESCRIPTION
Generate hydrogen bonds for the entire structure. Show hydrogen bonds for visible atoms. At present, some very simple geometric restrains are used to generate hydrogen bonds. Check the configuration file (.garlicrc) and the source file gen_hybonds.c to learn more about these restrains.

Keyword OFF may be used to hide hydrogen bonds.

For hydrogen bonds, there is no proportional ("nice") style. The only available styles are 0, 1, 2, 3, 4 and 5.

Default style used to draw hydrogen bonds is 1 (a single line of fixed width). You can change it by specifying the style. Examples:

hyb	Generate hydrogen bonds and show them using default style (1).
hyb 4	Generate hydrogen bonds and show them using style 4 (four lines).
hyb off	Hide hydrogen bonds

IGN, IGNORE

NAME
IGN, IGNORE - do nothing.

SYNOPSIS
IGN
IGNORE

DESCRIPTION
This command does nothing. It is absolutely useless. Do not use it to pause the program execution - PAUSE should be used for this purpose.

LAB, LABELS

NAME
LAB, LABELS - show or hide labels.

SYNOPSIS
LAB
LABELS
LAB OFF
LABELS OFF

DESCRIPTION
If used without keyword OFF, this command shows labels for selected atoms. If used with keyword OFF, this command hides labels. Each label contains:
(1) residue name;
(2) residue sequence number;
(3) chain identifier;
(4) atom name;
(5) alternate location indicator.

RELATED COMMANDS
TITLE adds the title to the main window. TAG assigns the specified tag to a structure. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

LOG

NAME
LOG - write interactive commands into the log file.

SYNOPSIS
LOG file_name
LOG OFF

DESCRIPTION
Use this command to log your garlic session into the specified file. The log file may be modified later and used as garlic script. LOG OFF closes the log file and stops logging.

NOTES
(1) If you logged the entire garlic session and want to use your log file as script, do not forget to remove the keyword QUIT (EXIT) which was used to end the garlic session!

(2) Lines which have # in the first column are treated as comments. Empty lines are ignored.

(3) Use PAUSE to pause the program execution. This is useful if preparing lecture or presentation, otherwise the script will run till the end without stopping.

(4) You can start and stop logging at any moment during your garlic session. Do not use the same log file name twice if you want to keep the old file - it will be overwritten.

RELATED COMMANDS
Exe executes the garlic script. PAUSE pauses the script execution.

MEM, MEMBRANE

NAME

MEM, MEMBRANE - generate and manipulate the membrane associated with the structure.

SYNOPSIS

SHORT FORM	LONG FORM
MEM	MEMBRANE
MEM BET	MEMBRANE BETA
MEM RAD value	MEMBRANE RADIUS value
MEM THI value	MEMBRANE THICKNESS value
MEM TRA value	MEMBRANE TRANSPARENCY value
MEM OFF	MEMBRANE OFF

DESCRIPTION

The command MEM (MEMBRANE) may be used to associate the membrane with a protein structure. By default, no membrane is associated with the structure when it is loaded into memory. The membrane is initialized after the first execution of the command membrane. The membrane is useful when analysing some membrane protein, but it does not make much sense when working with a soluble protein.

The experimental determination of the structure of fluid lipid bilayers in The Stephen White Laboratory at UC Irvine has revealed a significant thermal motion of lipid molecules. This means that there is no clear edge of the biological membrane. However, the model used in garlic is just the opposite: the membrane is represented by two parralel planes, with clear external edges. The membrane thickness is also precisely defined. The idea was to give at least a bad model of the membrane, to allow selection of the transmembrane region. Please be sure to read those beatifull pages from Steven White Laboratory!

The planes used to simulate the membrane are represented as elliptical surfaces. The inner sides are colored orange-red, while the outer sides of the membrane are colored blue. The transparency of these planes may be adjusted, but not individually. The allowed range of transparency from 0 to 1. If the transparency is equal to zero both planes will be opaque. Default transparency is 0.4 (hard-coded).

In addition to the transparency, the membrane thickness and the radius of both planes may be adjusted (keywords THICKNESS and RADIUS, short forms THI and RAD). Default radius will be 50% larger than the membrane thickness. Default membrane thickness is 30 angstroms. It is not possible to change default membrane thickness through .garlicrc file. If you want to change it, modify the hard-coded value in the source file defines.h and recompile the program.

If working with beta barrel protein (porin-like membrane proteins), the keyword BETA may be used to improve membrane placement.

KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
OFF	OFF	Hide membrane.
BET	BETA	Attach membrane to beta barrel protein (porin).
THI	THICKNESS	Set the membrane thickness (in angstroms).
RAD	RADIUS	Set the radius of both planes (use angstroms).
THI	THICKNESS	Set the membrane thickness (in angstroms).
TRA	TRANSPARENCY	Set the transparency of both planes (between 0 and 1).

EXAMPLES

COMMAND	DESCRIPTION
mem	Initialize the membrane and make it visible.
mem rad 20	Change the radius of both planes to 20 angstroms.
mem tra 0.3	Change the transparency of both planes (new value: 0.3).
mem thi 20 mem beta	Change membrane thickness and attach membrane to beta barrel protein.
mem off	Hide membrane.

NOTES

(1) By default, the membrane moves with the structure. If movement controls affect only the membrane, be sure to make it visible. Otherwise, you may push the membrane far away from the object to which this membrane belongs.

RELATED COMMANDS

LOAD is used to load the structure (PDB file). MOVE is used to define which object should be moved. POSITION is used to place the chosen object (structure, plane, membrane or all) to arbitrary position.

MON, MONO

NAME
MON, MONO - switch to mono mode.

SYNOPSIS
MON
MONO

DESCRIPTION
Switch to mono mode, i.e. switch stereo off.

RELATED COMMANDS
Use STEREO to switch to stereo mode. STEREO OFF does the same job as MONO.

MOV, MOVE

NAME
MOV, MOVE - define which object should be moved.

SYNOPSIS
MOV STR
MOV MEM
MOV PLA
MOV ALL
MOVE STRUCTURE
MOVE MEMBRANE
MOVE PLANE
MOVE ALL

DESCRIPTION
This command defines which object should be moved when rotation and translation controls or commands are used. When a PDB file is read, a new structure is stored into program memory. A single plane (initially invisible) is associated with each structure. On request (after the first execution of the command MEMBRANE), a single membrane may also be added to the structure. By default, the movement controls are affecting both the atomic structure and the associated objects (the plane and the membrane, if initialized). The command MOV (MOVE) may be used to change the action of the movement controls, to move only the choosen object.

The command MOVE affects only the molecule which is currently being handled (the structure which is "caught").

KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
STR	STRUCTURE	Move only the structure (atoms), leaving the plane and the membrane at the current position.
MEM	MEMBRANE	Move only the membrane, leaving the structure (atoms) and the plane at the current position.
PLA	PLANE	Move only the plane, leaving the structure (atoms) and the membrane at the current position.
ALL	ALL	Move all (atoms + plane + membrane).

EXAMPLES

COMMAND	DESCRIPTION

mov pla	Move the plane leaving the structure and the membrane at the current position.
mov all	Move structure, plane and membrane. This is default action.

NOTES

(1) The plane and the membrane are affected by rotation and translation controls and commands. Slab and color fading do not affect these objects.

(2) Never use two keywords with the command MOVE! If you want to move the plane and the membrane, for example, you should move it one by one!

RELATED COMMANDS

PLA (PLANE) is used to manipulate the plane associated with the molecular structure. MEM (MEMBRANE) is used to generate and manipulate the membrane. CATCH is used to catch the specified structure.

NEI, NEIGHBORHOOD

NAME
NEI, NEIGHBORHOOD - hide or show the sequence neighborhood.

SYNOPSIS
NEI
NEI OFF
NEIGHBORHOOD
NEIGHBORHOOD OFF

DESCRIPTION
Hide or show the sequence neighborhood of the residue covered by the pointer. When you cross an atom or bond with the mouse pointer, the output window will contain some useful information about this atom. In addition to this, the top portion of the main window will contain the list of the residues before and after the residue to which this atom belongs. The central residue will be enclosed in a small rectangle. The entire sequence neighborhood will be enclosed in a wide rectangle.

If you are not interested in the sequence neighborhood, execute the command:

nei off

If you want to remove the sequence neighborhood permanently, find this section in the configuration file .garlicrc and replace the keyword "yes" by "no":

```
# Sequence neighborhood of the residue under
# the pointer may be visible or hidden (yes/no):

show sequence neighborhood: yes
```

By default, the sequence neighborhood will be visible.

KEYWORDS
The only keyword is OFF. If used without any keyword, the command NEI will make the sequence neighborhood visible. If combined with the keyword OFF, the command will hide the sequence neighborhood.

EXAMPLES

COMMAND	DESCRIPTION

nei off	Hide the sequence neighborhood.
nei	Show the sequence neighborhood.

NOTES

(1) Residues in the sequence neighborhood are listed in direction from amino- to carboxyl-terminal residue.

(2) If the current residue is close to the polypeptide chain end, it will be displaced from the central position.

PAU, PAUSE

NAME
PAU, PAUSE - pause script execution.

SYNOPSIS
PAU
PAUSE

DESCRIPTION
Pause script execution. This may be useful if using garlic for lectures and conference presentations. The script execution will be paused until the return key is pressed.

RELATED COMMANDS
Use EXE (EXECUTE) to load and execute garlic script. Use LOG to log your garlic session. The log file may be modified into the script file later (or even left unchanged).

PLA, PLANE

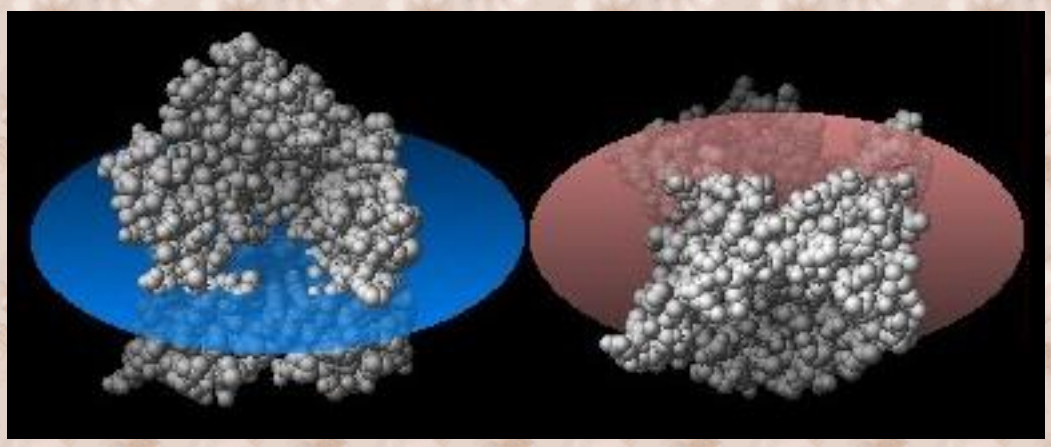
NAME
PLA, PLANE - manipulate the plane associated with the structure.

SYNOPSIS
PLA
PLA RAD value
PLA TRA value
PLA OFF
PLANE
PLANE RADIUS value
PLANE TRANSPARENCY value
PLANE OFF

DESCRIPTION
When a PDB file is read, a new structure is stored into program memory. A single plane is associated with this structure. By default, the plane is unvisible and movement controls are affecting both the structure and the associated plane. The command PLANE may be used to make the plane visible, to set the plane transparency or radius, or to hide the plane.

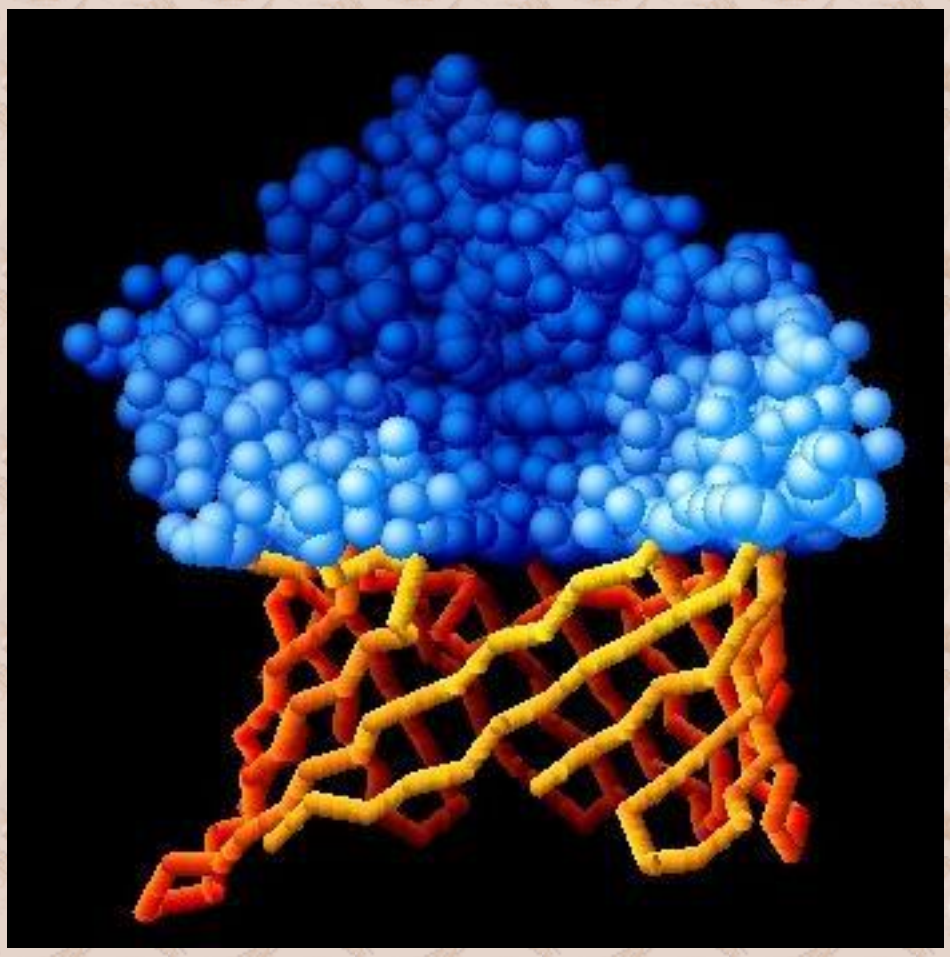
Plane is represented by an ellipse. One side of this ellipse will be colored blue and other side will be colored orange-red. Blue side is treated as top (upper) side, while orange-red side is treated as bottom side. Far side of the plane is dark.

The transparency value should be between 0 and 1. If the transparency is equal to zero the plane is opaque. Default plane transparency is 0.4 (hard-coded). The initial (default) plane radius is based on the spacial extent of the structure. The image below shows two semi-transparent planes: the left plane is seen from above, while the right plane is seen from below. The transparency is equal to 0.3 for both planes.



Plane may be used for different purposes:
(1) To distinguish protein domains. Many soluble proteins fold into two domains. Plane may be used to outline the border between these domains.

(2) Atoms may be selected according to their position with respect to plane. The command SEL ABO (SELECT ABOVE) selects atoms which are above the plane. The command SEL BEL (SELECT BELOW) selects atoms which are below the plane. The image below shows what may be achieved when applying different drawing styles to atoms on different sides of the plane.
(3) To represent the cellular membrane. Since version 1.2, garlic is capable to represent the membrane directly, so this usage of planes is obsolete.



KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
OFF	OFF	Hide plane.
RAD	RADIUS	Set plane radius (value should be given in angstroms).
TRA	TRANSPARENCY	Set plane transparency (between 0 and 1).

EXAMPLES

COMMAND	DESCRIPTION
plane	Make the plane visible.
pla rad 20	Change plane radius to 20 angstroms.

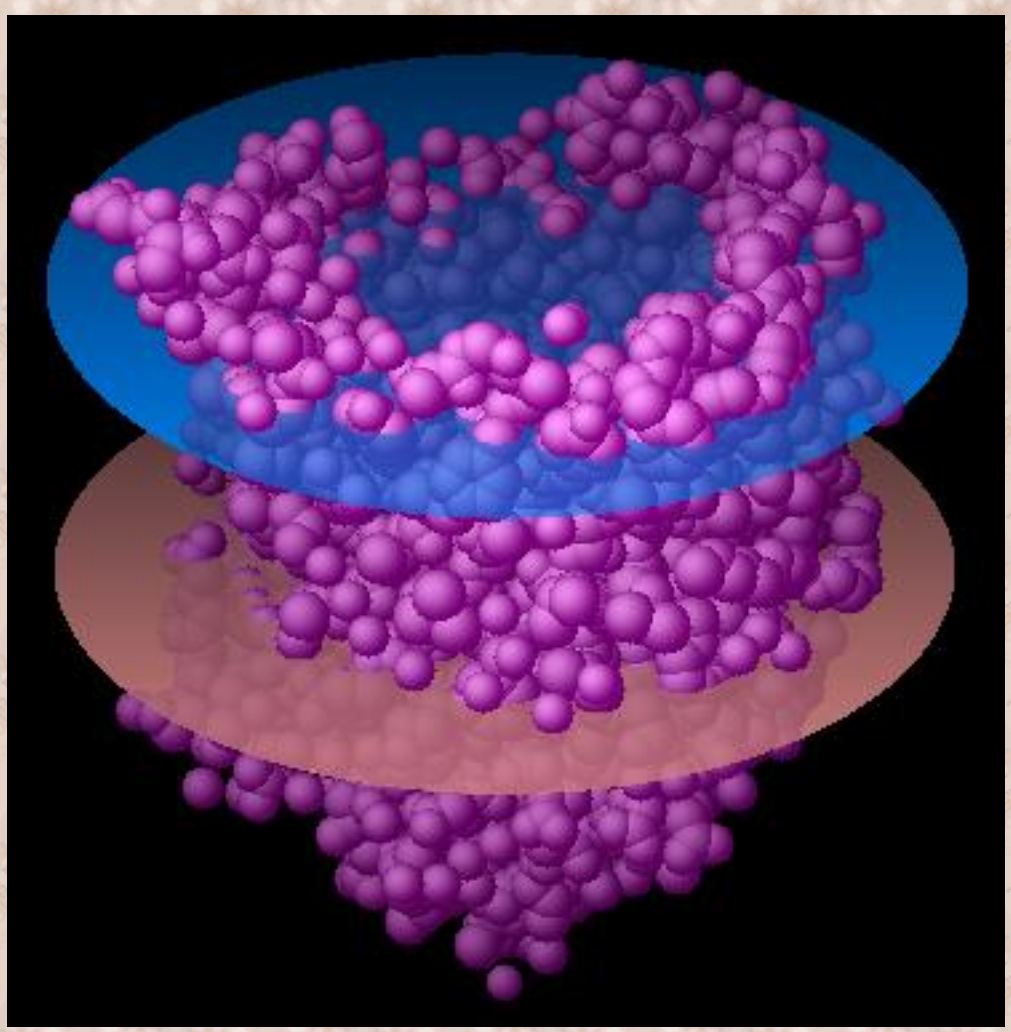
pla tra 0.3	Change plane transparency (new value: 0.3).
plane off	Hide plane.

NOTES

(1) By default, the plane moves with the structure. If movement controls affect only the plane, be sure to make it visible. Otherwise, you may push the plane far away from the object to which this plane belongs.

(2) In garlic source code, each plane is defined by the plane center (three coordinates) and by the normal vector (three-component vector).

(3) At present, garlic associates only one plane with each structure. If for some reason you need two planes (for example, to simulate the cellular membrane), use the following trick:
(3.1) Prepare the structure and its associated plane (the first plane).
(3.2) Load another structure (something small, like a single residue) and hide it.
(3.3) Make the plane (which is associated with this small structure) visible.
(3.4) Change radius and transparency for the second plane.
(3.5) Set the position and orientation of this plane.
If you learn this trick, you will be able to prepare images like this one:



RELATED COMMANDS

LOAD is used to load the structure (PDB file). MOVE is used to define which object should be moved. POSITION is used to place the chosen object (structure, plane, membrane or all) to arbitrary position. SELECT ABOVE selects atoms above the plane, while SELECT BELOW selects atoms below the plane.

PLO, PLOT

NAME
PLO, PLOT - draw averaged hydrophobicity and/or hydrophobic moment.

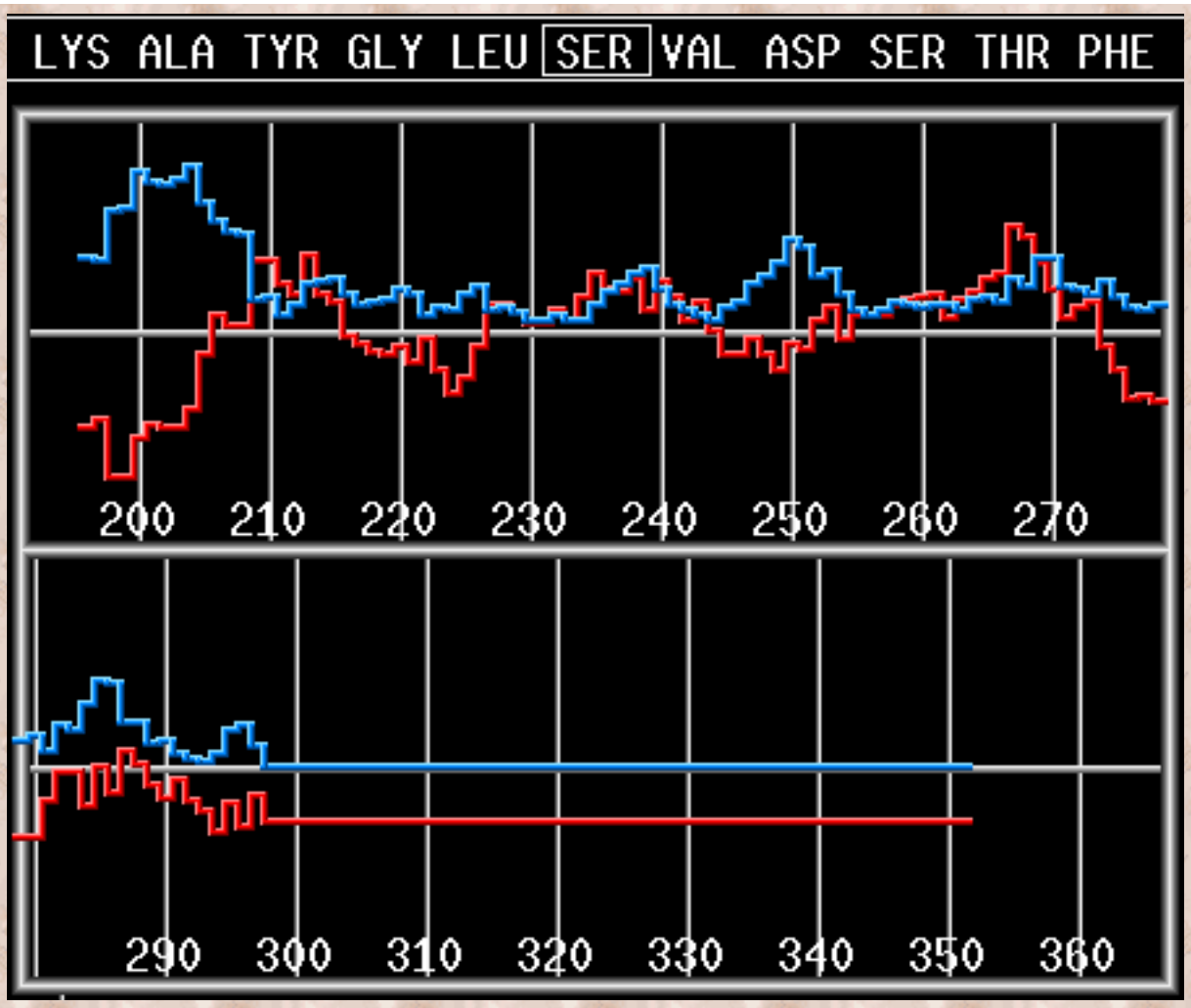
SYNOPSIS
PLO HYD
PLO HYD start_index end_index
PLO MOM
PLO MOM start_index end_index
PLO HYD MOM
PLO HYD MOM start_index end_index
PLO OFF
PLOT HYDROPHOBICITY
PLOT HYDROPHOBICITY start_index end_index
PLOT MOMENT
PLOT MOMENT start_index end_index
PLOT HYDROPHOBICITY MOMENT
PLOT HYDROPHOBICITY MOMENT start_index end_index
PLOT OFF

DESCRIPTION
Draw averaged hydrophobicity and/or hydrophobic moment. The averaged hydrophobicity and hydrophobic moment will be calculated using the sequence from the main sequence buffer, the current sliding window width and the current hydrophobicity scale. To calculate the hydrophobic moment one more parameter is required: the rotation angle between adjacent residues.

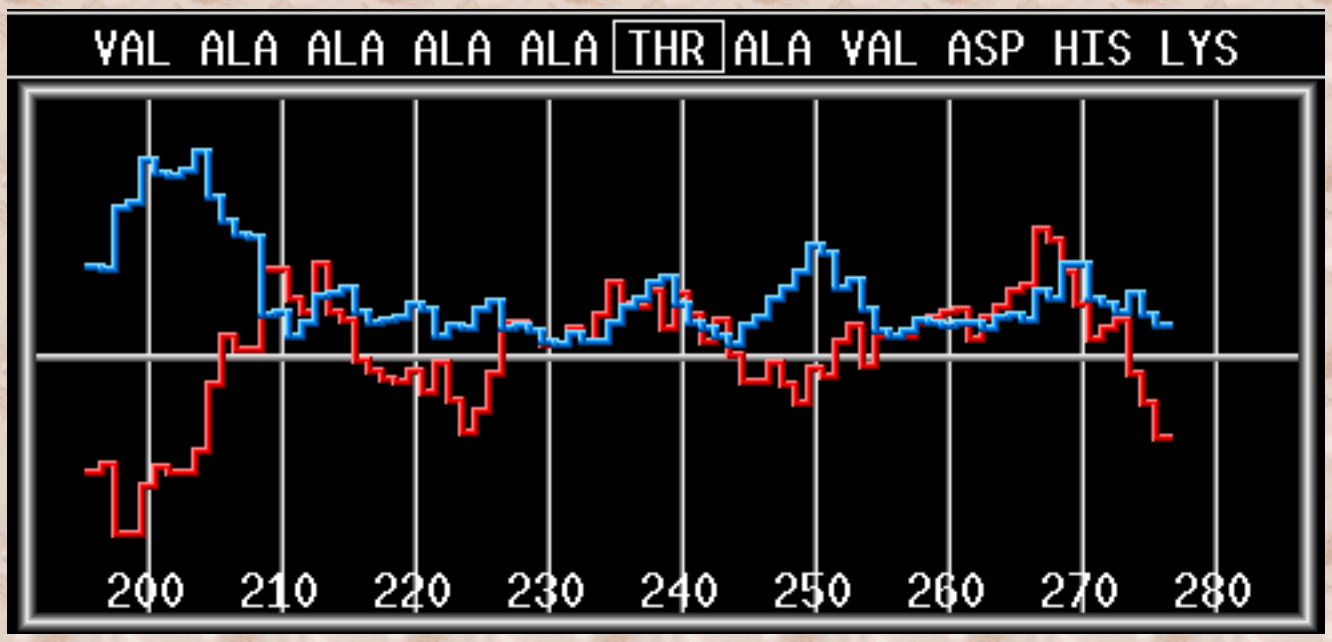
The averaged hydrophobicity will be shown as red line, while the hydrophobic moment will be shown as blue line. The information about the residue below or above the pointer (mouse) will be visible in the output window (bottom right corner of the main window), while the sequence neighborhood of the current residue will be visible above the plot (top of the main window).

If the entire sequence is used for calculation, there is a chance that plot will contain the straight line at the end. This portion of the plot refers to solvent molecules, which are typically stored to the end of PDB file. This trailing line may be easily removed by adjusting the residue range. Here are two examples:

The first image was prepared using all residues from 200 to the last one, including solvent molecules.



The second image was prepared using residues from 200 to 280, omitting the solvent molecules.



KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION

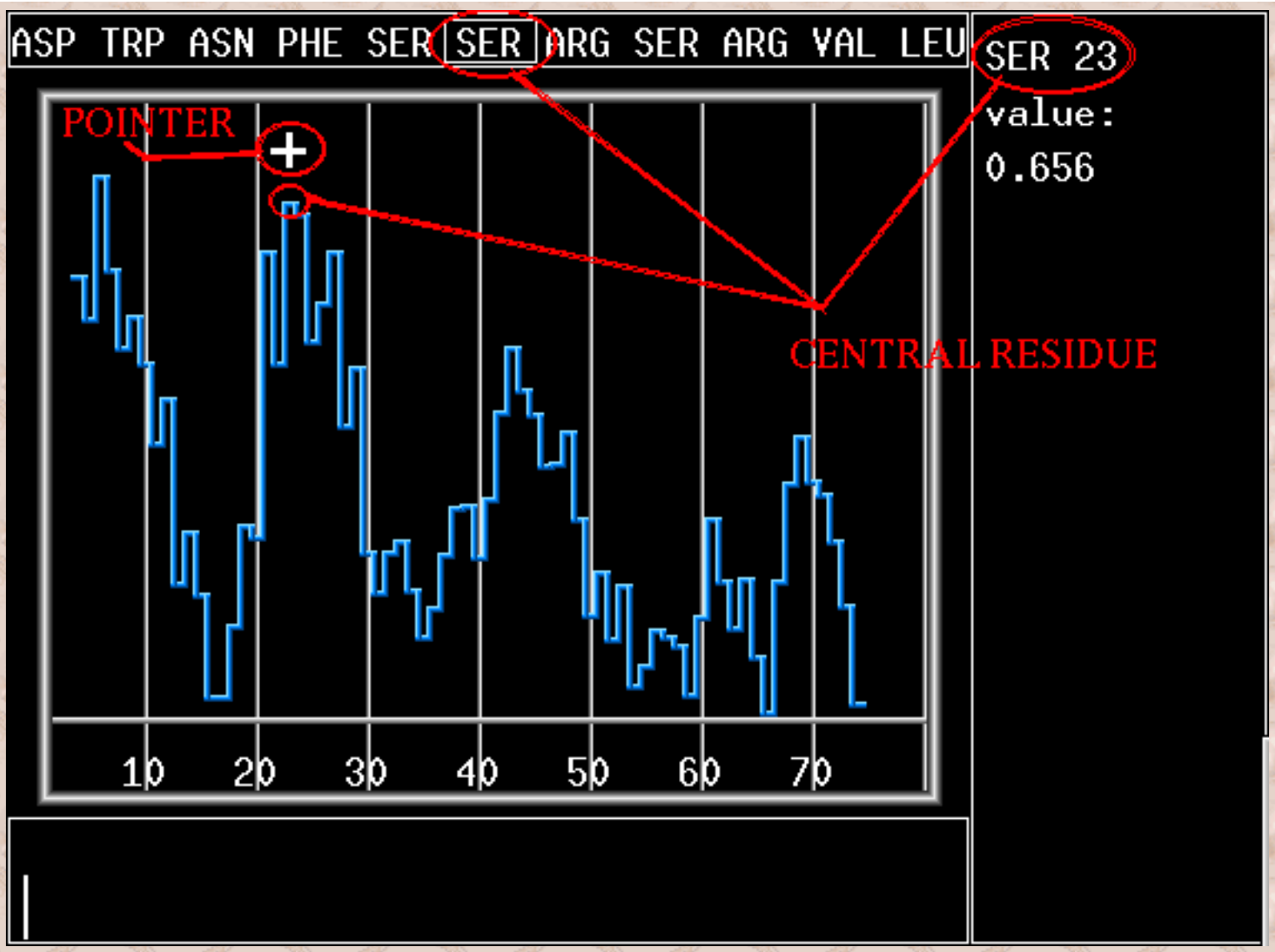
OFF	OFF	Return to the main drawing mode (draw atomic coordinates). Instead using this command, you can hit the ESCAPE key.
HYD	HYDROPHOBICITY	Draw averaged hydrophobicity.
MOM	MOMENT	Draw hydrophobic moment.

PARAMETERS

PARAMETER (SHORT)	DESCRIPTION
start_index	Serial index of the first residue.
end_index	Serial index of the last residue.

MOUSE USAGE

Mouse may be used to retrieve the information about averaged hydrophobicity and hydrophobic moment for a given residue. This residue is treated as the central residue of the current sliding window. The numerical data, along with residue name and serial number will be visible in the output window (bottom right corner). The sequence neighborhood of this residue will be visible above the plot. The information will be associated with the residue which has the same horizontal position (x coordinate) as the mouse pointer.



EXAMPLES

COMMAND	DESCRIPTION
load 2por.pdb seq from 1 scale eis win 7 angle 180 plot hyd mom 1-300	Load porin coordinates, copy sequence to the main sequence buffer, select Eisenberg hydrophobicity scale, set window width to 7 and set angle to 180 degrees. Draw averaged hydrophobicity and hydrophobic moment for residues from 1 to 300.
seq load sample.fasta scale eis angle 100 plot mom	Read the file sample.fasta, which contains the protein sequence in FASTA format (one letter code), select Eisenberg scale, set angle to 100 and draw hydrophobic moment.
plot off	Return to default drawing mode. Instead using this command, you can hit the ESCAPE key.

MATHEMATICAL BACKGROUND

Both the averaged hydrophobicity and the hydrophobic moment are calculated using a rectangular sliding window. If there are N residues in the sliding window, the averaged hydrophobicity is equal to:

$$\frac{1}{N}\sum_{i=0}^{N} h_i$$

Hydrophobic moment is equal to:

$$\frac{1}{N}\left\{\left[\sum_{i=1}^{N} h_i sin\,(i\alpha)\right]^2 + \left[\sum_{i=1}^{N} h_i cos\,(i\alpha)\right]^2\right\}^{\frac{1}{2}}$$

If you are searching for amphipatic alpha helices, set alpha to 100 degrees. To identify amphipatic beta strands, use 180 degrees. You can change alpha by using the command ANGLE.

NOTES

(1) Instead using the command PLOT OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) PLOT uses only the sequence stored to the main sequence buffer. Read description of the command SEQ (SEQUENCE) to learn how to initialize this buffer.

(3) If you plot both the averaged hydrophobicity and the hydrophobic moment, the output window (bottom right corner) will contain the hydrophobic moment of the central residue.

(3) Every time you change hydrophobicity scale, don't forget to refresh the plot (i.e., execute the command PLOT once more).

RELATED COMMANDS

SEQUENCE is used to copy, define or load the sequence. ANGLE defines the rotation angle between adjacent residues. SCALE is used to specify the hydrophobicity scale. WINDOW is used to set the sliding window width.

POS, POSITION

NAME

POS, POSITION - move the origin of the internal coordinate system to the specified position.

SYNOPSIS

POS x y z
POSITION x y z

DESCRIPTION

An internal coordinate system is assigned to each structure. The command POS (POSITION) sets the position of this origin. Three coordinates (x, y and z) should be specified.

Initially, the position of geometric center is used as the internal system origin for each structure. When loaded, this origin is set into the point (0, 0, 0).

RELATED COMMANDS

CEN (CENTER) redefines the internal system origin. MOV (MOVE) chooses the object which should be moved (structure, plane, membrane or all).

RAM, RAMACHANDRAN

NAME
RAM, RAMACHANDRAN - draw Ramachandran plot.

SYNOPSIS
RAM
RAM SEL
RAM OFF
RAMACHANDRAN
RAMACHANDRAN SEL
RAMACHANDRAN OFF

DESCRIPTION
Draw Ramachandran plot (only for proteins). The main chain torsion angles, phi and psi, are used to prepare two-dimensional scatter plot. Residues for which both phi and psi angle may be calculated will be shown as small circles. The horizontal axis (abscisa) is used for phi values, while the vertical axis (ordinate) is used for psi values. Blue color is used for trans residues, magenta for cis residues and red for bad residues. Trans residues are drawn first, followed by cis residues. Bad residues are drawn last. A residue is treated as bad if peptide unit associated with this residue is not planar. Peptide unit is considered as non-planar if it is twisted for more than 20 degrees. Terminal residues will be missing, because at least one of dihedral angles is not defined for such residues.

DIHEDRAL ANGLES
Click here for definitions of dihedral angles.

KEYWORDS
If used without any keyword, the command RAM will prepare the Ramachandran plot for protein structure(s) which are currently being handled ("caught"). Keyword OFF is used to switch off the Ramachandran plot, i.e. to return to the main drawing mode (atomic structure display). If keyword SEL (SELECTED) is used, only the residues which are currently selected will be visible in the Ramachandran plot. A residue is treated as selected if the first atom of this residue is selected. For proteins, this is usually N (nitrogen) atom. Here is the overview:

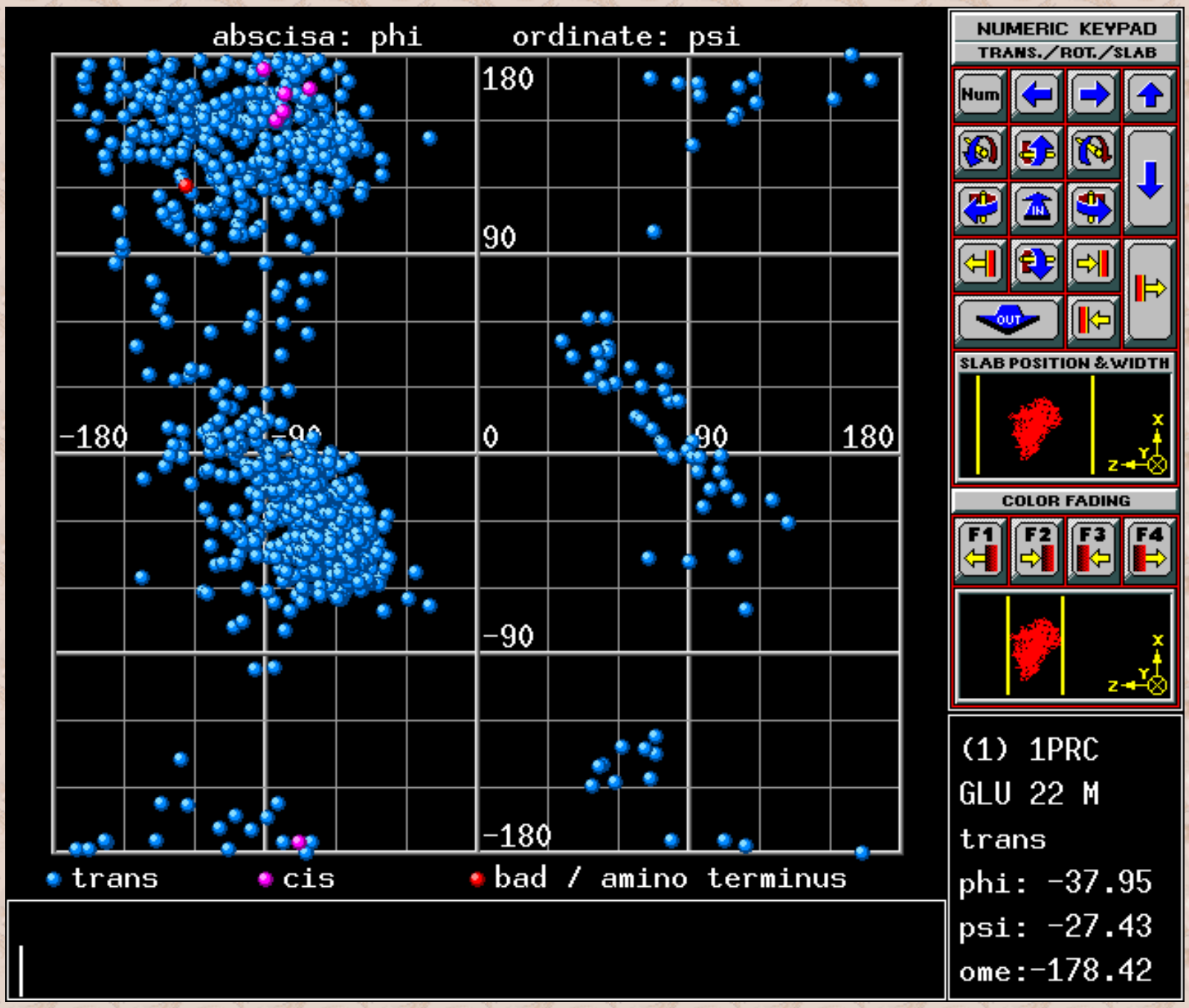
KEYWORD	DESCRIPTION
ram sel	Draw Ramachandran plot for selected residues.
ram off	Return to default drawing mode (atomic structure). Instead using this command, you can hit the ESCAPE key.

MOUSE USAGE
Pointing device (mouse) may be used to identify individual residues in Ramachandran plot. Just place the mouse pointer above the selected residue and the most important data for this residue will be shown in the output window. The output window will look like this:

```
(1) 1PRC
ALA 250 C
trans
phi: -52.91
psi:  -2.21
ome:-179.68
```

EXAMPLE OF RAMACHANDRAN PLOT

The example below show the Ramachandran plot for photosynthetic reaction center from Rhodopseudomonas viridis.



EXAMPLES

COMMAND	DESCRIPTION
ram	Draw Ramachandran plot for all residues.
ram off	Return to default drawing mode (atomic structure).
ram sel	Draw Ramachandran plot for selected residues.
sel pro ram sel	Select all prolines and draw Ramachandran plot for prolines.
sel cis ram sel	Select all residues in cis conformation and draw Ramachandran plot for them.
sel bad ram sel	Select bad residues (peptide unit not planar) and draw Ramachandran plot.
sel tra ram sel	Select all residues in trans conformation and draw Ramachandran plot.

NOTES

(1) Instead using the command RAMA OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) G. N. Ramachandran devised in the late 1960's the steric constraints for amino acid residues in proteins. As the number of high resolution structures is increasing, it appears evident that these old constrains are becoming obsolete. If you are interested in this problem, read this article:

http://xray.bmc.uu.se/~gerard/rama/ramarev.html

RELATED COMMANDS

SEL may be used to select a portion of protein structure, to reduce the amount of data in Ramachandran plot.

REF, REFRESH

NAME
REF, REFRESH - switch refreshing on or off.

SYNOPSIS
REF
REFRESH
REF OFF
REFRESH OFF

DESCRIPTION
Most of garlic commands require redrawing of the main window. This may slow down the execution of the program. To save some time, the refreshing may be switched off. Just execute the command:

ref off

(the long form is REFRESH OFF). After that, a number of time-consuming commands may be executed, and refreshing may be turned on again. To switch on refreshing, execute the command REF without the keyword OFF:

ref

This trick is very useful with scripts. Put the command REF OFF close to the top of the script and do not forget to put the command REF (without the keyword OFF!) to the bottom of the script. Try the sample scripts atoms.script , bonds.script and colors.script . The refreshing trick is used in these scripts.

If refreshing is switched off, you will see the message in the middle of the main garlic window (yellow text "Refreshing off" on red background).

Garlic Tutorial

Script 1 (atoms.script) - Drawing styles for atoms

This script shows the available drawing styles for atoms. Note that nothing is visible for style "0" (row one, column one)! The file trp.pdb is required as input. You can mark, copy and paste this script to your local host (create the file atoms.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe atoms.script

The sample image is at the bottom of this page.

```
# Show all drawing styles used to draw atoms. Bonds are hidden!
# This script requires garlic version 1.2 or later!

# Atom style 0:
load trp.pdb
pos -24 -15 0
ato 0
bon 0
tag "0"

# Now inform user that refreshing is off:
title 1 50 50 "Please be patient ..."

# Switch refreshing off:
refresh off

# Atom style 1:
load trp.pdb
pos -12 -15 0
ato 1
bon 0
tag "1"

# Atom style 2:
load trp.pdb
pos 0 -15 0
ato 2
```

```
bon 0
tag "2"

# Atom style 3:
load trp.pdb
pos 12 -15 0
ato 3
bon 0
tag "3"

# Atom style 4:
load trp.pdb
pos 24 -15 0
ato 4
bon 0
tag "4"

# Atom style 5:
load trp.pdb
pos -24 -5 0
ato 5
bon 0
tag "5"

# Atom style 6:
load trp.pdb
pos -12 -5 0
ato 6
bon 0
tag "6"

# Atom style 7:
load trp.pdb
pos 0 -5 0
ato 7
bon 0
tag "7"

# Atom style bal:
load trp.pdb
pos 12 -5 0
ato bal
bon 0
tag "bal (ball)"

# Atom style ba2:
```

```
load trp.pdb
pos 24 -5 0
ato ba2
bon 0
tag "ba2"

#Atom style small:
load trp.pdb
pos -24 5 0
ato sma
bon 0
tag "sma (small)"

# Atom style sm2:
load trp.pdb
pos -12 5 0
ato sm2
bon 0
tag "sm2"

# Atom style covalent:
load trp.pdb
pos 0 5 0
ato cov
bon 0
tag "cov (covalent)"

#Atom style co2:
load trp.pdb
pos 12 5 0
ato co2
bon 0
tag "co2"

#Atom style spacefill:
load trp.pdb
pos -24 15 0
ato spa
bon 0
tag "spa (spacefill)"

#Atom style sp2:
load trp.pdb
pos -12 15 0
ato sp2
bon 0
```

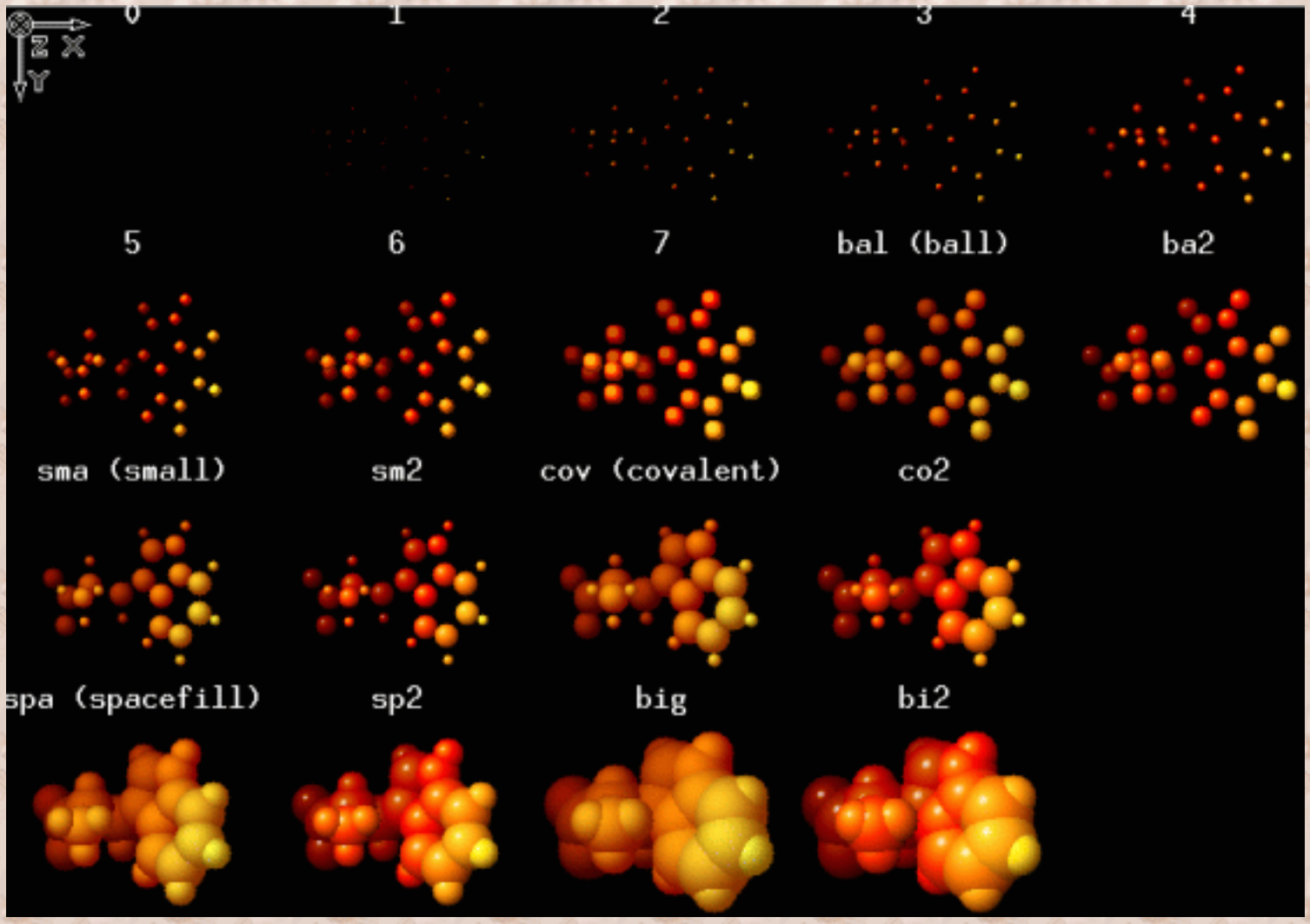
```
tag "sp2"

#Atom style big:
load trp.pdb
pos 0 15 0
ato big
bon 0
tag "big"

#Atom style bi2:
load trp.pdb
pos 12 15 0
ato bi2
bon 0
tag "bi2"

# Hide the title:
title 1 off

# Switch refreshing on:
refresh
```


0
1
2
3
4
Z X
Y
5
6
7
bal (ball)
ba2
sma (small)
sm2
cov (covalent)
co2
spa (spacefill)
sp2
big
bi2

Garlic Tutorial

Script 2 (bonds.script) - Drawing styles for bonds

This script shows the available drawing styles for bonds. The file trp.pdb is required as input. You can mark, copy and paste this script to your local host (create the file bonds.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe bonds.script

The sample image is at the bottom of this page.

```
# Show all drawing styles used to draw bonds. Atoms are hidden,
# except for nice bonds!
# This script will work if you use default .garlicrc script.
# This script requires garlic version 1.2 or later!

# Bond style 1:
load trp.pdb
pos -12 -6 -40
ato 0
bon 1
tag "1"

# Now inform user that refreshing is off:
title 1 50 50 "Please be patient ..."

# Switch refreshing off:
refresh off

# Bond style 2:
load trp.pdb
pos 0 -6 -40
ato 0
bon 2
tag "2"

# Bond style 3:
load trp.pdb
pos 12 -6 -40
ato 0
bon 3
tag "3"

# Bond style 4:
```

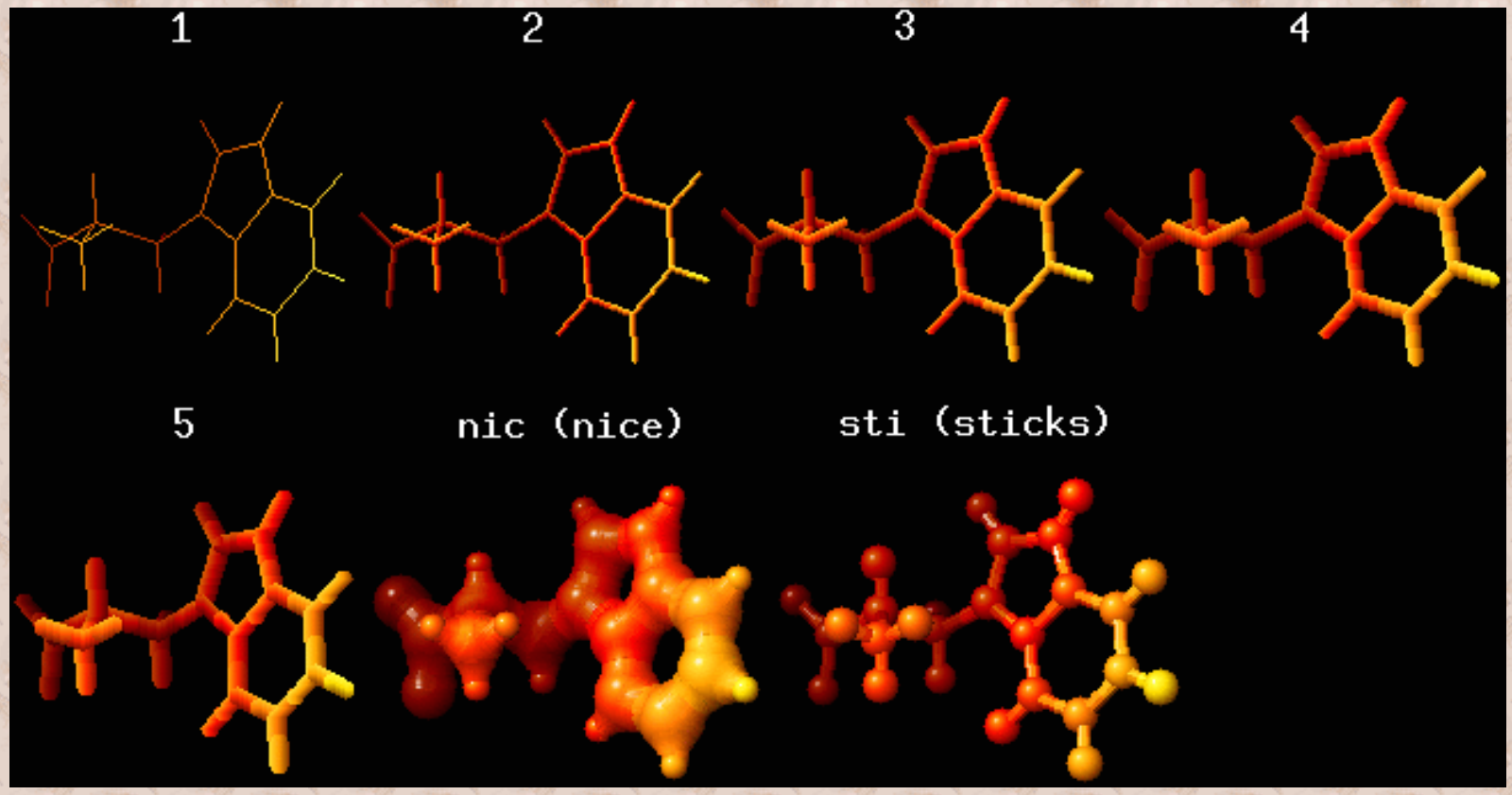
```
load trp.pdb
pos -12 6 -40
ato 0
bon 4
tag "4"

# Bond style 5:
load trp.pdb
pos 0 6 -40
ato 0
bon 5
tag "5"

# Bond style nice:
load trp.pdb
pos 12 6 -40
ato co2
bon nice
tag "nic (nice)"

# Hide the title:
title 1 off

# Switch refreshing on:
refresh
```



Garlic Tutorial

Script 3 (colors.script) - Predefined color schemes

This script shows some selected color schemes. All schemes shown here are hard-coded in the program. The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file colors.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe colors.script

The sample image is at the bottom of this page.

```
# Show predefined color schemes, version 1.2 and later versions.
# This script will work if you use default .garlicrc script.
# This script requires garlic version 1.2 or later!

load trp.pdb
pos -18 -15 0
ato sp2
bon nice
color red

# Now inform user that refreshing is off:
title 1 50 50 "Please be patient ..."

# Switch refreshing off:
refresh off

load trp.pdb
pos -6 -15 0
ato sp2
bon nice
color green

load trp.pdb
pos 6 -15 0
ato sp2
bon nice
color blue
```

```
load trp.pdb
pos 18 -15 0
ato sp2
bon nice
color yellow

load trp.pdb
pos -18 -5 0
ato sp2
bon nice
color cyan

load trp.pdb
pos -6 -5 0
ato sp2
bon nice
color magenta

load trp.pdb
pos 6 -5 0
ato sp2
bon nice
color white

load trp.pdb
pos 18 -5 0
ato sp2
bon nice
color yellow-green

load trp.pdb
pos -18 5 0
ato sp2
bon nice
color cyan-green

load trp.pdb
pos -6 5 0
ato sp2
bon nice
color cyan-blue

load trp.pdb
pos 6 5 0
ato sp2
```

```
bon nice
color magenta-blue

load trp.pdb
pos 18 5 0
ato sp2
bon nice
color magenta-red

load trp.pdb
pos -18 15 0
ato sp2
bon nice
color orange

load trp.pdb
pos -6 15 0
ato sp2
bon nice
color hot

load trp.pdb
pos 6 15 0
ato sp2
bon nice
color cold

load trp.pdb
pos 18 15 0
ato sp2
bon nice
color cpk

# Hide the title:
title 1 off

# Switch refreshing on:
refresh
```

REG, REGISTER

NAME
REG, REGISTER

SYNOPSIS
REG
REGISTER

DESCRIPTION
Register garlic: send a short e-mail to the author. This command will fail if your machine is not connected to the Internet. The only content of the message will be the word 'Hi!'. Your registration will not be abused, i.e. your e-mail address will not be given to spammers or anyone else. The registration will be used just to count garlic users.

If your machine is not connected to the Internet, send an e-mail from some other machine. Questions, comments and suggestions are welcome.

The author may be reached at:
zucic@garlic.mefos.hr
zucic@mia.os.carnet.hr

Author's home page:
http://garlic.mefos.hr/zucic

REGISTER GARLIC - by registering, you are supporting further development of this program!

RES, RESTRICT

NAME
RES, RESTRICT - restrict the current selection.

SYNOPSIS
RES chain_identifiers/residue_serials/residue_names/atom_names
RES residue_ranges
RES residue_names
RES ATO atomic_ranges
RES keyword
RES ELE chemical_symbol
RESTRICT chain_identifiers/residue_serials/residue_names/atom_names
RESTRICT residue_ranges
RESTRICT residue_names
RESTRICT ATOMS atomic_ranges
RESTRICT keyword
RESTRICT ELEMENT chemical_symbol

DESCRIPTION
Restrict the current selection. Atoms which do not satisfy the specified cryteria are excluded from selection. Four types of restriction cryteria may be used:

(1) detailed selection;
(2) restriction by residue serial numbers;
(3) restriction by residue names;
(4) restriction selection (by keyword);
(5) restriction by chemical symbol;
(6) restriction by atom serial number.

DETAILED RESTRICTION
In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The string should contain exactly three slashes, separating different data types:

chain_identifiers/residue_serials/residue_names/atom_names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to specify all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from restriction.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers.

For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from restriction.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from restriction. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to specify all atoms, while EXC may be used to exclude some atoms from this specification. Examples:

res a/*/*/*	Leave only atoms which belong to chain A.
res * exc m/*/*/ca	Leave only CA atoms which belong to chain M.
res */*/*/* exc ca,c,n,o	Remove CA, C, N and O atoms from the selection.
res a/* exc 72-112/*/ca	Leave only CA atoms which belong to chain A, but exclude residues 72-112.

RESTRICTION BY RESIDUE SERIAL NUMBERS

In this type of selection restriction, residue numbers, residue ranges or residue names may be specified. The restriction cryteria should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

res 1-100	Leave only atoms which belong to residues from 1 to 100.
res 1-100 exc 20-40	Leave only atoms which belong to residues 1-100, but exclude 20-40.
res 1, 4, 8, 11-48 exc 20-32	Leave atoms which belong to residues 1, 4, 8, 11-48 but exclude residues 20-32.

RESTRICTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

res phe,tyr,trp	Restrict selection to PHE, TYR and TRP.

RESTRICTION BY ATOMIC SERIAL NUMBERS

To restrict the current selection to a single atom by the atomic serial number, combine the command RES (RESTRICT) and the keyword ATO (ATOMS). For example, to restrict the selection to the atom number 102 type:

res ato 102

The same keyword may be used to restrict the current selection to a range of atoms or to two or more ranges. Examples:

res ato 1-100	Restrict the current selection to atoms which have serial numbers in the range between 1 and 100.
res 1-20 40-50	Restrict the current selection to atoms which have serial numbers between 1 and 20 and between 40 and 50.

Do not combine the keywords EXC (EXCLUDE) and ATO (ATOMS).

SPECIAL RESTRICTION KEYWORDS

Some special keywords may be combined with RES to specify residues or atoms according to some properties. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted. COM (COMPLEMENT) may be specified, but restriction to complement means that nothing will be left in the selection. Examples:

res * res all	Leave the selection unchanged (trivial, useless).
res abo res above	Restrict to atoms above the plane.
res aci res acidic	Leave only acidic amino-acids in the selection (GLU and ASP).
res ali res aliphatic	Leave only aliphatic amino acids (ILE, LEU and VAL).
res alt	Restrict to atoms at alternate positions.
res bad	Restrict selection to bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
res bas res basic	Leave only basic amino acids (ARG, LYS and HIS).
res bel res below	Restrict to atoms below the plane.
res cha res charged	Leave only charged amino acids (ARG, LYS, HIS, GLU and ASP).
res cis	Restrict selection to cis residues.
res com res complement	Leave only atoms which were not select previously.

res het res hetero	Leave only hetero atoms (heme groups, water etc.).
res pho res hydrophobic	Leave only hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
res mai res main_chain	Leave only main chain atoms (CA, C, N and O).
res mod serial_number res model serial_number	Restrict to a model specified by serial_number. NMR structure is a set of models. Example: res mod 1
res neg res negative	Leave only negatively charged amino acids (GLU and ASP).
res pol res polar	Leave only polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
res seq res sequence	Restrict to sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
res pos res positive	Leave only positively charged amino acids (ARG, LYS and HIS).
res sid res side_chains	Leave only atoms which belong to side chains (all except CA, C, N and O).
res sma res small	Leave only small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
res sph res sphere	Restrict to the atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
res tin res tiny	Leave only tiny amino acids (GLY,ALA and SER).
res tra res trans	Restrict selection to trans residues.
sel tri sel triplet	If there are three (or more) positively charged residues in a fragment of up to five protein residues, restrict the current set of selected atoms to these three residues. Detailed explanation may found in the article: D. Juretic, L. Zoranic and D. Zucic, Basic charge clusters and predictions of membrane protein topology, Journal of Chemical Information and Computer Sciences 42, No. 3, 620-632 (2002).

RESTRICTING SELECTION TO THE SPECIFIED CHEMICAL ELEMENT

To restrict the selection to certain chemical element, use the keyword ELEMENT (short form: ELE) and

the standard chemical symbol. To restrict your selection to iron atoms, for example, you should type the following command:

res ele fe

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and "quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1. The interatomic distance is not important! Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. Note that symbols J and Q are not used in the periodic table of elements.

NOTES

(1) The command RESTRICT resets the editing mode to default (no editing).

RELATED COMMANDS

SELECT overwrites the previous selection. ADD expands the previous selection.

ROT, ROTATE

NAME
ROT, ROTATE - rotate the structure for the given angle around the given axis.

SYNOPSIS
ROT axis angle

DESCRIPTION
Rotate the structure. The axis should be specified with one letter (x, y or z) and the angle should be given in degrees.

EXAMPLES

COMMAND	DESCRIPTION
rot z 90	Rotate around z for 90 degrees (counterclockwise).
rot x -0.5	Rotate around x for -0.5 degrees (clockwise).

SCA, SCALE

NAME
SCA, SCALE - select hydrophobicity scale.

SYNOPSIS
SCA keyword
SCALE keyword

DESCRIPTION
The command SCALE selects the specified hydrophobicity scale. At present, three scales are available: Eisenberg normalized consensus scale, Kyte-Doolittle hydropathy scale and White octanol scale (experimental). The scale is assigned to the structure which is currently being handled (the structure which was caught using the command CATCH). It is also used as default hydrophobicity scale for the sequence in the main sequence buffer. The hydrophobicity scale is used to calculate the averaged hydrophobicity and hydrophobic moment. It may be also used to color the protein structure according to hydrophobicity.

Hard-coded program default is Eisenberg scale.

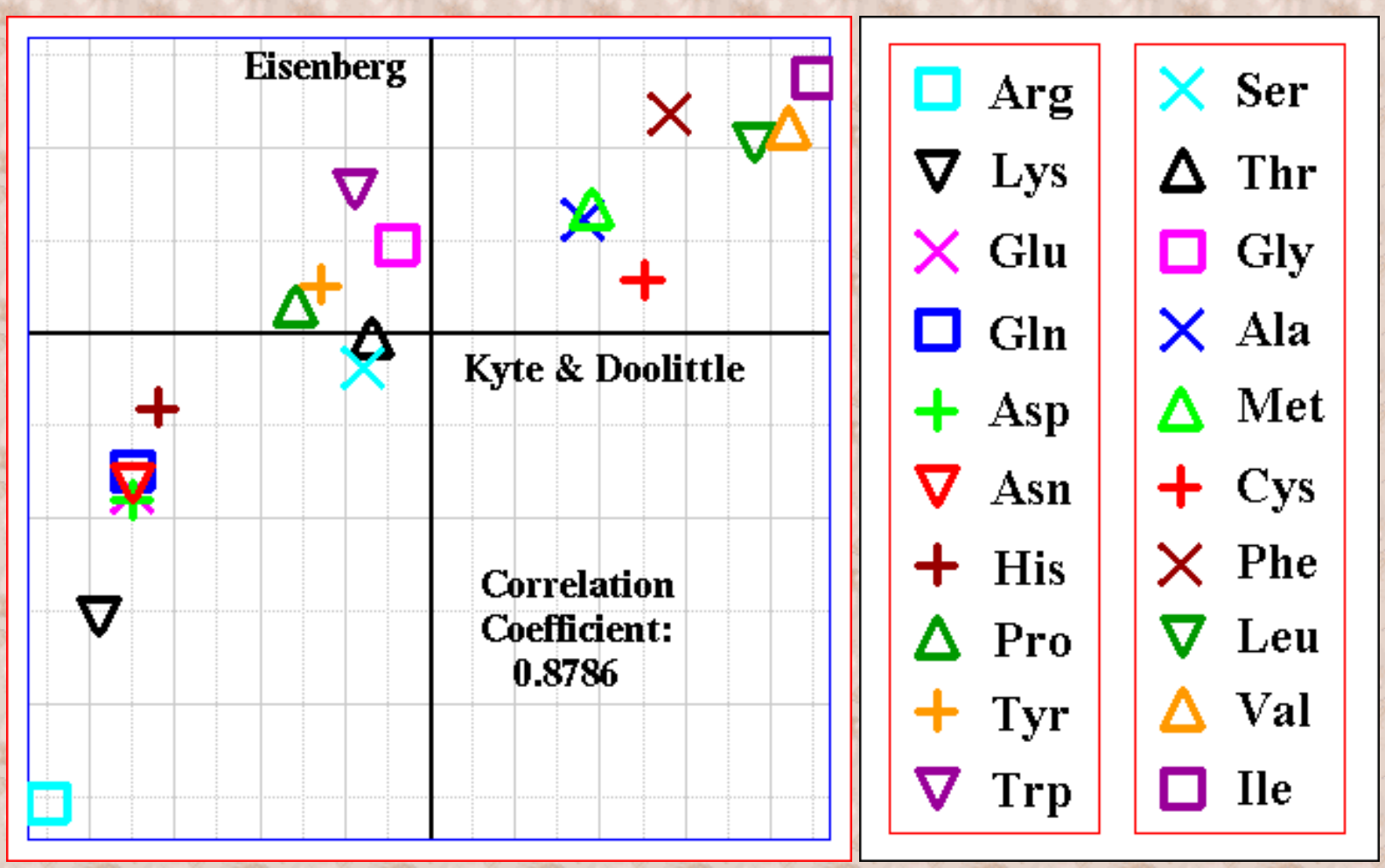
KEYWORDS

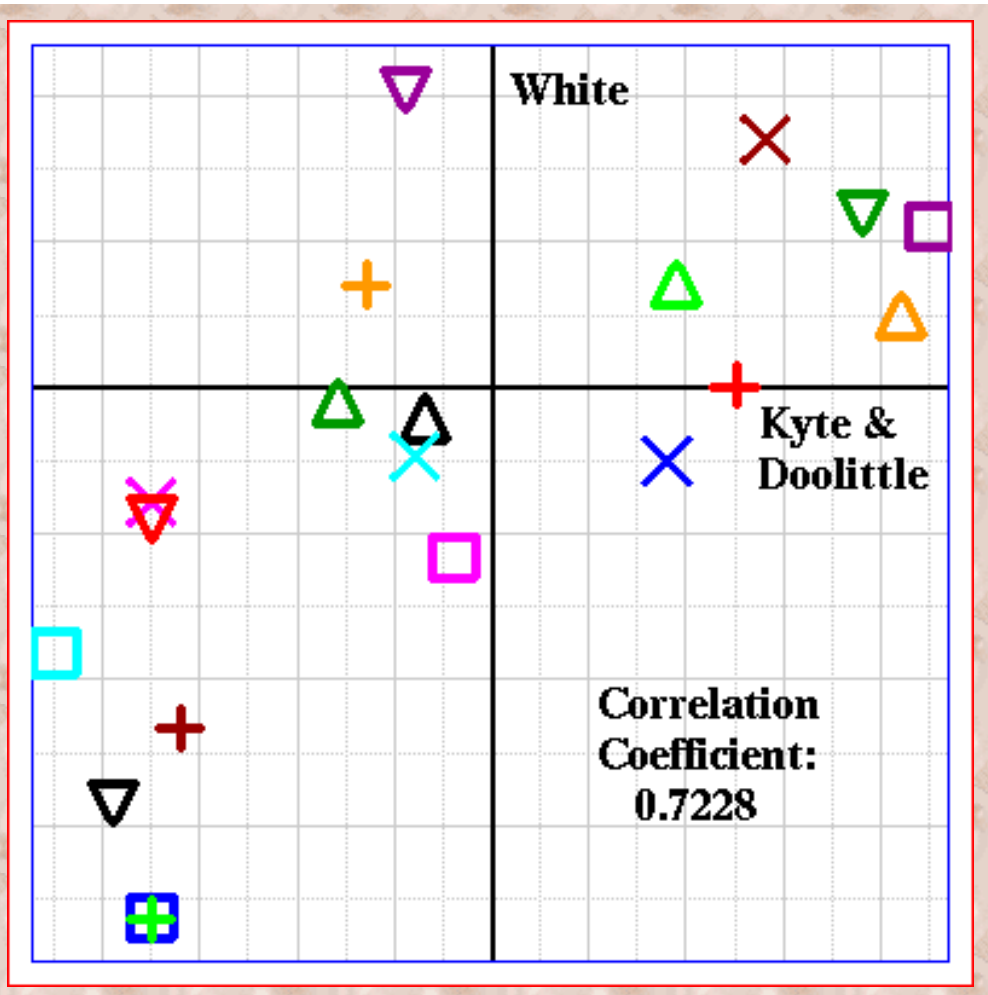
KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
EIS	EISENBERG	Use Eisenberg normalized consensus hydrophobicity scale.
KD	KD	Use Kyte-Doolittle hydropathicity scale.
WHI	WHITE	Use octanol scale (Steven White group, experimental data).

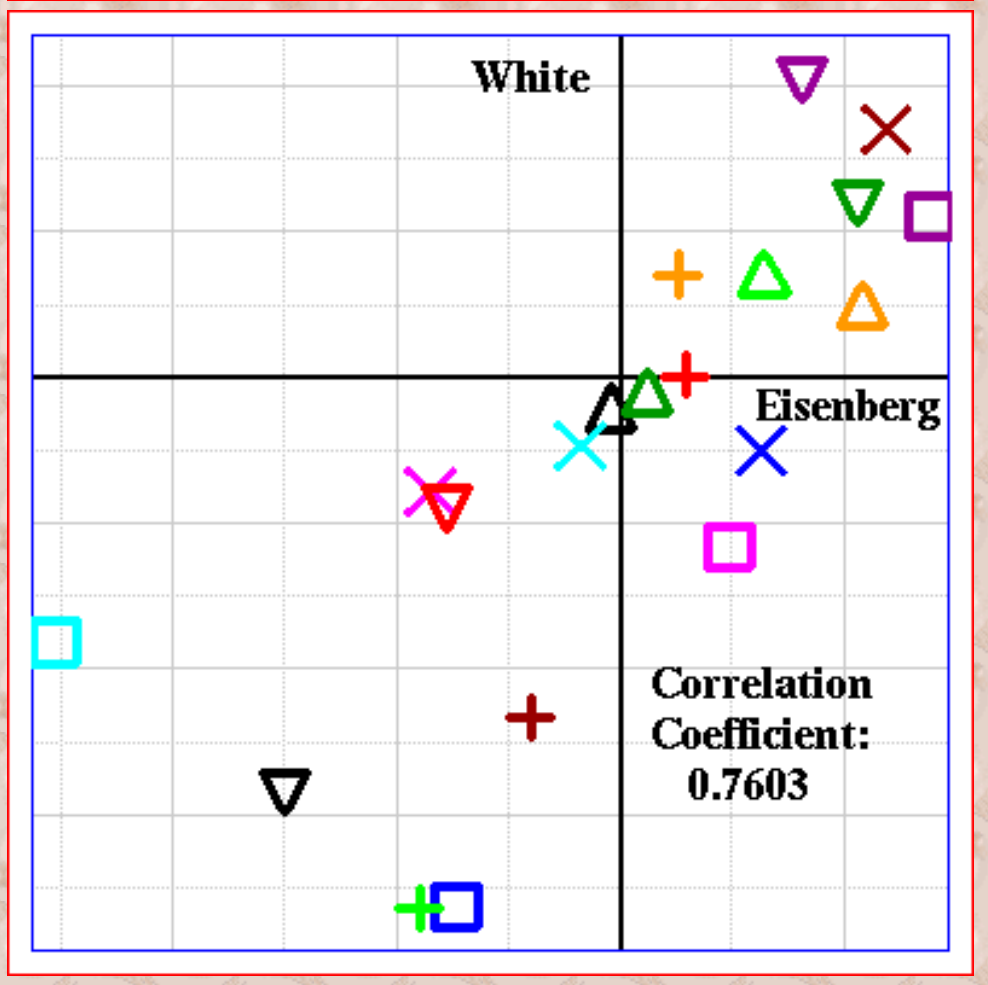
HYDROPHOBICITY SCALES
The table below contains numeric data for three hydrophobicity scales which are used in garlic. Correlation coefficients and plots are also given. The original White octanol scale contains free energy changes for a transfer of whole residues from water to octanol. In garlic, these free energy changes are multiplied by minus one and used as hydrophobicity values. The experimental values and nice theoretical explanations may be found at:
http://blanco.biomol.uci.edu/hydrophobicity_scales.html

NAME	EIS	KD	WHI
ALA	0.62	1.80	-0.50
ARG	-2.53	-4.50	-1.81
ASN	-0.78	-3.50	-0.85
ASP	-0.90	-3.50	-3.64
CYS	0.29	2.50	0.02
GLN	-0.85	-3.50	-0.77
GLU	-0.74	-3.50	-3.63
GLY	0.48	-0.40	-1.15
HIS	-0.40	-3.20	-2.33

ILE	1.38	4.50	1.12
LEU	1.06	3.80	1.25
LYS	-1.50	-3.90	-2.80
MET	0.64	1.90	0.67
PHE	1.19	2.80	1.71
PRO	0.12	-1.60	-0.14
SER	-0.18	-0.80	-0.46
THR	-0.05	-0.70	-0.25
TRP	0.81	-0.90	2.09
TYR	0.26	-1.30	0.71
VAL	1.08	4.20	0.46
ASX	-0.84	-3.50	-2.25
GLX	-0.80	-3.50	-2.20
UNK	0.00	-0.49	-0.52




White
Kyte &
Doolittle
Correlation
Coefficient:
0.7228


White
Eisenberg
Correlation
Coefficient:
0.7603

EXAMPLES

COMMAND	DESCRIPTION
sca eis	Use the scale made by David Eisenberg.
sca whi	Use the experimental scale made by Steven White and coworkers.

NOTES

(1) Many hydrophobicity scales may be found in literature. However, most of these scales are mutually highly correlated.

RELATED COMMANDS

PLOT is used to draw averaged hydrophobicity and hydrophobic moment. COLOR HYPHOB is used to color the structure according to hydrophobicity of residues.

REFERENCES

(1) Kyte, J. and Doolittle, R. F. (1982). J. Mol. Biol. 157, p. 105.
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(3) Wimley, W. C. and White, S. H. (1996). Nature Struct. Biol. 3, p. 842.
(4) Wimley, W. C., Creamer, T. P. and White, S. H. (1996). Biochemistry 35, p. 5109.
(5) White, S. H. and Wimley, W. C. (1998). Biochim. Biophys. Acta 1376, p 339.
(6) White, S. H. and Wimley, W. C. (1999). Annu. Rev. Biophys. Biomol. Struc. 28, p. 319.

SEL, SELECT

NAME
SEL, SELECT - select specified atoms. Overwrite the previous selection.

SYNOPSIS
SEL chain_identifiers/residue_serials/residue_names/atom_names
SEL residue_ranges
SEL residue_names
SEL ATO atomic_ranges
SEL keyword
SEL ELE chemical_symbol
SELECT chain_identifiers/residue_serials/residue_names/atom_names
SELECT residue_ranges
SELECT residue_names
SELECT ATOMS atomic_ranges
SELECT keyword
SELECT ELEMENT chemical_symbol

DESCRIPTION
Select specified atoms. Atoms are selected according to the specified cryteria. Six types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword);
(5) selection by chemical symbol;
(6) selection by atom serial number.

DETAILED SELECTION
In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain_identifiers/residue_serials/residue_names/atom_names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers.

For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

sel a/*/*/*	Select all atoms from chain A.
sel * exc m/*/*/ca	Select CA atoms from all chains except chain M.
sel */*/*/* exc ca,c,n,o	Select all atoms except CA, C, N and O.
sel a/* exc 72-112/*/ca	Select CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

sel 1-100	Select residues from 1 to 100.
sel 1-100 exc 20-40	Select residues 1-100 but exclude 20-40.
sel 1, 4, 8, 11-48 exc 20-32	Select residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY ATOMIC SERIAL NUMBERS

To select a single atom by the atomic serial number, combine the command SEL (SELECT) and the keyword ATO (ATOMS). For example, to select the atom number 102 type:

sel ato 102

The same keyword may be used to select a range of atoms or two or more ranges. Examples:

sel ato 1-100	Select atoms which have serial numbers in the range between 1 and 100.
sel 1-20 40-50	Select atoms which have serial numbers between 1 and 20 and between 40 and 50.

Do not combine the keywords EXC (EXCLUDE) and ATO (ATOMS).

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

sel phe,tyr,trp	Select PHE, TYR and TRP.

SPECIAL SELECTION KEYWORDS

Some special keywords may be combined with SEL (SELECT) to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

sel * sel all	Select all atoms (select all).
sel abo sel above	Select atoms above the plane.
sel aci sel acidic	Select acidic amino acids (GLU and ASP).
sel ali sel aliphatic	Select aliphatic amino acids (ILE, LEU and VAL).
sel alt	Select atoms at alternate positions.
sel bad	Select bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
sel bas sel basic	Select basic amino acids (ARG, LYS and HIS).
sel bel sel below	Select atoms below the plane.
sel cha sel charged	Select charged amino acids (ARG, LYS, HIS, GLU and ASP).
sel cis	Select cis residues.
sel com sel complement	Select atoms which were not selected previously.
sel het sel hetero	Select hetero atoms (heme groups, water etc.).
sel pho sel hydrophobic	Select hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).

sel mai sel main_chain	Select main chain atoms (CA, C, N and O).
sel mod serial_number sel model serial_number	Select model specified by serial_number. NMR structure is a set of models. Example: sel mod 1
sel neg sel negative	Select negatively charged amino acids (GLU and ASP).
sel pol sel polar	Select polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
sel pos sel positive	Select positively charged amino acids (ARG, LYS and HIS).
sel seq sel sequence	Select sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
sel sid sel side_chains	Select atoms which belong to side chains (all except CA, C, N and O).
sel sma sel small	Select small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
sel sph sel sphere	Select atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
sel tm	Select the transmembrane part (useful for membrane proteins).
sel abo sel above	Select atoms above the plane.
sel tra sel trans	Select trans residues.
sel tri sel triplet	If there are three (or more) positively charged residues in a fragment of up to five protein residues, select them. Detailed explanation may found in the article: D. Juretic, L. Zoranic and D. Zucic, Basic charge clusters and predictions of membrane protein topology, Journal of Chemical Information and Computer Sciences 42, No. 3, 620-632 (2002).

SELECTING CHEMICAL ELEMENTS

To select certain chemical element, use the keyword ELEMENT (short form: ELE) and the standard chemical symbol. To select iron, for example, you should type the following command:

sel ele fe

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and

"quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1. The interatomic distance is not important! Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. Note that symbols J and Q are not used in the periodic table of elements.

NOTES

(1) The command SELECT resets the editing mode to default (no editing).

(2) The keyword TM may be used to select the transmembrane part of the protein. In addition to the atoms which lay between two planes which define the membrane, some outside atoms will be taken into account, if they don't lay more than two anstroms from the nearest plane. This should ensure that some hydrophobic residues close to the edge will not be excluded from the selection. **RELATED COMMANDS**

ADD expands the previous selection. RESTRICT restrics the previous selection.

SEQ, SEQUENCE

NAME
SEQ, SEQUENCE - manipulate the content of the sequence buffer.

SYNOPSIS
SEQ = three_letters_code
SEQ LOAD filename
SEQ READ filename
SEQ FROM structure_identifier
SEQ COPY
SEQ SAVE filename
SEQ SWN filename
SEQ RESET

DESCRIPTION
The command SEQ (long form: SEQUENCE) manipulates the content of the main sequence buffer. Garlic mantains two sequence buffers: the main buffer and the reference buffer. The main sequence buffer is used to prepare the average hydrophobicity plot, the hydrophobic moment plot, helical wheel plot and for some other operations which require the sequence information. The reference sequence buffer is used for sequence comparison and other operations which require two sequences.

Both buffers store the following sequence information:
(1) The number of residues.
(2) The sequence in the form of three letters code. Uppercase letters are used.
(3) Disulfide bond flag, if information about disulfide bonds is available.
(4) Residue serial numbers.
(5) Raw hydrophobicity values (replaced by average value for exotic residues).

In addition, the main sequence buffer contains the following information:
(6) The average hydrophobicity. width.
(7) The hydrophobic moment.

As sequence information may be given independently from any structure, atomic coordinates are not required for most sequence manipulation routines. Thus, garlic may be used as the sequence analysing tool.

All version of the command SEQ, except one, are used to manipulate the content of the main sequence buffer. The only exception is SEQ COPY, which copies the content of the main sequence buffer to the reference buffer. This is the only way to store information to the reference buffer.

SEQ = three_letters_code
The command SEQ may be used with the keyword = (equal sign) to define sequence at garlic command prompt. This may be practical to define a short sequence fragment. This fragment may be used for helical

wheel plot, or to locate the given sequence fragment in a structure which is being investigated. The syntax:

SEQ = three_letters_code

Example:

seq = ala phe tyr trp asn

The sequence fragment will be converted to uppercase. The sequence is not checked for exotic residues so you can use the non-standard codes. However, the routine which assigns the hydrophobicity values will fail to recognize them. The average hydrophobicity value (calculated for the current scale) will be assigned to these residues. At present, 23 codes are recognized:

```
ALA, CYS, LEU, MET, GLU, GLN, HIS, LYS, VAL, ILE,
PHE, TYR, TRP, THR, GLY, SER, ASP, ASN, PRO, ARG,
ASX, GLX, UNK.
```

SEQ LOAD filename

The keyword LOAD (or READ, short forms LOA and REA) may be used to read the sequence from the specified file. Garlic is capable to recognize two types of input file formats: FASTA files (one letter code) and files which contain three letters code in a free format.

If input file contains the symbol > (greater than) in the first column of the first useful line, the file is treated as one letter protein code in FASTA format. Empty lines are ignored. The lines beginning with the symbol # (numbersign) in the first column are treated as comments (ignored too). Thus, the lines which are not empty and do not contain the symbol # in the first column are treated as useful.

If input file is not recognized as FASTA file, it is expected to contain the three letters code in a free format. Empty lines and all lines which contain # in the first column are ignored. All other lines are treated as useful. Digits (serial numbers, for example) are ignored. The following characters are threated as separators:
(1) space
(2) tab
(3) comma (,)
(4) semicolon (;)
(5) newline (line feed)

If input file contains at least one bad code (a residue name which consists of four letters, for example) the reading will fail. The hard-coded maximal number of residues is 20000, but it may be easily changed (see MAXRESIDUES in the header file defines.h).

Example:
load sample.fasta

SEQ FROM structure_identifier

The keyword FROM (short form: FRO) may be used to copy the sequence from the specified structure to the main sequence buffer. Only selected residues are copied. Residue is treated as selected if the first atom is selected. For proteins, this is typically N (nitrogen). Residue insertion codes are ignored! Thus, the same residue serial index (number) may appear more than once in the array of residue serial numbers.

Example:
seq from 1

SEQ COPY

The command SEQ COPY (short form: SEQ COP) copies the sequence from the main sequence buffer to the reference buffer. This is the only way to initialize the reference buffer. This command must be executed (i.e., the keyword COPY must be used) before executing commands which require two sequences for proper operation. The main sequence buffer may be initialized prior to SEQ COPY by using one of the keywords described above (=, LOAD or FROM).

Example:
seq copy

SEQ SAVE filename

The command SEQ SAVE (short form: SEQ SAV) saves the sequence to the specified file. Ten codes (each consisting of up to three letters) are written per line, separated by space. Serial numbers are not included (but see the keyword SWN).

Example:
seq save 9pap.seq

SEQ SWN filename

The command SEQ SWN saves the sequence to the specified file. Both residue names and serial numbers are written to the output file. Insertion codes will be missing! Five serial numbers and residue names are written per line, separated by space.

Example:
seq swn 9pap.seq

SEQ RESET

Reset (clear) the main sequence buffer. The command SEQ RESET (short form: SEQ RES) sets the number of residues in the main sequence buffer to zero. The storage is not freed, so the buffer may be used again later.

Example:
seq reset

RELATED COMMANDS

PLOT prepares the average hydrophobicity and/or hydrophobic moment plot. COMPARE compares two sequences. VENN draws Venn diagram. WHEEL draws helical wheel plot. SEL SEQ selects portions of the structure which contain the sequence stored to the main sequence buffer. To use any of these

commands, the main sequence buffer (to use COMPARE both buffers) must be initialized by using the command SEQ. STR defines the secondary structure and CREATE may be used to create a new peptide.

SHO, SHOW

NAME
SHO, SHOW - show selected atoms.

SYNOPSIS
SHO
SHOW

DESCRIPTION
Show selected atoms and associated bonds. Atoms and bonds drawn using style "0" will remain unvisible, but they are formally treated as visible.

RELATED COMMANDS
HIDE hides selected atoms and associated bonds.

SLA, SLAB

NAME
SLA, SLAB - change slab.

SYNOPSIS
SLA keyword
SLA FRONT shift
SLA BACK shift
SLAB keyword
SLAB FRONT shift
SLAB BACK shift

DESCRIPTION
Change the slab. Slab is used to cut the slice out from the structure and to hide the rest. Two slab surfaces are used: the front slab surface, which is the one closer to the observer and the back slab surface. There are three versions of this command:

(1) SLAB FRONT shift ----> move the front slab surface;
(2) SLAB BACK shift ----> move the back slab surface;
(3) SLAB keyword ----> switch slab off or change the type of the surfaces.

SLAB FRONT shift
This command moves the front slab surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys DEL and ENTER on numeric keypad). The shift value should be given in angstroms. Positive shift moves the front slab surface away from the observer. FRONT may be abbreviated to FRO.

SLAB BACK shift
This command moves the back slab surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys 1 and 3 on the numeric keypad). The shift value should be given in angstroms. Positive shift moves the back slab surface away from the observer. BACK may be abbreviated to BAC.

SLAB keyword
Some keywords may be used to change the type of slab surfaces and to switch slab off. Here is the list of keywords:

SHORT FORM	LONG FORM	DESCRIPTION
OFF	OFF	Switch slab off: all parts of the structure should be visible.
PLA	PLANE	Use planes as slab surfaces

SPH	SPHERE	Use spheres as slab surfaces
CYL	CYLINDER	Use cylinders as slab surfaces
HALF-SPH	HALF-SPHERE	Use spheres as slab surfaces, but hide the back half of the structure.
HALF-CYL	HALF-CYLINDER	Use cylinders as slab surfaces, but hide the back half of the structure.

For most structures, the planar slab is the best choice. Spherical and semi-spherical slab may be useful when working with large globular proteins, while cylindrical and semi-cylindrical slab is useful when working with beta-barrel proteins (like porins). The cylinder axis is parallel to y axis (vertical from users standpoint).

EXAMPLES

COMMAND	DESCRIPTION
slab off	Switch slab off
slab front 4.5	Move the front slab surface 4.5 angstroms away from the observer
slab back -2.8	Move the back slab surface 2.8 angstroms closer to the observer
slab half-sph	Change slab to semi-spherical

SSB

NAME
SSB - change drawing style for disulfide bonds.

SYNOPSIS
SSB style

DESCRIPTION
Change drawing style for disulfide bonds. Disulfide bond style is defined separately from atom style. This command does not affect the ordinary covalent bonds: the command BONDS should be used for that purpose. Note that there is no separate keyword for curved bonds and sticks (nice style): the bond curvature is defined by the command PROBE .

STYLE	THICKNESS	TYPE
0	Unvisible bonds.	Fixed width.
1	A single line.	Fixed width.
2	Three lines.	Fixed width.
3	Five lines.	Fixed width.
4	Seven lines.	Fixed width.
5	Nine lines.	Fixed width.
nic nice	Curved bonds, conical sticks or cylindrical sticks, depending both on the bond probe radius and the atomic radii. This bond style is available for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2. Do not combine the nice bond style with atomic styles 0, 1, 2, 3, 4, 5, 6, 7, BALL and BA2.	Proportional.
sti sticks	Cylindrical sticks. The command BONDS STICKS (short form: BON STI) is the most convenient way to draw bonds as sticks. Default stick radius may be changed by using the command STICKS (short form: STI).	Proportional.

NICE BONDS
Nice bonds may be curved or straight, cylindrical or conical, depending on bond probe radius. If this radius is small (like 0.8 angstroms), the bonds will be curved. Probe radius of 10 angstroms will give the straight bonds. If you want to draw the chemical bonds as cylindrical sticks, it is more convenient to use the command BONDS STICKS. If your atoms are drawn using different radii, the bonds will appear

conical. For more details, read also the text about the command BONDS .

NOTES

(1) Unvisible disulfide bonds (style 0) are not treated as hidden - they are just invisible.

(2) The nice bond style is allowed for ordinary covalent bonds and for disulfide bonds, but not for hydrogen bonds.

(4) Remember that the nice disulfide bond style works only for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2.

RELATED COMMANDS

PRO (PROBE) is used to set the probe radius. ATO (ATOMS) is used to change the drawing style for atoms. SSB is used to change the bond drawing style for disulfide bonds. STI (STICKS) is used to change the stick radius. BALLS is used to set the ball radius.

STE, STEREO

NAME
STE, STEREO - switch to stereo mode.

SYNOPSIS
STE
STEREO
STE OFF
STEREO OFF

DESCRIPTION
Switch to stereo mode. If keyword OFF is added, switch stereo off, i.e. switch to mono mode.

RELATED COMMANDS
Use MONO to switch to mono mode. It does exactly the same job as STEREO OFF.

STI, STICKS

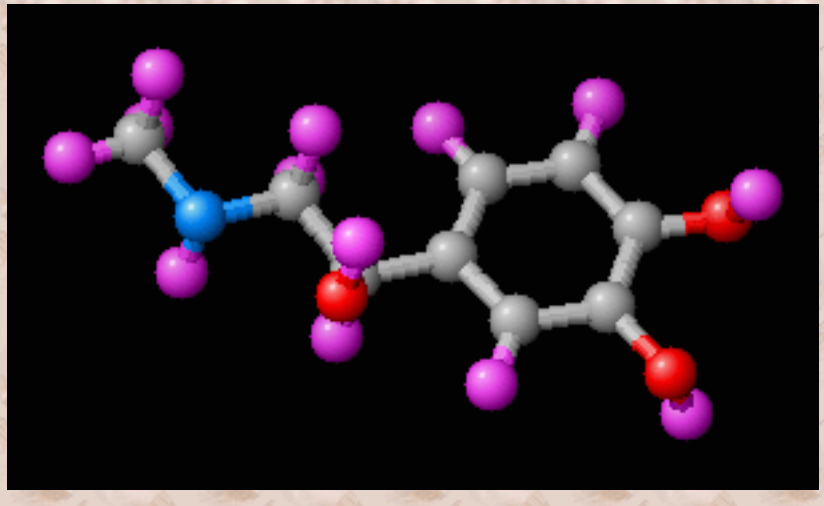
NAME
STI, STICKS - set the radius of sticks.

SYNOPSIS
STI value
STICKS value

DESCRIPTION
Set the stick radius. The stick radius is used to draw selected bonds as sticks. To draw bonds as sticks, execute the command BONDS STICKS (short form: BON STI). Default radius is 0.15 angstroms, but this may be changed in the configuration file .garlicrc .

One and only one stick radius is assigned to each loaded structure. Thus, after the command BONDS STICKS, all selected bonds will be drawn as sticks of the same radius. The stick radius may be changed separately for each structure. The command STICKS affects only the structure which is currently "caught" (see the command CATCH) .

EXAMPLES
The image below shows the adrenalin molecule drawn using default stick radius and default ball radius. Bonds were drawn as sticks (BON STI) while atoms were drawn as specular balls (ATO BA2).



RELATED COMMANDS
BONDS is used to define drawing style for bonds. SSB is used to define drawing style for disulfide bonds. ATOMS is used to define drawing style for atoms. PROBE is used to define the bond probe radius (the alternative way to draw bonds as sticks).

STR, STRUCTURE

NAME
STR, STRUCTURE - manipulate the content of the secondary structure buffer.

SYNOPSIS
STR = one_letter_code
STR LOAD filename
STR READ filename
STR FROM structure_identifier
STR COPY
STR SAVE filename
STR RESET

DESCRIPTION
The command STR (long form: STRUCTURE) manipulates the content of the main secondary structure buffer. Garlic mantains two secondary structure buffers: the main buffer and the reference buffer. The main secondary structure buffer is used to create a new structure and to replace a portion of an existing structure.

Both buffers store the following secondary structure information:
(1) The length of the secondary structure.
(2) The secondary structure (one letter codes). The codes are:

C = coil,
E = strand,
G = 3-10 helix,
H = alpha helix,
T = turn.

As the secondary structure information may be defined independently from any structure, atomic coordinates are not required for most secondary structure manipulation routines.

All version of the command STR, except one, are used to manipulate the content of the main secondary structure buffer. The only exception is STR COPY, which copies the content of the main secondary structure buffer to the reference buffer. This is the only way to initialize the reference buffer.

STR = one_letter_code
The command STR may be used with the keyword = (equal sign) to define the secondary structure at garlic command prompt. This may be practical to define the secondary structure of a short peptide or a small protein. The syntax:

STR = one_letter_code

Example:

str = ccccccchhhhhhhctttteeeeeccccccccccccccc

The secondary structure will be converted to uppercase. If at least one bad code is found, the command will fail and the main secondary structure buffer will be left empty. Space, comma and tab may be used as separators.

STR LOAD filename
The keyword LOAD (or READ, short forms LOA and REA) may be used to read the secondary structure from the specified file. The input file should be written in a format similar to FASTA. Empty lines and lines beginning with # will be ignored. The number of codes per line is arbitrary. Example:

```
1xxx_  mol:protein length:103     Sample secondary structure
CCCCCCCCCCCEEEEEEEEEEEECCCCCCCCCCCHHHHHHHHHHHHHHHHHHHHCCCCCEEEEEEEEECCCCCCCCC
CCCCCCCCHHHHHHHHHHHCCCCCCCCC
```

The following characters are threated as separators:
(1) space
(2) tab
(3) comma (,)

If input file contains at least one bad code (a residue name which consists of four letters, for example) the reading will fail. The hard-coded maximal number of residues is 20000, but it may be easily changed (see MAXRESIDUES in the header file defines.h).

Example:
load secstr.fasta

STR FROM structure_identifier
The keyword FROM (short form: FRO) may be used to copy the secondary structure from the specified atomic structure to the main secondary structure buffer. Only the structure of selected residues is copied. Residue is treated as selected if the first atom is selected. For proteins, this is typically N (nitrogen).

Example:
str from 1

STR COPY
The command STR COPY (short form: STR COP) copies the secondary structure from the main secondary structure buffer to the reference buffer. This is the only way to initialize the reference buffer. This command must be executed (i.e., the keyword COPY must be used) before executing commands which require two secondary structures for proper operation. The main secondary structure buffer may be initialized prior to STR COPY by using one of the keywords described above (=, LOAD or FROM).

Example:
str copy

STR SAVE filename
The command STR SAVE (short form: STR SAV) saves the secondary structure to the specified file. The output file will be written in FASTA format.

Example:
str save 9pap.secstr

STR RESET
Reset (clear) the main secondary structure buffer. The short form is STR RES. The command STR RESET sets the number of codes in the main secondary structure buffer to zero. The storage is not freed, so the buffer may be used again later.

Example:
str reset

RELATED COMMANDS
SEQ may be used to define the sequence. CREATE may be used to create a new peptide.

TAG

NAME
TAG - assign tag (short text) to a structure.

SYNOPSIS
TAG "tag"
TAG OFF

DESCRIPTION
If used without keyword OFF, this command assigns the specified tag to the structure which is currently handled. If used with keyword OFF, this command hides tag. Tag may contain up to 128 characters.

EXAMPLES

COMMAND	DESCRIPTION
tag "PORIN"	Add the tag "PORIN" to a structure which is currently handled (caught)
tag off	Hide tag

RELATED COMMANDS
The command LABELS assigns labels to selected atoms. TITLE adds the title to the main window. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

TBG

NAME
TBG - change the background color used to draw input and output window.

SYNOPSIS
TBG color

DESCRIPTION
Change the background color used to draw input and output window. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted.

This command does not affect the output window in the sequence comparison mode. Check the command COMPARE .

EXAMPLES

COMMAND	DESCRIPTION
tbg white	White
tbg DarkSlateGray	Dark dark slate gray
tbg #3000a0007000	Kind of green
tbg rgb:0/0/8	Dark blue
tbg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
TFG changes the foreground (text) color used in input and output window.

TFG

NAME
TFG - change the color used to draw text in input and output window.

SYNOPSIS
TFG color

DESCRIPTION
Change the color used to draw text in input and output window. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted.

This command does not affect the output window in the sequence comparison mode. Check the command COMPARE .

EXAMPLES

COMMAND	DESCRIPTION
tfg white	White
tfg DarkSlateGray	Dark dark slate gray
tfg #3000a0007000	Kind of green
tfg rgb:0/0/8	Dark blue
tfg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
TBG changes the background color used to draw input and output window.

TIT, TITLE

NAME
TIT, TITLE - add, move or remove the specified title.

SYNOPSIS
TIT identifier OFF
TIT identifier screen_x screen_y
TIT identifier screen_x screen_y "title_string"
TITLE identifier OFF
TITLE identifier screen_x screen_y
TITLE identifier screen_x screen_y "title_string"

DESCRIPTION
The keyword TITLE may be used to add, move or remove the title to or from the main window. Up to 100 titles may be added to the main window, to explain the content. The title position may be specified through screen_x and screen_y. Each title has the unique identifier. The identifier is a number between 0 and 99 (these two values are allowed too). The title string should be included into quotes.

EXAMPLES

COMMAND	DESCRIPTION
tit 8 50 50 "This is porin"	Add the title number 8 to the main window, close to the top left corner
tit 8 100 400	Move the title number 8 to a new position
tit 8 off	Remove (hide) the title number 8

RELATED COMMANDS
The command LABELS assigns labels to selected atoms. TAG assigns the specified tag to a structure. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

TRA, TRANSLATE

NAME
TRA, TRANSLATE - translate the structure for the given shift in the given direction.

SYNOPSIS
TRA axis shift

DESCRIPTION
Translate the structure. The axis should be specified with one letter (x, y or z) and the shift should be given in angstroms.

EXAMPLES

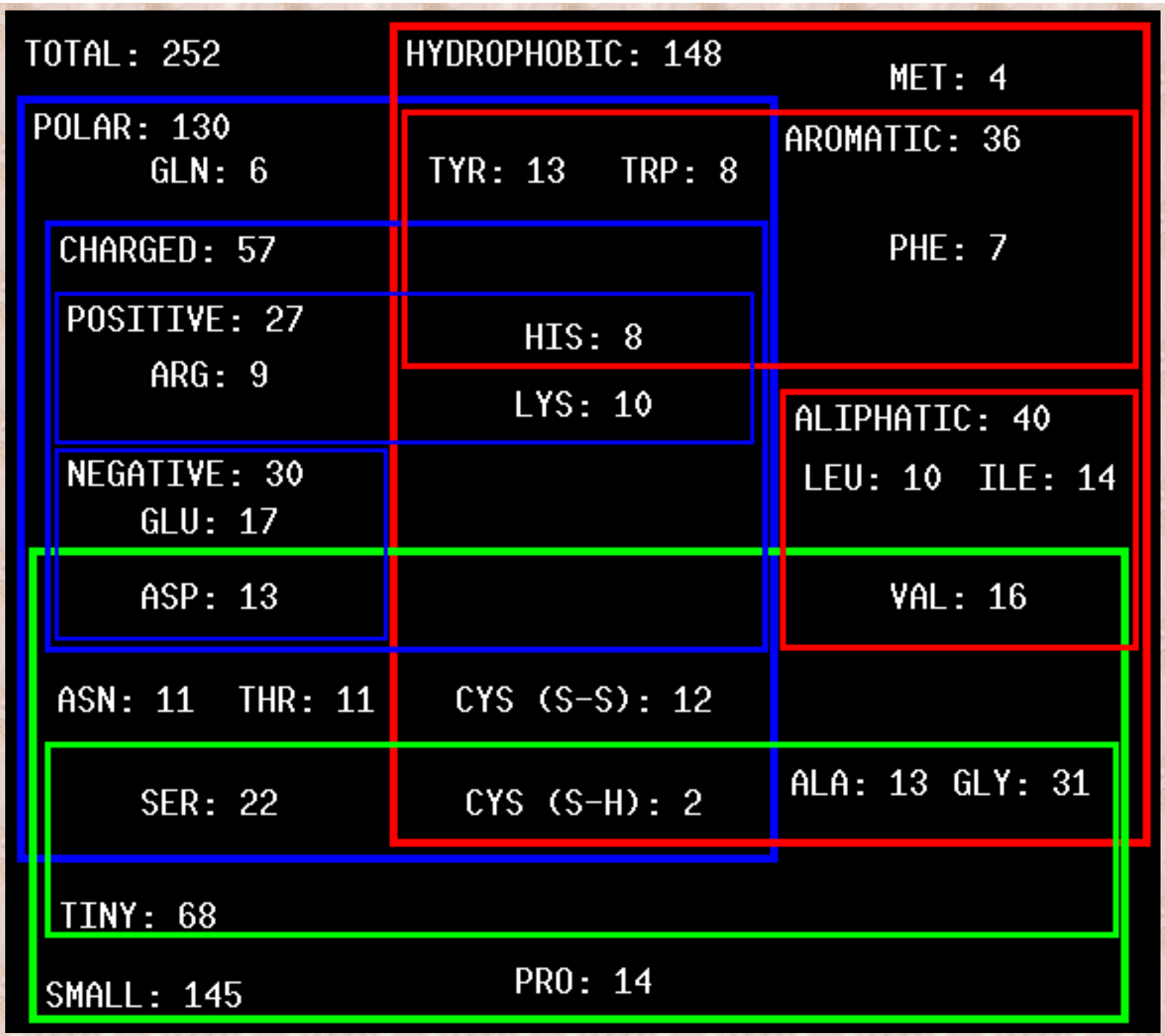
COMMAND	DESCRIPTION
tra x 40	Move to the right, 40 angstroms.
tra y -0.5	Move up, 0.5 angstroms (y points down).

VEN, VENN

NAME
VEN, VENN - draw Venn diagram.

SYNOPSIS
VEN
VEN OFF
VEN start_index end_index
VENN
VENN OFF
VENN start_index end_index

DESCRIPTION
Draw Venn diagram for the given protein sequence or sequence fragment. Venn diagram gives the quick statistical overview of the protein sequence: count of residues and residue types. It is primarily intended for students. Experts will not find this routine very interesting.



KEYWORDS AND PARAMETERS

The command VENN may be used alone, combined with the keyword OFF or with two residue serial indices. If used alone, the Venn diagram will be drawn for the entire sequence stored in the main sequence buffer. Two residue serial indices may be used to specify the residue range. The keyword OFF is used to return to the main drawing mode (structure drawing mode).

EXAMPLES

COMMAND	DESCRIPTION

load 2por.pdb seq from 1 ven	Load the specified structure (porin), copy the sequence from this structure to the main sequence buffer and draw Venn diagram.
ven 1-100	Prepare Venn diagram with counts, but only for residues with serial numbers from 1 to 100.
ven off	Return to default drawing mode. Instead using this command, you can hit the ESCAPE key.

NOTES

(1) Instead using the command VENN OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) Ven diagram is a term from the set theory, which is part of mathematics. Different sorts of Venn diagrams may be found in different branches of science.

(3) If used without any parameters, Venn diagram will be drawn for the entire sequence, including solvent molecules, which are typically included to PDB file after the protein structure. However, these residues will not be included into individual residue counts. If you want to exclude the solvent molecules from Venn diagram, check the serial index of the last protein residue. After that, use the range from residue 1 to this residue (use the actual residue number in the place of last_residue):

ven 1 last_residue

RELATED COMMANDS

SEQUENCE is used to copy, define or load the sequence.

WHE, WHEEL

NAME
WHE, WHEEL - draw helical wheel plot.

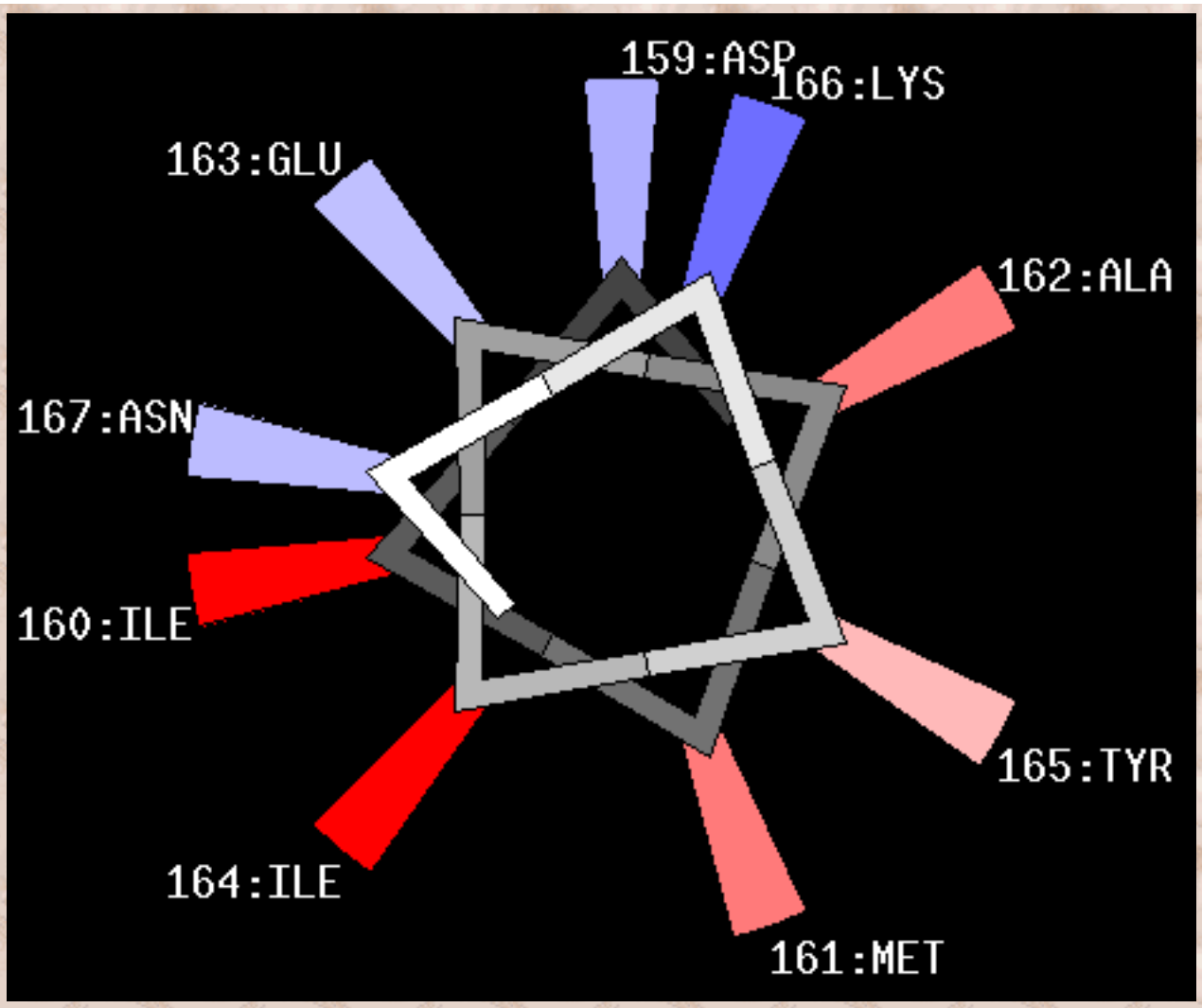
SYNOPSIS

SHORT FORM	LONG FORM
WHE	WHEEL
WHE CLO	WHEEL CLOCKWISE
WHE start_index end_index	WHEEL start_index end_index
WHE start_index end_index CLO	WHEEL start_index end_index CLOCKWISE
WHE OFF	WHEEL OFF

DESCRIPTION
Draw helical wheel plot for the given sequence or sequence fragment. Helical wheel may be used to recognize the amphiphilic character of the specified sequence fragment. The sequence from the main sequence buffer (or part of it) is used as input. Additional input: the rotation angle between adjacent residues and hydrophobicity values. The angle should correspond to certain structural motif. Default (hard-coded) angle is 100 degrees, which corresponds to alpha helix, but this may be changed to some arbitrary value, using the command ANGLE. The value of 160 degrees is suitable for beta strand and 115 or 125 is suitable for 3-10 helix.

While helical wheel may be drawn for any sequence length, it makes sense only for short sequence fragments (up to about twenty residues). Hydrophobic residues will be colored in shades of red, while hydrophilic residues will be colored blue. Color intensity depends on the hydrophobicity: very hydrophobic residues will be intensely red and weakly hydrophobic residues will be almost white. Very hydrophilic residues will be intensely blue and weakly hydrophilic residues will be almost white. The command SCALE may be used to select the hydrophobicity scale.

The command WHEEL is usually used in combination with some other commands. See the examples below.



KEYWORDS AND PARAMETERS

The command WHEEL may be used alone, combined with one of two keywords (OFF and CLOCKWISE) or with two residue serial indices. If used alone, the helical wheel will be drawn for the entire sequence stored in the main sequence buffer. If this sequence is large the plot will be useless. Two residue serial indices may be used to specify the residue range.

By default, residues are drawn counterclockwise. This arrangement of residues gives the top view of a helix. The keyword CLO (long form: CLOCKWISE) may be used to force clockwise arrangement of residues (the bottom view of a helix).

The keyword OFF is used to return to the main drawing mode (the structure drawing mode).

EXAMPLES

COMMAND	DESCRIPTION

seq = asp ile met ala glu ile scale eis angle 100 wheel	Initialize the sequence fragment, select Eisenberg hydrophobicity scale, set angle to 100 degrees and draw helical wheel. It is assumed that that the specified sequence fragment belongs to alpha helix.
load 2por.pdb seq from 1 scale eis angle 160 wheel 2-10	Load porin coordinates, copy the sequence of this protein to the main sequence buffer, select Eisenberg hydrophobicity scale, set angle to 160 degrees and draw helical wheel for residues from 2 to 10. It is assumed that the specified sequence fragment belongs to beta strand.
whe clo	Draw residues clockwise. This gives the bottom view of a helix, which is more common in books.
whe off	Return to default drawing mode. Instead using this command, you can hit the ESCAPE key.

NOTES

(1) Instead using the command WHEEL OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) Don't forget that WHEEL uses only the sequence stored to the main sequence buffer. Read description of the command SEQ (SEQUENCE) to learn how to initialize this buffer.

RELATED COMMANDS

SEQUENCE is used to copy, define or load the sequence. ANGLE defines the rotation angle between adjacent residues. SCALE is used to specify the hydrophobicity scale.

WIN, WINDOW

NAME
WIN, WINDOW - set the sliding window width.

SYNOPSIS
WIN value
WINDOW value

DESCRIPTION
Set the sliding window width. The value is stored as an internal variable and used to calculate and draw average hydrophobicity and hydrophobic moment. The hard-coded default value is 11 residues. The minimal value is 1. The command PLOT may be used to plot the averaged hydrophobicity and/or hydrophobic moment.

EXAMPLES

COMMAND	DESCRIPTION
win 20	Set the sliding window width to 20.
win 8 plot mom	Set the sliding window width to 8 and draw hydrophobic moment.

RELATED COMMANDS
PLOT is used to draw averaged hydrophobicity and/or the hydrophobic moment. ANGLE is used to set the rotation angle between adjacent residues (important for hydrophobic moment, not for averaged hydrophobicity).

Mouse Usage

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

MOUSE USAGE IN DEFAULT MODE

Move the mouse pointer over the structure and you will see the textual information about the atom covered by the pointer. This information will be visible in the output window (the bottom right corner of the main window).

If viewing some large structure (like protein or DNA), the sequence neighborhood of the residue covered by the mouse pointer will be visible in the top portion of the main window (see the example below).

The structure drawing mode is not the only mode where this trick may be used: try also Ramachandran plot, hydrophobicity plots and sequence comparison. The examples below show the content of the output window for all four cases:

Structure display

```
(1) 2POR
PHE 192
C  1426  C
t.f.: 55.22
phob:  1.19
selected
phi: -120.71
psi:   68.12
ome:  178.15
chi1: -62.06
chi2: -42.35
chi3:     -
x:    -5.550
y:   -15.344
z:   -18.352
```

Ramachandran plot

```
(1) 1PRC
ILE 145 H
trans
phi:  -87.26
psi:  128.68
omeg: 174.92
```

Averaged hydrophobicity

```
GLY 62
value:
0.767
```

Sequence comparison

HORIZ.	VERT.
23GLY	GLY27
24SER	SER28
25CYS	CYS29
26TRP	TRP30
27ALA	ALA31
28PHE	PHE32
29SER	GLY33
30ALA	ALA34
31VAL	VAL35
32VAL	GLU36
33THR	ALA37

The image below is an example of the sequence neighborhood. Read the text about the command NEIGHBORHOOD for more information about sequence neighborhood.

USING MOUSE INSTEAD OF KEYBOARD CONTROLS

Mouse clicks may be used for rotations, translations, and for slab and color adjustment. If you want to rotate or translate the structure, or to change slab and color fading, click on a selected button in the control window (the top right corner of the main window). Shift, alt and control play the same role as if keyboard is used for the same job.

Some desktop environments (like KDE and Gnome) use function keys to launch pop-up menus or for some other purpose. This means that function keys F1, F2, F3 and F4 will not work properly with garlic. You can use mouse to click on dummy buttons in a control window. Another approach will be to change the desktop environment settings.

MOUSE USAGE IN EDITING MODE

After executing the EDIT CLICK command, the mouse may be used to pick a single bond for editing. Read the page about the command EDIT to learn how to pick a single bond.

Garlic Reference Card, Version 1.3

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic reference card contains the list of commands and keywords, with short description of commands. Print this page and keep it at hand during your garlic sessions. Garlic reference card is not a learning tool, it is just a reminder. Newbies should start with garlic tutorial.

HTML version Make sure that your browser is properly configured for printing.

Garlic Tutorial

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Lessons

These lessons should help you to learn how to use garlic. Command are given in lowercase, in a short form, but you can use the long form as well as the uppercase letters. File names should be specified in the correct case.

RECOMMENDED USAGE: Print lessons.

In addition, you should read the pages describing garlic commands and controls !

Lesson 1 - Get familiar with garlic
Lesson 2 - Load a small structure
Lesson 3 - Playing with two structures
Lesson 4 - Drawing styles and color schemes
Lesson 5 - How to select atoms
Lesson 6 - Ramachandran plot
Lesson 7 - Helical wheel plot
Lesson 8 - Plot averaged hydrophobicity and hydrophobic moment
Lesson 9 - Venn diagram
Lesson 10 - Semitransparent plane
Lesson 11 - Create small structure
Lesson 12 - Replace selected residues

Scripts

The scripts listed below may be used to demonstrate the available drawing styles for atoms and bonds, as well as some predefined color schemes. These scripts were included into the garlic source package 28. March 2000. If you have an older package, copy these scripts to your local host. There are two ways to copy scripts:
(1) Click here to download them via ftp.
(2) Go to the page which contains the script you selected. Mark and copy the script. Paste it into a local file. Recommended file names: 1: atoms.script, 2: bonds.script, 3: colors.script, 4: dance.script .

Script 1 - Drawing styles for atoms
Script 2 - Drawing styles for bonds
Script 3 - Predefined (hard-coded) color schemes
Script 4 - Dancing tryptophan

Garlic Tutorial

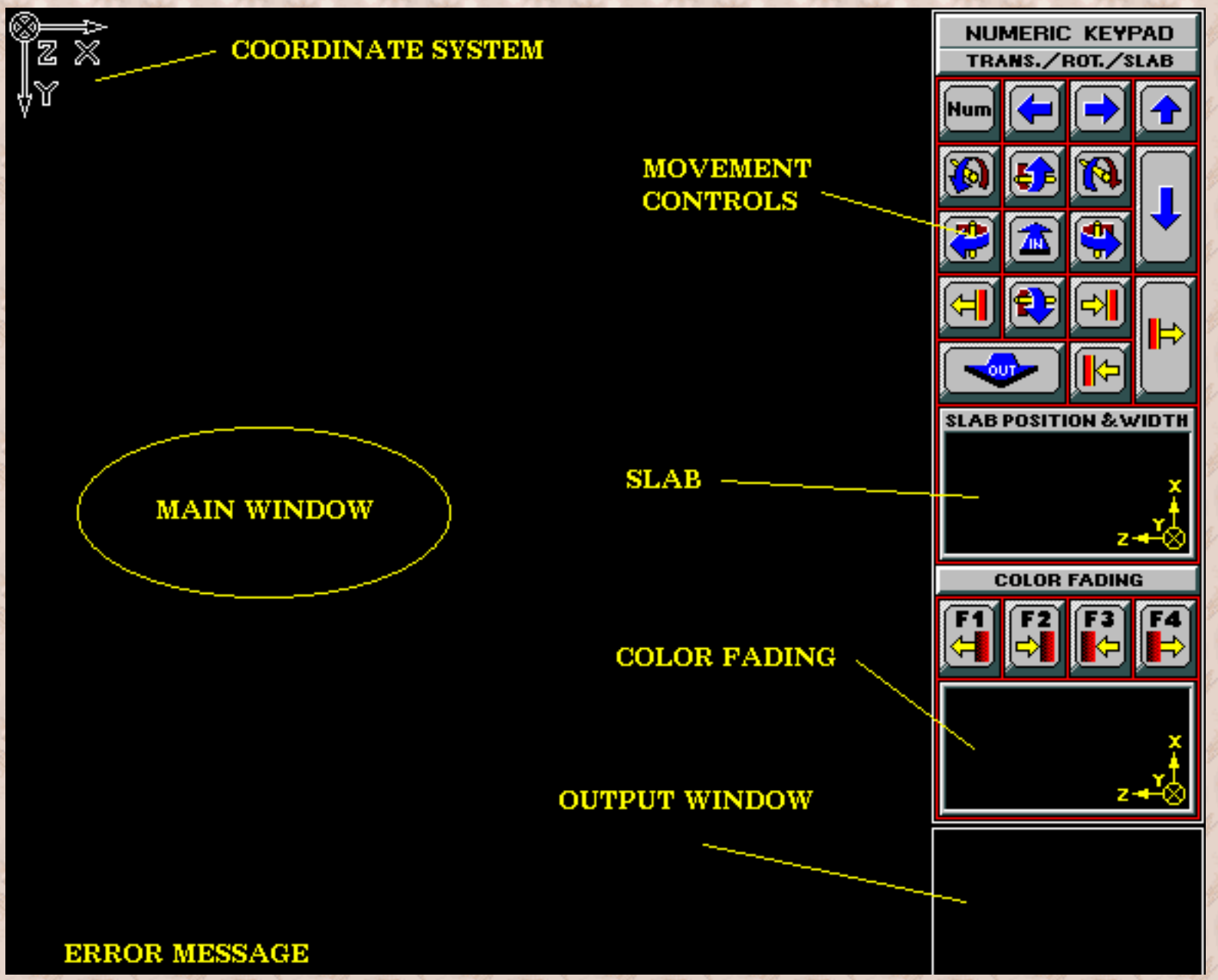
Lesson 1 - Get Familiar with Garlic

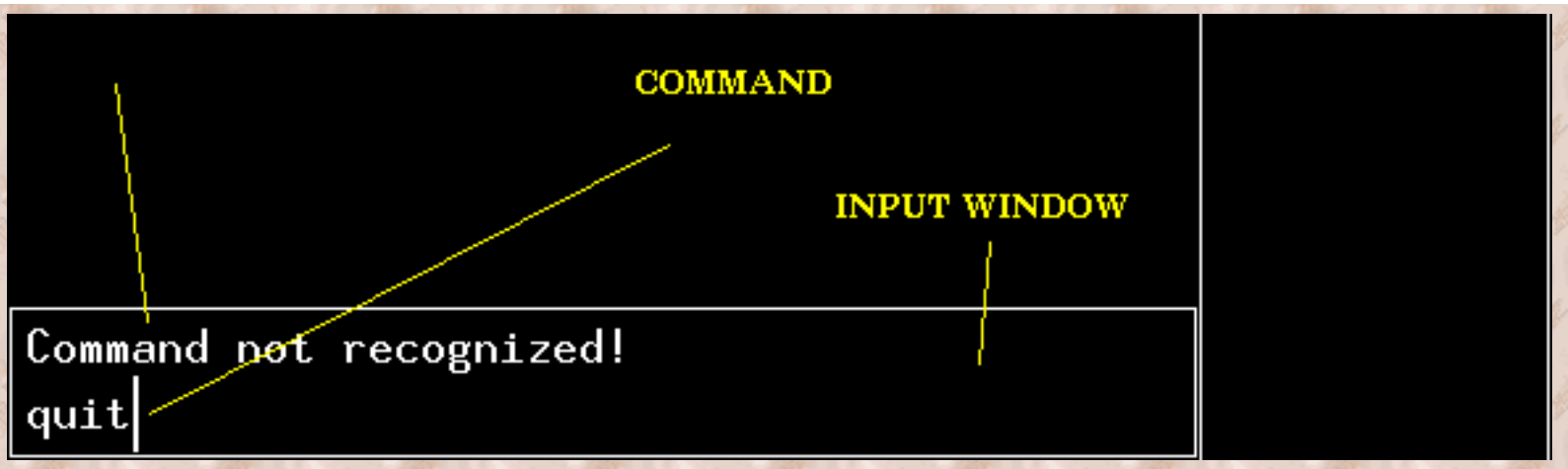
In this lesson, you will execute only one command at garlic prompt: exit, to quit the garlic session.

Start your X session. Use the terminal window to start garlic:

garlic

If garlic is in the path searched by your shell, the garlic window will appear on your screen. Try to remember what are the parts of the entire garlic window. The input window will be empty, but the image below is adapted to show the area reserved for error messages and the area reserved for commands.





When you have learned what are the main parts of the garlic window, quit your garlic session by typing exit or quit (exi or qui):

exit

Garlic Tutorial

Lesson 2 - Load a Small Structure

In this lesson, you will learn how to load a PDB file and how to move the structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load tryptophan (it should be included in the source package). This command should be executed at garlic prompt:

loa trp.pdb

Step 3 - how to use the pointing device (mouse):

Move the mouse pointer over atoms and bonds and read the text which appears in the output window (bottom right corner). Note that half of each bond is assigned to each of two atoms involved in bond formation.

Step 4 - use garlic controls (i.e. the keys on numeric keypad) to rotate the structure (just a single amino acid):

First play for a while with keys 4 and 6, then with 2 and 8, and finally with 7 and 9. Try the same while holding shift (alone), control (alone), alt and shift (simultaneously) and control and shift (simultaneously). Do not try control-alt combinations, unless you are very experienced with unix and X.

Step 5 - use garlic controls (numeric keypad) to translate the structure:

PC keyboard: use /, *, -, +, 5 and 0.
Terminal keyboard: use PF2, PF3, -, comma, 5 and 0.
Repeat while holding modifier keys (alone or in combination).

Step 6 - move the structure to the screen center again:

pos 0 0 0

Step 7 - rotate and translate the structure using commands instead of controls. Try the following set of commands:

rot x 90
tra x 4

tra y -4
tra z -50
rot y 180

Step 8 - move the color surfaces. As your structure is very small, be sure to hold the control key while pressing functions keys:

Hold control key and press F1.
Hold control key and press F4.
Note that color is changing.
Hold control key and play with F1, F2, F3 and F4 for a while.

Step 9 - move the slab surfaces. As your structure is very small, be sure to hold the control key:

Hold control key and 3 (numeric keypad). Repeat until some atoms and bonds disappear.
Hold control key and play with 1, 3, decimal separator (next to 0) and enter for a while. Note that (in control window) visible atoms are red and unvisible atoms are dark cyan.

Step 10 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 3 - Playing with Two Structures

In this lesson, you will learn how to work with two or more structures. The original source package contains two PDB files: trp.pdb and phe.pdb. Each contains a single amino acid: trp.pdb = tryptophan, phe.pdb = phenylalanine. In this lesson, tryptophan will be colored blue, while phenylalanine will be colored red. Note the role of the command cat (catch).

Step 1 - start garlic (if necessary):

garlic

Step 2 - load trypthophan:

loa trp.pdb

Step 3 - change TRP color to blue:

col blue

Step 4 - load phenylalanine:

loa phe.pdb

Step 5 - change PHE color to red:

col red

Two structures will be distinguished by color and by the identifier: tryptophan is treated as structure number 1, and phenylalanine is treated as structure number 2. Two structures are now overlapping.
Step 6 - move tryptophan to the left:

cat 1
pos -5 0 0

Step 7 - move phenylalanine to the right:

cat 2
pos 5 0 0

Step 8 etc. - use the command cat (catch) to rotate structures one by one:

Use cat 1 and cat 2 to catch and rotate structures, one by one.
Translate both structures to the position where they will be overlapped, but do not use keyword pos!

When finished, discard loaded structures:

dis all

Garlic Tutorial

Lesson 4 - Drawing Styles and Color Schemes

In this lesson, you will learn different drawing styles, used for atoms and bonds. Note that garlic uses separate styles for atoms and bonds. You will also try some predefined color schemes. Use the X server which offers 24 bits per pixel, if possible.

As you will often reuse some commands, just with a different argument, note that garlic has a history buffer, where commands which were previously used are stored. The arrow keys may be used to recall one of these commands.

Use the "UP" arrow to scan the history buffer backwards, "DOWN" arrow to scan it upwards, "LEFT" arrow to move the insertion mark left and "RIGHT" arrow to move the insertion mark to the right (if possible, of course). Backspace (or delete, if you have some unusual keyboard mapping) may be used to remove characters.

Step 1 - start garlic (if this wasn't done before):

garlic

Step 2 - load trypthophan and bring it closer to you:

loa trp.pdb
pos 0 0 -150

Step 3 - make bonds unvisible (i.e. set bond thickness to zero):

bon 0

Step 4 - learn which drawing styles are available for atoms.
Hint: use the arrow key "UP" to call the previous command.

ato 1
ato 2
ato 3
ato 4
ato 5
ato 6
ato 7
ato bal
ato ba2
ato big

ato bi2
ato spa
ato sp2

Step 5 - hide atoms:

ato 0

Step 6 - learn which drawing styles are available for bonds.
Hint: use the arrow key "UP" to call the previous command.

bon 1
bon 2
bon 3
bon 4
bon 5

Step 7 - learn how to draw balls and sticks:

bon 4
ato bal

Step 8 - try some predefined color schemes.
Hint: use the arrow key "UP" to call the previous command.
Warning: Always use the full color scheme name (do not abbreviate)!

col red
col green
col blue
col yellow
col cyan
col magenta
col white
col yellow-green
col cyan-green
col cyan-blue
col magenta-blue
col magenta-red
col orange
col hot
col cold
col cpk

Step 9 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 5 - How to Select Atoms

In this lesson, you will learn how to select atoms. The command select (or whatever command plays this role) is one of the most important commands in every molecular visualization program.

For this lesson, you will need a true protein structure, not just a single amino acid as in previous lessons.

Step 1 - obtain the protein structure:

Use you web browser to access The Protein Data Bank (www.rcsb.org) .
Type 1HUC into the small search field. Start the search and wait for the answer.
Choose the option "Download/Display File".
Finally, choose file format "PDB", compression "none" in the section "Download the Structure File" and wait.

Step 2 - start garlic (if necessary):

garlic

Step 3 - load the structure. You should have the file 1HUC.pdb somewhere in the path searched by garlic (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 4 - draw backbone, to simplify the picture:

bac

Step 5 - use different colors for different chains:

col chain

Step 6 - select chain A, draw balls and sticks and change color scheme to CPK:

```
sel a/*/*/*
bac off
bon 4
ato bal
col cpk
```

Step 7 - redefine the internal system origin (the rotation center) and move chain A to the screen center:

```
cen
pos 0 0 0
```

Step 8 - restrict the selection to aliphatic amino acids and change color to yellow (chain A):

```
res ali
col yellow
```

Step 9 - select all, make it visible, show only backbone but reduce the backbone thickness:

```
sel *
sho
bac 3
```

Step 10 - hide side chains:

Step 10 - select cysteine residues, but only for chains A and C; make them visible, use spacefill style:

```
sel a,c/*/cys/*
show
ato spa
```

Step 11 - discard loaded structure:

```
dis all
```

Garlic Tutorial

Lesson 6 - Draw Ramachandran Plot

In this lesson, you will learn how to prepare Ramachandran plot. This plot shows the pairs of dihedral angles phi and psi. You can find more details here .

You can use any protein structure for this lesson. Here we are going to use 1HUC.pdb, retrieved in the previous lesson.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure. You should have the file 1HUC.pdb somewhere in the path searched by garlic (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 3 - prepare Ramachandran plot.

rama

Step 4 - Identify some residues.

Use mouse (pointing device) to identify individual residues. Just move the pointer over the choosen residue symbol and you will see the residue name, serial number and dihedral angles in the output window.

Step 5 - draw Ramachandran plot for glycines.

sel gly
rama sel

Step 6 - return to the main drawing mode. You can either type the command rama off or hit the escape key.

rama off

Step 7 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 7 - Draw Helical Wheel

In this lesson, you will learn how to prepare the helical wheel plot. This plot may be used to identify amphipatic segments in a protein sequence, i.e. the amphipatic helices. In this lesson, the solved structure will be used for demonstration. For more details, read this (WHEEL command description).

You can use any protein structure for this lesson. In this example 1HUC.pdb is used, though you can use any protein structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure. You should have your PDB file (here 1HUC.pdb) somewhere in the search path (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 3 - select all atoms except hetero atoms. If this is not done the hetero "residues" (i.e., solvent molecules) will corrupt the helical wheel plot. The trick is to select hetero residues, and then to select complement. You don't have to hide hetero residues, so you can skip the command hide.

sel het
hide
sel com

Step 4 - check the number of chains in human cathepsin B. If there are two or more chains, the residue serial number should not be used as unique residue identifier.

color chain

Step 5 - there are obviously four chains. Hide all chains except B. Hide everything, after that select only the chain B and make it visible. Hetero residues will not be included into selection, so the step 3 was in fact unnecessary.

sel all
hide
sel b/*/*/*
show

Step 6 - try to find one helix at the chain B surface. Helices may be easily recognized if using backbone

representation of the protein. It is also practical to use the geometric center of the chain B as the rotation center, and to move it to the screen center.

bac
cen
pos 0 0 0

Step 7 - play with the chain B to find this helix:

76	77	78	79	80	81	82	83	84	85	86
PRO	ALA	GLU	ALA	TRP	ASN	PHE	TRP	THR	ARG	LYS

Step 8 - copy the sequence of the chain B to the main sequence buffer. Note that the helical wheel plot uses the sequence which is stored in the main sequence buffer. Right now this buffer is empty!

seq from 1

Step 9 - draw helical wheel for residues from 76 to 86:

wheel 76-86

Step 10 - return to the main drawing mode. Hit the escape key or type the following command:

whe off

Step 11 - discard loaded structure:

dis all

Step 12 - clear the main sequence buffer:

seq reset

Do not forget that for helical wheel plot, the main sequence buffer should be initialized!

Garlic Tutorial

Lesson 8 - Draw Averaged Hydrophobicity and Hydrophobic Moment

---

In this lesson, you will learn how to draw the averaged hydrophobicity and hydrophobic moment for the sequence which is stored in the main sequence buffer.

In this lesson no atomic coordinates will be used. The only information available will be the sample protein sequence stored in FASTA format. The sample sequence may be found in the original garlic package or downloaded via ftp . Save this sequence as ASCII text, not as HTML.

In this example, mouse may be used to identify residues and their imminent sequence neighborhood. The residue information will be visible in the output window (bottom right corner), while the neighboring residues will be listed in the upper part of the main window. The central residue (the one choosen by the mouse) will be enclosed in a small rectangle.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the sequence.

seq load sample.fasta

Step 3 - plot the averaged hydrophobicity. Use mouse to identify the residues in the plot. The residue information will be visible in the output window (bottom right corner).

plot hyd

Step 4 - plot the hydrophobic moment. Use mouse to identify residues.

plot mom

Step 5 - plot both averaged hydrophobicity and hydrophobic moment. Note that the numeric value in the output window will be equal to the hydrophobic moment in this case!

plot hyd mom

Step 6 - return to the main drawing mode. You can either type the command plot off or hit the escape key.

plot off

Step 7 - clear the sequence buffer. You can skip this step, it is not very important.

seq reset

Garlic Tutorial

Lesson 9 - Venn Diagram

In this simple lesson, you will learn how to prepare the Venn diagram with some residue counts. There is nothing special in this routine and experts will not find it very useful. It is primarily intended for students and other newbies, which are interested in the residue composition of the given protein.

The only information required to prepare the Venn diagram is the protein sequence. In this example, the sequence will be extracted from PDB data. Another approach will be to load the sequence from some FASTA file. The PDB file used here is 1HUC.pdb, but you can replace it with any PDB file which contains the protein structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure.

load 1HUC.pdb

Step 3 - discard all hetero atoms:

sel het
sel com

Step 4 - restrict your selection to chains A and B:

res a,b/*/*/*

Step 5 - extract sequence:

seq from 1

Step 6 - draw Venn diagram with residue counts:

venn

Step 7 - discard the structure:

dis all

Step 8 - clear the sequence buffer. You can omit this command.

seq reset

Garlic Tutorial

Lesson 10 - The Semitransparent Plane

This lesson explains how to control the plane associated with the structure. More precisely, you will learn how to show, hide or move the plane and how to change the plane properties. The plane may be used to divide the structure in two parts, for selection and to model the cellular membrane.

It might be good idea to read the text about the command PLANE before you start with this lesson.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load some the structure. In this lesson the papain structure is used, but you can use any other structure.

load 9PAP.pdb

Step 3 - make the plane visible:

pla

Now you should see an ellipsa which represents the plane. If you have not rotated the structure before making the plane visible, the ellipsa will be blue. The near edge will be bright, while the far edge will be dark.

Step 4 - rotate both the structure and the plane about x axis:

Hold the [shift] key and press 8 on numeric keypad.

Note the change of the ellipsa color: now you see another face of the plane. The blue face is treated as the upper side, while the orange-red face is treated as bottom side.

Step 5 - change the plane radius.

pla rad 20

Step 6 - Change the plane transparency (make it opaque):

pla tra 0

Step 7 - select all atoms above the plane:

sel above

Step 8 - change color for the current selection:

color cold

Step 9 - attach movement controls to the plane:

mov pla

Step 10 - rotate the plane, leaving the structure in its current orientation:

Use numeric keypad (keys 2, 8, 4 and 6) and modifier keys (shift, alt, control) to rotate the plane.

Step 11 - attach controls to both structure and plane:

mov all

Step 12 - hide the plane:

pla off

Step 13 - discard the structure:

dis all

Garlic Tutorial

Lesson 11 - Creating Small Structure

In this lesson you will learn how to create a short alpha helix. The structure created using the method described here may be saved as any other structure.

Before starting with this lesson, read something about the command CREATE .

Step 1 - start garlic (if not started already):

garlic

Step 2 - prepare a short sequence (polyalanine, eight residues):

seq = ala ala ala ala ala ala ala ala

Step 3 - initialize the secondary structure (let's play with an alpha helix):

str = hhhh hhhh

Step 4 - create a short alpha helix:

create

Step 5 - save your structure:

save test.pdb

Step 6 - discard the structure:

dis all

That's all!

Garlic Tutorial

Lesson 12 - Replace Selected Residues

In this lesson you will learn how to replace selected residues. The structure used in this example will be 1HUC.pdb, but you can use any other protein structure.

Before starting with this lesson, read something about the command REPLACE .

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure:

load 1HUC.pdb

Step 3 - change color:

color cold

Step 4 - select the residue 26 in the chain A:

sel a/26/*/*

Step 5 - define the replacement for this residue:

seq = ser

Step 6 - replace CYS 26 by SER:

replace

Move the residue 26 closer to check the replacement (use numeric keys).

Step 7 - discard structure:

dis all

Garlic Tutorial

Script 4 - Dancing tryphophan

Just try it!

Type the following command at garlic prompt:

exe dance.script

```
load trp.pdb
bon 4
pos 0 0 1000
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
```

```
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
```

COM.	ARGUMENTS	APPLIES TO	DESCRIPTION
ADD	the same as for SEL	structure	Add to selection
ANG	angle (degrees)	helical wheel, hydrophobic moment	Angle for helical wheel and hydrophobic moment calculation
ATO	0, 1, 2, 3, 4, 5, 6, 7, BAL, BA2, SMA, SM2, COV, CO2, SPA, SP2, BIG, BI2	selection	Set drawing style for atoms
BAC	0, 1, 2, 3, 4, 5, OFF	selection	Draw backbone
BAL	radius (angstroms)	structure	Set ball radius (balls & sticks)
BG	color_specification	main window	Change background color
BLU	width height, OFF	main window	Blur (soften) image
BON	0, 1, 2, 3, 4, 5, NICE	selection	Set drawing style for bonds
CAT	structure_identifier	structure	Catch structure
CEN	none	structure, selection	Redefine system origin
COL	detailed_color_specification, red, green, blue, yellow, cyan, magenta, white, yellow-green, cyan-green, cyan-blue, magenta-blue, magenta-red, orange, hot, cold, monochrome, cpk, zebra, chain, hyphob	selection	Assign color; do not abbreviate color scheme name!
COM	none, OFF, minimal_score segment_width, CORNER serial1 serial2, ZOOM zoom_factor	both sequence buffers	Compare two sequences
CRE	none	main sequence buffer, main structure buffer	Create new structure
DIS	structure_identifier *, all	structure	Discard structure
DOC	identifier_1 identifier_2 OFF	Two structures	Prepare two structures for docking
EDI	OFF, ATO, BON atom1 atom2, CLI, DIM, MAI, OME, PHI, PSI, SID	structure	Edit structure
EXE	file_name	script file	Execute script
EXI	none	garlic session	Quit garlic session
FAD	FRO shift, BAC shift, OFF, PLA, SPH, CYL, HALF-SPH, HALF-CYL	structure	Change color fading
FG	color_specification	main window	Change text color

FON	font_name	all windows	Change font
GRO	id1 id2 ... idN, ALL, SAV filename, SSC filename	structure(s)	Group structures
HID	none	selection	Hide atoms and bonds
HYB	none, OFF	structure	Generate hydrogen bonds
LAB	none, OFF	selection	Show labels
LOA	file_name	structure_file	Load structure (file)
LOG	file_name, OFF	commands	Log garlic commands
MEM	none, OFF, BET, RAD radius, THI thickness, TRA transparency	membrane	Show or hide membrane, set properties
MON	none	main window	Switch to mono mode
MOV	ALL, MEM, PLA, STR	struct., memb., plane	Attach controls to given object
NEI	none, OFF	main window	Show or hide seq. neighborhood
PAU	none	garlic script	Pause script execution
PLA	none, OFF, RAD radius, TRA transparency	plane	Show or hide plane, set properties
PLO	HYD, MOM, OFF, HYD start_residue end_residue, MOM_start_residue end_residue	sequence buffer	Plot hydrophobicity and/or hydrophobic moment
POS	x, y, z	structure	Move to (x, y, z)
PRO	radius (angstroms)	structure	Set probe radius
QUI	none	garlic session	Quit garlic session
RAD	radius (angstroms)	Selection sphere	Change selection sphere radius
RAM	none, SEL, OFF	structure	Draw Ramachandran plot
REF	none, OFF	main window	Refreshing on/off
REG	none	mail	Register garlic
REP	none	structure, sequence buffer	Replace selected residues
RES	the same as for SEL	selection	Restrict selection
ROT	axis angle (degrees)	structure	Rotate
SAV	file_name file_name SEL	structure, selection	Save atomic data to file (SEL = selection only)
SCA	EIS, KD, WHI	hydrophobicity scale	Choose hydrophobicity scale: Eisenberg, Kyte-Doolittle, White

SEL	chains/res_nums/res_names/atom_names, residue_numbers, residue_names, *, ALL, ABO, ACI, ALI, ALT, BAD, BAS, BEL, CHA, CIS, COM, HET, PHO, MAI, MOD model_number, NEG, POL, POS, SEQ, SID, SMA, SPH, TIN, TM, TRA, TRI	structure, selection	Define new selection (overwrite previous)
SEQ	= three_letters_code, LOAD filename, FROM structure_identifier, COPY, SAVE filename, SWN filename, RESET	sequence buffer, reference seq. buffer	Manipulate sequence buffer
SET	PHI, PSI, OME, CHI1, CHI2, CHI3, CHI4, CHI5 (angle required, degrees)	structure	Set the specified dihedral angle
SHO	none	selection	Show atoms and bonds
SLA	FRO shift, BAC shift, OFF, PLA, SPH, CYL, HALF-SPH, HALF-CYL	structure	Change slab
SSB	0, 1, 2, 3, 4, 5, NICE	disulfide bonds	Set draw. style for disulf. bonds
STE	none, OFF	main window	Switch to stereo mode
STI	radius (angstroms)	structure	Set stick radius (balls & sticks)
STR	= one_letter_code, LOAD filename, FROM structure_identifier, COPY, SAVE filename, RESET	sec. struct. buffer, ref. sec. struct. buffer	Manipulate sec. structure buffer
TAG	"string", OFF	structure	Assign or remove tag
TBG	color_specification	input&output window	Change text background
TFG	color_specification	input&output window	Change text color
TIT	identifier x y "string" identifier x y identifier OFF	main window	Add, move or remove title
TRA	axis shift	structure	Translate
VEN	none, OFF, start_residue end_residue	sequence buffer	Draw Venn diagram with statistics
WHE	none, OFF, CLOCKWISE, start_index end_index, start_index end_index CLOCKWISE	sequence buffer	Draw helical wheel
WIN	number_of_residues	sliding window	Set sliding window width

Garlic Command Line Options

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page explains the command line options. To see this list, type one of the following commands:

garlic -h
garlic -h | less

```
==============================================================================
                Garlic - free molecular viewer and editor
==============================================================================

Garlic was written by Damir Zucic (zucic@garlic.mefos.hr) as a complement
to other molecular visualization  programs, like rasmol (by Roger Sayle).
It was written to simplify  the analysis of membrane proteins, but it can
be used as general purpose molecular visualization program, provided that
molecular coordinates are available in  PDB format, version 2.1 or older.
Garlic may also be used to analyze protein sequences.

Some of the  features, which  distinguish this program from  others, are:
(1) Coordinates, labels and  other data are  automatically displayed  for
    the atom nearest to the current pointer (mouse) position.
(2) Additional numeric data,  like  hydrophobicity, may be associated  to
    each amino acid. The  whole  structure  may be  colored  according to
    these values.
(3) Selection mechanism is different.
(4) Two bonds at different distance from  observer have different colors.
------------------------------------------------------------------------------
Usage:              garlic [true_garlic_options] [X11_options] [filename]
------------------------------------------------------------------------------
Command line options may be divided in two groups: true (specific) garlic
options and X11 options.  Options may be given in any order.  All options
and hard-coded  default values are listed  in the table  below.  For each
parameter, the value defined through command line is used,  if available.
If not, the value defined in .garlicrc file is used. If .garlicrc file is
not  available,  or there is  no corresponding  entry in  this file,  the
hard-coded default value is used.  The sample  .garlicrc file included in
the original package contains  the values equal to  hard-coded  defaults.
------------------------------------------------------------------------------
garlic option:        Description:
------------------------------------------------------------------------------
-h, --help            Print help and exit.
```

-v, --version	Print version and exit.
-r, --register	Register garlic: inform author that your site has garlic installed and that someone is going to use this program. By registering, you are encouraging author to continue development of garlic. You can also help author to ensure support for further development. This option sends an e-mail message, containing only the e-mail message header and the word 'Hi!',to zucic@garlic.mefos.hr. Please execute garlic -r if you are going to use this program. If your system is not connected to the Internet, you can send short e-mail from some other system.
-nosys	Hide the coordinate system icon (top left corner).
-no-control	Hide the control window (upper right corner).
-stereo	Display stereo image.
-slab mode	Default slab mode. Available slab modes are: off, planar (default), sphere, half-sphere, cylinder and half cylinder.
-fading mode	Default color fading mode. Available modes: off, planar (default), sphere, half-sphere, cylinder and half cylinder.
-as number	Default atom drawing style (hard-coded default: 2).
-bs number	Default bond drawing style (hard-coded default: 3).
-fs number	Default number of color fading surfaces. Parallel planes, concentric spheres or conc. cylinders may be used as fading surfaces. Three RGB triplets are assigned to each surface. Surfaces are evenly spaced; at least one and at most eight should be defined. At least three colors (left, middle and right) are assigned to each visible atom. These three colors are based on the position of a given atom relative to the nearest fading surface(s) and on colors assigned to these surfaces. Colors are combined using linear weighting.
-lc[i] color	Left color at the i-th surface; i is between zero and seven. The color string should be compliant with X11R5. Blue, for example, may be specified as blue or as RGB:0000/0000/FFFF etc. For example -lc4 RGB:BBBB/8888/4444 defines the left color at the surface whose index is equal to four.
-mc[i] color	Middle color at the i-th surface.
-rc[i] color	Right color at the i-th surface.
-pc, --print-config	Print configuration data and exit.
-pcn	Print cursor names to stdout and exit.
-log logfile	Write commands and messages to log file. The file will be created in the current working directory. If this is not possible, log file will be created in users home directory.

```
-----------------------------------------------------------------------
X11 option:            Description:
-----------------------------------------------------------------------
-display displayname   X server to contact.
-geometry geom         Window geometry (default: almost the whole screen).
-bg color              Main window background color (default is black).
-fg color              Main window foreground color (default: white).
-fn fontname           Text font; (default is 10x20).
-tbg color             Text background color (default is black).
-tfg color             Text color (default is white).
-cursor cursorname     Cursor name; see  /usr/include/X11/cursorfont.h for
                          names; remove the XC_ prefix.
-----------------------------------------------------------------------
filename:              The input file name.  Full pathname may be used. If
                       filename does not contain the path, garlic will try
                       to find  the specified file in  the current working
                       directory.  If the first attempt  to open  the file
                       fails,  the filename  is appended to the content of
                       the environment  variable  MOL_DIR  for  the second
                       attempt.  If this fails too, garlic will search all
                       directories  specified in  the environment variable
                       MOL_PATH.
-----------------------------------------------------------------------
Personal initializations may be written to .garlicrc file. Normally, this
file should be kept in users home directory.  Note that this is  not  the
first directory to be searched for  .garlicrc file!  Up to six  pathnames
are tryed in the following order:

.garlicrc                       .garlicrc  in current  working directory.
$HOME/.garlicrc                 .garlicrc in home directory.  This is the
                                   recommended location.
$HOME/garlic/.garlicrc          ./garlicrc,  subdirectory garlic of users
                                   home directory.
/etc/garlicrc                  garlicrc in /etc, Debian linux; note that
                                   file name is garlicrc in this case!
/usr/local/lib/garlic/.garlicrc .garlicrc  in  /usr/local/lib/garlic dir.
/usr/lib/garlic/.garlicrc       .garlicrc in /usr/lib/garlic; this is the
                                   last attempt; if it failes, hard-coded
                                   default values will be used.
-----------------------------------------------------------------------
Environment variables:
-----------------------------------------------------------------------
MOL_DIR                Defines where to look for the specified file if not
                          found in the current working directory.
MOL_PATH               The list of directories to be searched.  It is used
                          if attempt with MOL_DIR failes  or if MOL_DIR is
                          not defined. Use space  or colon (:) to separate
                          directory names. MOL_PATH is quite useful; it is
```

```
                        recommended to define  this environment variable
                        through  .login,  .bashrc or  some other script.
                        MOL_PATH  is more useful  than  MOL_DIR so it is
                        recommended  to define only  MOL_PATH  variable.
DISPLAY               X server to which  the program should be connected.
-----------------------------------------------------------------------------
garlic home page:                          http://garlic.mefos.hr/garlic
Damir Zucic home page:                     http://garlic.mefos.hr/zucic
E-mail:                                    zucic@garlic.mefos.hr
=============================================================================
```

Garlic Versions

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains a list of garlic versions, with links.

- 1.0 March 2000.
- 1.1 February 2001.
- 1.2 September 2002.
- 1.3 April 2003.
- 1.4 Under development.

Garlic

Free Molecular Visualization Program

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

This is the home of garlic - free, open source molecular visualization program. Garlic is the most portable molecular visualization program in unix world. Follow the links below to find more about garlic. Don't forget to visit the screenshot gallery !

Since March 10. 2000 till January 11. 2001 garlic was downloaded 1879 times!

Mirrors: Canada United Kingdom

What is garlic?	Download garlic	Tutorial	Mouse usage
Garlic features	Installation	Reference card	Bug fixes
Announcements	Garlic commands	Configuration file	Changes
Screenshot Gallery	Garlic controls	License	Support garlic!
Technical info	Garlic options	Author	Competition

Questions, Bug Reports, Comments and Suggestions

The form below may be used to send bug reports, comments and suggestions, or to ask question about garlic. You can also send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) .

Name and institution:

e-mail address (please type it carefully):

Message:

SEND CLEAR

User comments

Dear Dr. Zucic,

This is to express my appreciation for creating this wonderful molecular graphics program, perhaps the only one which I can run without being irritated on my Linux/Alpha.

Thank you so much,

With best regards,

Ansuman Lahiri, University of Stockholm, Sweden

Garlic

The Most Portable Molecular Visualization Program in Unix World

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

The statement that garlic is the most portable molecular visualization program in unix world might look quite bold at the first sight, but it is based on serious arguments. Garlic requires only three libraries to run: the standard C library (libc), the standard math library (libm), and the standard X11 library (libX11). These libraries are available on every serious unix or unix compatible system. All other programs, (except one: mdxv) require some additional binary libraries.

Compiling and/or installing a program which requires numerous libraries may turn into nightmare. Not only that all these libraries must be present on your system: a version number is important too! And if you manage to compile and/or install the program, it may behave strange when you try to use it: there is a chance that one or more libraries were not tested enough before shipping, causing core dumps and other runtime problems.

Check the list of freely available molecular visualization programs for unix and unix clones. This page lists also the libraries required to run each of these programs.

Free Molecular Visualization Programs for Unix and/or Linux

---

free molecular visualization programs, free molecular viewers, list of molecular visualization programs, list of molecular viewers, molecular rendering, protein visualization tools, molecular visualization resources, download page, download source, download executable, download binary, B, Chime, Chimera, Cn3D, Deep View Swiss-PDBViever, DINO, Flex, Garlic, gdpc, gOpenMol, Jmol, Kinemage, mdxvu, MOIL-View, MOLEKEL, MOLMOL, MolScript, Moviemol, NAMOT, QMOL, PREPI, Protein Explorer, PyMOL, RasMol, Raster3D, VEGA, Viewmol, VMD, WinMGM, XMakemol, XMol, Ymol, biological macromolecule, protein structure, DNA structure, PDB, unix, linux, free software download, open source software, Damir Zucic.

This page contains the list of free molecular visualization programs, complete with links. Only freely available programs which run on unix or unix compatible platform are listed. Some of these programs are available only as binary code for some specific platform(s).

Most programs were found using AltaVista and Lycos, while some others were suggested by readers of this list. Thanks to all of them!

Some of the programs listed below have a very limited license. Be sure to read the license before using such program!

The time-limited trial versions of commercial programs were omitted from the list.

The programs listed here were not evaluated and no comparison was made.

If you have your own free molecular visualization program for unix or linux, or if you know for such program which is not included in the list below, please send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) . Please send corrections and changes to the same address.

Last updated: October 16, 2001.

The information contained here was valid at that time. As developing is going on, it is likely that some additional libraries may become necessary for some of the programs listed here. However, it is almost certain that libraries listed here will be required in future versions too.

PROGRAM	LIBRARIES REQUIRED	PROGRAM TYPE
B	Java based package	Your browser should support Java Virtual Machine
Chime	libc, libm, libX11, libXt, libXext, libXm, libC, libgen	browser plug-in, SGI machine required
Chimera	many libraries, still under development	stand alone program, online registration required
Cn3D	libc, libm, libX11, libXt, libXext, libXmu, libXp	both browser plug-in and stand alone program
Deep View Swiss-PdbViewer	libc, libm, libX11, libXt, libXext, libXmu, libXi, libXp, libMesaGL, libMesaGLU, libpthread, libz	stand alone program, IRIX or linux required

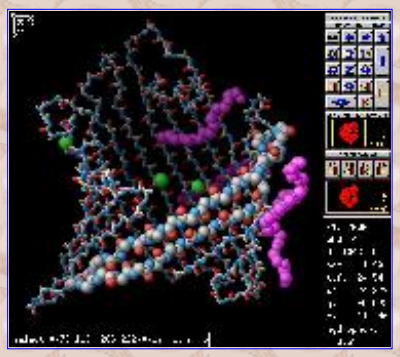
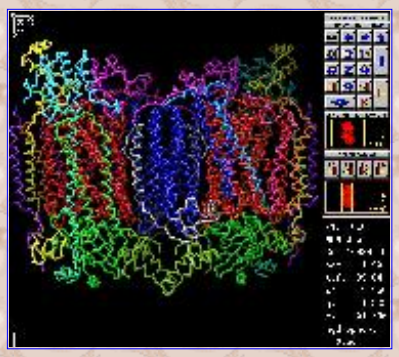
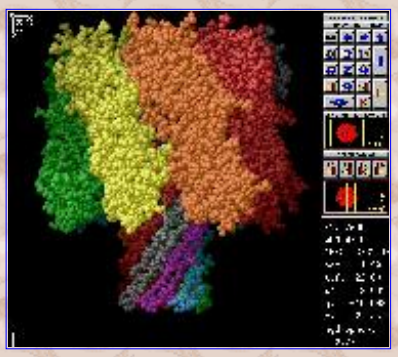
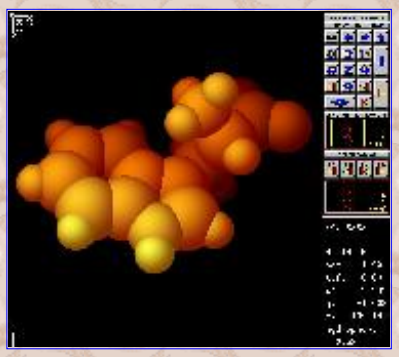
DINO	libc, libm, libX11, libXt, libXext, libXmu, libXi, libgdbm, libGL, libGLU	stand alone program
Flex	libc, libm, libX11, libxview, libolgx, xlibflexdraw	stand alone, binaries for DEC/alpha, DEC/MIPS, IBM RS, SGI, Sun
Garlic	libc, libm, libX11	stand alone program, GNU GPL license
gdpc	libc, libm, libX11, libXext, libXi, libgtk, libgdk, libgmodule, libglib, libdl, libpthread	stand alone program
gOpenMol	libc, libm, libX11, libXt, libXext, libXmu, libXi, libdl, libXaw, Tcl/Tk, + Mesa or Open GL libraries	graphics interface to the OpenMol set of programs GNU GPL license
Jmol	Java-based application	stand alone program (Java-based application)
Kinemage	libc, libm, libX11, libXt, libXm	stand alone program
mdxvu	libc, libm, libX11, precompiled for some systems	stand alone program
MOIL-View	FORTRAN program, binaries available for Silicon Graphics workstations	stand alone program, registration expected
MOLEKEL	libc, libm, libX11, libXext, libXmu, libXi, libMesaGL, libMesaGLU, libtiff, libjpeg	precompiled for SGI IRIX, linux PC and SunOS, registration required
MOLMOL	libc, libm, libX11, libXt, libXext, libXm, libGL, libGLU, libGLcore, libC, libgen, libgen, libpng, libz	stand alone, binaries for DEC/MIPS, DEC/alpha, SGI, SPARC and RS/6000
MolScript	libc, libm, libX11, libXt, libXext, libXmu, libGL, libGLU, libGLcore, libmedia, libC, libgen, libvice, libjpeg, libpng, libz	stand alone, online registration required
Moviemol	libc, libm, libX11, libXext, libYgl or OpenGL	stand alone program
NAMOT	libc, libm, libX11, libxview, libolgx	stand alone program
QMOL	libc, libm, libX11, libXt, libXext, libXm, libGLw, libMesaGL, libMesaGLU, libstdc++, libSM, libICE	stand alone program
PREPI	Precompiled binary for Silicon Graphics IRIX	stand alone, registration required (written agreement)

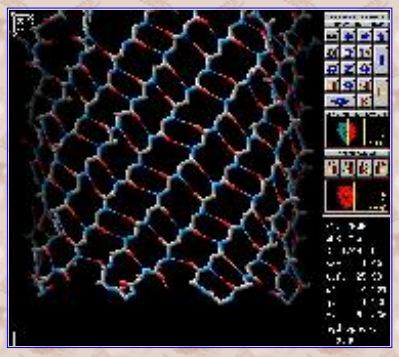
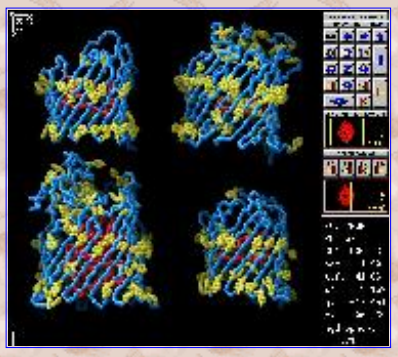
Protein Explorer	Works under linux, but in a Windows subsystem: requires Win4Lin or WMWare	requires Chime 2 and commercial Windows subsystem for linux, online registration required
PyMOL	libc, X libs, libpng, zlib, python, Mesa	Requires Python, an intepreted programming language
RasMol	libc, libm, libX11 libXext, libXi	stand alone program
Raster3D	Mixed FORTRAN 77 and C code, requires both compilers	stand alone program
VEGA	libc, libm, libz, liblocale	No OpenGL support for linux version
Viewmol	libc, libm, libX11, libXt, libXext, libXm, libXi, libXp, libGL, libGLU, libtiff, libtiff, libpthread, libdb, libdl, libutil	graphical front end for comp. chemistry programs, GNU GPL license
VMD	Statically linked binaries for AIX, HPUX, IRIX, linux, Solaris and TRU64	stand alone, online registration required
WinMGM	libc, libm, libMesaGL, libsubplex, libchelpers, libmgmcalctools, libmolecules, libmolenergy	stand alone, some custom libraries required
XMakemol	libc, libm, libX11, libXt, libXm, libXpm, libGL, libGLU	stand alone program, GNU GPL license
XMol	Precompiled binaries for DEC/MIPS, DEC/alpha, Silicon Graphics IRIX, SPARC, Sun-3 and RS/6000	The link is broken! Where is this program?
Ymol	libc, libm, libX11, libXext	stand alone program

Garlic Screenshot Gallery

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

This page contains eight garlic screenshots reduced to a size suitable for fast downloading. Click the selected image to load the full-sized version. All images are stored in JPG format; color quality is slightly reduced by compression. True-color display is recommended for viewing this page.

What is Garlic?

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

Garlic is a free molecular visualization program written for unix and unix clones.

Garlic was born September 30, 1998. At that time I needed a good molecular visualization program and almost the only thing at hand was RasMol. I had some hard time with RasMol so I tryed to adapt it to my needs. However, I realized that it is very hard to read and change RasMol source code, so I decided to write my own molecular visualization program.

Further, I decided to learn programming for the X window system, and this is my first serious program written for X11.

Since 1997 I use GNU/Linux software, so I concluded that it would be fair to add something useful and modern to the existing collection of free software because this software significantly improved my working conditions.

Garlic was forgotten few times, for months, as I had some other things to do, but now it is finaly operative.

Though the version which is currently available is just a prerelease version, it is very stable and robust, at least on systems which were available for testing here at University of Osijek, Croatia.

The name garlic was choosen because my original intention was to write a modular program, which will be capable to call a number of modules via system calls. I also like garlic. Later, I reallized that this name may be reinterpreted as follows:
G stands for GNU (license),
AR for analysis and rendering,
LI for linux,
C for C (the computer language).

Who might be interested to use this program?

Students
As garlic is free, students may find it interesting as a learning tool. Garlic may be installed on a cheap, no-name PC (running linux, of course), or even on a laptop (very handy!).

University assistents and professors
It is somewhat delicate to use a commercial software for lectures and seminars (assignments). In their later carrier students may be boosted toward a software which they used during their study just because they have some experience with it. Universities should not influence the software market by choosing certain commercial product just because it is cheap or for some other reason suitable for university assignments.
Garlic may also be used for lectures, presentations and for scientific work.

Professionals
Many professionals would like to use some molecular visualization program at home or on a portable computer. Some others may be interested to adapt the program to their own needs. Software makers are unwilling to give the source code and to allow modification of their product. They also try to drain

as much money as possible for additional (home) copies. Anyone wishing to cut the rope is invited to use and modify garlic, but the final product has to remain free and open, in agreement with GNU General Public License .

Others

Anyone interested to learn something about proteins and DNA may find garlic useful.

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Version 2, June 1991

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Updated: 3 Jan 2000 rms

Download garlic

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

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http://garlic.mefos.hr/sources/garlic-1.0

Garlic Tutorial

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

Lessons

These lessons should help you to learn how to use garlic. Command are given in lowercase, in a short form, but you can use the long form as well as the uppercase letters. File names should be specified in the correct case.

RECOMMENDED USAGE: Print these lesson before use.

In addition, you should read the pages describing garlic commands and controls !

Lesson 1 - Get familiar with garlic
Lesson 2 - Load a small structure
Lesson 3 - Playing with two structures
Lesson 4 - Drawing styles and color schemes
Lesson 5 - How to select atoms

Scripts

The scripts listed below may be used to demonstrate the available drawing styles for atoms and bonds, as well as some predefined color schemes. These scripts were included into the garlic source package 28. March 2000. If you have an older package, copy these scripts to your local host. There are two ways to copy scripts:
(1) Click here to download them via ftp.
(2) Go to the page which contains the script you selected. Mark and copy the script. Paste it into a local file. Recommended file names: 1: atoms.script, 2: bonds.script, 3: colors.script, 4: dance.script .

Script 1 - Drawing styles for atoms
Script 2 - Drawing styles for bonds
Script 3 - Predefined (hard-coded) color schemes
Script 4 - Dancing tryptophan

Garlic Commands

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

The image in the main window is controled by CONTROLS and by COMMANDS. This page contains the list of garlic commands.

Garlic commands are strings, consisting of one or more words. A command is executed when you press the RETURN key (this key is labeled ENTER on some keyboards). Note that ENTER key on the numeric keypad (the one in the bottom right corner of your keyboard) is NOT the right key! Commands will be displayed in the area called "input window".

Input window is placed at the bottom of the main garlic window, left justified. You don't have to the click into this area to enter the command string - just type it. The input window is capable to display a single error message (top) and a single command (bottom).

You can access previously executed commands by using arrow keys on your keyboard (the UP arrow scans the history buffer backwards and DOWN arrow in the opposite direction).

This page contains the alphabetic list of garlic commands with a short description and with link to detailed description.

Commands are generally case insensitive, but file names are case sensitive because unix (linux) is case sensitive.

SHORT FORM	LONG FORM	SHORT DESCRIPTION
ADD	ADD	Expand current selection
ATO	ATOMS	Change atom drawing style
BAC	BACKBONE	Draw backbone
BACKG	BACKGROUND	The same as BG
BG	BACKGROUND	Change main window background color
BON	BONDS	Change bond drawing style
CAT	CATCH	Catch the specified structure
CEN	CENTER	Change the internal coordinate system origin
COL	COLOR	Set color
DIS	DISCARD	Discard macromolecular complex
EXE	EXECUTE	Execute garlic script
EXI	EXIT	Quit garlic session
EXP	EXPAND	The same as ADD
FAD	FADING	Change color fading style or parameter(s)

FG	FOREGROUND	Change main window foreground color
FON	FONT	Change font
FOREG	FOREGROUND	The same as FG
HID	HIDE	Hide selected atoms
HYB	HYBONDS	Generate hydrogen bonds
IGN	IGNORE	Ignore (this command does nothing)
LAB	LABELS	Show labels
LOA	LOAD	Load the specified file
LOG	LOG	Write commands to log file
MON	MONO	Switch to mono mode
PAU	PAUSE	Pause execution (useful in scripts)
POS	POSITION	Move structure to specified position
QUI	QUIT	The same as exit
REA	READ	The same as LOAD
REG	REGISTER	Register garlic
RES	RESTRICT	Restrict current selection
ROT	ROTATE	Rotate structure
SAV	SAVE	Save atomic data to file
SEL	SELECT	Select atoms
SHO	SHOW	Show selected atoms
SLA	SLAB	Change slab style or parameter(s)
STE	STEREO	Switch to stereo mode
TAG	TAG	Assign tag (short text) to structure
TAK	TAKE	The same as CATCH
TBG	TEXT_BACKGROUND	Change text background color
TFG	TEXT_FOREGROUND	Check text foreground color
TIT	TITLE	Add title to the main window
TRA	TRANSLATE	Translate structure

Garlic Controls

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

The image in the main window is controled by CONTROLS and by COMMANDS . This page contains description of garlic controls.

Garlic controls are reserved keys, which may be used to rotate and translate the structure, to change the position of slab surfaces and to change the way color depends on distance from the observer. At present, the reserved keys are numeric keypad keys and four function keys (F1, F2, F3 and F4).

Numeric keypad	Function keys

For each control, five steps are available: normal, large, very large, small and very small. If you press the control without holding a modifier key (shift, alt or control), the normal step will be used.

Modifier keys may be used in combination with reserved keys to select large, very large, small or very small step. Here is the table of modifier keys:

MODIFIER KEYS	STEP	EXAMPLE
none	Normal	
shift	Large	
alt_shift	Very large	
control	Small	
shift_control	Very small	

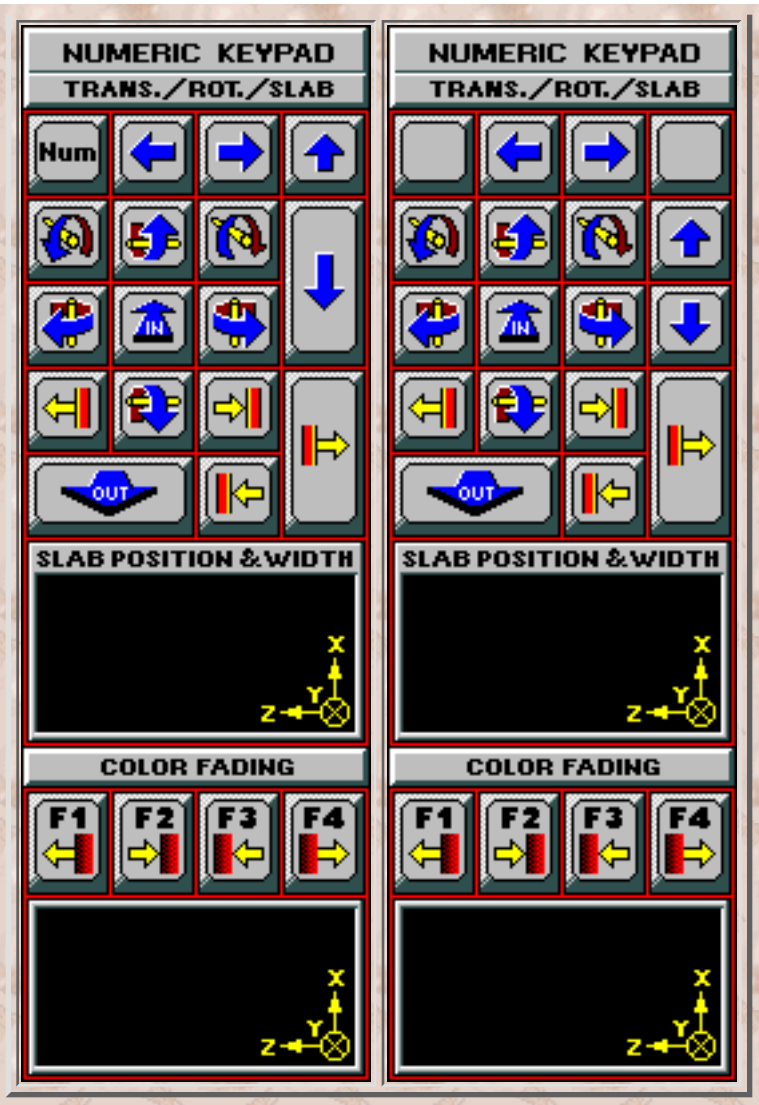
Be sure to avoid ctrl_alt combinations, because some of these combinations may have a very interesting effect (try, for example, ctrl_alt_del or ctrl_alt_F1).

The table below contains the list of controls and corresponding action upon the structure which is currently handled (held, catched). The table refers to PC (101/102) keyboard. There are slight differences between PC and terminal keyboard; three terminal keys are listed in the table (KP_F2, KP_F3, KP_Separator). If you have some exotic keyboard, use the program xshowkey to check the mapping of keys and send this list to the author: zucic@garlic.mefos.hr

KEY	LOCATION	ACTION
0	Numeric keypad	Translate structure along z in negative direction
1	Numeric keypad	Move back (distant) slab surface along z in positive direction
2	Numeric keypad	Rotate structure clockwise around x
3	Numeric keypad	Move back (distant) slab surface along z in negative direction
4	Numeric keypad	Rotate structure clockwise around y
5	Numeric keypad	Translate structure along z in positive direction
6	Numeric keypad	Rotate structure counterclockwise around y
7	Numeric keypad	Rotate structure counterclockwise around z
8	Numeric keypad	Rotate structure counterclockwise around x
9	Numeric keypad	Rotate structure clockwise around z
delete	Numeric keypad	Move front (close) slab surface along z in positive direction
enter	Numeric keypad	Move front (close) slab surface along z in negative direction
/ (slash) KP_F2	Numeric keypad	Translate structure left
* (asterisk) KP_F3	Numeric keypad	Translate structure right
- (minus)	Numeric keypad	Translate structure up
+ (plus) KP_Separator	Numeric keypad	Translate structure down
F1	Function keys	Move back (distant) color surface along z in positive direction
F2	Function keys	Move back (distant) color surface along z in negative direction
F3	Function keys	Move front (close) color surface along z in positive direction
F4	Function keys	Move front (close) color surface along z in negative direction
Num Lock	Numeric keypad	Unused

Here are the illustrations:

PC keyboard	Terminal keyboard


NUMERIC KEYPAD
TRANS./ROT./SLAB
Num
IN
OUT
SLAB POSITION & WIDTH
X
Y
Z
COLOR FADING
F1
F2
F3
F4
NUMERIC KEYPAD
TRANS./ROT./SLAB
IN
OUT
SLAB POSITION & WIDTH
X
Y
Z
COLOR FADING
F1
F2
F3
F4

ADD, EXP, EXPAND

NAME
ADD, EXP, EXPAND - add specified atoms to current selection.

SYNOPSIS
ADD chain identifiers/residue serials/residue names/atom names
ADD residue_ranges
ADD residue_names
ADD keyword

DESCRIPTION
Add specified atoms to current selection. Atoms are added according to the specified cryteria. The command EXPAND does exactly the same job as ADD. The essential difference between ADD and SELECT is that ADD does not overwrite the previous selection. Four types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword).

DETAILED SELECTION
In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain identifiers/residue serials/residue names/atom names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

add a/*/*/*	Add all atoms from chain A to current selection.
add * exc m/*/*/ca	Add CA atoms from all chains except chain M.
add */*/*/* exc ca,c,n,o	Add all atoms except CA, C, N and O.

add a/* exc 72-112/*/ca	Add CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

add 1-100	Add residues from 1 to 100 to current selection.
add 1-100 exc 20-40	Add residues 1-100 but exclude 20-40.
add 1, 4, 8, 11-48 exc 20-32	Add residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

add phe,tyr,trp	Add PHE, TYR and TRP to current selection.

SPECIAL SELECTION

Some special keywords may be combined with ADD to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

add *	Add all atoms to current selection, i.e. select all.
add all	The same as ADD *
add aci add acidic	Add acidic amino acids (GLU and ASP).
add ali add aliphatic	Add aliphatic amino acids (ILE, LEU and VAL).
add bas add basic	Add basic amino acids (ARG, LYS and HIS).
add cha add charged	Add charged amino acids (ARG, LYS, HIS, GLU and ASP).
add com add complement	Add atoms which were not select previously.
add het add hetero	Add hetero atoms (heme groups, water etc.).
add pho add hydrophobic	Add hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
add mai add main_chain	Add main chain atoms (CA, C, N and O).
add neg add negative	Add negatively charged amino acids (GLU and ASP).

add pol **add polar**	**Add polar amino acids** **(ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).**
add pos **add positive**	**Add positively charged amino acids (ARG, LYS and HIS).**
add sid **add side_chains**	**Add atoms which belong to side chains (all except CA, C, N and O).**
add sma **add small**	**Add small amino acids** **(GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).**
add tin **add tiny**	**Add tiny amino acids (GLY,ALA and SER).**

RELATED COMMANDS

EXPAND does exactly the same job as ADD. SELECT overwrites the previous selection. RESTRICT restrics the previous selection.

ATO, ATOMS

NAME
ATO, ATOMS - change drawing style for atoms.

SYNOPSIS
ATO style
ATOMS style

DESCRIPTION
Change drawing style for atoms. Atom style is defined separately from bond style. For BALLS, BIG and SPACEFILL style, atom sizes are read from .garlicrc file. If this file is not available, hard-coded defaults are used.

STYLE	DESCRIPTION	SIZE
0	Unvisible atoms	Fixed
1	A single pixel	Fixed
2	3x3 cross (5 pixels)	Fixed
3	3x3 square (9 pixels)	Fixed
4	5x5 circle (21 pixel)	Fixed
5	7x7 square (37 pixels)	Fixed
6	9x9 circle (61 pixel)	Fixed
7	11x11 circle (109 pixels)	Fixed
bal balls	Balls (suitable to draw balls and sticks)	Proportional
big	Big (oversized atoms)	Proportional
spa spacefill	Spacefill style; the size of atom depends on atom type	Proportional

NOTES
(1) Unvisible atoms (style 0) are not treated as hidden - they are just invisible.
(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

RELATED COMMANDS
BON (BONDS) changes drawing style for bonds.

BAC, BACKBONE

NAME
BAC, BACKBONE - draw backbone.

SYNOPSIS
BAC
BAC OFF
BAC bond_style

DESCRIPTION
Draw polypeptide (protein) backbone, by connecting neighbouring CA (C alpha) atoms. All other atoms in the selected portion of the structure will be hidden. At present, five bond styles are available, all of them fixed in size.

If this command is specified without any arguments, default bond style (5) will be used.

The command BAC OFF hides the backbone and shows atoms and bonds which were visible before.

STYLE	THICKNESS	TYPE
0	Unvisible bonds	Fixed
1	single, thin line	Fixed
2	Three lines	Fixed
3	Five lines	Fixed
4	Seven lines	Fixed
5	Nine lines	Fixed

NOTES
(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.

RELATED COMMANDS
BON (BONDS) changes drawing style for bonds, but does not affect the backbone. ATO (ATOMS) command may be used to add atoms to the backbone. It is recommended to show only CA atoms, using BALL or SPACEFILL style.

BG, BACKG, BACKGROUND

NAME

BG, BACKG, BACKGROUND - change the main window background color.

SYNOPSIS

BG color
BACKG color
BACKGROUND color

DESCRIPTION

Change the main window background color. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted. Examples:

COMMAND	DESCRIPTION
bg white	White
bg DarkSlateGray	Dark dark slate gray
bg #3000a0007000	Kind of green
bg rgb:0/0/8	Dark blue
bg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS

FG (FOREG, FOREGROUND) changes the main window foreground (text) color.

BON, BONDS

NAME
BON, BONDS - change drawing style for bonds.

SYNOPSIS
BON style
BONDS style

DESCRIPTION
Change drawing style for bonds. Bond style is defined separately from atom style. At present, proportionally sized styles are not available.

STYLE	THICKNESS	TYPE
0	Unvisible bonds	Fixed
1	A single line	Fixed
2	Three lines	Fixed
3	Five lines	Fixed
4	Seven lines	Fixed
5	Nine lines	Fixed

NOTES
(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.
(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

RELATED COMMANDS
ATO (ATOMS) changes drawing style for atoms.

CAT, CATCH

NAME
CAT, CATCH - catch the specified macromolecular complex.

SYNOPSIS
CAT identifier
CATCH identifier

DESCRIPTION
Catch the specified structure (macromolecular complex). The structure is a set of atoms read from a single file. Thus, every file is treated as a separate structure. The structure identifier is positive integer. The value zero is not used; structures are numbered 1, 2, 3, etc. When you catch a single structure, all transformations (rotations, translations etc.) are applied to this structure, leaving other structures intact. Selection (commands SELECT, ADD, RESTRICT) are also applied only to this structure. The command CATCH is used when working with more than one structure - for example, when docking an inhibitor to a substrate. When only one structure (file) is loaded, this command has no purpose. Examples:

COMMAND	DESCRIPTION
cat 1	Catch the structure number 1.
cat 7	Catch the structure number 7.

NOTES
(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure you want to catch. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
ALA 125
CA  941  C
occ.:  1.00
t.f.: 28.40
x:    16.261
y:    -4.719
z:   -18.285
hydrophob.:
 -0.50

selected
```

RELATED COMMANDS

TAK (TAKE) does exactly the same job as CATCH.

CEN, CENTER

NAME

CEN, CENTER - change the origin of the internal coordinate system.

SYNOPSIS

CEN
CENTER

DESCRIPTION

An internal coordinate system is assigned to each structure. The command CEN (CENTER) redefines the position of this origin. A new origin will be equal to the geometric center position calculated for selected atoms. This may be quite useful if working with a large structure. By selecting a small portion of the structure, or even a single atom, the internal system origin may be set to a place which contains the most interesting part of the structure. Rotations, slab changes and color changes will be done with respect to new origin. This will keep the interesting part in the same part of the screen. It is recommended to hide the uninteresting part of the structure, to make rotations and other transformations faster. When you load the structure the geometric center of the whole structure is used as the internal system origin. If you displaced the origin but now you want to move it back to the original position, you should these two commands:

sel all
cen

This command is applied to the structure which is currently hangled, i.e. the one to which the command CATCH was applied last.

RELATED COMMANDS

POS sets the origin of the internal system to the specified position in the main (global) coordinate system.

COL, COLOR

NAME
COL, COLOR - change the color of selected atoms and their corresponding bonds.

SYNOPSIS
COL color_scheme_name
COL left_1 middle_1 right_1 ... ... left_N, middle_N, right_N

DESCRIPTION
Change the color used to draw selected atoms and their corresponding bonds. Half of each bond belongs to one atom, while half of the same bond belongs to another atom. The easy way to specify color is to use the predefined color scheme. The powerfull (but more complicated) way to specify color is to issue detailed color specification.

COLOR USAGE
In garlic, colors are used to create 3D illusions. In most color schemes, the atoms close to the observer have bright colors, while distant atoms have dark colors. Atoms and bonds look like three-dimensional objects because one side is brighter than the other. Here are some technical details about color usage:

At least one and at most eight surfaces are assigned to each structure. These surfaces are equidistant planes, spheres or cylinders. The surface which is nearest to the observer is called "front surface", while the most distant surface is called "back surface". To each surface, three colors are assigned: left, middle and right color. In most color schemes, left color is bright and right color is dark. Atoms may be divided in three groups:

(1) Atoms which are in front of the front surface;
(2) Atoms which are behind the back surface;
(3) All other atoms, positioned in the sandwich between two surfaces.

All atoms which are in front of the front surface are drawn using the same set of three colors which assigned to front surface. Atoms behind the back surface are colored using three colors assigned to back surface. Colors for atoms laying between two surfaces are prepared by linear interpolation of colors assigned to these two surfaces. This is what I call color fading (this term was not the best choice I could make, sorry).

In a special case, when only one surface is used, color does not depend on distance.

Almost all predefined color schemes typically define two surfaces, i.e. a total of six colors. There are some exceptions: color schemes HOT and COLD use three surfaces, while MONOCHROME uses only one.

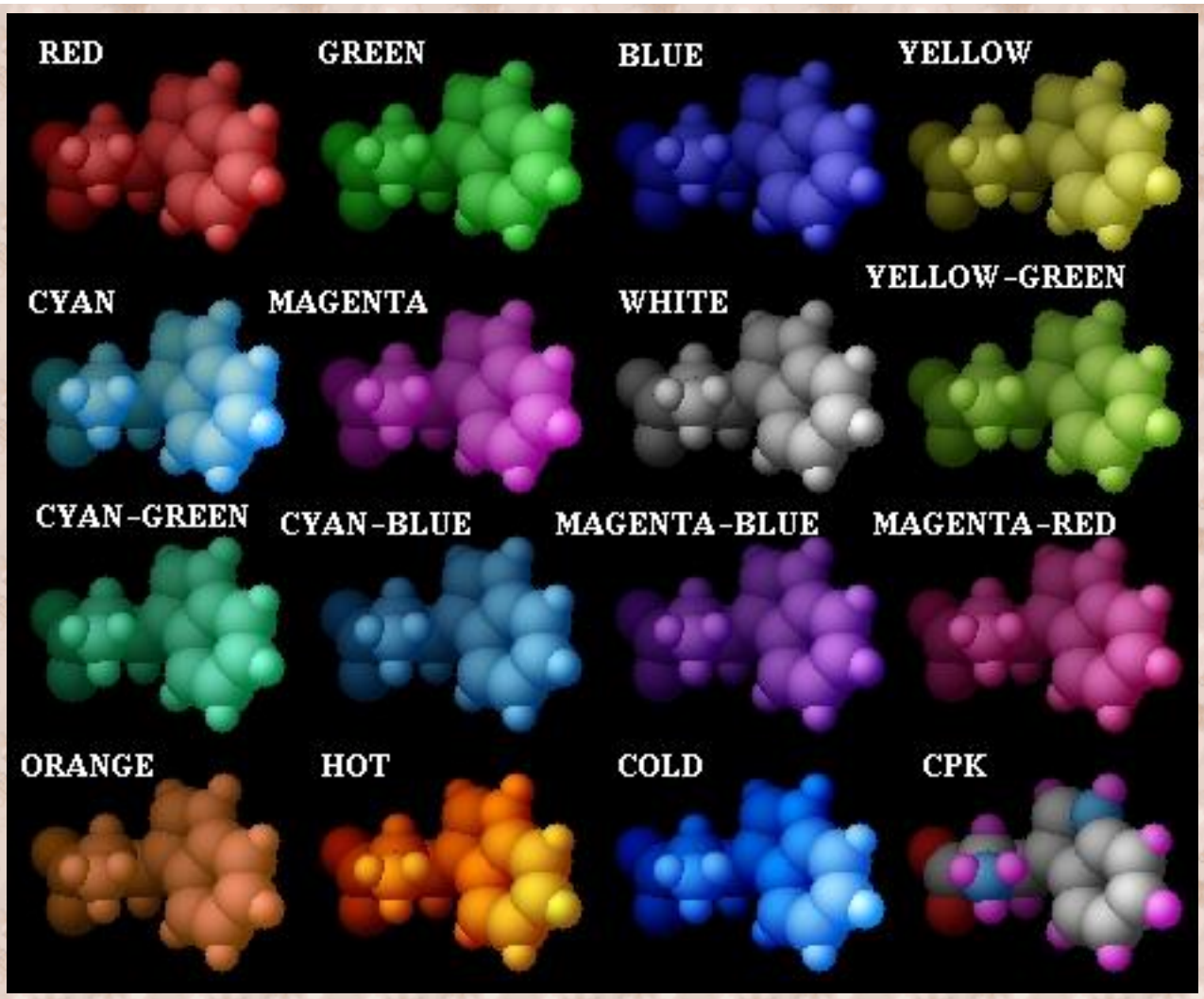
Planes, spheres and cylinders
For most proteins and other molecules, planar fading is the best choice. In this case, a set of planes, perpendicular to z axis is used. Concentric spheres may be used when working with large globular proteins, while cylinders may be used for beta-barrel proteins, like porins. The axis of concentric cylinders is parallel to y.

USING PREDEFINED COLOR SCHEMES
Twenty predefined color schemes are available:

SCHEME NAME	DESCRIPTION

RED	**Red color scheme; distant atoms are dark**
GREEN	**Green, distant atoms are dark**
BLUE	**BLUE (deep sea), distant atoms are dark**
YELLOW	**Yellow, distant atoms are dark**
CYAN	**Cyan (cloudless sky), distant atoms are dark**
MAGENTA	**Magenta, distant atoms are dark**
WHITE	**Shades of gray, distant atoms almost black**
YELLOW-GREEN	**Somewhere between yellow and green, distant atoms dark**
CYAN-GREEN	**Somewhere between green and blue-green, distant atoms dark**
CYAN-BLUE	**Somewhere between blue and blue-green, distant atoms dark**
MAGENTA-BLUE	**Somewhere between blue and magenta, distant atoms are dark**
MAGENTA-RED	**Somewhere between red and magenta, distant atoms are dark**
ORANGE	**Orange, distant atoms are dark**
HOT	**The nearest atoms are yellow, atoms in the middle are orange and distant atoms are dark red**
COLD	**The nearest atoms are cyan, atoms in the middle are cyan-blue and distant atoms are dark blue**
MONOCHROME	**Edge black, central region white, distance independent**
CPK	**Modified Corey-Pauling-Kultun color scheme, distant atoms are dark**
ZEBRA	**Residues with even serial number are red, odd residues cyan-blue, distant atoms are dark**
CHAIN	**Use color to distinguish chains; distant atoms are should be dark**
HYPHOB	**Assign color according to hydrophobicity; distant atoms are dark**

Do not abbreviate the color scheme name! Case is not important. Some selected schemes are shown here:



DETAILED COLOR SPECIFICATION

Most users should be satisfied with predefined color schemes. Anyway, it is fairly easy to use colors which are not available through predefined schemes. To define N color planes (up to eight), you have to define 3 * N colors. The keyword OLD may be used to leave the previous value unchanged. Here are some examples:

col yellow orange red red DarkRed black	Define two color surfaces with six colors.
col rgb:ffff/ffff/4444 rgb:ffff/dddd/0000 DarkRed	One color surface, three colors.
col old old old black black black	Leave the front colors unchanged, set all back colors to black.

Be careful with the keyword OLD - it may be used only if the currently used color scheme has at least as many colors as a new one.

RELATED COMMANDS

FADING may be used to change the position of outer color surfaces and to switch color fading on and off.

DIS, DISCARD

NAME

DIS, DISCARD - discard the specified macromolecular complex.

SYNOPSIS

DIS identifier
DIS ALL
DIS *
DISCARD identifier
DISCARD ALL
DISCARD *

DESCRIPTION

Discard the specified structure (macromolecular complex). The memory used to store the structure is freed. If keyword ALL is used (or asterisk, *), all structures will be discarded. Examples:

COMMAND	DESCRIPTION
dis 1	Discard the structure number 1.
dis 7	Discard the structure number 7.
dis *	Discard all. Nothing will be loaded after this command.

NOTES

(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure which should be discarded. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
ALA 125
CA  941  C
occ.:  1.00
t.f.: 28.40
x:    16.261
y:    -4.719
z:   -18.285
hydrophob.:
 -0.50

selected
```

(2) If you discard everything, the indexing will be reset too. The first structure you load after discarding everything will be assigned index "1" (one).

RELATED COMMANDS

LOAD (READ) loads the specified file.

EXE, EXECUTE

NAME

EXE, EXECUTE - load and execute garlic script.

SYNOPSIS

EXE file_name
EXECUTE file_name

DESCRIPTION

Load and execute the specified garlic script. The garlic script file should contain garlic commands. There is only one command which is not executed if added into garlic script: the EXE command. This is done to avoid endless loops; the script which executes itself will generate an endless loop. If you don't like it, change to source file execute_command1.c (use the source, Luke!). Examples:

COMMAND	DESCRIPTION
exe tango.script	Execute the script which loads trp.pdb and forces this molecule to play something similar to Argentinian tango.

RELATED COMMANDS

LOG may be used to store commands used during a garlic session. The log file may be used later as a script.

EXI, EXIT, QUI, QUIT

NAME

EXI, EXIT, QUI, QUIT - quit garlic session (exit from garlic).

SYNOPSIS

EXI
EXIT
QUI
QUIT

DESCRIPTION

Quit garlic session, i.e. exit from garlic. The main garlic window will be closed, memory freed etc. At present, garlic is not capable to save any data (this will be changed, of course), so there are no warning messages.

FAD, FADING

NAME
FAD, FADING - change the color dependence on a distance from the observer.

SYNOPSIS
FAD keyword
FAD FRONT shift
FAD BACK shift
FADING keyword
FADING FRONT shift
FADING BACK shift

DESCRIPTION
Change the way color depends on distance. Distance is measured from the atom to the observer. This command comes in three versions:

(1) FADING FRONT shift ----> move the front color surface;
(2) FADING BACK shift ----> move the back color surface;
(3) FADING keyword ----> switch fading off or change the type of the surfaces.

FADING FRONT shift
This command moves the front fading surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys F1 and F2). The shift value should be given in angstroms. Positive shift moves the front color surface away from the observer. With most color schemes, the front (closer) portion of the structure will be brighter after the positive shift. FRONT may be abbreviated to FRO.

FADING BACK shift
This command moves the back fading surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys F3 and F4). The shift value should be given in angstroms. Positive shift moves the back color surface away from the observer. With most color schemes, the contrast will be reduced after the positive shift. Negative shift results in better contrast, i.e. distant atoms will become darker. BACK may be abbreviated to BAC.

FADING keyword
Some keywords may be used to change the type of color surfaces and to switch color fading off. Here is the list of keywords:

SHORT FORM	LONG FORM	DESCRIPTION
OFF	OFF	Switch fading off: colors should become distance independent.
PLA	PLANE	Use planes as color surfaces.
SPH	SPHERE	Use spheres as color surfaces.
CYL	CYLINDER	Use cylinders as color surfaces.
HALF-SPH	HALF-SPHERE	Use spheres as color surfaces, but apply only to the front half of the structure.
HALF-CYL	HALF-CYLINDER	Use cylinders as color surfaces, but apply only to the front half of the structure.

For most structures, the planar fading is the best choice. Spherical and semi-spherical fading may be useful when working with large globular proteins, while cylindrical and semi-cylindrical fading is useful when working with beta-barrel proteins (like porins). The cylinder axis is parallel to y axis (vertical from users standpoint).

EXAMPLES

COMMAND	DESCRIPTION
fading off	Switch color fading off.
fading pla	Switch fading to planar.
fading front 4.5	Move the front color surface 4.5 angstroms away from the observer.
fading back -2.8	Move the back color surface 2.8 angstroms closer to the observer.
fading half-sph	Change fading to semi-spherical.

RELATED COMMANDS

COLOR defines the color for selected atoms.

FG, FOREG, FOREGROUND

NAME

FG, FOREG, FOREGROUND - change the main window foreground color.

SYNOPSIS

FG color
FOREG color
FOREGROUND color

DESCRIPTION

Change the main window foreground color. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted. This color is used to draw labels and titles. Note that this color is not used to draw atoms and bonds. Examples:

COMMAND	DESCRIPTION
fg white	White
fg DarkSlateGray	Dark dark slate gray
fg #3000a0007000	Kind of green
fg rgb:0/0/8	Dark blue
fg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS

BG (BACKG, BACKGROUND) changes the main window background color.

FON, FONT

NAME

FON, FONT - change font.

SYNOPSIS

FON font_name
FONT font_name

DESCRIPTION

Change font. At present, garlic uses only one font for input, output and main window. Try to execute xlsfonts on your system, to obtain a list of fonts. Default font is set in .garlicrc file. Examples:

```
fon 10x20
fon olglyph-19
```

RELATED COMMANDS

FG changes the text color used to draw strings in the main window. TFG changes the text color used to draw strings in input and output window.

HID, HIDE

NAME
HID, HIDE - hide selected atoms.

SYNOPSIS
HID
HIDE

DESCRIPTION
Hide selected atoms and associated bonds.

RELATED COMMANDS
SHOW shows selected atoms and associated bonds.

HYB, HYBONDS

NAME

HYB, HYBONDS - generate hydrogen bonds.

SYNOPSIS

HYB
HYB style
HYB OFF
HYBONDS
HYBONDS style
HYBONDS OFF

DESCRIPTION

Generate hydrogen bonds for the entire structure. Show hydrogen bonds for visible atoms. At present, some very simple geometric restrains are used to generate hydrogen bonds. Check the configuration file (.garlicrc) and the source file gen_hybonds.c to learn more about these restrains.

Keyword OFF may be used to hide hydrogen bonds.

Default style used to draw hydrogen bonds is 1 (a single line, fixed). You can change it by specifying the style. Examples:

hyb	**Generate hydrogen bonds and show them using default style (1).**
hyb 4	**Generate hydrogen bonds and show them using style 4 (four lines).**
hyb off	**Hide hydrogen bonds**

IGN, IGNORE

NAME

IGN, IGNORE - do nothing.

SYNOPSIS

IGN
IGNORE

DESCRIPTION

This command does nothing. It is absolutely useless. Do not use it to pause the program execution - PAUSE should be used for this purpose.

LAB, LABELS

NAME

LAB, LABELS - show or hide labels.

SYNOPSIS

LAB
LABELS
LAB OFF
LABELS OFF

DESCRIPTION

If used without keyword OFF, this command shows labels for selected atoms. If used with keyword OFF, this command hides labels. Each label contains:
(1) residue name;
(2) residue sequence number;
(3) chain identifier;
(4) atom name;
(5) alternate location indicator.

RELATED COMMANDS

TITLE adds the title to the main window. TAG assigns the specified tag to a structure. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

LOA, LOAD, REA, READ

NAME
LOA, LOAD, REA, READ - load the specified file.

SYNOPSIS
LOA file_name
LOAD file_name
REA file_name
READ file_name

DESCRIPTION
Load and display the specified file. The file content will be treated as a separate structure. The unique structure identifier (positive integer) will be assigned to this structure. The structure will be placed in the middle of the screen.

You can load any file more than once. A total number of structures which may be simultaneously loaded depends on the available memory. The hard-coded maximum is 1000, which should be more than enough.

The command LOAD may be written in uppercase, lowercase or mixed case, but the file name should be specified in correct case - unix file names are case sensitive.

SEARCH PATH
The file is searched in one or more directories, in the following order:

(1) the current working directory;
(2) directory specified in the environment variable MOL_DIR;
(3) all directories specified in the environment variable MOL_PATH.

The recommended environment variable is MOL_PATH.

RELATED COMMANDS
DIS (DISCARD) discards the specified structure. SAV (SAVE) saves the atomic data to a file.

LOG

NAME

LOG - write interactive commands into the log file.

SYNOPSIS

LOG file_name
LOG OFF

DESCRIPTION

Use this command to log your garlic session into the specified file. The log file may be modified later and used as garlic script. LOG OFF closes the log file and stops logging.

NOTES

(1) If you logged the entire garlic session and want to use your log file as script, do not forget to remove the keyword QUIT (EXIT) which was used to end the garlic session!

(2) Lines which have # in the first column are treated as comments. Empty lines are ignored.

(3) Use PAUSE to pause the program execution. This is useful if preparing lecture or presentation, otherwise the script will run till the end without stopping.

(4) You can start and stop logging at any moment during your garlic session. Do not use the same log file name twice if you want to keep the old file - it will be overwritten.

RELATED COMMANDS

Exe executes the garlic script. PAUSE pauses the script execution.

MON, MONO

NAME
MON, MONO - switch to mono mode.

SYNOPSIS
MON
MONO

DESCRIPTION
Switch to mono mode, i.e. switch stereo off.

RELATED COMMANDS
Use STEREO to switch to stereo mode. STEREO OFF does the same job as MONO.

PAU, PAUSE

NAME

PAU, PAUSE - pause script execution.

SYNOPSIS

PAU
PAUSE

DESCRIPTION

Pause script execution. This may be useful if using garlic for lectures and conference presentations. The script execution will be paused until the return key is pressed.

RELATED COMMANDS

Use EXE (EXECUTE) to load and execute garlic script. Use LOG to log your garlic session. The log file may be modified into the script file later (or even left unchanged).

POS, POSITION

NAME

POS, POSITION - move the origin of the internal coordinate system to the specified position.

SYNOPSIS

POS x y z
POSITION x y z

DESCRIPTION

An internal coordinate system is assigned to each structure. The command POS (POSITION) sets the position of this origin. Three coordinates (x, y and z) should be specified.

Initially, the position of geometric center is used as the internal system origin for each structure. When loaded, this origin is set into the point (0, 0, 0).

RELATED COMMANDS

CEN redefines the internal system origin.

REG, REGISTER

NAME
REG, REGISTER

SYNOPSIS
REG
REGISTER

DESCRIPTION
Register garlic: send a short e-mail to the author. This command will fail if your machine is not connected to the Internet. The only content of the message will be the word 'Hi!'. Your registration will not be abused, i.e. your e-mail address will not be given to spammers or anyone else. The registration will be used just to count garlic users.

If your machine is not connected to the Internet, send an e-mail from some other machine. Questions, comments and suggestions are welcome.

The author may be reached at:
zucic@garlic.mefos.hr
zucic@drava.etfos.hr
zucic@mia.os.carnet.hr

Author's home page:
http://garlic.mefos.hr/zucic

REGISTER GARLIC - by registering, you are supporting further development of this program!

RES, RESTRICT

NAME
RES, RESTRICT - restrict the current selection.

SYNOPSIS
RES chain identifiers/residue serials/residue names/atom names
RES residue_ranges
RES residue_names
RES keyword

DESCRIPTION
Restrict the current selection. Atoms which do not satisfy the specified cryteria are excluded from selection. Four types of restriction cryteria may be used:

(1) detailed restriction;
(2) restriction by residue serial numbers;
(3) restriction by residue names;
(4) special restriction (by keyword).

DETAILED RESTRICTION
In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The string should contain exactly three slashes, separating different data types:

chain identifiers/residue serials/residue names/atom names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to specify all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from restriction.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from restriction.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from restriction. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to specify all atoms, while EXC may be used to exclude some atoms from this specification. Examples:

res a/*/*/*	**Leave only atoms which belong to chain A.**
res * exc m/*/*/ca	**Leave only CA atoms which belong to chain M.**
res */*/*/* exc ca,c,n,o	**Remove CA, C, N and O atoms from the selection.**
res a/* exc 72-112/*/ca	**Leave only CA atoms which belong to chain A, but exclude residues 72-112.**

RESTRICTION BY RESIDUE SERIAL NUMBERS

In this type of selection restriction, residue numbers, residue ranges or residue names may be specified. The restriction cryteria should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

res 1-100	Leave only atoms which belong to residues from 1 to 100.
res 1-100 exc 20-40	Leave only atoms which belong to residues 1-100, but exclude 20-40.
res 1, 4, 8, 11-48 exc 20-32	Leave atoms which belong to residues 1, 4, 8, 11-48 but exclude residues 20-32.

RESTRICTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

res phe,tyr,trp	Restrict selection to PHE, TYR and TRP.

SPECIAL RESTRICTION

Some special keywords may be combined with RES to specify residues or atoms according to some properties. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted. COM (COMPLEMENT) may be specified, but restriction to complement means that nothing will be left in the selection. Examples:

res *	Leave the selection unchanged (trivial, useless).
res all	The same as RES *
res aci res acidic	Leave only acidic amino-acids in the selection (GLU and ASP).
res ali res aliphatic	Leave only aliphatic amino acids (ILE, LEU and VAL).
res bas res basic	Leave only basic amino acids (ARG, LYS and HIS).
res cha res charged	Leave only charged amino acids (ARG, LYS, HIS, GLU and ASP).
res com res complement	Leave only atoms which were not select previously.
res het res hetero	Leave only hetero atoms (heme groups, water etc.).
res pho res hydrophobic	Leave only hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
res mai res main_chain	Leave only main chain atoms (CA, C, N and O).
res neg res negative	Leave only negatively charged amino acids (GLU and ASP).

res pol **res polar**	**Leave only polar amino acids** **(ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).**
res pos **res positive**	**Leave only positively charged amino acids (ARG, LYS and HIS).**
res sid **res side_chains**	**Leave only atoms which belong to side chains (all except CA, C, N and O).**
res sma **res small**	**Leave only small amino acids** **(GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).**
res tin **res tiny**	**Leave only tiny amino acids (GLY,ALA and SER).**

RELATED COMMANDS

SELECT overwrites the previous selection. ADD expands the previous selection.

ROT, ROTATE

NAME

ROT, ROTATE - rotate the structure for the given angle around the given axis.

SYNOPSIS

ROT axis angle

DESCRIPTION

Rotate the structure. The axis should be specified with one letter (x, y or z) and the angle should be given in degrees.

EXAMPLES

COMMAND	DESCRIPTION
rot z 90	Rotate around z for 90 degrees (counterclockwise).
rot x -0.5	Rotate around x for -0.5 degrees (clockwise).

SAV, SAVE

NAME

SAV, SAVE - save atomic data to the specified file.

SYNOPSIS

SAV file_name
SAV file_name SEL
SAVE file_name
SAVE file_name SEL

DESCRIPTION

Save atomic data to the specified file. By default, all atoms are saved. If keyword SEL is used, only selected atoms are saved. No header is written, just ATOM and HETATM records. You may copy and paste the header from the original (input) file. Coordinates will be expressed in the internal coordinate system (the geometric center used as the origin). Don't forget that unix (linux) file names are case sensitive. If the specified file exists already, it will be overwritten without warning!

RELATED COMMANDS

LOA (LOAD) loads the specified structure. DIS (DISCARD) discards the specified structure.

SEL, SELECT

NAME

SEL, SELECT - select specified atoms. Overwrite the previous selection.

SYNOPSIS

SEL chain identifiers/residue serials/residue names/atom names
SEL residue_ranges
SEL residue_names
SEL keyword

DESCRIPTION

Select specified atoms. Atoms are selected according to the specified cryteria. Four types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword).

DETAILED SELECTION

In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain identifiers/residue serials/residue names/atom names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

sel a/*/*/*	Select all atoms from chain A.
sel * exc m/*/*/ca	Select CA atoms from all chains except chain M.
sel */*/*/* exc ca,c,n,o	Select all atoms except CA, C, N and O.
sel a/* exc 72-112/*/ca	Select CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

sel 1-100	Select residues from 1 to 100.
sel 1-100 exc 20-40	Select residues 1-100 but exclude 20-40.
sel 1, 4, 8, 11-48 exc 20-32	Select residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

sel phe,tyr,trp	Select PHE, TYR and TRP.

SPECIAL SELECTION

Some special keywords may be combined with SEL (SELECT) to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

sel *	Select all atoms (select all).
sel all	The same as SEL *
sel aci sel acidic	Select acidic amino acids (GLU and ASP).
sel ali sel aliphatic	Select aliphatic amino acids (ILE, LEU and VAL).
sel bas sel basic	select basic amino acids (ARG, LYS and HIS).
sel cha sel charged	Select charged amino acids (ARG, LYS, HIS, GLU and ASP).
sel com sel complement	Select atoms which were not selected previously.
sel het sel hetero	Select hetero atoms (heme groups, water etc.).
sel pho sel hydrophobic	Select hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
sel mai sel main_chain	Select main chain atoms (CA, C, N and O).
sel neg sel negative	Select negatively charged amino acids (GLU and ASP).
sel pol sel polar	Select polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).

sel pos **sel positive**	**Select positively charged amino acids (ARG, LYS and HIS).**
sel sid **sel side_chains**	**Select atoms which belong to side chains (all except CA, C, N and O).**
sel sma **sel small**	**Select small amino acids** **(GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).**
sel tin **sel tiny**	**Select tiny amino acids (GLY, ALA and SER).**

RELATED COMMANDS

ADD expands the previous selection. RESTRICT restrics the previous selection.

SHO, SHOW

NAME
SHO, SHOW - show selected atoms.

SYNOPSIS
SHO
SHOW

DESCRIPTION
Show selected atoms and associated bonds. Atoms and bonds drawn using style "0" will remain unvisible, but they are formally treated as visible.

RELATED COMMANDS
HIDE hides selected atoms and associated bonds.

SLA, SLAB

NAME
SLA, SLAB - change slab.

SYNOPSIS
SLA keyword
SLA FRONT shift
SLA BACK shift
SLAB keyword
SLAB FRONT shift
SLAB BACK shift

DESCRIPTION
Change the slab. Slab is used to cut the slice out from the structure and to hide the rest. Two slab surfaces are used: the front slab surface, which is the one closer to the observer and the back slab surface. There are three versions of this command:

(1) SLAB FRONT shift ----> move the front slab surface;
(2) SLAB BACK shift ----> move the back slab surface;
(3) SLAB keyword ----> switch slab off or change the type of the surfaces.

SLAB FRONT shift
This command moves the front slab surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys DEL and ENTER on numeric keypad). The shift value should be given in angstroms. Positive shift moves the front slab surface away from the observer. FRONT may be abbreviated to FRO.

SLAB BACK shift
This command moves the back slab surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys 1 and 3 on the numeric keypad). The shift value should be given in angstroms. Positive shift moves the back slab surface away from the observer. BACK may be abbreviated to BAC.

SLAB keyword
Some keywords may be used to change the type of slab surfaces and to switch slab off. Here is the list of keywords:

SHORT FORM	LONG FORM	DESCRIPTION
OFF	OFF	Switch slab off: all parts of the structure should be visible.
PLA	PLANE	Use planes as slab surfaces
SPH	SPHERE	Use spheres as slab surfaces
CYL	CYLINDER	Use cylinders as slab surfaces
HALF-SPH	HALF-SPHERE	Use spheres as slab surfaces, but hide the back half of the structure.
HALF-CYL	HALF-CYLINDER	Use cylinders as slab surfaces, but hide the back half of the structure.

For most structures, the planar slab is the best choice. Spherical and semi-spherical slab may be useful when working with large globular proteins, while cylindrical and semi-cylindrical slab is useful when working with beta-barrel proteins (like porins). The cylinder axis is parallel to y axis (vertical from users standpoint).

EXAMPLES

COMMAND	DESCRIPTION
slab off	Switch slab off
slab front 4.5	Move the front slab surface 4.5 angstroms away from the observer
slab back -2.8	Move the back slab surface 2.8 angstroms closer to the observer
slab half-sph	Change slab to semi-spherical

STE, STEREO

NAME
STE, STEREO - switch to stereo mode.

SYNOPSIS
STE
STEREO
STE OFF
STEREO OFF

DESCRIPTION
Switch to stereo mode. If keyword OFF is added, switch stereo off, i.e. switch to mono mode.

RELATED COMMANDS
Use MONO to switch to mono mode. It does exactly the same job as STEREO OFF.

TAG

NAME

TAG - assign tag (short text) to a structure.

SYNOPSIS

TAG "tag"
TAG OFF

DESCRIPTION

If used without keyword OFF, this command assigns the specified tag to the structure which is currently handled. If used with keyword OFF, this command hides tag. Tag may contain up to 128 characters.

EXAMPLES

COMMAND	DESCRIPTION
tag "PORIN"	Add the tag "PORIN" to a structure which is currently handled (caught)
tag off	Hide tag

RELATED COMMANDS

The command LABELS assigns labels to selected atoms. TITLE adds the title to the main window. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

TBG

NAME
TBG - change the background color used to draw input and output window.

SYNOPSIS
TBG color

DESCRIPTION
Change the background color used to draw input and output window. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted. Examples:

COMMAND	DESCRIPTION
tbg white	White
tbg DarkSlateGray	Dark dark slate gray
tbg #3000a0007000	Kind of green
tbg rgb:0/0/8	Dark blue
tbg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
TFG changes the foreground (text) color used in input and output window.

TFG

NAME
TFG - change the color used to draw text in input and output window.

SYNOPSIS
TFG color

DESCRIPTION
Change the color used to draw text in input and output window. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted. Examples:

COMMAND	DESCRIPTION
tfg white	White
tfg DarkSlateGray	Dark dark slate gray
tfg #3000a0007000	Kind of green
tfg rgb:0/0/8	Dark blue
tfg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
TBG changes the background color used to draw input and output window.

TIT, TITLE

NAME

TIT, TITLE - add, move or remove the specified title.

SYNOPSIS

TIT identifier OFF
TIT identifier screen_x screen_y
TIT identifier screen_x screen_y "title_string"
TITLE identifier OFF
TITLE identifier screen_x screen_y
TITLE identifier screen_x screen_y "title_string"

DESCRIPTION

The keyword TITLE may be used to add, move or remove the title to or from the main window. Up to 100 titles may be added to the main window, to explain the content. The title position may be specified through screen_x and screen_y. Each title has the unique identifier. The identifier is a number between 0 and 99 (these two values are allowed too). The title string should be included into quotes.

EXAMPLES

COMMAND	DESCRIPTION
tit 8 50 50 "This is porin"	Add the title number 8 to the main window, close to the top left corner
tit 8 100 400	Move the title number 8 to a new position
tit 8 off	Remove (hide) the title number 8

RELATED COMMANDS

The command LABELS assigns labels to selected atoms. TAG assigns the specified tag to a structure. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

TRA, TRANSLATE

NAME

TRA, TRANSLATE - translate the structure for the given shift in the given direction.

SYNOPSIS

TRA axis shift

DESCRIPTION

Translate the structure. The axis should be specified with one letter (x, y or z) and the shift should be given in angstroms.

EXAMPLES

COMMAND	DESCRIPTION
tra x 40	Move to the right, 40 angstroms.
tra y -0.5	Move up, 0.5 angstroms (y points down).

Garlic Tutorial

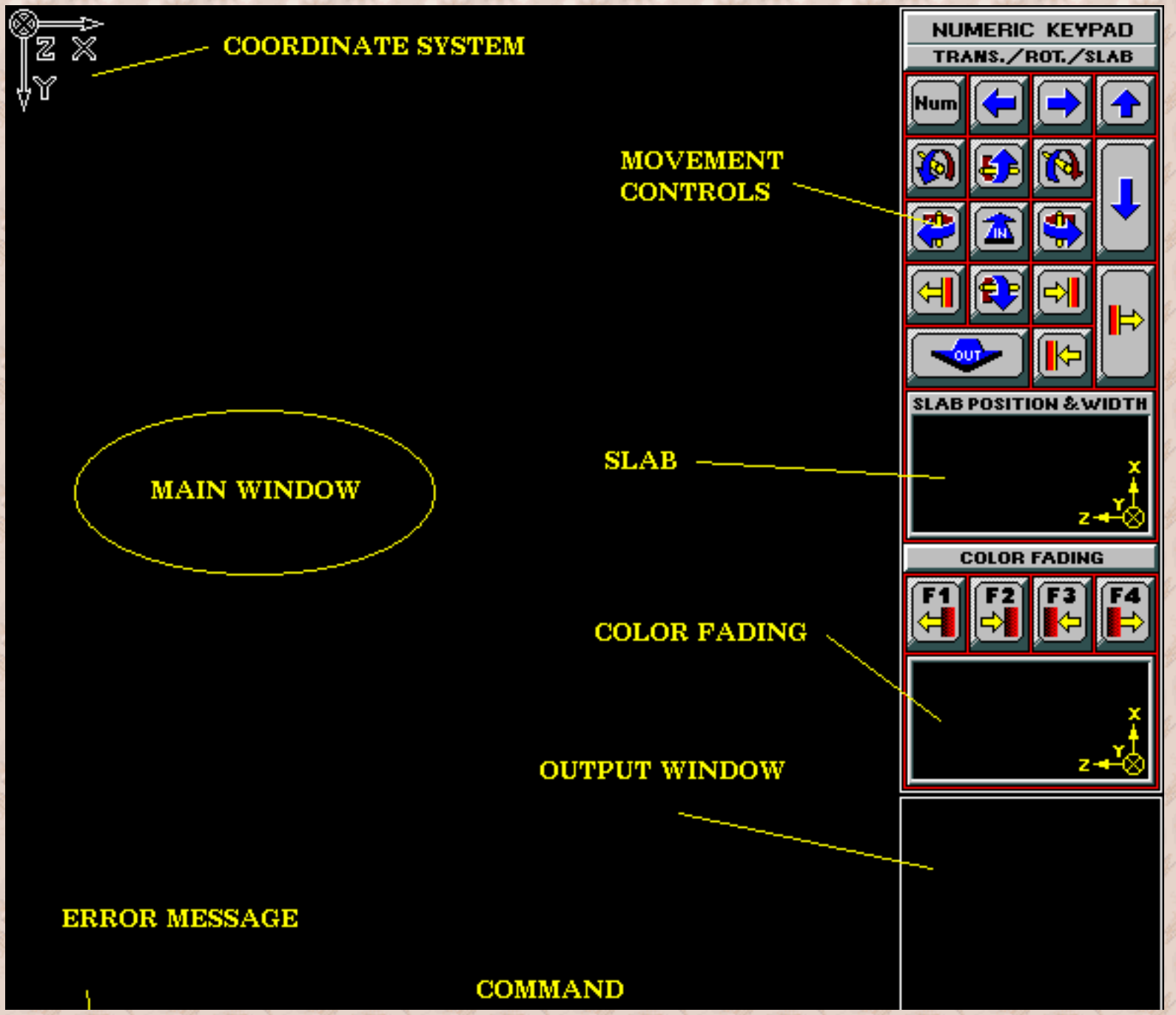
Lesson 1 - Get familiar with garlic

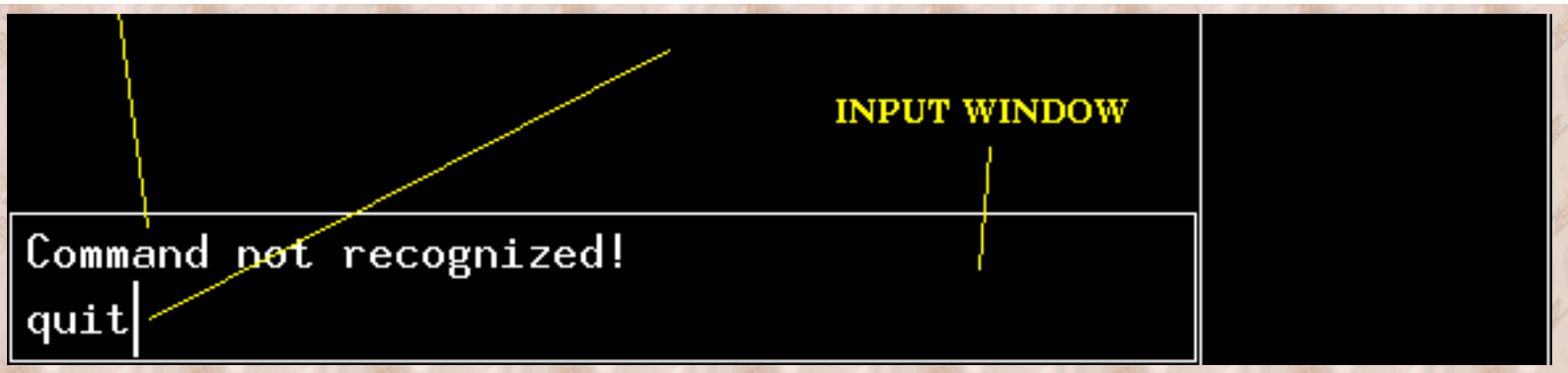
In this lesson, you will execute only one command at garlic prompt: exit, to quit the garlic session.

Start your X session. Use the terminal window to start garlic:

garlic

If garlic is in the path searched by your shell, the garlic window will appear on your screen. Try to remember what are the parts of the entire garlic window. The input window will be empty, but the image below is adapted to show the area reserved for error messages and the area reserved for commands.





When you have learned what are the main parts of the garlic window, quit your garlic session by typing exit or quit (exi or qui):

exit

Garlic Tutorial

Lesson 2 - Load a small structure

In this lesson, you will learn how to load a PDB file and how to move the structure.

Step 1 - start garlic:

garlic

Step 2 - load tryptophan (it should be included in the source package). This command should be executed at garlic prompt:

loa trp.pdb

Step 3 - the role of mouse pointer

Move the mouse pointer over atoms and bonds and read the text which appears in the output window (bottom right corner). Note that half of each bond is assigned to each of two atoms involved in bond formation.

Step 4 - use garlic controls (i.e. the keys on numeric keypad) to rotate the structure (just a single amino acid):

First play for a while with keys 4 and 6, then with 2 and 8, and finally with 7 and 9. Try the same while holding shift (alone), control (alone), alt and shift (simultaneously) and control and shift (simultaneously). Do not try control-alt combinations, unless you are very experienced with unix and X.

Step 5 - use garlic controls to translate the structure:

PC keyboard: use /, *, -, +, 5 and 0.
Terminal keyboard: use PF2, PF3, -, comma, 5 and 0.
Repeat while holding modifier keys (alone or in combination).

Step 6 - move the structure to the screen center again:

pos 0 0 0

Step 7 - rotate and translate the structure using commands instead of controls. Try the following set of commands:

rot x 90
tra x 4
tra y -4
tra z -50
rot y 180

Step 8 - move the color surfaces. As your structure is very small, be sure to hold the control key while pressing functions keys:

Hold control key and press F1.
Hold control key and press F4.
Note that color is changing.

Hold control key and play with F1, F2, F3 and F4 for a while.

Step 9 - move the slab surfaces. As your structure is very small, be sure to hold the control key:

Hold control key and 3 (numeric keypad). Repeat until some atoms and bonds disappear.
Hold control key and play with 1, 3, decimal separator (next to 0) and enter for a while. Note that (in control window) visible atoms are red and unvisible atoms are dark cyan.

Step 10 - end your garlic session:

exit

Garlic Tutorial

Lesson 3 - Playing with two structures

In this lesson, you will learn how to work with two or more structures. The original source package contains two PDB files: trp.pdb and phe.pdb. Each contains a single amino acid: trp.pdb = tryptophan, phe.pdb = phenylalanine. In this lesson, tryptophan will be colored blue, while phenylalanine will be colored red. Note the role of the command cat (catch).

Step 1 - start garlic:

garlic

Step 2 - load trypthophan:

loa trp.pdb

Step 3 - change TRP color to blue:

col blue

Step 4 - load phenylalanine:

loa phe.pdb

Step 5 - change PHE color to red:

col red

Two structures will be distinguished by color and by the identifier: tryptophan is treated as structure number 1, and phenylalanine is treated as structure number 2. Two structures are now overlapping.
Step 6 - move tryptophan to the left:

cat 1
pos -5 0 0

Step 7 - move phenylalanine to the right:

cat 2
pos 5 0 0

Step 8 etc. - use the command cat (catch) to rotate structures one by one

Now use cat 1 and cat 2 to catch and rotate structures, one by one.
Translate both structures to the position where they will be overlapped, but do not use keyword pos!
When finished, end your garlic session.

Garlic Tutorial

Lesson 4 - Drawing styles and color schemes

In this lesson, you will learn different drawing styles, used for atoms and bonds. Note that garlic uses separate styles for atoms and bonds. You will also try some predefined color schemes. Use the X server which offers 24 bits per pixel, if possible.

As you will often reuse some commands, just with a different argument, note that garlic has a history buffer, where commands which were previously used are stored. The arrow keys may be used to recall one of these commands.

Use the "UP" arrow to scan the history buffer backwards, "DOWN" arrow to scan it upwards, "LEFT" arrow to move the insertion mark left and "RIGHT" arrow to move the insertion mark to the right (if possible, of course). Backspace (or delete, if you have some unusual keyboard mapping) may be used to remove characters.

Step 1 - start garlic:

```
garlic
```

Step 2 - load trypthophan and bring it closer to you:

```
loa trp.pdb
pos 0 0 -150
```

Step 3 - make bonds unvisible (i.e. set bond thickness to zero):

```
bon 0
```

Step 4 - learn which drawing styles are available for atoms.
Hint: use the arrow key "UP" to call the previous command.

```
ato 1
ato 2
ato 3
ato 4
ato 5
ato 6
ato 7
ato bal
ato big
ato spa
```

Step 5 - hide atoms:

```
ato 0
```

Step 6 - learn which drawing styles are available for bonds.
Hint: use the arrow key "UP" to call the previous command.

```
bon 1
bon 2
```

bon 3
bon 4
bon 5

Step 7 - learn how to draw balls and sticks:

bon 4
ato bal

Step 8 - try some predefined color schemes.
Hint: use the arrow key "UP" to call the previous command.
Warning: Always use the full color scheme name (do not abbreviate)!

col red
col green
col blue
col yellow
col cyan
col magenta
col white
col yellow-green
col cyan-green
col cyan-blue
col magenta-blue
col magenta-red
col orange
col hot
col cold
col cpk

Step 9 - quit this garlic session:

exit

Garlic Tutorial

Lesson 5 - How to select atoms

In this lesson, you will learn how to select atoms. The command select (or whatever command plays this role) is one of the most important commands in every molecular visualization program.

For this lesson, you will need a true protein structure, not just a single amino acid as in previous lessons.

Step 1 - obtain the protein structure:

Use you web browser to access The Protein Data Bank (www.rcsb.org) .
Type 1HUC into the small search field. Start the search and wait for the answer.
Choose the option "Download/Display File".
Finally, choose file format "PDB", compression "none" in the section "Download the Structure File" and wait.

Step 2 - start garlic:

garlic

Step 3 - load the structure. You should have the file 1HUC.pdb somewhere in the path searched by garlic (if you defined the environment variable MOL_DIR), or in your current working directory.

loa 1HUC.pdb

Step 4 - draw backbone, to simplify the picture:

bac

Step 5 - use different colors for different chains:

col chain

Step 6 - select chain A, draw balls and sticks and change color scheme to CPK:

sel a/*/*/*
bac off
bon 4
ato bal
col cpk

Step 7 - redefine the internal system origin (the rotation center) and move chain A to the screen center:

cen
pos 0 0 0

Step 8 - restrict the selection to aliphatic amino acids and change color to yellow (chain A):

res ali
col yellow

Step 9 - select all, make it visible, show only backbone but reduce the backbone thickness:

```
sel *
sho
bac 3
```

Step 10 - hide side chains:

Step 10 - select cysteine residues, but only for chains A and C; make them visible, use spacefill style:

```
sel a,c/*/cys/*
show
ato spa
```

Step 11 - quit your garlic session:

```
exi
```

Garlic Tutorial

Script 1 - Drawing styles for atoms

This script shows the available drawing styles for atoms. Note that nothing is visible for style "0" (first row, first column)! The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file atoms.script). Or, click here to download the script.

Type the following command at garlic prompt:

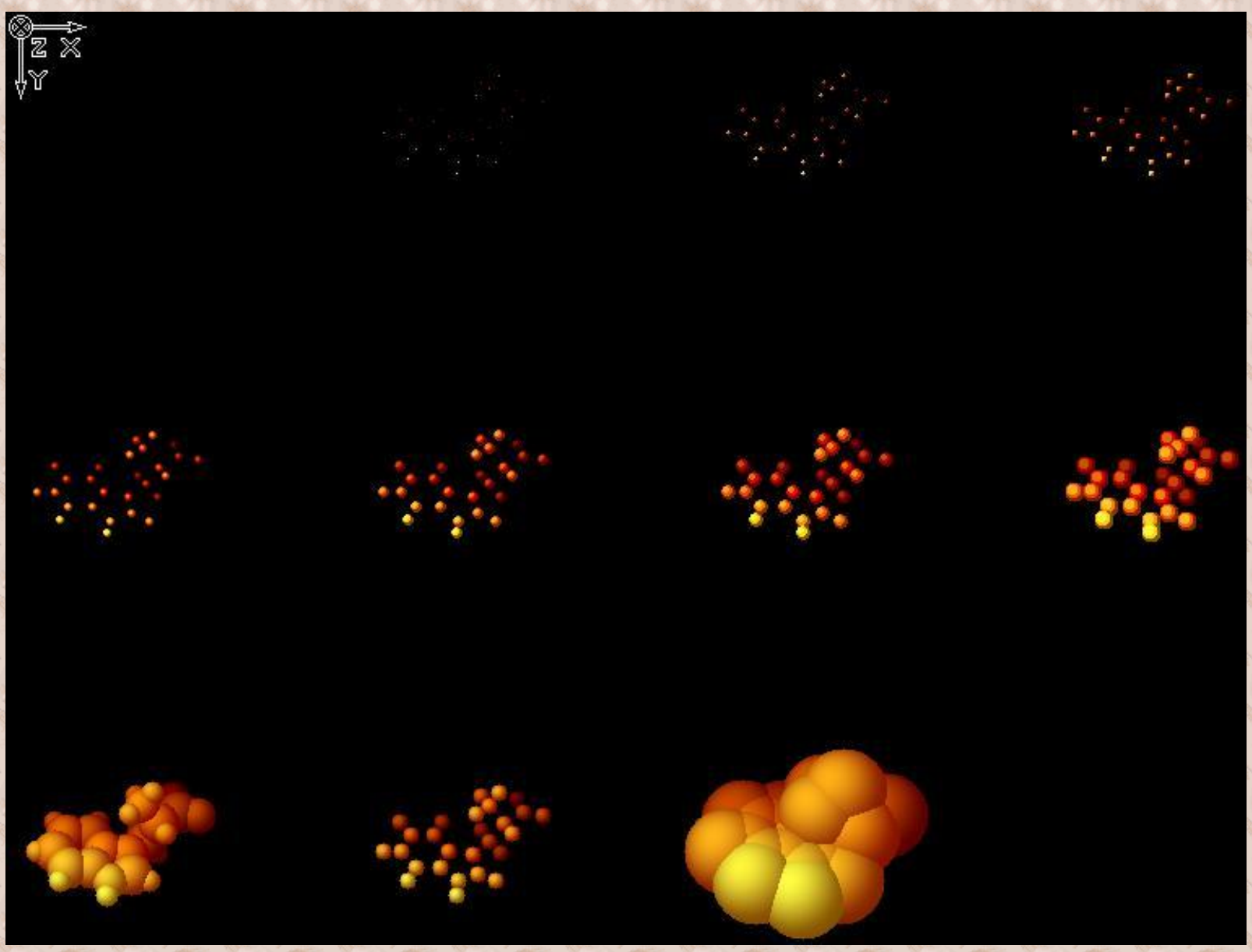
exe atoms.script

The sample image is at the bottom of this page.

```
# Show all drawing styles used to draw atoms. Hide all bonds!

# Atom style 0 (univisible):
load trp.pdb
pos -30 -20 0
ato 0
bon 0
# Atom style 1:
load trp.pdb
pos -10 -20 0
ato 1
bon 0
# Atom style 2:
load trp.pdb
pos 10 -20 0
ato 2
bon 0
# Atom style 3:
load trp.pdb
pos 30 -20 0
ato 3
bon 0
# Atom style 4:
load trp.pdb
pos -30 0 0
ato 4
bon 0
# Atom style 5:
load trp.pdb
pos -10 0 0
ato 5
bon 0
# Atom style 6:
load trp.pdb
pos 10 0 0
ato 6
bon 0
# Atom style 7:
load trp.pdb
pos 30 0 0
ato 7
bon 0
```

```
# Atom style spa:
load trp.pdb
pos -30 20 0
ato spa
bon 0
# Atom style bal:
load trp.pdb
pos -10 20 0
ato bal
bon 0
# Atom style big:
load trp.pdb
pos 10 20 0
ato big
bon 0
```



Garlic Tutorial

Script 2 - Drawing styles for bonds

This script shows the available drawing styles for bonds. Note that nothing is visible for style "0" (first row, first column)! The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file bonds.script). Or, click here to download the script.

Type the following command at garlic prompt:

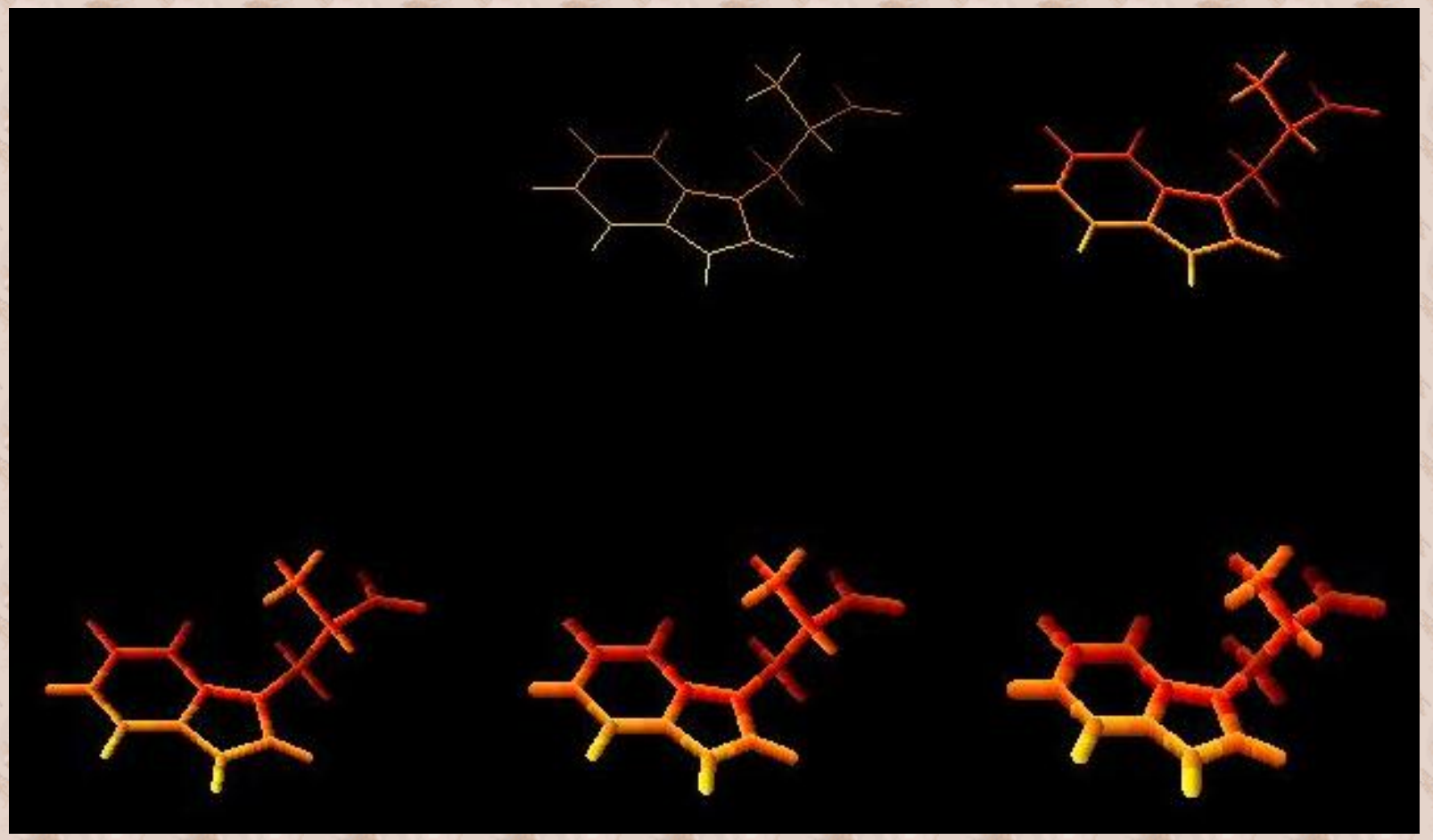
exe bonds.script

The sample image is at the bottom of this page.

```
# Show all drawing styles used to draw bonds. Atoms are hidden!
# This script will work if you use default .garlicrc configuration file.

# Bond style 0:
load trp.pdb
pos -12 -6 -100
ato 0
bon 0
# Bond style 1:
load trp.pdb
pos 0 -6 -100
ato 0
bon 1
# Bond style 2:
load trp.pdb
pos 12 -6 -100
ato 0
bon 2
# Bond style 3:
load trp.pdb
pos -12 6 -100
ato 0
bon 3
# Bond style 4:
load trp.pdb
pos 0 6 -100
ato 0
bon 4
# Bond style 5:
load trp.pdb
pos 12 6 -100
```

```
ato 0
bon 5
```



Garlic Tutorial

Script 3 - Predefined color schemes

This script shows some selected color schemes. All schemes shown here are hard-coded in the program. The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file colors.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe colors.script

The sample image is at the bottom of this page.

```
# Show predefined color schemes.
# This script will work if you use default .garlicrc configuration file.

load trp.pdb
pos -18 -18 0
bon 0
ato spa
color red

load trp.pdb
pos -6 -18 0
bon 0
ato spa
color green

load trp.pdb
pos 6 -18 0
bon 0
ato spa
color blue

load trp.pdb
pos 18 -18 0
bon 0
ato spa
color yellow

load trp.pdb
pos -18 -6 0
```

```
bon 0
ato spa
color cyan

load trp.pdb
pos -6 -6 0
bon 0
ato spa
color magenta

load trp.pdb
pos 6 -6 0
bon 0
ato spa
color white

load trp.pdb
pos 18 -6 0
bon 0
ato spa
color yellow-green

load trp.pdb
pos -18 6 0
bon 0
ato spa
color cyan-green

load trp.pdb
pos -6 6 0
bon 0
ato spa
color cyan-blue

load trp.pdb
pos 6 6 0
bon 0
ato spa
color magenta-blue

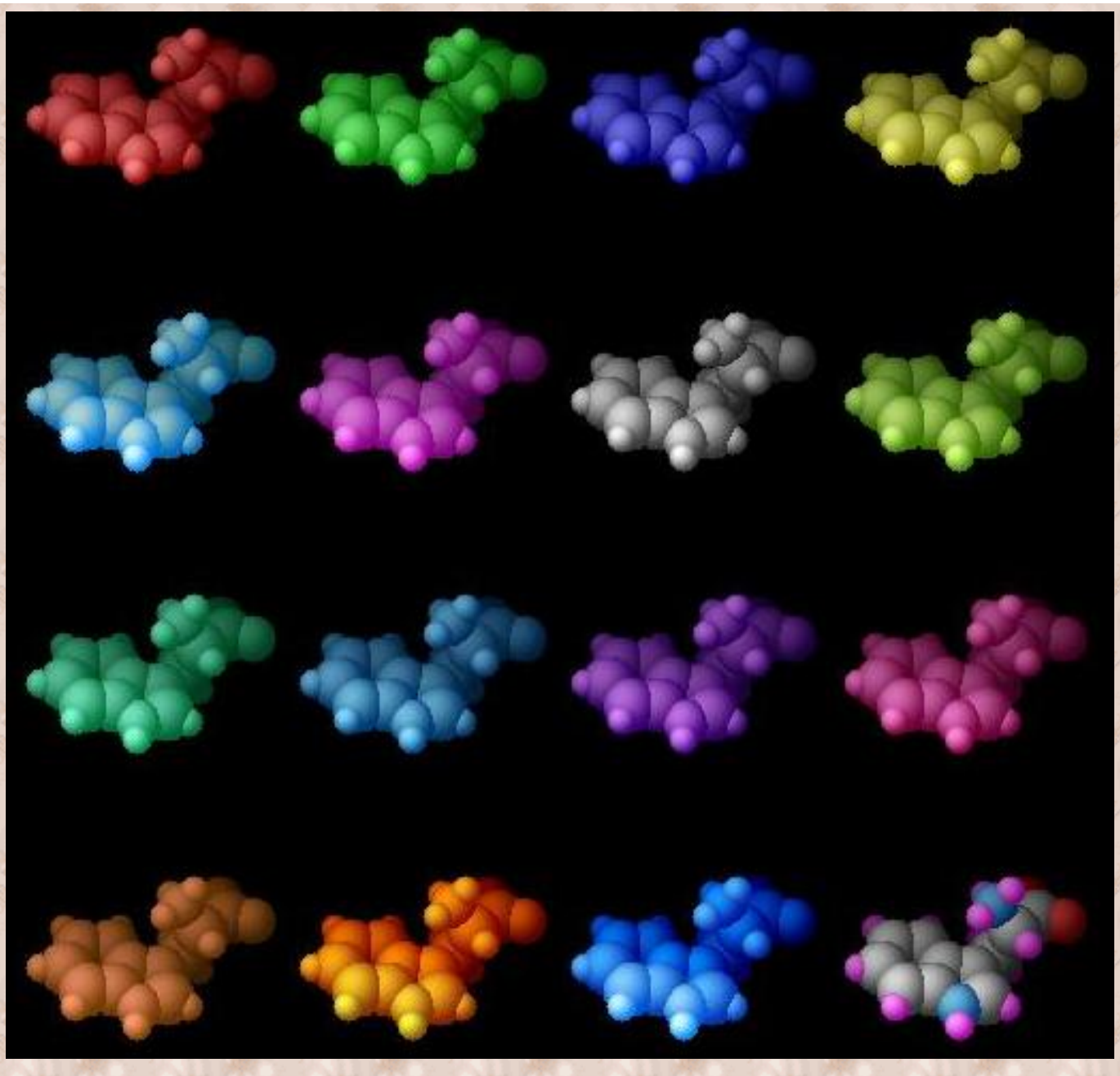
load trp.pdb
pos 18 6 0
bon 0
ato spa
color magenta-red
```

```
load trp.pdb
pos -18 18 0
bon 0
ato spa
color orange

load trp.pdb
pos -6 18 0
bon 0
ato spa
color hot

load trp.pdb
pos 6 18 0
bon 0
ato spa
color cold

load trp.pdb
pos 18 18 0
bon 0
ato spa
color cpk
```



Garlic Tutorial

Script 4 - Dancing tryphophan

Just try it!

Type the following command at garlic prompt:

exe dance.script

```
load trp.pdb
bon 4
pos 0 0 1000
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
```

```
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
```

Mouse Usage

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

Move the mouse pointer over the structure and you will see the textual information about the atom covered by the pointer.

Since 10. April 2000 (garlic version 1.0), mouse clicks may be used for rotations and translations and also for slab and color adjustment. Click on a selected button in a control window (top right corner of the main window). Shift, alt and control play the same role as if keyboard is used for the same job.

Perhaps it will be good idea to use right mouse button for some kind of menu and left mouse button for selection. If you have some ideas, write to me. The address is: zucic@garlic.mefos.hr .

Garlic Features

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

Features which are already implemented are marked DONE.
Features which are still unavailable are marked TODO.
Partially available features are marked PARTIAL.

DONE	Garlic is free. The source code is available to everyone.
DONE	Five types of slab are available: planar, spherical, semi-spherical, cylindrical and semi-cylindrical.
DONE	The slab position and thickness are visible in a small window.
DONE	Atomic bonds as well as atoms are treated as independent drawable objects.
DONE	The atomic and bond colors depend on position. Five mapping modes are available (as for slab).
DONE	Garlic is capable to display stereo image.
TODO	Garlic will be capable to display other geometric objects, like membrane, for example.
DONE	Atomic information is available for atom covered by the mouse pointer. No click required, just move the mouse pointer over the structure!
DONE	Garlic is capable to load more than one structure.
TODO	It will be possible to replace the original residues by some others. Torsion angles will be adjustable.
PARTIAL	It will be possible to color the residues according to hydrophobicity and other properties.
DONE	The command prompt is available at the bottom of the main window. It is capable to display one error message and one command string.

How to install garlic

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

Once in the future I will prepare the configure script. Until then, follow these instructions:

(1)	Put garlic package (garlic.tar.gz) into some empty directory.
(2)	Uncompress the package: gzip -d garlic.tar.gz
(3)	Unpack sources: tar xf garlic.tar
(4)	Check which C compiler is available on your system. If you don't know how to find this information, try this: man -k compiler to obtain the list of available compilers.
(5)	If gcc (GNU C) compiler is not available on your system, use your favorite editor to edit Makefile. Replace gcc in: CC = gcc line with the name of your compiler (this may be cc, for example). If gcc is available on your system, do not change the CC line.
(6)	Find a directory which contains the Xlib library. Try this: cd / find . -name libX11* Check where is the file libX11.so (sharable library - prefered) or libX11.a (static library - reserve option). If your directory is different from /usr/X11R6/lib, modify the line: LIBPATH = -L/usr/X11R6/lib in Makefile. For example, if libX11.so is stored in /usr/shlib directory on your system, the LIBPATH should be changed to: LIBPATH = -L/usr/shlib
(7)	Compile the package - just type: make and wait some time.
(8)	If everything worked fine, copy the executable to a choosen directory. /usr/local/bin may be a good choice. This job should be done by root (system administrator): cp garlic /usr/local/bin If you don't have root privileges, ask your local administrator to install garlic, or just leave it in one of your directories.
(9)	Now the .garlicrc configuration file should be copyed to a directory where it will be accessible to everyone as the public configuration script. If this is not done, garlic will work anyway, using hard-coded defaults. The recommended directory is /usr/local/lib/garlic but if /usr/local/lib does not exist on your system, /usr/lib/garlic may be used. This should be done by root (system administrator): mkdir /usr/local/lib/garlic cp .garlicrc /usr/local/lib/garlic

(10)	It may be good idea to copy the configuration file to your home directory. If you do this, you can personalize your garlic sessions, because your private configuration file overrides the system-wide defaults. Of course, you don't need root privileges for this: cp .garlicrc $HOME
(11)	If you store structures in some reserved directores, you may add this line into your .login, .tcshrc, .cshrc or some other startup file: setenv MOL_PATH $HOME/directory1:$HOME/directory2 In this example, PDB files are kept in directory1 and directory2, and both directories are subdirectories of your home directory.
(12)	Clean up the mess (sources and .o files). Be sure to leave trp.pdb .pdb for later practice (this is the only PDB file included in the original garlic package). Do not delete files with extension .script (tutorial scripts).

If garlic refuses to work because it fails to get the TrueColor visual, try to execute xdpyinfo and xwininfo (click into root window); check the list of supported visuals and the current color depth. Choose the color depth for which the TrueColor visual is available!

Protein and DNA coordinates may be found at The Protein Data Bank .

If you can't compile, install or run garlic, write to me (Damir Zucic), my address is zucic@garlic.mefos.hr .

Garlic Reference Card

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

Garlic reference card contains the list of commands and keywords, with short description of commands. Print this page and keep it at hand during your garlic sessions. Garlic reference card is not a learning tool, it is just a reminder.

CLICK HERE !

COM.	ARGUMENTS	APPL. TO	DESCRIPTION
ADD	the same as for SEL	structure	Add to selection
ATO	0, 1, 2, 3, 4, 5, 6, 7, BAL, BIG, SPA	selection	Drawing style for atoms
BAC	0, 1, 2, 3, 4, 5, OFF	selection	Draw backbone
BG	color_specification	main window	Change background color
BON	0, 1, 2, 3, 4, 5	selection	Drawing style for bonds
CAT	structure_identifier	structure	Catch structure
CEN	none	structure, selection	Redefine internal system origin
COL	detailed_color_specification, RED, GREEN, BLUE, YELLOW, CYAN, MAGENTA, WHITE, YELLOW-GREEN, CYAN-GREEN, CYAN-BLUE, MAGENTA-BLUE, MAGENTA-RED, ORANGE, HOT, COLD, MONOCHROME, CPK, ZEBRA, CHAIN, HYPHOB	selection	Assign color; do not abbreviate color scheme name!
DIS	structure_identifier *, all	structure	Discard structure
EXE	file_name	script file	Execute script
EXI	none	garlic session	Quit garlic session
FAD	FRO shift, BAC shift, OFF, PLA, SPH, CYL, HALF-SPH, HALF-CYL	structure	Change color fading
FG	color_specification	main window	Change text color
FON	font_name	all windows	Change font
HID	none	selection	Hide atoms and bonds
HYB	none, OFF	structure	Generate hydrogen bonds
LAB	none, OFF	selection	Show labels
LOA	file_name	structure_file	Load structure (file)
LOG	file_name, OFF	commands	Log garlic commands
MON	none	main window	Switch to mono mode
PAU	none	garlic script	Pause script execution
POS	x, y, z	structure	Move to (x, y, z)
REG	none	mail	Register garlic
RES	the same as for SEL	selection	Restrict selection
ROT	axis angle	structure	Rotate
SAV	file_name file_name SEL	structure or selection	Save atomic data to file (SEL = selection only)
SEL	chains/res_nums/res_names/atom_names residue_numbers residue_names *, all, aci, bas, cha, com, het, pho, mai, neg, pol, pos, sid, sma, tin	structure, selection	Define new selection (overwrite previous)
SHO	none	selection	Show atoms and bonds

SLA	**FRO shift, BAC shift, OFF, PLA, SPH, CYL, HALF-SPH, HALF-CYL**	**structure**	**Change slab**
STE	**none, OFF**	**main window**	**Switch to stereo mode**
TAG	**"string" OFF**	**structure**	**Assign or remove tag**
TBG	**color_specification**	**input+output window**	**Change text background color**
TFG	**color_specification**	**input+output window**	**Change text color**
TIT	**identifier x y "string" identifier x y identifier OFF**	**main window**	**Add, move or remove title**
TRA	**axis shift**	**structure**	**Translate**

Bug Fixes

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

This page contains the list of bugs and bug fixes.

BUG DESCRIPTION	STATUS
Occasional floating point exception. Spotted on Digital Alpha, does not affect Intel Pentium, 486 and some other machines. Caused by a bug in function which is refreshing the control window. If some structure is loaded, program works fine.	fixed 24/Mar/2000

Garlic Release Announcements

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

The current version of garlic is 1.0 (the very first after the original 1x).
It was released on 10. April 2000.
Read changes to see the latest news on garlic development.
Major versions will be announced trough these Usenet newsgroups:

bionet.molbio.proteins
bionet.software
bionet.software.www
bionet.announce
bionet.biology
bionet.computational
bionet.software.sources
comp.os.linux.announce

Changes

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

This page contains the list of changes. Bug fixes are not included here!

DATE	CHANGE
2000/03/28	Five scripts included into garlic source package.
2000/04/10	Version 1.0 released (see below for changes)
2000/04/10	The keyword ALL may be used with the command DISCARD, to discard all structures.
2000/04/10	The history buffer is now capable to store the commands executed from the script.
2000/04/10	The command TAG added. With this command, a short text may be associated with a structure. Tag is bound to the structure, so it moves along with it.
2000/04/10	Color handling sligthly improved.
2000/04/10	Mouse clicks may be used for translations and rotations as well as for slab and color adjustment. Click on a selected button in a control window (top right).
2000/04/10	A simple startup logo (text) added.

Garlic Configuration File

.garlicrc

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

This page contains the sample configuration file for garlic. When started, garlic will try to find the configuration file called .garlicrc in the following directories:

(1) the current working directory;
(2) users home directory ($HOME);
(3) garlic subdirectory of user's home directory ($HOME/garlic);
(4) /usr/local/lib/garlic ;
(5) /usr/lib/garlic .

If all attempts fail, the hard-coded defaults will be used. The configuration file .garlicrc should be included in the original garlic package. Most parameters are explained below (read the comments). Anyway, if you have some questions, send an e-mail to me:
zucic@garlic.mefos.hr

```
# Personal initialization file for garlic (molecular visualization program).
# Created on January 2. 1999 by Damir Zucic.
# Modified and/or expanded many times since then.
# Last modification: March 22, 2000.


# Geometry of the main window. Use the keyword default, or specify the
# geometry string (for example 780x560+10+10).

main window geometry: default


# Margins; used only if geometry string is not given. Geometry string may be
# given through command line arguments.

main window left margin: 15 pixels
main window right margin: 15 pixels
main window top margin: 30 pixels
main window bottom margin: 15 pixels


# Main font:

main font: 10x20


# Main window cursor. If you don't like default cursor, replace it; read
# the file /usr/include/X11/cursorfont.h ; remove the XC_ prefix to obtain
# the cursor name.
```

```
main window cursor: default


# A small coordinate system may be displayed in the top left corner (yes/no):

show coordinate system: yes


# Stereo flag (yes/no):

display stereo image: no


# Parameters for stereo image:

stereo internal margin (screen units): 10 pixels
stereo angle: 5.0 degrees


# Light source theta and phi angle (theta is defined with respect to z axis,
# phi with respect to x axis:

light source theta angle: 150 degrees
light source phi angle:   225 degrees


# Default slab mode (possible modes are off, planar, sphere, half-sphere,
# cylinder and half-cylinder):

default slab mode: planar


# Default color fading mode (off, planar, sphere, half-sphere, cylinder and
# half-cylinder):

default color fading mode: planar


# Default drawing style for atoms:

default atom drawing style: 2


# Default drawing style for bonds:

default bond drawing style: 2


# Window colors:

main window background color: black
```

```
main window foreground color: white
text background color: black
text foreground color: white


# The number of color fading surfaces:

number of color fading surfaces: 3


# Colors at given fading surface(s). The surface index is given in brackets.
# The largest surface index is (number of color fading surfaces) - 1.

left   color 0: RGB:FFFF/FFFF/4444
middle color 0: RGB:FFFF/DDDD/0000
right  color 0: RGB:8888/5555/0000

left   color 1: RGB:FFFF/8888/0000
middle color 1: RGB:FFFF/0000/0000
right  color 1: RGB:8888/0000/0000

left   color 2: RGB:8888/0000/0000
middle color 2: RGB:4444/0000/0000
right  color 2: RGB:2222/0000/0000


# Rotation steps. Normal steps is used if numeric key is pressed without
# any modifier. Large step is selected by holding [shift] while pressing
# the key, and very large step is selected by using both [alt] and [shift].
# Small step is selected by holding [control] while pressing the key, and
# very small step by using both [alt] and [control].

rotations steps: 0.2 1.0 5.0 30.0 90.0


# Five translation steps (very small, small, normal, large and very large).
# Use angstrom units.

translation steps: 0.2 1.0 5.0 25.0 100.0


# Five slab steps (very small, small, normal, large and very large).
# Use angstrom units.

slab steps: 0.2 1.0 5.0 20.0 80.0


# Five fading steps (very small, small, normal, large and very large).
# Use angstrom units.

fading steps: 0.2 1.0 5.0 20.0 80.0
```

```
# Window size limits: used only if screen width and/or height are larger
# than values specified here. By default, screen width and height are used.

maximal main window width: 3000 pixels
maximal main window height: 2500 pixels


# The nearest line (bond) thickness; used only if drawing bonds as lines
# and line thickness is used for perspective.

the nearest line thickness: 5 pixels


# Screen dimensions and position of garlic user in real world. Use realistic
# values. Do not change units (mm). Strange values may cause image distortions.

screen width in real world: 270 millimeters
screen height in real world: 195 millimeters
distance between user and screen in real world: 700 millimeters


# Scaling information: used to scale user and screen down to atomic scale.
# Only screen width is required, in angstrom units.

screen width in atomic world: 0.5 angstroms


# User z coordinate in atomic coordinate system. It must be negative
# and absolute value should be quite large. The x axis points to the right,
# y axis downward and z axis in direction opposite to observers direction.

user position in atomic coordinate system: -250.0 angstroms


# Maximal bond length is used to check which atoms and bonds are invisible.
# It is assumed that there are no atoms with radius larger than this length.

maximal bond length: 2.2 angstroms


# Crude limits for bond lengths. No distinction between N-CA and C-N is made.
# Use angstrom units. Be tolerant, there are many bad structures around.
# Generic bond length is used for atomic pairs which are not recognized.

approximate C-C bond length: from 1.3 to 1.8 angstroms
approximate C-N bond length: from 1.0 to 1.7 angstroms
approximate C-O bond length: from 1.0 to 1.5 angstroms
approximate C-S bond length: from 1.5 to 2.1 angstroms
approximate C-H bond length: from 0.8 to 1.2 angstroms
```

```
approximate N-H bond length: from 0.9 to 1.3 angstroms
approximate O-H bond length: from 0.7 to 1.3 angstroms
approximate S-H bond length: from 0.9 to 1.6 angstroms
approximate O-P bond length: from 1.2 to 1.8 angstroms
generic bond length:         from 0.8 to 2.0 angstroms
hydrogen bond length:        from 2.4 to 4.0 angstroms


# Hydrogen bond C-O...N angle range:

hydrogen bond C-O...N angle: from 130 to 180 degrees


# The upper limit for CA-CA distance for neighbouring residues. Used to
# draw backbone, connection neighbouring CA atoms.

maximal CA-CA distance: 4.0 angstroms


# Atomic radii, used for spacefill style. Radius equal to 70% of Van der
# Waals radius may be a good choice.

radius of H atom: 0.70 angstroms
radius of C atom: 1.20 angstroms
radius of N atom: 1.05 angstroms
radius of O atom: 1.00 angstroms
radius of S atom: 1.25 angstroms
generic radius:   1.20 angstroms


# Ball radius, used to draw balls and sticks:

ball radius: 0.45 angstroms


# Big sphere radius, used to draw oversized atoms:

big radius: 2.50 angstroms


# For a given atom, the chemical bonds are identified by inspecting
# distances to the neighboring atoms. The array with atomic data should
# be scanned in forward and backward direction (with respect to the given atom)
# to find which atoms are bound to a given atom. The following parameters
# define how many neighboring atoms should be checked in each direction.

number of bond candidates: 30 before and 30 after the given atom
```

Support Garlic!

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

You can support garlic development in different ways. Some options are listed here, sorted by complexity (the simplest one is the first). Though garlic is a free software, someone has to pay for it. The author will need strong arguments to ensure support for a program which makes no money. If you like garlic, support it!

REGISTER GARLIC

The fact that you use garlic doesn't help much if I don't know that there is one more user. The easiest way to register is to execute the command:
reg
at garlic prompt. This requires that your machine is connected to the Internet. A short message will be send to zucic@garlic.mefos.hr; the only content of this message will be the word 'Hi!'. I will use the header of this message to extract your address. The address will be added to the list. Your address will not be abused, it will be kept secret and used only to count garlic users.

You can also send a more verbose message to zucic@garlic.mefos.hr with comments and suggestions.

There is one more way to register garlic: at your shell (terminal) prompt, type:
garlic -r
(if connected to the Internet, of course).

SEND A POSTCARD

You can also register by sending a postcard. I like stamps!
Here is the address:

Damir Zucic
ETF Osijek
Kneza Trpimira 2B
31000 Osijek
Croatia
Europe

INFORM OTHERS

Inform your colleagues and friends about garlic. Many potential users do not read Usenet news, so it is difficult to reach all those who might be interested to use garlic. I don't like spam and other aggressive forms of communication so I wouldn't use such methods to attract users.

ADD LINK TO YOUR WEB PAGES

Add link to your personal web page(s), pointing to garlic.

MIRROR GARLIC

If you like garlic and you can set aside few megabytes of disk space, you can establish a mirror site with garlic sources and related material. This should not be very complicated - there is only one source

package and few dozens of web pages. The national academic network (CARNet) here in Croatia is pretty good, but communication lines to some countries (like U.K. and Germany) are overcrowded most of the time.

USE IT FOR LECTURES AND PRESENTATIONS

An experienced user may use garlic for lectures and presentations. There is a command pau (pause) which makes it easy to control script execution.

MAKE A DONATION

Donations are welcome, of course. Contact the author for technical details (zucic@garlic.mefos.hr).

Technical Requirements

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

Garlic tends to be POSIX compliant. It is also ANSI C compliant, to the maximum possible extent. Xlib functions are the only non-ANSI functions used by this program.

OPERATING SYSTEM
Unix or unix clone and the X window system. Linux and XFree86 recommended.

SUPPORTED HARDWARE PLATFORMS
Desktop PC, laptop, notebook, unix workstation equipped with a color monitor with a color depth of at least 8 bits per pixel. No dials required. Some X servers do not support TrueColor visual at 8 bits per pixel: try to switch to higher color depth (12, 15, 24, ...)!

CPU
Intel, Digital Alpha, SUN MIPS and some others. This program has no special hardware requirements.

GRAPHICS INTERFACE
Garlic requires the X window system. The recommended version is X11R6, but older versions may work too.
THE X SERVER SHOULD BE CAPABLE TO SUPPORT TrueColor VISUAL!
Some older servers may be unable to support the TrueColor visual; if you have such X server, garlic will refuse to work. Some modern X servers do not support the TrueColor visual at 8 bits per pixel, but these are usually running on a hardware which may offer 12 or more bits per pixel.

COMPILER
GNU C compiler is recommended, but other compilers compliant with ANSI C standard should work too.

REQUIRED LIBRARIES
The only required libraries are libc (C), libm (mathematical) and libX11 (the standard X11 library).

KEYBOARD
The standard PC 101/102 keyboard should work fine. The laptop keyboard may be used too. If you have some kind of unix workstation with terminal keyboard, this may work too.

MOUSE
Any mouse should serve well.

THE LIST OF COMPATIBLE SYSTEMS
Up to now, it is confirmed that garlic may be compiled and used on these systems:
Intel (486, Pentium MMX)
Digital Alpha
Sun Solaris
SGI (Iris Indigo)

Please inform me (zucic@garlic.mefos.hr) if you successfully compiled and used garlic on a system which is not listed here. Anyone tryed to compile garlic on HP system?

Garlic Command Line Options

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, unofficial release, Damir Zucic.

This page explains the command line options. To see this list, type one of the following commands:

garlic -h
garlic -h | less

```
==============================================================================
                Garlic - free molecular visualization program
==============================================================================

Garlic was written by  Damir Zucic  (zucic@garlic.mefos.hr) as a complement
to other molecular visualization  programs, like rasmol (by Roger Sayle).
It was written to simplify  the analysis of membrane proteins, but it can
be used as general purpose molecular visualization program, provided that
molecular coordinates are available in  PDB format, version 2.1 or older.

Some of the  features, which  distinguish this program from  others, are:
(1) Coordinates, labels and  other data are  automatically displayed  for
    the atom nearest to the current pointer (mouse) position.
(2) Additional numeric data,  like  hydrophobicity, may be associated  to
    each amino acid. The  whole  structure  may be  colored  according to
    these values.
(3) Selection mechanism is different.
(4) Two bonds at different distance from  observer have different colors.
------------------------------------------------------------------------------
Usage:              garlic [true_garlic_options] [X11_options] [filename]
------------------------------------------------------------------------------
Command line options may be divided in two groups: true (specific) garlic
options and X11 options.  Options may be given in any order.  All options
and hard-coded  default values are listed  in the table  below.  For each
parameter, the value defined through command line is used,  if available.
If not, the value defined in .garlicrc file is used. If .garlicrc file is
not  available,  or there is  no corresponding  entry in  this file,  the
hard-coded default value is used.  The sample  .garlicrc file included in
the original package contains  the values equal to  hard-coded  defaults.
------------------------------------------------------------------------------
garlic option:        Description:
------------------------------------------------------------------------------
-h, --help            Print help and exit.
-v, --version         Print version and exit.
-r, --register        Register garlic:  inform author that  your site has
                        garlic installed and that someone is going to use
```

```
                        this program. By registering, you are encouraging
                        author to continue development of garlic. You can
                        also help  author to  ensure support  for further
                        development. This option sends an e-mail message,
                        containing only the e-mail message header and the
                        word 'Hi!',to zucic@garlic.mefos.hr. Please execute
                        garlic -r   if you are going to use this program.
                        If your system is  not connected to the Internet,
                        you can send short e-mail from some other system.
-nosys                  Hide the coordinate system icon  (top left corner).
no-control              Hide the control window (upper right corner).
-stereo                 Display stereo image.
-slab mode              Default slab mode.  Available slab modes are:  off,
                        planar (default),  sphere, half-sphere,  cylinder
                        and half cylinder.
-fading mode            Default color fading mode.  Available  modes:  off,
                        planar (default),  sphere, half-sphere,  cylinder
                        and half cylinder.
-as number              Default atom drawing style (hard-coded default: 2).
-bs number              Default bond drawing style (hard-coded default: 2).
-fs number              Default number of  color fading surfaces.  Parallel
                        planes, concentric spheres or conc. cylinders may
                        be used as  fading surfaces.  Three  RGB triplets
                        are assigned to each surface. Surfaces are evenly
                        spaced;  at least one and at most eight should be
                        defined. At least three colors  (left, middle and
                        right) are assigned to  each visible atom.  These
                        three colors are based on the position of a given
                        atom  relative to  the nearest  fading surface(s)
                        and on colors assigned to these surfaces.  Colors
                        are combined using linear weighting.
-lc(i) color            Left color at the  i-th surface;  i is between zero
                        and seven.  The color string should be  compliant
                        with X11R5.  Blue, for example,  may be specified
                        as blue or as RGB:0000/0000/FFFF etc. For example
                        -lc4 RGB:BBBB/8888/4444    defines the left color
                        at the surface whose index is equal to four.
-mc(i) color            Middle color at the i-th surface.
-rc(i) color            Right color at the i-th surface.
-pc, --print-config     Print configuration data and exit.
-pcn                    Print cursor names to stdout and exit.
-log logfile            Write commands and messages to  log file.  The file
                        will be created in the current working directory.
                        If this is not possible, log file will be created
                        in users home directory.
-----------------------------------------------------------------------------
X11 option:             Description:
-----------------------------------------------------------------------------
```

```
-display displayname  X server to contact.
-geometry geom        Window geometry (default: almost the whole screen).
-bg color             Main window background color (default is black).
-fg color             Main window foreground color (default: white).
-fn fontname          Text font; (default is 10x20).
-tbg color            Text background color (default is black).
-tfg color            Text color (default is white).
-cursor cursorname    Cursor name; see  /usr/include/X11/cursorfont.h for
                        names; remove the XC_ prefix.
-----------------------------------------------------------------------
filename:             The input file name.  Full pathname may be used. If
                      filename does not contain the path, garlic will try
                      to find  the specified file in  the current working
                      directory.  If the first attempt  to open  the file
                      fails,  the filename  is appended to the content of
                      the environment  variable  MOL_DIR  for  the second
                      attempt.  If this fails too, garlic will search all
                      directories  specified in  the environment variable
                      MOL_PATH.
-----------------------------------------------------------------------
Personal initializations may be written to .garlicrc file. Normally, this
file should be kept in users home directory.  Note that this is  not  the
first directory to be searched for .garlicrc file! Up to five directories
are searched in the following order:

.                        Current working directory.
$HOME                    Users home directory (recommended).
$HOME/garlic             Subdirectory garlic (of users home directory).
/usr/local/lib/garlic    Public  initialization file  should be  there.
/usr/lib/garlic          The last  attempt;  if this fails,  hard-coded
                           default values are used.
-----------------------------------------------------------------------
Environment variables:
-----------------------------------------------------------------------
MOL_DIR               Defines where to look for the specified file if not
                        found in the current working directory.
MOL_PATH              The list of directories to be searched.  It is used
                        if attempt with  MOL_DIR failes or if  MOL_DIR is
                        not defined.  Use space  or colon (:) to separate
                        directory names. MOL_PATH is quite useful;  it is
                        recommended to define  this environment  variable
                        through .login or some other login script.
DISPLAY               X server to which  the program should be connected.
-----------------------------------------------------------------------
garlic home page:                        http://garlic.mefos.hr/garlic
Damir Zucic home page:                   http://garlic.mefos.hr/zucic
E-mail:                                  zucic@garlic.mefos.hr
=======================================================================
```

Garlic - Version 1.1

Free Molecular Visualization Program

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This is the home of garlic - free, open source molecular visualization program. Garlic is the most portable molecular visualization program in unix world. Follow the links below to find more about garlic. Don't forget to visit the screenshot gallery !

Release date: March 06, 2001. All versions are listed here .

Garlic home: [Croatia] Auto-mirrors: [Australia] [Canada] [United Kingdom] [United States]

HPUX archives (check the program version!): [Canada] [France] [Germany] [Italy] [Japan] [Netherlands] [South Africa] [United Kingdom] [USA (Utah)]

What is garlic?	Screenshot gallery	License
Download garlic	Installation guide	Documentation
Similar programs	Support garlic!	Author

Questions, Bug Reports, Comments and Suggestions

The form below may be used to send bug reports, comments and suggestions, or to ask question about garlic. You can also send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) .

Name and institution:

e-mail address (please type it carefully):

Message:

SEND CLEAR

User comments

Dear Dr. Zucic,

This is to express my appreciation for creating this wonderful molecular graphics program, perhaps the only one which I can run without being irritated on my Linux/Alpha.

Thank you so much,

With best regards,

Ansuman Lahiri, University of Stockholm, Sweden

Garlic

The Most Portable Molecular Visualization Program in Unix World

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

The statement that garlic is the most portable molecular visualization program in unix world might look quite bold at the first sight, but it is based on serious arguments. Garlic requires only three libraries to run: the standard C library (libc), the standard math library (libm), and the standard X11 library (libX11). These libraries are available on every serious unix or unix compatible system. All other programs, (except one: mdxvu) require some additional binary libraries.

Compiling and/or installing a program which requires numerous libraries may turn into nightmare. Not only that all these libraries must be present on your system: a version number is important too! And if you manage to compile and/or install the program, it may behave strange when you try to use it: there is a chance that one or more libraries were not tested enough before shipping, causing core dumps and other runtime problems.

Check the list of freely available molecular visualization programs for unix and unix clones. This page lists also the libraries required to run each of these programs.

Free Molecular Visualization Programs for Unix and/or Linux

---

free molecular visualization programs, free molecular viewers, list of molecular visualization programs, list of molecular viewers, molecular rendering, protein visualization tools, molecular visualization resources, download page, download source, download executable, download binary, AMMP, B, BRAGI, Cn3D, Deep View Swiss-PDBViever, DINO, Flex, garlic, gdpc, Ghemical, gOpenMol, Grasp, ICMlite, Jmol, Kinemage, mdxvu, Mercury, MOIL-View, MOLDEN, MOLEKEL, MOLMOL, MolScript, Moviemol, NAMOT, QMOL, PREPI, PyMOL, RasMol, Raster3D, spock, VEGA, Viewmol, WinMGM, VMD, XMakemol, XmMol, XMol, Ymol, biological macromolecule, protein structure, DNA structure, PDB, unix, linux, free software download, open source software, Damir Zucic.

This page contains the list of free molecular visualization programs, complete with links. Only freely available programs which run on unix or unix compatible platform are listed. Some of these programs are available only as binary code for some specific platform(s).

Most programs were found using AltaVista, Lycos and Google, while some others were suggested by readers of this list. Thanks to all of them!

Some of the programs listed below have a very limited license. Be sure to read the license before using such program!

The time-limited trial versions of commercial programs were omitted from the list.

The programs listed here were not evaluated and no comparison was made.

If you have your own free molecular visualization program for unix or linux, or if you know for such program which is not included in the list below, please send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) . Please send corrections and changes to the same address.

Last updated: June 14, 2002.

The information contained here was valid before that day. As developing is going on, it is likely that some additional libraries may become necessary for some of the programs listed here. However, it is almost certain that libraries listed here will be required in future versions too.

PROGRAM	LIBRARIES REQUIRED	PROGRAM TYPE / LICENSE
AMMP	libc, libm, libX11, libXt, libXext, libXmu, libXm, libSM, libICE, libNoVersion	Stand alone program, modified GNU GPL license.
B	Java based package.	Your browser should support Java Virtual Machine.
BRAGI	It seems that this program is still under development.	The license has to be negotiated.
Chimera	Needs Python, Tcl/Tk, Tix, Togl, PIL, Numeric, Grail, Pmw, msms, VRML, JPEG, Info-ZIP, TR, ScientificPython; still under development.	Stand alone program, online registration required. Requires many libraries.

Cn3D	libc, libm, libX11, libXt, libXext, libXmu, libXp	Both browser plug-in and stand alone program.
Deep View Swiss-PdbViewer	libc, libm, libX11, libXt, libXext, libXmu, libXi, libXp, libMesaGL, libMesaGLU, libpthread, libz	Stand alone program, IRIX or linux required.
DINO	libc, libm, libX11, libXt, libXext, libXmu, libXi, libgdbm, libGL, libGLU	Stand alone program.
Flex	libc, libm, libX11, libxview, libolgx, xlibflexdraw	Stand alone, binaries for DEC/alpha, DEC/MIPS, IBM RS, SGI, Sun.
garlic	libc, libm, libX11	Stand alone program, GNU GPL license.
Ghemical	requires g++ compiler, f2c compiler, glut, GNOME, gtkglarea, mpich, MPQC ...	Stand alone program, GNU GPL license.
gdpc	libc, libm, libX11, libXext, libXi, libgtk, libgdk, libgmodule, libglib, libdl, libpthread	Stand alone program.
gOpenMol	libc, libm, libX11, libXt, libXext, libXmu, libXi, libdl, libXaw, Tcl/Tk, + Mesa or Open GL libraries	Graphics interface to the OpenMol set of programs; GNU GPL license.
Grasp	This program has been written for Silicon Graphics computers.	Under special circumstances, the $500 fee will be waived.
ICMlite	Binaries: SGI, DEC Alpha, SUN, Linux; libc, libm, libX11, libXt, libXext, libXmu, libSM, libICE, libpthread	Stand alone program, free for academic use.
Jmol	Java-based application.	Stand alone program (Java-based application).
Kinemage	libc, libm, libX11, libXt, libXm	Stand alone program.
mdxvu	libc, libm, libX11, precompiled for some systems	Stand alone program.
Mercury	libc, libm, libX11, libXt, libXext, libXmu, libXi, libXft, libXRender, libMesaGLU, libMesaGL, libSM, libICE, libjpeg, libpng, libmng, libdialogs, libwidgets, libqt, libqtspecific, libguiindep, libtoolkit, libcsd, libCif, libKCC-eh, libz, libfreetype, liblcms	Stand alone program, read conditions of use carefully.
MOIL-View	FORTRAN program, binaries available for Silicon Graphics workstations.	Stand alone program, registration expected.

MOLDEN	FORTRAN 77, libc, libm, libX11	Stand alone, free for academic use.
MOLEKEL	libc, libm, libX11, libXext, libXmu, libXi, libMesaGL, libMesaGLU, libtiff, libjpeg	Precompiled for SGI IRIX, linux PC and SunOS, registration required.
MOLMOL	libc, libm, libX11, libXt, libXext, libXm, libGL, libGLU, libGLcore, libC, libgen, libgen, libpng, libz	Stand alone, binaries for DEC/MIPS, DEC/alpha, SGI, SPARC and RS/6000.
MolScript	libc, libm, libX11, libXt, libXext, libXmu, libGL, libGLU, libGLcore, libmedia, libC, libgen, libvice, libjpeg, libpng, libz	Stand alone, online registration required.
Moviemol	libc, libm, libX11, libXext, libYgl or OpenGL	Stand alone program.
NAMOT	libc, libm, libX11, libxview, libolgx	Stand alone program.
QMOL	libc, libm, libX11, libXt, libXext, libXm, libGLw, libMesaGL, libMesaGLU, libstdc++, libSM, libICE	Stand alone program.
PREPI	Precompiled binary for Silicon Graphics IRIX.	Stand alone, registration required (written agreement).
PyMOL	libc, X libs, libpng, zlib, python, Mesa	Requires Python, an intepreted programming language.
RasMol	libc, libm, libX11 libXext, libXi	Stand alone program.
Raster3D	Mixed FORTRAN 77 and C code, requires both compilers.	Stand alone program.
spock	libc, libm, libX11, libXt, libXext, libXmu, libXm, libXi, libXpm, libMesaGL, libMesaGLU, libSM, libICE, libjpeg, libtiff, libcrypt, libz, libNoVersion	Stand alone program, free for some users, registration required.
VEGA	libc, libm, libz, liblocale	No OpenGL support for linux version.
Viewmol	libc, libm, libX11, libXt, libXext, libXm, libXi, libXp, libGL, libGLU, libtiff, libtiff, libpthread, libdb, libdl, libutil	Graphical front end for comp. chemistry programs, GNU GPL license.
WinMGM	libc, libm, libMesaGL, libsubplex, libchelpers, libmgmcalctools, libmolecules, libmolenergy	Stand alone, some custom libraries required.
VMD	Statically linked binaries for AIX, HPUX, IRIX, linux, Solaris and TRU64.	Stand alone, online registration required.

XMakemol	**libc, libm, libX11, libXt, libXm, libXpm, libGL, libGLU**	**Stand alone program, GNU GPL license.**
XmMol	**libc, libm, libX11, libXt, libXext, libXm, libXp, libSM, libICE; Motif or openMotif required.**	**Free for academic use, registration required (written agreement).**
XMol	**Precompiled binaries for SGI, Sun-3, Sun-4 and RS/6000.**	**Some other binaries may be found in some other archives; development seems to be halted.**
Ymol	**libc, libm, libX11, libXext**	**Stand alone program.**

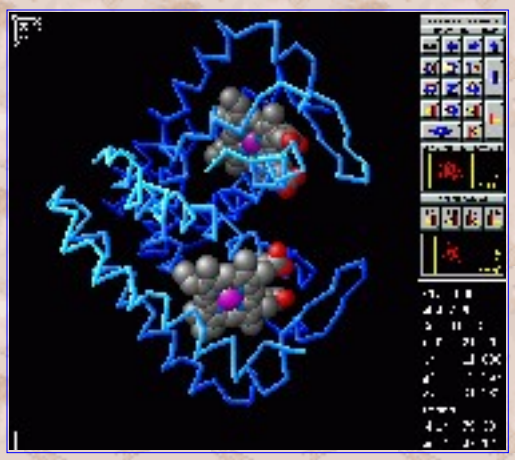
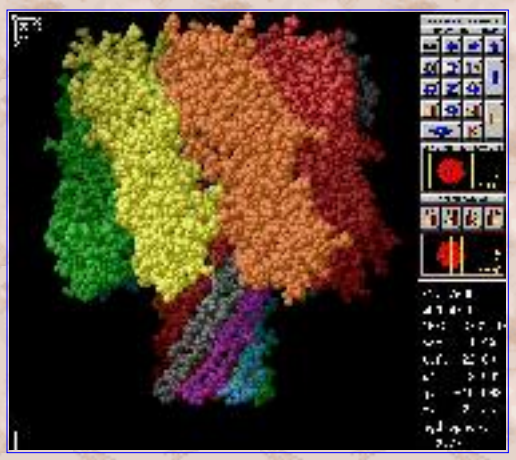
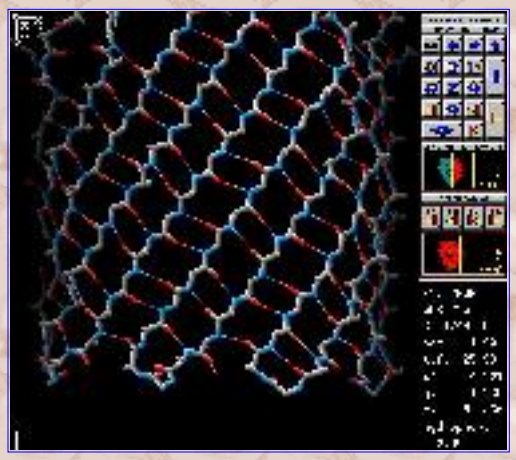
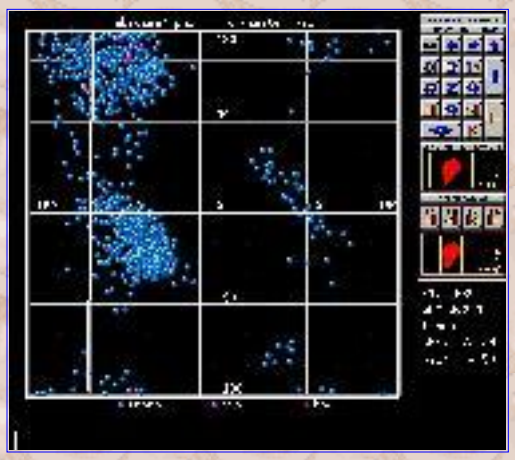
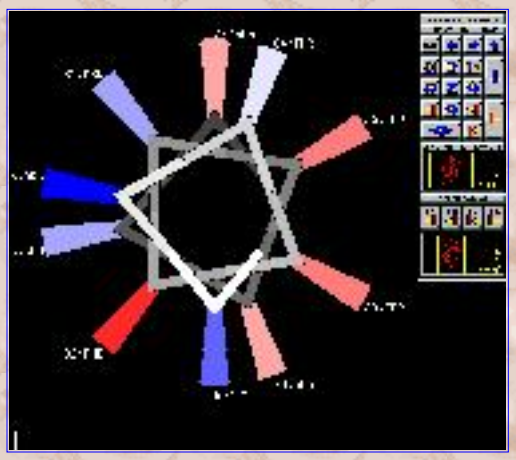
Garlic Screenshot Gallery

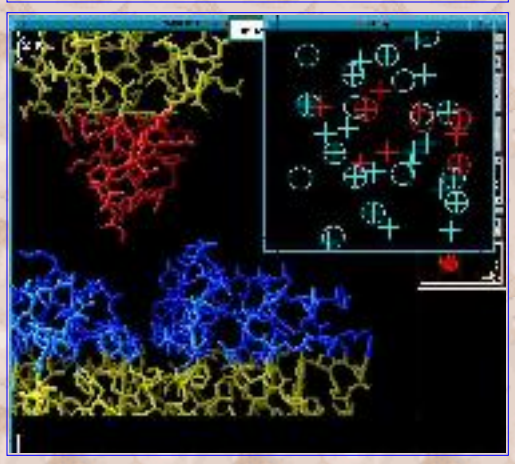
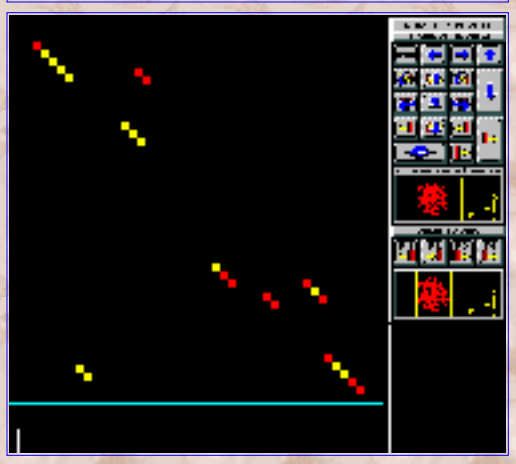
Version 1.1

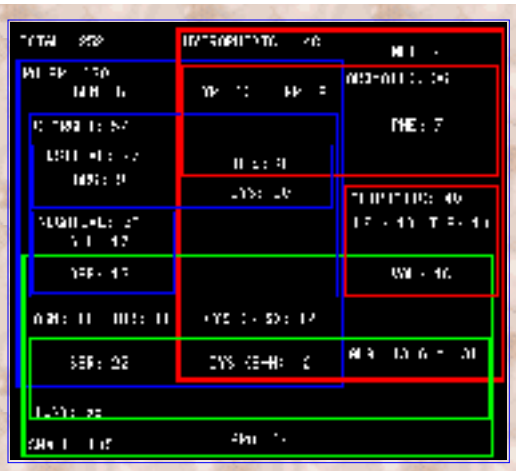
---

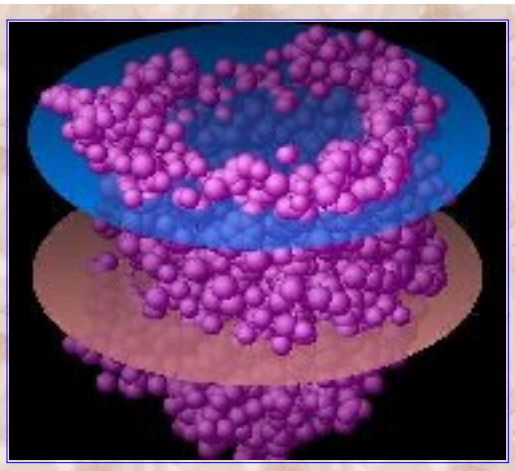
garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

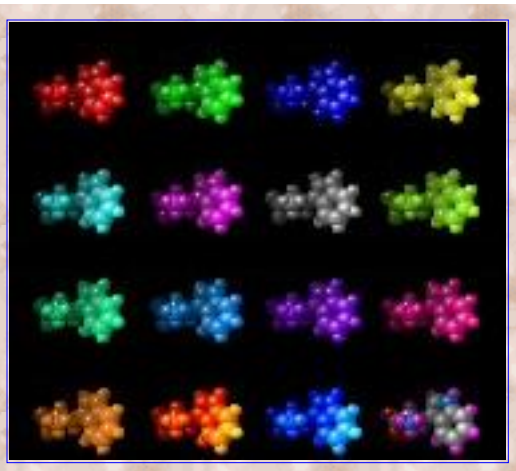
This page contains twelve garlic screenshots reduced to a size suitable for fast downloading. Click the selected image to load the full-sized version. Most images are stored in JPG format; color quality is slightly reduced by compression. True-color display is recommended for viewing this page.







Garlic Versions

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains a list of garlic versions, with links.

- **1.0** **March 2000.**
- **1.1** **February 2001.**
- **1.2** **September 2002.**
- **1.3** **Under development.**

Garlic - Version 1.2

Free Molecular Viewer and Editor

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This is the home of garlic - free, open source molecular viewer and editor. Garlic is the most portable molecular viewer in the unix world. Follow the links below to find more about garlic. Don't forget to visit the screenshot gallery !

Release date: September 20, 2002. All versions are listed here .

Garlic home: [Croatia] Auto-mirrors: [Australia] [Canada] [United Kingdom] [United States]

What is garlic?	Screenshot gallery	License
Download garlic	Installation guide	Documentation
Similar programs	Support garlic!	Author

Linux distributions with precompiled garlic: [Debian] [Mandrake] [SuSE]

HPUX archives (check the program version!): [Canada] [France] [Germany] [Italy] [Japan] [Netherlands] [South Africa] [United Kingdom] [USA (Utah)]

AIX archive (check the program version!): [The Henry Samueli School, UCLA]

2003/01/20: FTP site closed. HTTP download will be the only download method.

2002/09/20: Version 1.2 released. Garlic is now capable to create and edit molecular structures.

2002/09/18: Garlic development will be supported by the Ministry of Science of Republic of Croatia.

Questions, Bug Reports, Comments and Suggestions

The form below may be used to send bug reports, comments and suggestions, or to ask question about garlic. You can also send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) .

Name and institution:

e-mail address (please type it carefully):

Message:

SEND CLEAR

Garlic

The Most Portable Molecular Viewer and Editor in Unix World

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

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Check the list of freely available molecular visualization programs for unix and unix clones. This page lists also the libraries required to run each of these programs.

Free Molecular Visualization Programs for Unix and/or Linux

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free molecular visualization programs, free molecular viewers, list of molecular visualization programs, list of molecular viewers, molecular rendering, protein visualization tools, molecular visualization resources, download page, download source, download executable, download binary, AMMP, B, BRAGI, Cn3D, Deep View Swiss-PDBViever, DINO, Flex, garlic, gdpc, Ghemical, gOpenMol, Grasp, ICMlite, Jmol, Kinemage, mdxvu, Mercury, MOIL-View, MOLDEN, MOLEKEL, MOLMOL, MolScript, Moviemol, NAMOT, QMOL, PREPI, PyMOL, RasMol, Raster3D, spock, VEGA, Viewmol, WinMGM, VMD, XMakemol, XmMol, XMol, Ymol, biological macromolecule, protein structure, DNA structure, PDB, unix, linux, free software download, open source software, Damir Zucic.

This page contains the list of free molecular visualization programs, complete with links. Only freely available programs which run on unix or unix compatible platform are listed. Some of these programs are available only as binary code for some specific platform(s).

Most programs were found using AltaVista, Lycos and Google, while some others were suggested by readers of this list. Thanks to all of them!

Some of the programs listed below have a very limited license. Be sure to read the license before using such program!

The time-limited trial versions of commercial programs were omitted from the list.

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If you have your own free molecular visualization program for unix or linux, or if you know for such program which is not included in the list below, please send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) . Please send corrections and changes to the same address.

Last updated: September 20, 2002.

The information contained here was valid before that day. As developing is going on, it is likely that some additional libraries may become necessary for some of the programs listed here. However, it is almost certain that libraries listed here will be required in future versions too.

PROGRAM	LIBRARIES REQUIRED	PROGRAM TYPE / LICENSE
AMMP	libc, libm, libX11, libXt, libXext, libXmu, libXm, libSM, libICE, libNoVersion	Stand alone program, modified GNU GPL license.
B (where is it now?)	Java based package.	Your browser should support Java Virtual Machine.
BRAGI	It seems that this program is still under development.	The license has to be negotiated.
Chimera	Needs Python, Tcl/Tk, Tix, Togl, PIL, Numeric, Grail, Pmw, msms, VRML, JPEG, Info-ZIP, TR, ScientificPython; still under development.	Stand alone program, online registration required. Requires many libraries.

Cn3D	libc, libm, libX11, libXt, libXext, libXmu, libXp	Both browser plug-in and stand alone program.
Deep View Swiss-PdbViewer	libc, libm, libX11, libXt, libXext, libXmu, libXi, libXp, libMesaGL, libMesaGLU, libpthread, libz	Stand alone program, IRIX or linux required.
DINO	libc, libm, libX11, libXt, libXext, libXmu, libXi, libgdbm, libGL, libGLU	Stand alone program.
Flex	libc, libm, libX11, libxview, libolgx, xlibflexdraw	Stand alone, binaries for DEC/alpha, DEC/MIPS, IBM RS, SGI, Sun.
garlic	libc, libm, libX11	Stand alone program, GNU GPL license.
Ghemical	requires g++ compiler, f2c compiler, glut, GNOME, gtkglarea, mpich, MPQC ...	Stand alone program, GNU GPL license.
gdpc	libc, libm, libX11, libXext, libXi, libgtk, libgdk, libgmodule, libglib, libdl, libpthread	Stand alone program.
gOpenMol	libc, libm, libX11, libXt, libXext, libXmu, libXi, libdl, libXaw, Tcl/Tk, + Mesa or Open GL libraries	Graphics interface to the OpenMol set of programs; GNU GPL license.
Grasp	This program has been written for Silicon Graphics computers.	Under special circumstances, the $500 fee will be waived.
ICMlite	Binaries: SGI, DEC Alpha, SUN, Linux; libc, libm, libX11, libXt, libXext, libXmu, libSM, libICE, libpthread	Stand alone program, free for academic use.
Jmol	Java-based application.	Stand alone program (Java-based application).
Kinemage	libc, libm, libX11, libXt, libXm	Stand alone program.
mdxvu	libc, libm, libX11, precompiled for some systems	Stand alone program.
Mercury	libc, libm, libX11, libXt, libXext, libXmu, libXi, libXft, libXRender, libMesaGLU, libMesaGL, libSM, libICE, libjpeg, libpng, libmng, libdialogs, libwidgets, libqt, libqtspecific, libguiindep, libtoolkit, libcsd, libCif, libKCC-eh, libz, libfreetype, liblcms	Stand alone program, read conditions of use carefully.
MOIL-View	FORTRAN program, binaries available for Silicon Graphics workstations.	Stand alone program, registration expected.

MOLDEN	FORTRAN 77, libc, libm, libX11	Stand alone, free for academic use.
MOLEKEL	libc, libm, libX11, libXext, libXmu, libXi, libMesaGL, libMesaGLU, libtiff, libjpeg	Precompiled for SGI IRIX, linux PC and SunOS, registration required.
MOLMOL	libc, libm, libX11, libXt, libXext, libXm, libGL, libGLU, libGLcore, libC, libgen, libgen, libpng, libz	Stand alone, binaries for DEC/MIPS, DEC/alpha, SGI, SPARC and RS/6000.
MolScript	libc, libm, libX11, libXt, libXext, libXmu, libGL, libGLU, libGLcore, libmedia, libC, libgen, libvice, libjpeg, libpng, libz	Stand alone, online registration required.
Moviemol	libc, libm, libX11, libXext, libYgl or OpenGL	Stand alone program.
NAMOT	libc, libm, libX11, libxview, libolgx	Stand alone program.
QMOL	libc, libm, libX11, libXt, libXext, libXm, libGLw, libMesaGL, libMesaGLU, libstdc++, libSM, libICE	Stand alone program.
PREPI	Precompiled binary for Silicon Graphics IRIX.	Stand alone, registration required (written agreement).
PyMOL	libc, X libs, libpng, zlib, python, Mesa	Requires Python, an intepreted programming language.
RasMol	libc, libm, libX11 libXext, libXi	Stand alone program.
Raster3D	Mixed FORTRAN 77 and C code, requires both compilers.	Stand alone program.
spock	libc, libm, libX11, libXt, libXext, libXmu, libXm, libXi, libXpm, libMesaGL, libMesaGLU, libSM, libICE, libjpeg, libtiff, libcrypt, libz, libNoVersion	Stand alone program, free for some users, registration required.
VEGA	libc, libm, libz, liblocale	No OpenGL support for linux version.
Viewmol	libc, libm, libX11, libXt, libXext, libXm, libXi, libXp, libGL, libGLU, libtiff, libtiff, libpthread, libdb, libdl, libutil	Graphical front end for comp. chemistry programs, GNU GPL license.
WinMGM	libc, libm, libMesaGL, libsubplex, libchelpers, libmgmcalctools, libmolecules, libmolenergy	Stand alone, some custom libraries required.
VMD	Statically linked binaries for AIX, HPUX, IRIX, linux, Solaris and TRU64.	Stand alone, online registration required.

XMakemol	**libc, libm, libX11, libXt, libXm, libXpm, libGL, libGLU**	**Stand alone program, GNU GPL license.**
XmMol	**libc, libm, libX11, libXt, libXext, libXm, libXp, libSM, libICE; Motif or openMotif required.**	**Free for academic use, registration required (written agreement).**
XMol	**Precompiled binaries for SGI, Sun-3, Sun-4 and RS/6000.**	**Some other binaries may be found in some other archives; development seems to be halted.**
Ymol	**libc, libm, libX11, libXext**	**Stand alone program.**

Garlic Screenshot Gallery

Version 1.2

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains twelve garlic screenshots reduced to a size suitable for fast downloading. Click the selected image to load the full-sized version. All images are stored in PNG format. The true-color display is recommended for viewing this page.

Garlic Versions

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains a list of garlic versions, with links.

- **1.0** **March 2000.**
- **1.1** **February 2001.**
- **1.2** **September 2002.**
- **1.3** **Under development.**

Garlic - Version 1.3

Free Molecular Viewer and Editor

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This is the home of garlic - free, open source molecular viewer and editor. Garlic is the most portable molecular viewer in the unix world. Follow the links below to find more about garlic. Don't forget to visit the screenshot gallery !

Garlic is supported by the Ministry of Science and Technology, Republic of Croatia, as Project #0219031.

What is garlic? **Screenshot gallery** **Download garlic** **Installation guide**

Documentation **Similar programs** **License (GNU GPL)** **Author**

Release date: April 01, 2003. All versions are listed here .

Garlic home: [Croatia]

Auto-mirrors: [Australia] [Canada] [United Kingdom] [United States]

Linux distributions with precompiled garlic: [Debian] [Mandrake] [SuSE]

HPUX archives (check the program version!): [Canada] [France] [Germany] [Italy] [Japan] [Netherlands] [South Africa] [United Kingdom] [USA (Utah)]

AIX archive (check the program version!): [The Henry Samueli School, UCLA]

2003/04/01: Version 1.3 released.

Questions, Bug Reports, Comments and Suggestions

Send an e-mail message to Damir Zucic (zucic@garlic.mefos.hr) .

Garlic Versions

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains a list of garlic versions, with links.

- 1.0 March 2000.
- 1.1 February 2001.
- 1.2 September 2002.
- 1.3 April 2003.
- 1.4 Under development.

What is Garlic?

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic is a free molecular viewer and editor written for unix and unix clones.

Garlic was born September 30, 1998. At that time I needed a good molecular visualization program and almost the only thing at hand was RasMol. I had some hard time with RasMol so I tryed to adapt it to my needs. However, I realized that it is very hard to read and change RasMol source code, so I decided to write my own molecular visualization program.

Further, I decided to learn programming for the X window system, and this is my first serious program written for X11.

Since 1997 I use GNU/Linux software, so I concluded that it would be fair to add something useful and modern to the existing collection of free software because this software significantly improved my working conditions.

Garlic was forgotten few times, for months, as I had some other things to do, but now it is finaly operative.

Though the version number of the current version (1.2) is not very high, the program is very stable and robust, at least on systems which were available for testing here at University of Osijek, Croatia.

The name garlic was choosen because my original intention was to write a modular program, which will be capable to call a number of modules via system calls. In fact, I did the opposite thing: garlic now consists of a single unit which integrates all functions. Anyway, back in 1998 I thought that this program will be similar to garlic - a small core with a number of units packed around this core. I also like garlic.

Later, I reallized that program name may be reinterpreted as follows:
G stands for GNU (license),
AR for analysis and rendering,
LI for linux,
C for C (the computer language).

Who might be interested to use this program?

Students
As garlic is free and open, students may find it interesting as a learning tool. Garlic may be installed on a cheap, no-name PC (running a free linux distribution) or even on a laptop (very handy!).

University assistents and professors
It is somewhat delicate to use commercial software for lectures and seminars (assignments). In their later carrier students may be boosted toward the software which they used during their study just because they have some experience with it. Universities should not influence the software market by choosing certain commercial product just because it is cheap or for some other reason suitable for university assignments.

Professionals

Many professionals would like to use some molecular visualization program at home or on a portable computer. Some others may be interested to adapt the program to their own needs. Software makers are unwilling to give the source code and to allow modification of their product. They also try to drain as much money as possible for additional (home) copies. Anyone wishing to cut the rope is invited to use and modify garlic, but the final product has to remain free and open, in agreement with the GNU General Public License .

Others

Anyone interested to learn something about proteins, DNA and some other molecules may find garlic useful.

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Version 2, June 1991

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Download garlic

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

If your browser failes to recognize what should be done with the choosen file, please try the following:

(1) Click the right mouse button while pointing at the choosen file.

(2) Select the option "Save Link As ..." (from the pop-up menu).

(3) A dialog box will be opened - change directory and file name if necessary.

HTTP DOWNLOAD

Croatia: http://garlic.mefos.hr/sources/garlic-1.2

DEBIAN PACKAGES

Program: http://packages.debian.org/stable/science/garlic.html

Documentation: http://packages.debian.org/stable/doc/garlic-doc.html

---

RPM PACKAGES

The RPM package may be found at at.rpmfind.net . Use the search engine (at this site) to find the appropriate RPM package.

At least two RPM-based linux distributions contain garlic:

[Mandrake] [SuSE]

Garlic Installation

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic is the most portable molecular viewer/editor in the unix world, because the only libraries required by this program are the standard C library (libc), the standard math library (libm) and the standard X library (libX11). All other molecular visualization programs require some additional libraries.

Before starting the installation, you might be interested to check the technical requirements . Most contemporary unix and unix-like systems (like linux) meet these requirements without need to change the configuration, so you can skip this text if you are impatient.

If you have Apple McIntosh running Xtools from Tenon, please read these hints , contributed by Chris from Macinchem.

To compile and install garlic, follow these instructions:

(1)	Put garlic package (garlic-1.2.tar.gz) into some empty directory.
(2)	Uncompress and unpack the package: gzip -d garlic-1.2.tar.gz tar xf garlic-1.2.tar
(3)	Change your working directory: cd garlic-1.2
(4)	Check which C compiler is available on your system. If you don't know how to find this information, try this: man -k compiler to obtain the list of available compilers.
(5)	If gcc (GNU C) compiler is not available on your system, use your favorite editor to edit Makefile. Replace gcc in: CC = gcc line with the name of your compiler (this may be cc, for example). If gcc is available on your system, do not change the CC line.
(6)	Find a directory which contains the Xlib library. Try this: cd / find . -name libX11* Check where is the file libX11.so (sharable library - prefered) or libX11.a (static library - reserve option). If your directory is different from /usr/X11R6/lib, modify the line: LIBPATH = -L/usr/X11R6/lib in Makefile. For example, if libX11.so is stored in /usr/shlib directory on your system, the LIBPATH should be changed to: LIBPATH = -L/usr/shlib
(7)	Compile the package - just type: make and wait, it will take some time.

(8)	If everything worked fine, copy the executable to a choosen directory. /usr/local/bin may be a good choice. This job should be done by root (system administrator): cp garlic /usr/local/bin If you don't have root privileges, ask your local administrator to install garlic, or just leave it in one of your directories.
(9)	Now the .garlicrc configuration file and the file which contains the template residues should be copied to a directory where these files will be accessible to everyone. If this is not done, garlic will work anyway, using hard-coded default configuration, but you will be unable to replace residues and to create peptides. The recommended directory is /usr/local/lib/garlic but if directory /usr/local/lib does not exist on your system, /usr/lib/garlic may be may be used. This should be done by root (system administrator): mkdir /usr/local/lib/garlic cp .garlicrc /usr/local/lib/garlic cp residues.pdb /usr/local/lib/garlic
(10)	It may be good idea to copy the configuration file to your home directory or to the subdirectory garlic of your home directory. The same may be done with the file residues.pdb. If you do this, you will be able to personalize your garlic sessions, because your private files will override the system-wide defaults. Of course, you don't need root privileges to do this: cp .garlicrc $HOME cp residues.pdb $HOME or: mkdir $HOME/garlic cp .garlicrc $HOME/garlic cp residues.pdb $HOME/garlic
(11)	It is recommended to set the environment variable MOL_PATH, so garlic will search all directories listed in this variable to find the specified file. Click here for detailed instructions.
(12)	Clean up the mess (sources and .o files). Be sure to leave all .pdb files for later practice. Leave also the files with the extension .script, these are some garlic tutorial scripts.

If garlic refuses to work because it fails to get the TrueColor visual, try to execute xdpyinfo and xwininfo (click into the root window); check the list of supported visuals and the current color depth. Choose the color depth for which the TrueColor visual is available. If you have the SGI Octane workstation, please read this text , contributed by Randal R. Ketchem. If you have IBM RS6000 with AIX, read this hint, contributed by Nicolas Ferre.

The list of sites with proteins, nucleic acids and hetero compounds is here .

If you can't compile, install or run garlic, write to me (Damir Zucic), my address is zucic@garlic.mefos.hr .

Technical Requirements

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic tends to be POSIX compliant. It is also ANSI C compliant, to the maximum possible extent. Xlib functions are the only non-ANSI functions used by this program.

OPERATING SYSTEM
Unix or unix clone and the X window system. Linux and XFree86 recommended.

SUPPORTED HARDWARE PLATFORMS
Desktop PC, laptop, notebook, unix workstation equipped with a color monitor with a color depth of at least 8 bits per pixel. Garlic may also be used on Apple MacIntosh running Xtools from Tenon . Click here for instructions if you have such system. No dials are required. Some X servers do not support TrueColor visual at 8 bits per pixel: try to switch to higher color depth (12, 15, 24, ...)! If you have the SGI Octane workstation, you might be interested to read this text. If you have IBM RS6000 with AIX, read this hint.

CPU
Intel, Digital Alpha, HP, SUN MIPS, SGI and some others. This program has no special hardware requirements.

GRAPHICS INTERFACE
Garlic requires the X window system. The recommended version is X11R6, but older versions may work too.
THE X SERVER SHOULD BE CAPABLE TO SUPPORT TrueColor VISUAL!
Some older servers may be unable to support the TrueColor visual; if you have such X server, garlic will refuse to work. Some modern X servers do not support the TrueColor visual at 8 bits per pixel, but these are usually running on a hardware which may offer 12 or more bits per pixel.

COMPILER
GNU C compiler is recommended, but other compilers compliant with ANSI C standard should work too.

REQUIRED LIBRARIES
The only required libraries are libc (C), libm (mathematical) and libX11 (the standard X11 library).

KEYBOARD
The standard PC 101/102 keyboard should work fine. The laptop keyboard may be used too. If you have some kind of unix workstation with terminal keyboard, this may work too.

MOUSE
Any mouse should serve well.

THE LIST OF COMPATIBLE SYSTEMS
Up to now, it is confirmed that garlic may be compiled and used on these systems:
Intel and compatible processors;
Digital Alpha;
Sun Solaris;
SGI (Silicon Graphics);
HPUX (Hewlett-Packard).

Please inform me (zucic@garlic.mefos.hr) if you successfully compiled and used garlic on a system which is not listed here.

Compiling Garlic on Apple McIntosh

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Here you can read how to compile garlic for Apple MacIntosh running Xtools from Tenon . I would like to thank Chris from Macinchem for this contribution. Chris is also porting other chemistry related programs to Apple MaxIntosh. Please visit his Macinchem site: http://www.macinchem.fsnet.co.uk/macosx.htm

---

If you don't have access to Chris site, here is the important part:

```
... This was my first port, it requires X-Tools from Tenon.
Minor modifications of the Makefile (highlighted in red below) allow
compilation ...

        CC = gcc

        CCOPT = -O -I/usr/X11R6/include

        #CCOPT = -O3

        #CCOPT = -ansi -pedantic -O -Wall -Wstrict-prototypes -g3

        HEADERS = defines.h typedefs.h

        LIBPATH = -L/usr/X11R6/lib

        LINKOPT = -lX11 -lm
```

Setting the Color Depth on SGI Octane

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Some people are using SGI Octane in 8 bits per pixel mode. The TrueColor visual is not available at this color depth on this system. If you have such system, think of using it at its full power. I have no access to SGI Octane, so I had no idea how to change the color depth. I would like to thank Mr. Randal R. Ketchem for contributing the answer to this question.

Edit /usr/lib/X11/xdm/Xservers and change the argument list passed to /usr/bin/X11/X.

e.g.
To change the default configuration from the 8-bit pseudomap visual to the 24-bit TrueColor visual, change the single line:
:0 secure /usr/bin/X11/X -bs -nobitscale -c -pseudomap 4sight -solidroot sgilightblue -cursorFG red -cursorBG white

to a single line with:
:0 secure /usr/bin/X11/X -bs -nobitscale -c -class TrueColor -depth 24 -solidroot sgilightblue -cursorFG red -cursorBG white

---

Setting the Color Depth on IBM RS6000 with AIX4.3

---

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To use the X window system with 24 bits per pixel, run the following command:

xinit -- -x dbe -x abx -layer 0 -d 24 -cc TrueColor

I would like to thank Mr. Nicolas Ferre (Nancy, France) for this hint.

Environment Variable MOL_PATH

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The environment varible MOL_PATH may be used to define the list of directories which should be searched when you are trying to load certain PDB file. It is not mandatory to define this environment variable, but it is very practical.

MOL_PATH is not the only environment variable recognized by garlic. There is also MOL_DIR, but it is capable to specify only one directory, so it is not recommended.

The exact procedure which should be used to define the environment variable MOL_PATH depends on the shell you use. The procedure is described here for some commonly used shells.

If you don't know what is you shell, execute these commands:

```
echo $shell
echo $SHELL
```

Bourne Shell

If you are using the Bourne shell (sh) or the GNU clone called Bourne-again shell (bash), use the example bellow to create your own MOL_PATH variable. Use colon (:) to separate directories. It is important to export the variable! You should define this variable through your .bash_profile or .bashrc resource file in your home directory. Don't forget to replace the user name and directories.

```
MOL_PATH="/home/zucic/pdb:/home/zucic/glob:/home/zucic/memb"
export MOL_PATH
```

C Shell

If you are using the C shell (csh) or it's clone tcsh, use the command setenv to define the environment variable MOL_PATH. Use colon (:) to separate directories. You should define this variable through your .cshrc, .tcshrc or .login resource file in your home directory. The user name and directories should be replaced, of course.

```
setenv MOL_PATH /home/zucic/pdb:/home/zucic/glob:/home/zucic/memb
```

Other Shells

For other shells, read the manual page to learn how to define the environment variable MOL_PATH. In most cases, the method is similar to one of the methods described above.

Molecular Structures

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This page contains the list of sites with molecular structures. This list contains only the sites which contain data in PDB format. Note that links are subject to changes. If this happens, use Google or some other search engine to find the site. Use the words (or even entire titles) from the middle column as search terms.

DATA	LINK	REFERENCE
Proteins and nucleic acids	The Protein Data Bank, http://www.rcsb.org/pdb/	H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov, P.E.Bourne, The Protein Data Bank, Nucleic Acids Research 28, pp. 235-242 (2000).
Hetero compounds	Hetero-compound Information Centre - Uppsala, http://xray.bmc.uu.se/hicup/	Kleywegt, G.J. and Jones, T.A. (1998). Databases in protein crystallography. Acta Cryst D54, 1119-1131 (CCP4 Proceedings).
Many Small Molecules	Molecular Models from Chemistry at Okanagan University College, http://people.ouc.bc.ca/woodcock/molecule/molecule.html	Prepared by Dr. Dave Woodcock.

Garlic Documentation

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic documentation is written in HTML format. The sections are listed below, with a brief description. Newbies are recommended to read at least parts of each section.

Garlic Features	An overview of garlic features.
Controls	Reserved keys: rotations, translations, slab and color.
Commands	Detailed description of garlic commands.
Mouse Usage	Mouse tricks specific for garlic.
Reference Card	A quick reminder, both for newbies and experienced users.
Tutorial	A collection of lessons and demonstration scripts.
Options	Command line options.
Configuration File	Configuration file for garlic, called .garlicrc (for experts).
Environment Variables	Environment variables recognized by garlic.
Molecular Structures	Proteins, nucleic acids and hetero compounds.

Garlic Features

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Features which are already implemented are marked as DONE.
Partially implemented ideas are marked PARTIAL.

DONE	Garlic is free. The source code is available to everyone.
DONE	With garlic, you will be able to replace residues, to create new structures and to adjust bond angles.
DONE	Atoms may be drawn as spheres of different sizes. Bonds may be drawn as cylindrical sticks, conical sticks or as curved surfaces.
DONE	Five types of slab are available: planar, spherical, semi-spherical, cylindrical and semi-cylindrical.
DONE	The slab position and thickness are visible in a small window.
DONE	Atomic bonds as well as atoms are treated as independent drawable objects.
DONE	The atomic and bond colors depend on position. Five mapping modes are available (as for slab).
DONE	Garlic is capable to display stereo image.
DONE	Garlic is capable to display other geometric objects, like membrane, for example.
DONE	In addition to standard chemical elements, garlic allows the usage of two imaginary elements, called "jellium" (J) and "quarkonium" (Q). These elements may be used to draw some special objects. Jellium never forms any bonds, while quarkonium binds to neighboring atoms in the list (so it forms no bond, one bond or two bonds at most). Imaginary atoms may be used to adapt garlic for medical imaging, for example.
DONE	Atomic information is available for atom covered by the mouse pointer. No click required, just move the mouse pointer over the structure!
DONE	Garlic is capable to load more than one structure.
PARTIAL	It will be possible to color the residues according to hydrophobicity and other properties.
DONE	Garlic is capable to draw Ramachandran plot, helical wheel, Venn diagram, averaged hydrophobicity, hydrophobic moment plot and sequence comparison plot.
DONE	The command prompt is available at the bottom of the main window. It is capable to display one error message and one command string.

Garlic Controls

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The image in the main window is controled by CONTROLS and by COMMANDS . This page contains description of garlic controls.

Garlic controls are reserved keys, which may be used to rotate and translate the structure, to rotate bonds, to shift selected atoms and to change the position of slab surfaces and to change the way color depends on distance from the observer. At present, the reserved keys are numeric keypad keys and four function keys (F1, F2, F3 and F4).

Some desktop environments are reserving function keys for some special purposes. This means that some function keys will fail to work properly with garlic. To avoid this problem, you can use mouse to click on dummy buttons in control window. Another solution will be to change your desktop environment settings.

Numeric keypad	Function keys

For each control, five steps are available: normal, large, very large, small and very small. If you press the control without holding a modifier key (shift, alt or control), the normal step will be used.

Modifier keys may be used in combination with reserved keys to select large, very large, small or very small step. Here is the table of modifier keys:

MODIFIER KEYS	STEP	EXAMPLE
none	Normal	
shift	Large	
alt_shift	Very large	
control	Small	
shift_control	Very small	

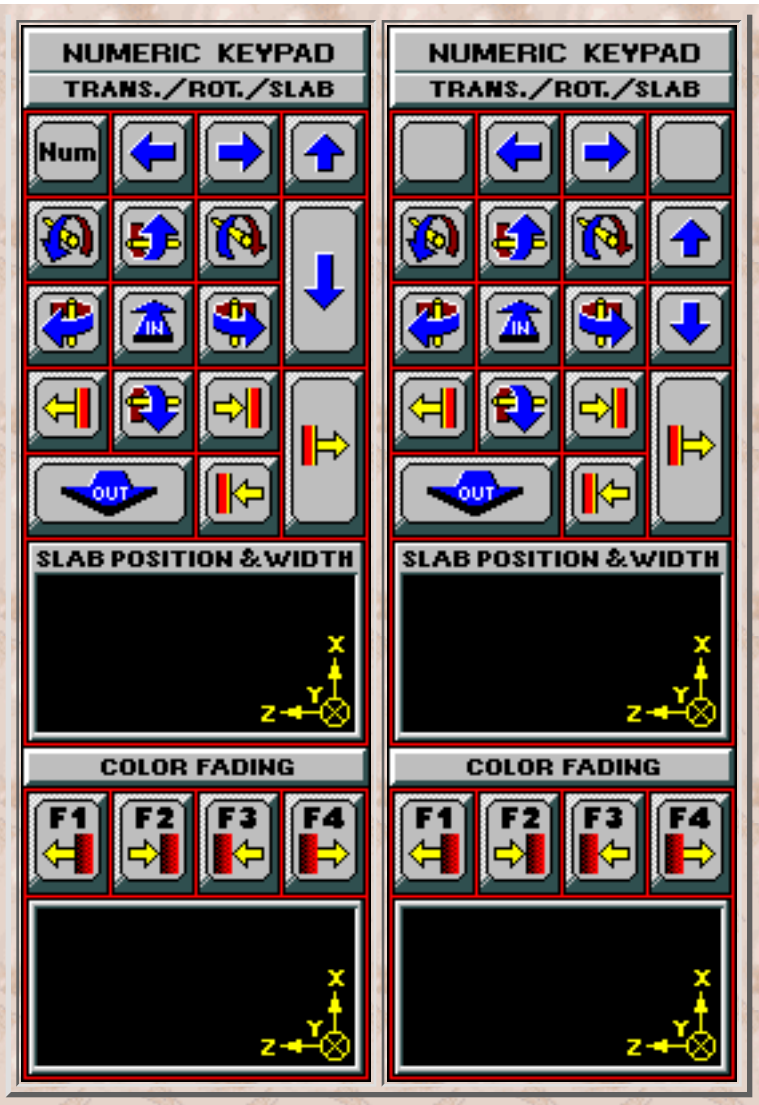
Be sure to avoid ctrl_alt combinations, because some of these combinations may have a very interesting effect (try, for example, ctrl_alt_del or ctrl_alt_F1).

The table below contains the list of controls and the corresponding default actions upon the structure which is currently handled (held, catched). These default actions will be active in default editing mode (no editing at all, just viewing the structure). If editing atoms or bonds some of the controls will have different role. The table refers to PC (101/102) keyboard. There are slight differences between PC and terminal keyboard; three terminal keys are listed in the table (KP_F2, KP_F3, KP_Separator). If you have some exotic keyboard, use the program xshowkey to check the mapping of keys and send this list to the author: zucic@garlic.mefos.hr

KEY	LOCATION	ACTION
0	Numeric keypad	Translate structure along z in negative direction.
1	Numeric keypad	Move back (distant) slab surface along z in positive direction.
2	Numeric keypad	Rotate structure clockwise around x.
3	Numeric keypad	Move back (distant) slab surface along z in negative direction.
4	Numeric keypad	Rotate structure clockwise around y.
5	Numeric keypad	Translate structure along z in positive direction.
6	Numeric keypad	Rotate structure counterclockwise around y.
7	Numeric keypad	Rotate structure counterclockwise around z.
8	Numeric keypad	Rotate structure counterclockwise around x.
9	Numeric keypad	Rotate structure clockwise around z.
delete	Numeric keypad	Move front (close) slab surface along z in positive direction.
enter	Numeric keypad	Move front (close) slab surface along z in negative direction.
/ (slash) KP_F2	Numeric keypad	Translate structure left.
* (asterisk) KP_F3	Numeric keypad	Translate structure right.
- (minus)	Numeric keypad	Translate structure up.
+ (plus) KP_Separator	Numeric keypad	Translate structure down.
F1	Function keys	Move back (distant) color surface along z in positive direction.
F2	Function keys	Move back (distant) color surface along z in negative direction.
F3	Function keys	Move front (close) color surface along z in positive direction.
F4	Function keys	Move front (close) color surface along z in negative direction.
Num Lock	Numeric keypad	Unused key.
Escape	Top left corner	Return to the main drawing mode (display structure).

Here are the illustrations:

PC keyboard	Terminal keyboard


NUMERIC KEYPAD
TRANS./ROT./SLAB
Num
IN
OUT
SLAB POSITION & WIDTH
X
Y
Z
COLOR FADING
F1
F2
F3
F4
NUMERIC KEYPAD
TRANS./ROT./SLAB
IN
OUT
SLAB POSITION & WIDTH
X
Y
Z
COLOR FADING
F1
F2
F3
F4

Garlic Commands

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The image in the main window is controled by CONTROLS and by COMMANDS. This page contains the list of garlic commands.

Garlic commands are strings, consisting of one or more words. A command is executed when you press the RETURN key (this key is labeled ENTER on some keyboards). Note that ENTER key on the numeric keypad (the one in the bottom right corner of your keyboard) is NOT the right key! Commands will be displayed in the area called the input window.

The input window is placed at the bottom of the main garlic window, left justified. You don't have to the click into this area to enter the command string - just type it. The input window is capable to display a single error message (top) and a single command (bottom).

You can access previously executed commands by using arrow keys on your keyboard (the UP arrow scans the history buffer backwards and DOWN arrow in the opposite direction).

This page contains the alphabetic list of garlic commands with a short description and with link to detailed description.

Commands are generally case insensitive, but file names are case sensitive because unix (linux) is case sensitive.

SHORT FORM	LONG FORM	SHORT DESCRIPTION
ADD	ADD	Expand current selection.
ANG	ANGLE	Define angle.
ATO	ATOMS	Change atom drawing style.
BAC	BACKBONE	Draw backbone.
BACKG	BACKGROUND	The same as BG.
BG	BACKGROUND	Change main window background color.
BON	BONDS	Change bond drawing style.
CAT	CATCH	Catch the specified structure.
CEN	CENTER	Change the internal coordinate system origin.
COL	COLOR	Set color.
COM	COMPARE	Compare two sequences.
CRE	CREATE	Create structure.
DIS	DISCARD	Discard structure.
DOC	DOCK	Prepare two structures for docking.

EDI	EDIT	Edit structure.
EXE	EXECUTE	Execute garlic script.
EXI	EXIT	Quit garlic session.
EXP	EXPAND	The same as ADD.
FAD	FADING	Change color fading style or parameter(s).
FG	FOREGROUND	Change main window foreground color.
FON	FONT	Change font.
FOREG	FOREGROUND	The same as FG.
HID	HIDE	Hide selected atoms.
HYB	HYBONDS	Generate hydrogen bonds.
IGN	IGNORE	Ignore (this command does nothing).
LAB	LABELS	Show labels.
LOA	LOAD	Load the specified file.
LOG	LOG	Write commands to log file.
MEM	MEMBRANE	Membrane manipulation.
MON	MONO	Switch to mono mode.
MOV	MOVE	Define which object should be moved.
NEI	NEIGHBORHOOD	Show or hide the sequence neighborhood.
PAU	PAUSE	Pause execution (useful in scripts).
PLA	PLANE	Plane manipulation.
PLO	PLOT	Plot averaged hydrophob. and/or hydrophobic moment.
POS	POSITION	Move structure to specified position.
PRO	PROBE	Set the probe radius (used to draw nice bonds).
QUI	QUIT	The same as exit.
RAD	RADIUS	Define sphere radius (used for selection).
RAM	RAMACHANDRAN	Draw Ramachandran plot.
REA	READ	The same as LOAD.
REF	REFRESH	Switch graphics refreshing on or off.
REG	REGISTER	Register garlic.
REP	REPLACE	Replace selected residues.
RES	RESTRICT	Restrict current selection.
ROT	ROTATE	Rotate structure.
SAV	SAVE	Save atomic data to file.
SCA	SCALE	Select hydrophobicity scale.
SEL	SELECT	Select atoms.

SEQ	SEQUENCE	Sequence buffer manipulation.
SET	SET	Set the specified dihedral angle.
SHO	SHOW	Show selected atoms.
SLA	SLAB	Change slab style or parameter(s).
SSB	SSB	Change drawing style for disulfide bonds.
STE	STEREO	Switch to stereo mode.
STR	STRUCTURE	Secondary structure manipulation.
TAG	TAG	Assign tag (short text) to structure.
TAK	TAKE	The same as CATCH.
TBG	TEXT_BACKGROUND	Change text background color.
TFG	TEXT_FOREGROUND	Check text foreground color.
TIT	TITLE	Add title to the main window.
TRA	TRANSLATE	Translate structure.
VEN	VENN	Draw Venn diagram.
WHE	WHEEL	Draw helical wheel.
WIN	WINDOW	Set sliding window width.

ADD, EXP, EXPAND

NAME
ADD, EXP, EXPAND - add specified atoms to current selection.

SYNOPSIS
ADD chain_identifiers/residue_serials/residue_names/atom_names
ADD residue_ranges
ADD residue_names
ADD ATO atomic_ranges
ADD ATOMS atomic_ranges
ADD keyword
ADD ELE chemical_symbol
ADD ELEMENT chemical_symbol

DESCRIPTION
Add specified atoms to current selection. Atoms are added according to the specified cryteria. The command EXPAND does exactly the same job as ADD. The essential difference between ADD and SELECT is that ADD does not overwrite the previous selection. Four types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword);
(5) selection by chemical symbol;
(6) selection by atom serial number.

DETAILED SELECTION
In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain_identifiers/residue_serials/residue_names/atom_names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

add a/*/*/*	Add all atoms from chain A to current selection.
add * exc m/*/*/ca	Add CA atoms from all chains except chain M.
add */*/*/* exc ca,c,n,o	Add all atoms except CA, C, N and O.
add a/* exc 72-112/*/ca	Add CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

add 1-100	Add residues from 1 to 100 to current selection.
add 1-100 exc 20-40	Add residues 1-100 but exclude 20-40.
add 1, 4, 8, 11-48 exc 20-32	Add residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY ATOMIC SERIAL NUMBERS

To add a single atom by the atomic serial number, combine the command ADD and the keyword ATO (ATOMS). For example, to add the atom number 102 to the current selection type:

add ato 102

The same keyword may be used to add a range of atoms or to add two or more ranges. Examples:

add ato 1-100	Add atoms which have serial numbers in the range between 1 and 100.
add 1-20 40-50	Add atoms which have serial numbers between 1 and 20 and between 40 and 50.

Do not combine the keywords EXC (EXCLUDE) and ATO (ATOMS).

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

add phe,tyr,trp	Add PHE, TYR and TRP to current selection.

SPECIAL SELECTION KEYWORDS

Some special keywords may be combined with ADD to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

add * add all	Add all atoms to current selection, i.e. select all.
add abo add above	Add atoms above the plane.

add aci add acidic	Add acidic amino acids (GLU and ASP).
add ali add aliphatic	Add aliphatic amino acids (ILE, LEU and VAL).
add alt	Add atoms at alternate positions.
add bad	Add bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
add bas add basic	Add basic amino acids (ARG, LYS and HIS).
add bel add below	Add atoms below the plane.
add cha add charged	Add charged amino acids (ARG, LYS, HIS, GLU and ASP).
add cis	Add cis residues.
add com add complement	Add atoms which were not select previously.
add het add hetero	Add hetero atoms (heme groups, water etc.).
add pho add hydrophobic	Add hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
add mai add main_chain	Add main chain atoms (CA, C, N and O).
add mod serial_number add model serial_number	Add model specified by serial_number. NMR structure is a set of models. Example: add mod 1
add neg add negative	Add negatively charged amino acids (GLU and ASP).
add pol add polar	Add polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
add pos add positive	Add positively charged amino acids (ARG, LYS and HIS).
add seq add sequence	Add sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
add sid add side_chains	Add atoms which belong to side chains (all except CA, C, N and O).
add sma add small	Add small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
add sph add sphere	Add atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
add tin add tiny	Add tiny amino acids (GLY,ALA and SER).
add tra add trans	Add trans residues.

sel tri **sel triplet**	**If there are three (or more) positively charged residues in a fragment of up to five protein residues, add these residues to the current set of selected atoms. Detailed explanation may found in the article:** **D. Juretic, L. Zoranic and D. Zucic,** **Basic charge clusters and predictions of membrane protein topology,** **Journal of Chemical Information and Computer Sciences 42, No. 3, 620-632 (2002).**

EXPANDING SELECTION WITH THE SPECIFIED CHEMICAL ELEMENT

To add certain chemical element to the selection, use the keyword ELEMENT (short form: ELE) and the standard chemical symbol. To expand your selection with iron atoms, for example, you should type the following command:

add ele fe

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and "quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1. The interatomic distance is not important! Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. Note that symbols J and Q are not used in the periodic table of elements.

NOTES

(1) The command ADD resets the editing mode to default (no editing).

RELATED COMMANDS

EXPAND does exactly the same job as ADD. SELECT overwrites the previous selection. RESTRICT restrics the previous selection.

RAD, RADIUS

NAME

RAD, RADIUS - set sphere radius.

SYNOPSIS

RAD value
RADIUS value

DESCRIPTION

Set the sphere radius for selection. The value should be given in angstroms. The command SELECT SPHERE may be used to select only the atoms which fit into the sphere of a given radius around the current geometric center.

EXAMPLES

COMMAND	DESCRIPTION
rad 4.5	Set radius value to 4.5 angstroms.
sel 210-212 cen rad 10 sel sphere sel com hide	Select residues from 210 to 212, redefine the geometric center, set sphere radius to 10 angstroms and select atoms in a given sphere. Select all atoms outside the given sphere and hide them.

RELATED COMMANDS

SELECT SPHERE is used to select atoms in a sphere around the current geometric center. CENTER is used to redefine the position of the geometric center.

ANG, ANGLE

NAME
ANG, ANGLE - set angle.

SYNOPSIS
ANG value
ANGLE value

DESCRIPTION
Set the rotation angle between adjacent residues. This angle is stored as an internal variable and used to draw helical wheel or hydrophobic moment plot. The value should be specified in degrees. Default value is 100 degrees, which corresponds to alpha helix rotation angle. To prepare helical wheel or hydrophobic moment plot you have to make the assumption about the secondary structure. The assumption is made by setting the rotation angle for adjacent residues. The table below lists the common structural motifs and the corresponding angles.

STRUCTURAL MOTIF	RESIDUES PER TURN	ANGLE (DEGREES)
alpha helix	3.6	100
3-10 helix	3	120
beta strand	2.3	160

3-10 helices are usually short, but if you assume that more than three residues fold into 3-10 helix, modify the angle used to draw the helical wheel. If you use the realistic angle (120 degrees), some residues will be obscured (hidden behind the residues which are drawn later). Use 115 or 125 instead of 120 degrees, to avoid overlapping of residues.

RELATED COMMANDS
WHEEL draws the helical wheel. PLOT draws the hydrophobic moment plot.

ATO, ATOMS

NAME

ATO, ATOMS - change drawing style for atoms.

SYNOPSIS

ATO style
ATOMS style

DESCRIPTION

Change drawing style for atoms. Atom style is defined separately from bond style. For BALLS, BA2, BIG, BI2, COVALENT, CO2, SMALL, SM2, SPACEFILL and SP2 style, atomic radii are read from .garlicrc file. If this file is not available, hard-coded defaults are used. The styles listed above may be used to produce nice output but require more CPU time than other styles. The list of realistic, nice styles, sorted by size, from the smallest to the largest:
(1) SMALL and SM2;
(2) COVALENT and CO2;
(3) SPACEFILL and SP2;
(4) BIG and BI2.

Note that BALLS and BA2 style are not included in this list. All atoms drawn using this style will have the same size.

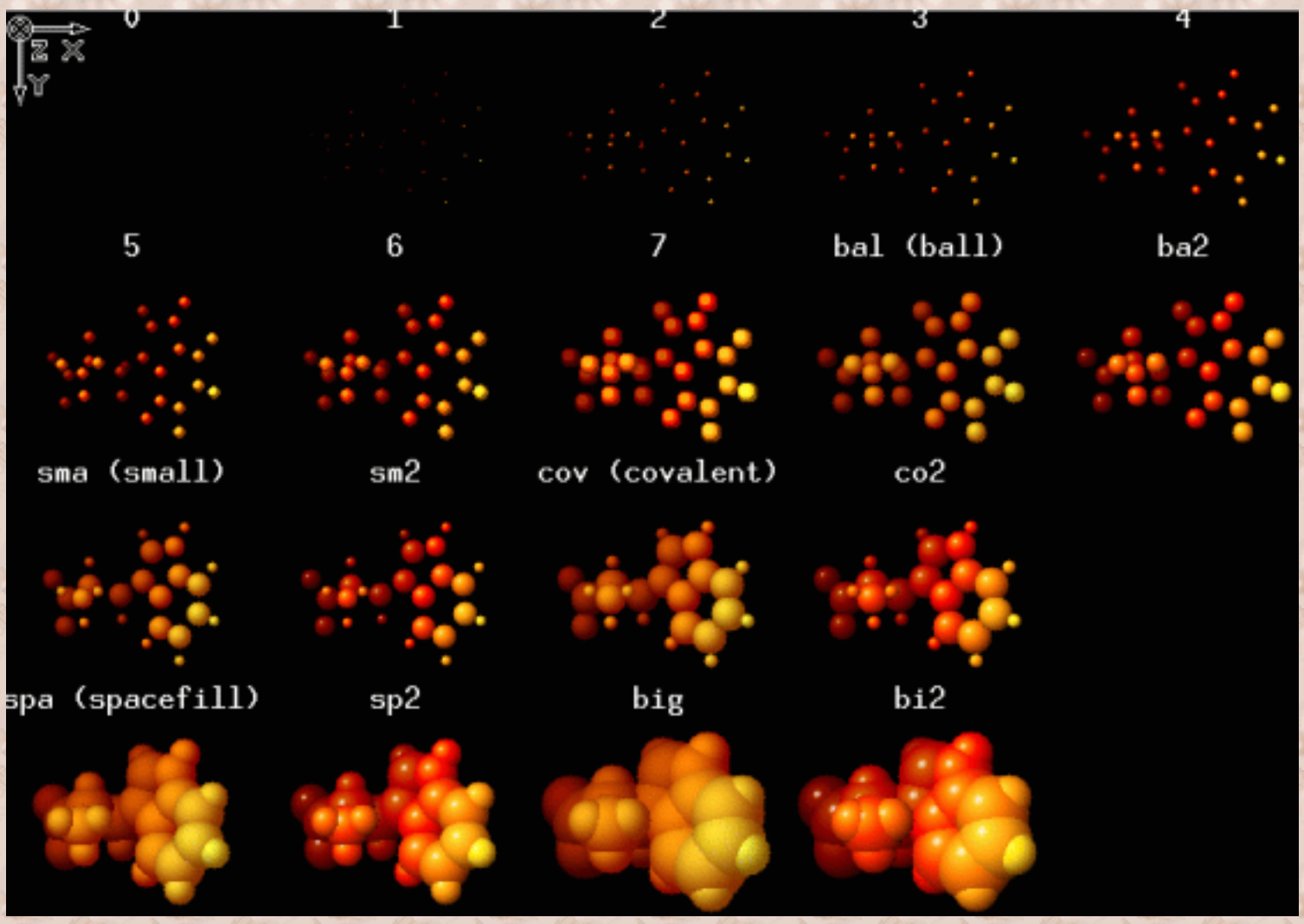
The second version of a given style has more enhanced contrast and more specular look than the first version (BA2 vs. BALL, BI2 vs. BIG etc). See the image at the bottom of this page to understand this difference.

STYLE	DESCRIPTION	SIZE
0	Unvisible atoms.	Fixed.
1	A single pixel.	Fixed.
2	3x3 cross (5 pixels).	Fixed.
3	3x3 square (9 pixels).	Fixed.
4	5x5 circle (21 pixel).	Fixed.
5	7x7 square (37 pixels).	Fixed.
6	9x9 circle (61 pixel).	Fixed.
7	11x11 circle (109 pixels).	Fixed.
bal balls	Balls (suitable to draw balls and sticks).	Proportional.
ba2	Balls with enhanced contrast.	Proportional.
sma small	Small style (default: 70% of covalent radius).	Proportional.
sm2	Small style, enhanced contrast.	Proportional.
cov covalent	Covalent style (default: covalent radius).	Proportional.
co2	Covalent style, enhanced contrast.	Proportional.

spa spacefill	Spacefill style (default: 70% of van der Waals radius).	Proportional.
sp2	Spacefill style, enhanced contrast.	Proportional.
big	Big style (default: van der Waals radius).	Proportional.
bi2	Big style, enhanced contrast.	Proportional.

EXAMPLES

The image below shows all drawing styles for atoms. To reproduce this image, execute the script atoms.script; the file trp.pdb (tryptophan) is required as input.



NOTES

(1) Unvisible atoms (style 0) are not treated as hidden - they are just invisible.

(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

(3) The ATOM keywords SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2 may be combined with the command BONDS NICE to produce very nice images. All other atomic styles (0 - 7, BALL, BA2) will not work with BONDS NICE.

RELATED COMMANDS

BON (BONDS) changes drawing style for bonds. PRO (PROBE) changes the probe radius (this probe is used to draw nice bonds).

BAC, BACKBONE

NAME
BAC, BACKBONE - draw backbone.

SYNOPSIS
BAC
BAC OFF
BAC bond_style

DESCRIPTION
Draw polypeptide (protein) backbone, by connecting neighbouring CA (C alpha) atoms. All other atoms in the selected portion of the structure will be hidden. At present, five bond styles are available, all of them fixed in size.

If this command is specified without any arguments, default bond style (5) will be used.

The command BAC OFF hides the backbone and shows atoms and bonds which were visible before.

STYLE	THICKNESS	TYPE
0	Unvisible bonds	Fixed
1	single, thin line	Fixed
2	Three lines	Fixed
3	Five lines	Fixed
4	Seven lines	Fixed
5	Nine lines	Fixed

NOTES
(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.

RELATED COMMANDS
BON (BONDS) changes drawing style for bonds, but does not affect the backbone. ATO (ATOMS) command may be used to add atoms to the backbone. It is recommended to show only CA atoms, using BALL or SPACEFILL style.

BG, BACKG, BACKGROUND

NAME

BG, BACKG, BACKGROUND - change the main window background color.

SYNOPSIS

BG color
BACKG color
BACKGROUND color

DESCRIPTION

Change the main window background color. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted.

This command does not affect the main window in the sequence comparison mode. Check the command COMPARE .

Examples:

COMMAND	DESCRIPTION
bg white	White
bg DarkSlateGray	Dark dark slate gray
bg #3000a0007000	Kind of green
bg rgb:0/0/8	Dark blue
bg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS

FG (FOREG, FOREGROUND) changes the main window foreground (text) color.

COM, COMPARE

NAME

COM, COMPARE - compare two sequences.

SYNOPSIS

COM
COM minimal_score segment_width
COM OFF
COM COR serial1 serial2
COM ZOO zoom_factor
COMPARE
COMPARE minimal_score segment_width
COMPARE OFF
COMPARE CORNER serial1 serial2
COMPARE ZOOM zoom_factor

DESCRIPTION

Compare two sequences. Garlic mantains two sequence buffers: the main sequence buffer and the reference sequence buffer. After initializing both buffers, the command COMPARE may be used to prepare the plot with comparison of these two sequences. Matching residues will be marked by dots or squares, depending on the zoom factor. Dots or squares which represent residue pairs which match exactly will be colored yellow, while residues which are different but have similar properties will be colored red. The reference sequence will be assigned to the horizontal (x) axis, while another (investigated) sequence will be assigned to the vertical (y) axis.

The plot will contain only residues which belong to the segments for which the score of matching residues is equal to or larger than minimal score. The minimal score (the number of matching pairs) and the width of the segment used for comparison may be specified by the user. Hard-coded defaults are SEGMENT_WIDTH and MINIMAL_SCORE, defined in defines.h file. The values used in the original garlic package: SEGMENT_WIDTH=5, MINIMAL_SCORE=5.

SCORING

Two sequences are compared using fixed width segments. The matrix shown below is used to identify matching residues. It was inspired by Dayhoff PAM250 matrix. However, while PAM250 matrix contains a range of values, both positive and negative, the only values used in the substitution matrix below are zero and one. One is used to identify matching residue pairs and zero for pairs which do not match.

		A	B	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	Z	X
ALA	A	1	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0
ASX	B	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	0	0	0	0	0	0	1	0
CYS	C	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	D	0	1	0	1	1	0	1	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
GLU	E	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
PHE	F	0	0	0	0	0	1	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0	0
GLY	G	1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
HIS	H	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	1	0	0	0	0	0	1	0
ILE	I	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
LYS	K	0	1	0	0	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	0
LEU	L	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
MET	M	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
ASN	N	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	0	1	0	0	0	0	1	0
PRO	P	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0
GLN	Q	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	1	0	0	0	0	0	1	0
ARG	R	0	0	0	0	0	0	0	1	0	1	0	0	0	0	1	1	0	0	0	1	0	0	0
SER	S	1	0	0	0	0	0	1	0	0	0	0	0	1	1	0	0	1	1	0	0	0	0	0
THR	T	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
VAL	V	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
TRP	W	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0
TYR	Y	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
GLX	Z	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
UNK	X	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

The scoring scheme used in garlic is much simpler than the elaborate schemes used in advanced programs for sequence alignments. However, this scheme is still quite useful and I believe that many users will like to play with the various segment widths and scores.

KEYWORDS AND PARAMETERS

All keywords and associated parameters are explained in the table below. Note that the minimal score may not exceed the segment width.

KEYWORD AND/OR PARAMETERS	DESCRIPTION
None	Draw sequence comparison, using default segment width and default minimal score.
OFF	Return to the main drawing mode. The same may be achieved by hiting the ESCAPE key.

minimal_score segment_width	Draw sequence comparison, using the specified segment width and the specified minimal score. Both parameters should be positive.
CORNER ref_offset main_offset	Draw sequence comparison, but skip some leading residues. Skip (ref_offset - 1) residues of the reference sequence and (main_offset - 1) residues of the main sequence.

MOUSE USAGE

The pointing device (mouse) may be used to find the residue serial numbers and names for matching pairs and residues which follow after them. After a chosen pair is reached with the pointer, the information about this pair and residues which follow them will be available in the output window (the bottom right corner). Color codes: yellow is used for residues which are equal, magenta for acceptable substitutions and red for mismatching residues.

HORIZ.	VERT.
23GLY	GLY27
24SER	SER28
25CYS	CYS29
26TRP	TRP30
27ALA	ALA31
28PHE	PHE32
29SER	GLY33
30ALA	ALA34
31VAL	VAL35
32VAL	GLU36
33THR	ALA37

EXAMPLES

COMMAND	DESCRIPTION
load 9PAP.pdb sel het sel com seq from 1 seq copy	Load the structure of papain, select all hetero atoms and then select the complement of this selection. The purpose of this trick is to exclude all hetero atoms from selection. Extract the sequence and copy it to the reference buffer.
load 1HUC.pdb sel a,b/*/*/* seq from 2 compare 8 10	After that, load the structure of human cathepsin B, select chains A and B (one molecules consists of two chains), extract the sequence and compare it with the content of the reference buffer. The minimal score is 8 and the segment width is 10.

load 9PAP.pdb **sel het** **sel com** **seq from 1** **seq copy** **seq load sample.fasta** **compare 6 7**	**Load the structure of papain and copy the sequence to the reference buffer using the same method as in the previous example. Read the second sequence from the specified FASTA file (one letter codes). Compare two sequences, using the specified minimal score and segment width (5/7).** **This is the typical usage of sequence comparison: compare a fresh sequence with the sequence of a solved structure.**
com zoom 4	**Change zoom factor to 4.**
com cor 100 100	**Skip the first hundred residues of both sequences.**

NOTES

(1) You don't need protein 3D structures to compare two sequences. The minimal information required for protein comparison is the primary structure, i.e. the protein sequence.

RELATED COMMANDS

The command SEQ (SEQUENCE) is used to manipulate the content of the main sequence buffer and of the reference sequence buffer. LOAD is used to load the PDB file. SELECT, ADD and RESTRICT are used for selection.

BON, BONDS

NAME

BON, BONDS - change drawing style for bonds.

SYNOPSIS

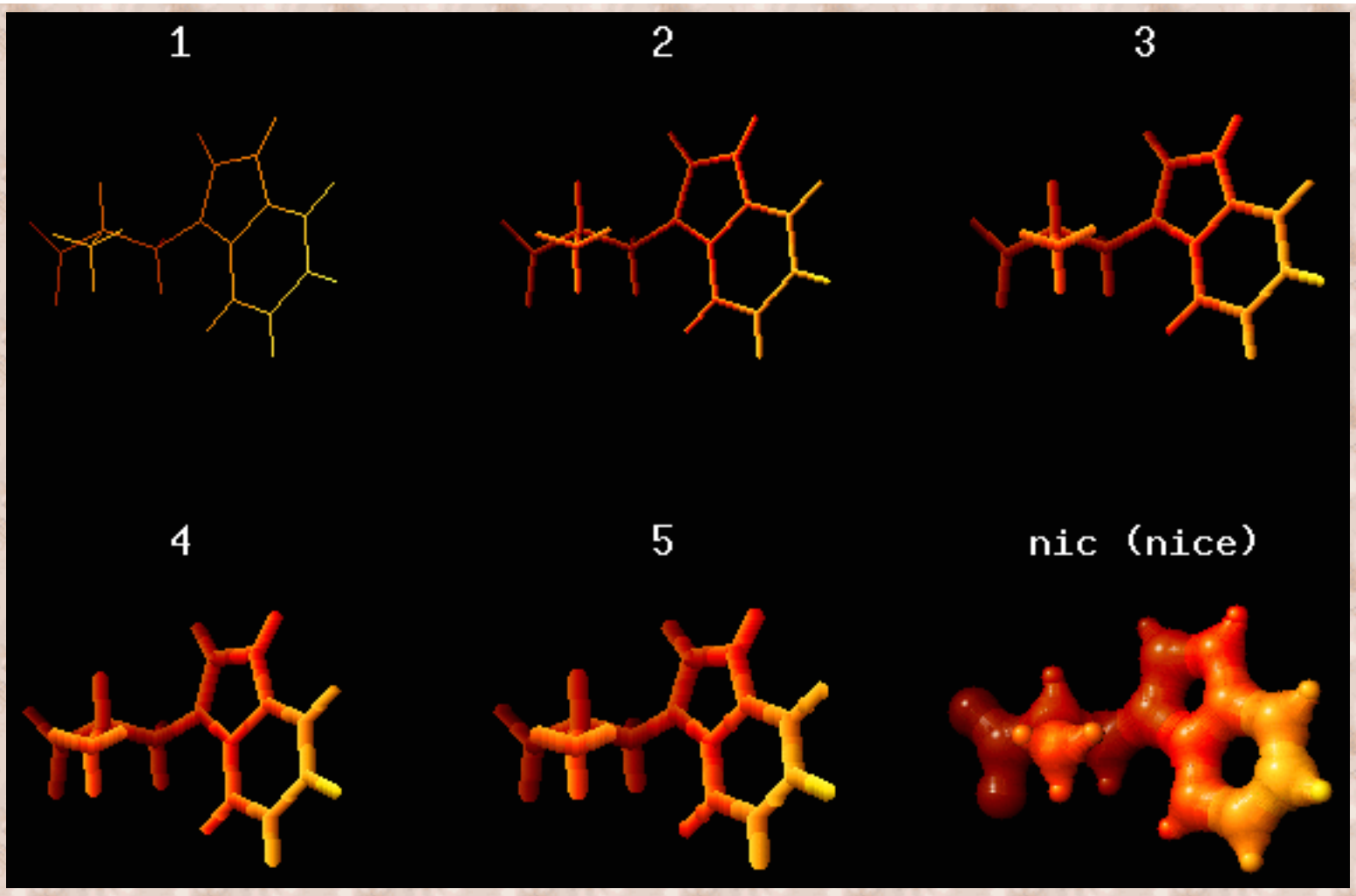
BON style
BONDS style

DESCRIPTION

Change drawing style for bonds. Bond style is defined separately from atom style. This command does not affect disulfide bonds: the command SSB should be used for that purpose. Note that there is no separate keyword for curved bonds and sticks (nice style): the bond curvature is defined by the command PROBE .

STYLE	THICKNESS	TYPE
0	Unvisible bonds.	Fixed.
1	A single line.	Fixed.
2	Three lines.	Fixed.
3	Five lines.	Fixed.
4	Seven lines.	Fixed.
5	Nine lines.	Fixed.
nic nice	Curved bonds, conical sticks or cylindrical sticks, depending both on the probe radius and the atomic radii. This bond style is available for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2. Do not combine the nice bond style with atomic styles 0, 1, 2, 3, 4, 5, 6, 7, BALL and BA2.	Proportional.

The image below shows all drawing styles for bonds. To reproduce this image, execute the script bonds.script; the file trp.pdb (tryptophan) is required as input.

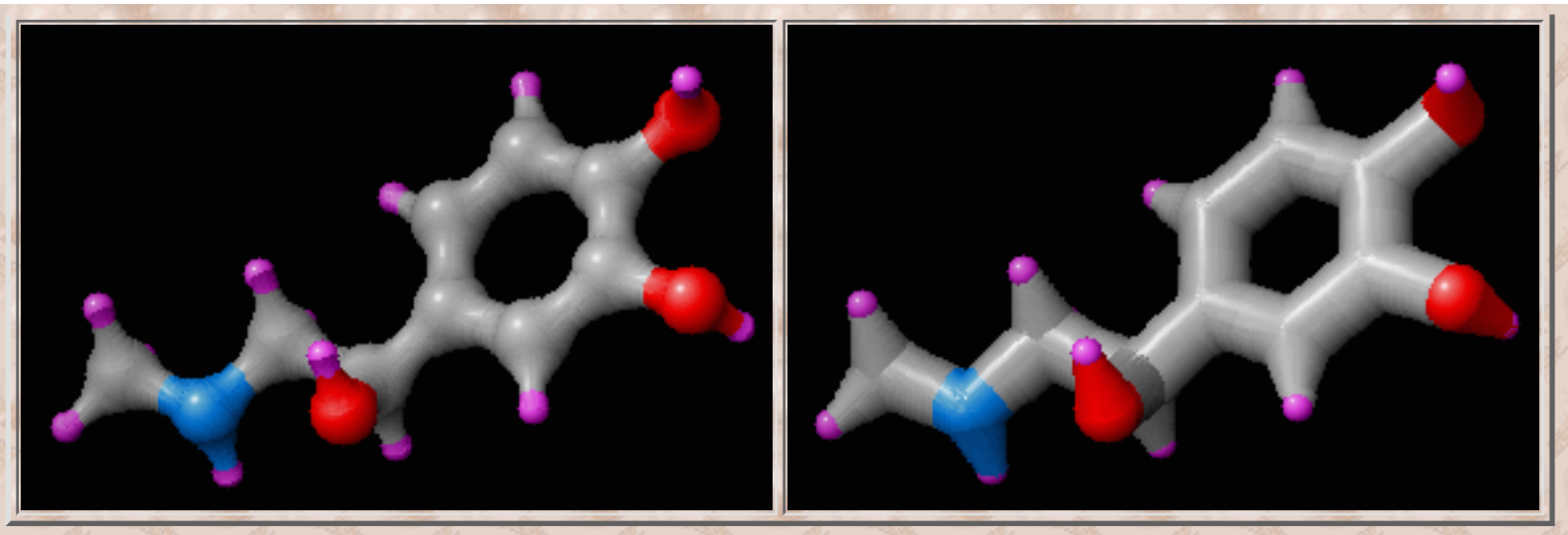


NICE BONDS

Nice bonds may be curved or straight, cylindrical or conical, depending on probe radius. If this radius is small (like 0.8 angstroms), the bonds will be curved. Probe radius of 10 angstroms will give the straight bonds. If you want to draw the chemical bonds as cylindrical sticks, use the same atomic radius for all atoms and a relatively large probe. The only way to set the same radius for all atoms is to edit the configuration file (.garlicrc). If your atoms are drawn using different radii, the bonds will appear conical. This is one of the things which make garlic different from most other programs: in garlic, sticks are just the special case of nice bonds. Most other programs are capable to draw just simple cylindrical sticks.

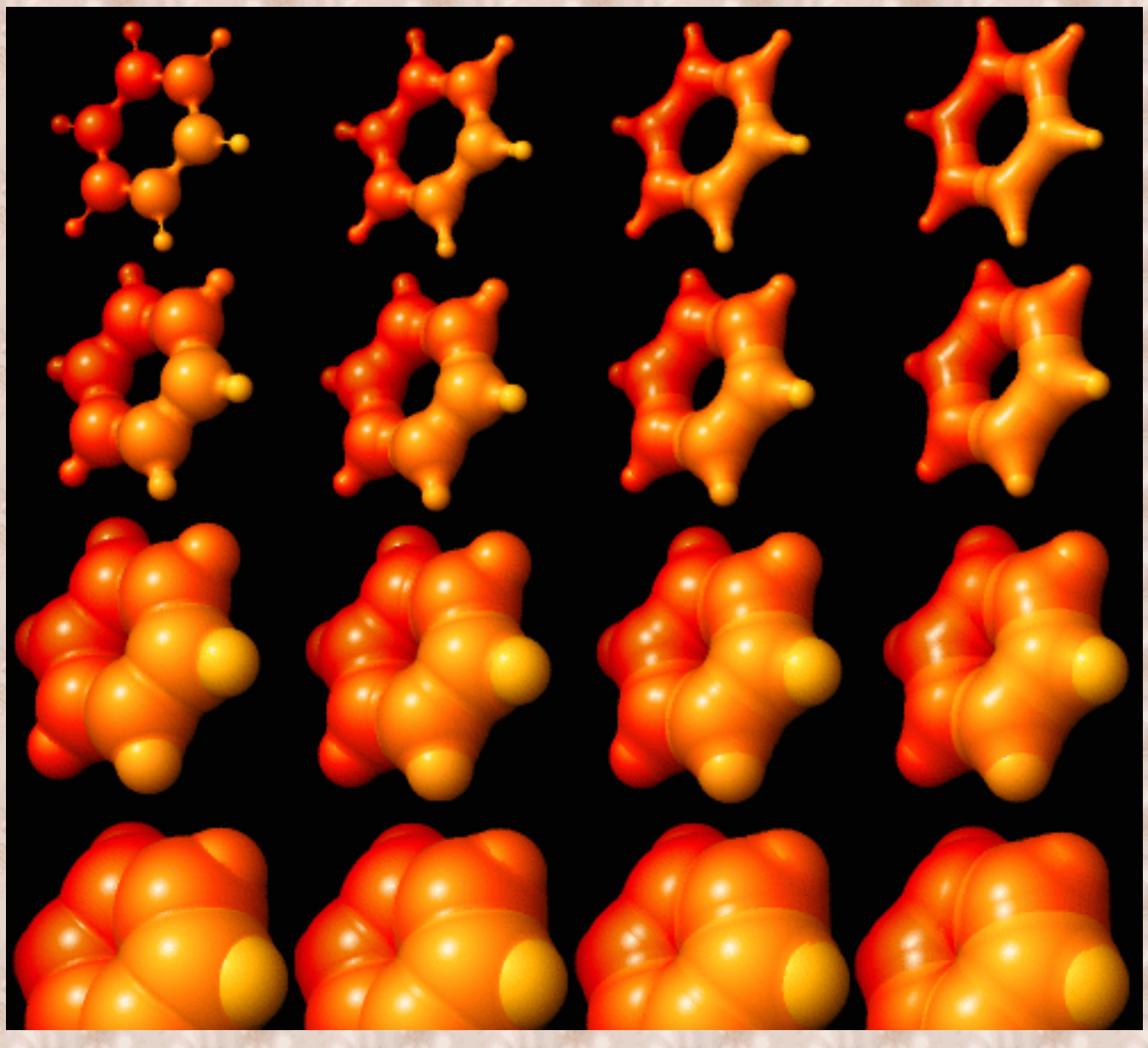
The images below shows the same structure (adrenalin) drawn using two different probes: 0.8 angstroms (curved bonds, the left image) and 10 angstroms (conical sticks, the right image). In both cases all atoms were drawn using the small atomic style with enhanced contrast (ATOMS SM2).

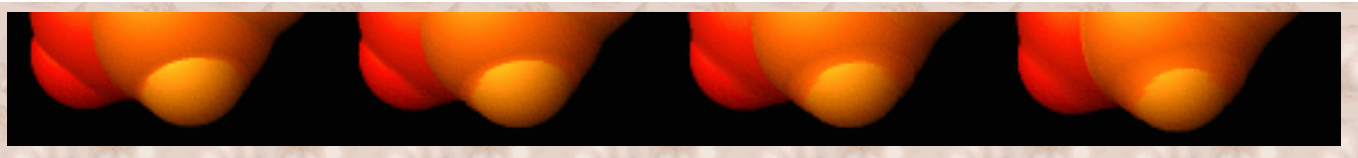
probe 0.8	probe 10



EXAMPLES

In this example, four drawing styles for atoms were combined with four different probes. The following drawing styles were used (vertical, from top to bottom): sm2, co2, sp2 and bi2. Probe radii (angstroms, from left to right): 0.25, 0.50, 1.00 and 2.00. A single benzene molecule was used to prepare this image.





NOTES

(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.

(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

(3) The nice bond style is allowed for ordinary covalent bonds and for disulfide bonds, but not for hydrogen bonds.

(4) Remember that the nice bond style works only for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2.

RELATED COMMANDS

PRO (PROBE) is used to set the probe radius. ATO (ATOMS) is used to change the drawing style for atoms. SSB is used to change the bond drawing style for disulfide bonds.

PRO, PROBE

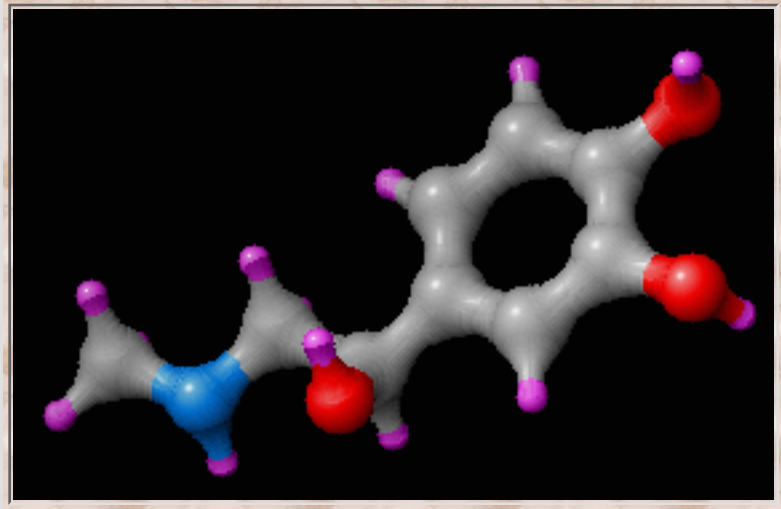
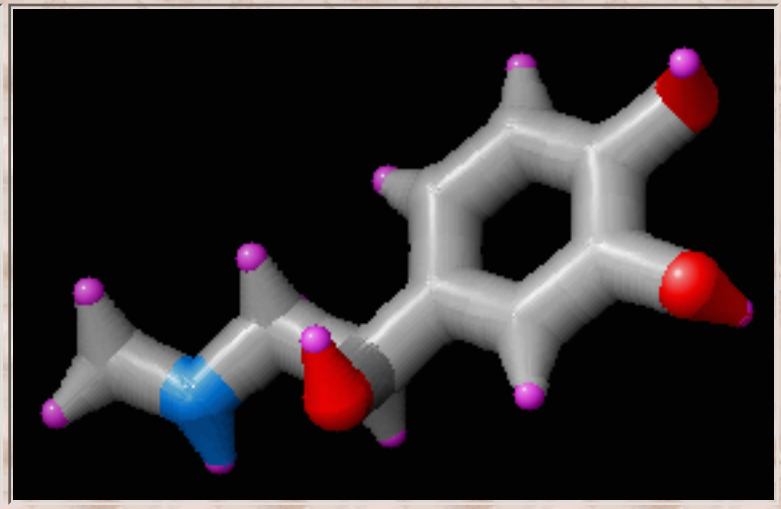
NAME
PRO, PROBE - set the probe radius.

SYNOPSIS
PRO value
PROBE value

DESCRIPTION
Set the probe radius. The probe is used to draw nice bonds (cones and sticks, curved or straight). Small probe (about 0.8 angstroms) is used to obtain curved bond shapes, while large probe (about 10 angstroms) may be used to draw cones or sticks. Be sure to read the text about the command BONDS to learn how to create nice images, playing with commands PROBE, ATOMS and BONDS. Default probe radius is 0.8 angstroms, but this may be changed in the configuration file .garlicrc .

One and only one probe radius is assigned to each loaded structure. The probe radius may be changed separately for each structure. The command PROBE affects only the structure which is currently "caught" (see the command CATCH) .

EXAMPLES
The images below show the same structure (adrenalin) drawn using two different probes: 0.8 angstroms (curved bonds, the left image) and 10 angstroms (conical sticks, the right image). In both cases all atoms were drawn using the small atomic style with enhanced contrast (ATOMS SM2). Bonds were drawn using the nice bond style (BONDS NICE).

probe 0.8	probe 10
	

RELATED COMMANDS
BONDS is used to define drawing style for bonds. SSB is used to define drawing style for disulfide bonds. ATOMS is used to define drawing style for atoms.

Garlic Configuration File - Version 1.2

.garlicrc

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains the sample configuration file for garlic. When started, garlic will try to find the configuration file called .garlicrc (or garlicrc, in one case!) in up to six directories, in the following order:

(1) in the current working directory (file .garlicrc);
(2) in user's home directory ($HOME/.garlicrc);
(3) in garlic subdirectory of user's home directory ($HOME/garlic/.garlicrc);
(4) in /etc directory (Debian GNU/Linux style, /etc/garlicrc, without dot!);
(5) in /usr/local/lib/garlic directory (file /usr/local/lib/garlic/.garlicrc);
(6) in /usr/lib/garlic directory (file /usr/lib/garlic/.garlicrc).

The recommended pathnames:

/usr/local/lib/garlic/.garlicrc (system-wide configuration file),
$HOME/.garlicrc (private configuration file).

If all attempts fail, the hard-coded defaults will be used. The configuration file .garlicrc should be included in the original garlic package. Most parameters are explained below (read the comments). Anyway, if you have some questions, send an e-mail to me:
zucic@garlic.mefos.hr

```
# Personal initialization file for garlic,
# free molecular viewer and editor.
# Version 1.2.
# Last modification: September 17, 2002.


# Geometry of the main window. Use the keyword default, or specify the
# geometry string (for example 780x560+10+10).

main window geometry: default


# Margins; used only if geometry string is not given. Geometry string may be
# given through command line arguments.

main window left margin: 50 pixels
main window right margin: 50 pixels
main window top margin: 50 pixels
main window bottom margin: 70 pixels


# Main font:

main font: 10x20
```

```
# Main window cursor. If you don't like default cursor, replace it; read
# the file /usr/include/X11/cursorfont.h ; remove the XC_ prefix to obtain
# the cursor name.

main window cursor: default


# A small coordinate system may be displayed in the top left corner (yes/no):

show coordinate system: yes


# Control window (top right corner) may be visible or hidden (yes/no):

show control window: yes


# Sequence neighborhood of the residue under
# the pointer may be visible or hidden (yes/no):

show sequence neighborhood: yes


# Stereo flag (yes/no):

display stereo image: no


# Parameters for stereo image:

stereo internal margin (screen units): 10 pixels
stereo angle: 5.0 degrees


# Light source theta and phi angle (theta is defined with respect to z axis,
# phi with respect to x axis:

light source theta angle: 150 degrees
light source phi angle:   225 degrees


# Default slab mode (possible modes are off, planar, sphere, half-sphere,
# cylinder and half-cylinder):

default slab mode: planar


# Default color fading mode (off, planar, sphere, half-sphere, cylinder and
# half-cylinder):
```

```
default color fading mode: planar


# Default drawing style for atoms (0, 1, 2, 3, 4, 5, 6 or 7):

default atom drawing style: 2


# Default drawing style for bonds (0, 1, 2, 3, 4 or 5):

default bond drawing style: 3


# Default drawing style for backbone:

default backbone drawing style: 5


# Window colors:

main window background color: black
main window foreground color: white
text background color: black
text foreground color: white


# The number of color fading surfaces:

number of color fading surfaces: 3


# Colors at given fading surface(s). The surface index is given in brackets.
# The largest surface index is (number of color fading surfaces) - 1.

left   color 0: RGB:FFFF/FFFF/4444
middle color 0: RGB:FFFF/DDDD/0000
right  color 0: RGB:8888/5555/0000

left   color 1: RGB:FFFF/8888/0000
middle color 1: RGB:FFFF/0000/0000
right  color 1: RGB:8888/0000/0000

left   color 2: RGB:8888/0000/0000
middle color 2: RGB:4444/0000/0000
right  color 2: RGB:2222/0000/0000


# Rotation steps. Normal steps is used if numeric key is pressed without
# any modifier. Large step is selected by holding [shift] while pressing
# the key, and very large step is selected by using both [alt] and [shift].
```

```
# Small step is selected by holding [control] while pressing the key, and
# very small step by using both [alt] and [control].

rotations steps: 0.2 1.0 5.0 30.0 90.0


# Five translation steps (very small, small, normal, large and very large).
# Use angstrom units.

translation steps: 0.2 1.0 5.0 25.0 100.0


# Five slab steps (very small, small, normal, large and very large).
# Use angstrom units.

slab steps: 0.2 1.0 5.0 20.0 80.0


# Five fading steps (very small, small, normal, large and very large).
# Use angstrom units.

fading steps: 0.2 1.0 5.0 20.0 80.0


# Window size limits: used only if screen width and/or height are larger
# than values specified here. By default, screen width and height are used.

maximal main window width: 3000 pixels
maximal main window height: 2500 pixels


# The nearest line (bond) thickness; used only if drawing bonds as lines
# and line thickness is used for perspective.

the nearest line thickness: 5 pixels


# Screen dimensions and position of garlic user in real world. Use realistic
# values. Do not change units (mm). Strange values may cause image distortions.

screen width in real world: 270 millimeters
screen height in real world: 195 millimeters
distance between user and screen in real world: 500 millimeters


# Scaling information: used to scale user and screen down to atomic scale.
# Only screen width is required, in angstrom units.

screen width in atomic world: 1.0 angstroms
```

```
# User z coordinate in atomic coordinate system. It must be negative
# and absolute value should be quite large. The x axis points to the right,
# y axis downward and z axis in direction opposite to observers direction.

user position in atomic coordinate system: -150.0 angstroms


# Maximal bond length is used to check which atoms and bonds are invisible.
# It is assumed that there are no atoms with radius larger than this length.

maximal bond length: 2.3 angstroms


# Crude limits for bond lengths. No distinction between N-CA and C-N is made.
# Use angstrom units. Be tolerant, there are many bad structures around.
# Generic bond length is used for atomic pairs which are not recognized.

approximate C-C bond length: from 1.3 to 1.8 angstroms
approximate C-N bond length: from 1.0 to 1.7 angstroms
approximate C-O bond length: from 1.0 to 1.5 angstroms
approximate C-S bond length: from 1.4 to 2.1 angstroms
approximate C-H bond length: from 0.8 to 1.2 angstroms
approximate N-O bond length: from 1.2 to 1.7 angstroms
approximate N-H bond length: from 0.9 to 1.3 angstroms
approximate O-H bond length: from 0.7 to 1.3 angstroms
approximate S-H bond length: from 0.9 to 1.6 angstroms
approximate O-P bond length: from 1.2 to 1.8 angstroms
approximate S-S bond length: from 1.8 to 2.3 angstroms
generic bond length:         from 0.8 to 2.0 angstroms
hydrogen bond length:        from 2.6 to 3.8 angstroms


# Hydrogen bond C-O...N angle range:

hydrogen bond C-O...N angle: from 125 to 180 degrees


# The upper limit for CA-CA distance for neighbouring residues. Used to
# draw backbone, connection neighbouring CA atoms.

maximal CA-CA distance: 4.1 angstroms


# Atomic radii, used for spacefill style. 70% of van der Waals radius may be
# a good choice.

hydrogen radius:   0.70 angstroms
carbon radius:     1.20 angstroms
nitrogen radius:   1.05 angstroms
oxygen radius:     1.00 angstroms
sulfur radius:     1.25 angstroms
```

```
phosphorus radius: 1.25 angstroms
generic radius:    1.40 angstroms


# Covalent atomic radii, used for covalent style.

hydrogen covalent radius:   0.30 angstroms
carbon covalent radius:     0.77 angstroms
nitrogen covalent radius:   0.70 angstroms
oxygen covalent radius:     0.66 angstroms
sulfur covalent radius:     1.04 angstroms
phosphorus covalent radius: 1.10 angstroms
generic covalent radius:    1.20 angstroms


# Small atomic radii. 70% of covalent radius may be a good choice.

hydrogen small radius:   0.21 angstroms
carbon small radius:     0.54 angstroms
nitrogen small radius:   0.49 angstroms
oxygen small radius:     0.46 angstroms
sulfur small radius:     0.73 angstroms
phosphorus small radius: 0.77 angstroms
generic small radius:    0.84 angstroms


# Van der Waals radii.

hydrogen van der Waals radius:   1.00 angstroms
carbon van der Waals radius:     1.70 angstroms
nitrogen van der Waals radius:   1.50 angstroms
oxygen van der Waals radius:     1.40 angstroms
sulfur van der Waals radius:     1.80 angstroms
phosphorus van der Waals radius: 1.80 angstroms
generic van der Waals radius:    2.00 angstroms


# Ball radius, used to draw balls and sticks:

ball radius: 0.45 angstroms


# Default probe radius, used to draw nice bonds with curved surfaces:

default probe radius: 0.80 angstroms


# For a given atom, the chemical bonds are identified by inspecting
# distances to the neighboring atoms. The array with atomic data should
# be scanned in forward and backward direction (with respect to the given atom)
# to find which atoms are bound to a given atom. The following parameters
```

 # define how many neighboring atoms should be checked in each direction.

number of bond candidates: 50 before and 50 after the given atom

---

CAT, CATCH

NAME

CAT, CATCH - catch the specified macromolecular complex.

SYNOPSIS

CAT identifier
CATCH identifier

DESCRIPTION

Catch the specified structure (macromolecular complex). The structure is a set of atoms read from a single file. Thus, every file is treated as a separate structure. The structure identifier is positive integer. The value zero is not used; structures are numbered 1, 2, 3, etc. When you catch a single structure, all transformations (rotations, translations etc.) are applied to this structure, leaving other structures intact. Selection (commands SELECT, ADD, RESTRICT) are also applied only to this structure. The command CATCH is used when working with more than one structure - for example, when docking an inhibitor to a substrate. When only one structure (file) is loaded, this command has no purpose. Examples:

COMMAND	DESCRIPTION
cat 1	Catch the structure number 1.
cat 7	Catch the structure number 7.

NOTES

(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure you want to catch. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
PHE 192
CE2  1433  C
t.f.: 64.06
trans
phi:-120.71
psi:  72.93
phob:  1.19
selected
x:    -3.276
y:   -18.665
z:   -13.754
```

(2) The command CATCH resets the editing mode to default (no editing).

RELATED COMMANDS

TAK (TAKE) does exactly the same job as CATCH.

CEN, CENTER

NAME
CEN, CENTER - change the origin of the internal coordinate system.

SYNOPSIS
CEN
CENTER

DESCRIPTION
An internal coordinate system is assigned to each structure. The command CEN (CENTER) redefines the position of this origin. A new origin will be equal to the geometric center position calculated for selected atoms. This may be quite useful if working with a large structure. By selecting a small portion of the structure, or even a single atom, the internal system origin may be set to a place which contains the most interesting part of the structure. Rotations, slab changes and color changes will be done with respect to new origin. This will keep the interesting part in the same part of the screen. It is recommended to hide the uninteresting part of the structure, to make rotations and other transformations faster. When you load the structure the geometric center of the whole structure is used as the internal system origin. If you displaced the origin but now you want to move it back to the original position, you should these two commands:

sel all
cen

This command is applied to the structure which is currently hangled, i.e. the one to which the command CATCH was applied last.

NOTES
(1) The command CEN (CENTER) does not move the structure to the screen center. To do this, use the command POS (POSITION).

RELATED COMMANDS
POS sets the origin of the internal system to the specified position in the main (global) coordinate system.

COL, COLOR

NAME
COL, COLOR - change the color of selected atoms and their corresponding bonds.

SYNOPSIS
COL color_scheme_name
COL left_1 middle_1 right_1 ... ... left_N, middle_N, right_N

DESCRIPTION
Change the color used to draw selected atoms and their corresponding bonds. Half of each bond belongs to one atom, while half of the same bond belongs to another atom. The easy way to specify color is to use the predefined color scheme. The powerfull (but more complicated) way to specify color is to issue detailed color specification.

COLOR USAGE
In garlic, colors are used to create 3D illusions. In most color schemes, the atoms close to the observer have bright colors, while distant atoms have dark colors. Atoms and bonds look like three-dimensional objects because one side is brighter than the other. Here are some technical details about color usage:

At least one and at most eight surfaces are assigned to each structure. These surfaces are equidistant planes, spheres or cylinders. The surface which is nearest to the observer is called "front surface", while the most distant surface is called "back surface". To each surface, three colors are assigned: left, middle and right color. In most color schemes, left color is bright and right color is dark. Atoms may be divided in three groups:

(1) Atoms which are in front of the front surface;
(2) Atoms which are behind the back surface;
(3) All other atoms, positioned in the sandwich between two surfaces.

All atoms which are in front of the front surface are drawn using the same set of three colors which assigned to front surface. Atoms behind the back surface are colored using three colors assigned to back surface. Colors for atoms laying between two surfaces are prepared by linear interpolation of colors assigned to these two surfaces. This is what I call color fading (this term was not the best choice I could make, sorry).

In a special case, when only one surface is used, color does not depend on distance.

Almost all predefined color schemes typically define two surfaces, i.e. a total of six colors. There are some exceptions: color schemes HOT and COLD use three surfaces, while MONOCHROME uses only one.

Planes, spheres and cylinders
For most proteins and other molecules, planar fading is the best choice. In this case, a set of planes, perpendicular to z axis is used. Concentric spheres may be used when working with large globular proteins, while cylinders may be used for beta-barrel proteins, like porins. The axis of concentric cylinders is parallel to y.

USING PREDEFINED COLOR SCHEMES
Twenty predefined color schemes are available:

SCHEME NAME	DESCRIPTION

RED	Red color scheme; distant atoms are dark
GREEN	Green, distant atoms are dark
BLUE	BLUE (deep sea), distant atoms are dark
YELLOW	Yellow, distant atoms are dark
CYAN	Cyan (cloudless sky), distant atoms are dark
MAGENTA	Magenta, distant atoms are dark
WHITE	Shades of gray, distant atoms almost black
YELLOW-GREEN	Somewhere between yellow and green, distant atoms dark
CYAN-GREEN	Somewhere between green and blue-green, distant atoms dark
CYAN-BLUE	Somewhere between blue and blue-green, distant atoms dark
MAGENTA-BLUE	Somewhere between blue and magenta, distant atoms are dark
MAGENTA-RED	Somewhere between red and magenta, distant atoms are dark
ORANGE	Orange, distant atoms are dark
HOT	The nearest atoms are yellow, atoms in the middle are orange and distant atoms are dark red
COLD	The nearest atoms are cyan, atoms in the middle are cyan-blue and distant atoms are dark blue
MODEL	Use different colors for different NMR models
MONOCHROME	Edge black, central region white, distance independent
CPK	Modified Corey-Pauling-Kultun color scheme, distant atoms are dark
ZEBRA	Residues with even serial number are red, odd residues cyan-blue, distant atoms are dark
CHAIN	Use color to distinguish chains; distant atoms are should be dark
HYPHOB	Assign color according to hydrophobicity; distant atoms are dark

Do not abbreviate the color scheme name! Case is not important. Some selected schemes are shown below.

DETAILED COLOR SPECIFICATION

Most users should be satisfied with predefined color schemes. Anyway, it is fairly easy to use colors which are not available through predefined schemes. To define N color planes (up to eight), you have to define 3 * N colors. The keyword OLD may be used to leave the previous value unchanged. Here are some examples:

col yellow orange red red DarkRed black	**Define two color surfaces with six colors.**
col rgb:ffff/ffff/4444 rgb:ffff/dddd/0000 DarkRed	**One color surface, three colors.**
col old old old black black black	**Leave the front colors unchanged, set all back colors to black.**

Be careful with the keyword OLD - it may be used only if the currently used color scheme has at least as many colors as a new one.

RELATED COMMANDS

FADING may be used to change the position of outer color surfaces and to switch color fading on and off.

CRE, CREATE

NAME
CRE, CREATE - create structure

SYNOPSIS
CRE
CREATE

DESCRIPTION
Create structure, using the sequence from the main sequence buffer and the secondary structure from the main secondary structure buffer. At present (version 1.2), garlic is capable to create polypeptides only. Do not use this command to create DNA or RNA structure.

Both buffers have to be initialized before issuing the command CREATE. A typical use will be to create a short peptide, which will be tryed as an inhibitor for a larger, experimentally determined structure.

The present version (garlic 2.1) will correctly interpret the secondary structure codes for alpha helix (H), 3-10 helix (G) and beta strand (E), while coil (C) and turn (T) will be treated the same way as beta strand.

TEMPLATE RESIDUES
The new structure will be created using the residues from the template file. The template file contains 20 standard residues. This file should be named residues.pdb and stored to at least one of the following directories (listed in the search order):
(1) The current working directory.
(2) $HOME/garlic (garlic subdirectory of user's home directory).
(3) /usr/local/lib/garlic (the system-wide template).

If you want to add some extra residues (like modified amino-acids) to the template file, make your own copy of the file residues.pdb and keep it either in $HOME/garlic subdirectory or in your favorite working directory. It is very easy to add residues to the template file: just copy and paste the chosen exotic residue from the PDB file where you have it to the end of garlic template file. Be sure to include hydrogen atoms! There is one more thing: be sure that your residue does not have the same residue serial number as the preceding residue. You don't have to worry about the position and the orientation of your residue.

If you don't have the file residues.pdb, click here for HTML version. It is very easy to convert this version to the plain PDB, just save it as the plain text.

EXAMPLE

seq = asp ala phe tyr trp asn str = eeeeee cre	Define a short sequence (six residues), use extended structure for all residues and create the short peptide.

NOTES
(1) The command CREATE resets the editing mode to default (no editing).

RELATED COMMANDS
Use SEQUENCE to prepare the protein sequence and STRUCTURE to prepare the secondary structure.

Garlic Template File

residues.pdb

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains the template file for garlic. This file contains the template residues, which are used as basic building blocks required to create a new polypeptide. If you don't have the template file, save this HTML file as text and remove all lines which do not contain the string ATOM at the beginning. Don't forget to check the bottom lines.

Recommended locations (listed in search order):

Special template file	residues.pdb in the current working directory
User's private template file	$HOME/garlic/residues.pdb
System-wide template file	/usr/local/lib/garlic/residues.pdb

Garlic uses only one template file. The program first looks in the current working directory, then in $HOME/garlic, and last in /usr/local/lib/garlic.

```
ATOM      1  N    ALA     1      -20.307  17.277  25.298  1.00  0.18
ATOM      2  CA   ALA     1      -20.293  16.365  24.112  1.00  0.19
ATOM      3  C    ALA     1      -18.873  16.278  23.541  1.00  0.20
ATOM      4  O    ALA     1      -18.190  17.275  23.428  1.00  0.25
ATOM      5  CB   ALA     1      -21.238  16.916  23.045  1.00  0.24
ATOM      6  H    ALA     1      -19.804  18.120  25.278  1.00  0.19
ATOM      7  HA   ALA     1      -20.622  15.383  24.409  1.00  0.18
ATOM      8  HB   ALA     1      -21.767  17.771  23.437  1.00  1.03
ATOM      9  HB   ALA     1      -20.670  17.215  22.176  1.00  1.00
ATOM     10  HB   ALA     1      -21.949  16.156  22.760  1.00  1.09
ATOM     11  N    ARG     2      -18.461  15.068  23.192  1.00  0.36
ATOM     12  CA   ARG     2      -17.108  14.831  22.625  1.00  0.36
ATOM     13  C    ARG     2      -17.200  13.824  21.484  1.00  0.30
ATOM     14  O    ARG     2      -17.868  12.814  21.598  1.00  0.30
ATOM     15  CB   ARG     2      -16.196  14.274  23.713  1.00  0.44
ATOM     16  CG   ARG     2      -15.991  15.334  24.791  1.00  0.76
ATOM     17  CD   ARG     2      -15.008  14.797  25.834  1.00  1.23
ATOM     18  NE   ARG     2      -15.444  15.244  27.185  1.00  1.90
ATOM     19  CZ   ARG     2      -14.847  14.759  28.240  1.00  2.72
ATOM     20  NH1  ARG     2      -13.673  14.207  28.102  1.00  3.38
ATOM     21  NH2  ARG     2      -15.449  14.840  29.395  1.00  3.41
ATOM     22  H    ARG     2      -19.080  14.321  23.320  1.00  0.39
ATOM     23  HA   ARG     2      -16.702  15.755  22.254  1.00  0.40
ATOM     24  HB   ARG     2      -16.648  13.394  24.149  1.00  0.54
ATOM     25  HB   ARG     2      -15.243  14.004  23.284  1.00  0.52
ATOM     26  HG   ARG     2      -15.593  16.232  24.346  1.00  1.17
ATOM     27  HG   ARG     2      -16.935  15.559  25.265  1.00  1.11
ATOM     28  HD   ARG     2      -14.990  13.717  25.799  1.00  1.78
```

ATOM	29	HD	ARG	2	-14.018	15.178	25.632	1.00	1.69
ATOM	30	HE	ARG	2	-16.171	15.891	27.280	1.00	2.34
ATOM	31	HH1	ARG	2	-13.244	14.162	27.199	1.00	3.40
ATOM	32	HH1	ARG	2	-13.202	13.832	28.898	1.00	4.14
ATOM	33	HH2	ARG	2	-16.349	15.268	29.460	1.00	3.47
ATOM	34	HH2	ARG	2	-15.007	14.474	30.213	1.00	4.18
ATOM	35	N	ASN	3	-16.516	14.122	20.389	1.00	0.23
ATOM	36	CA	ASN	3	-16.511	13.242	19.206	1.00	0.22
ATOM	37	C	ASN	3	-15.108	13.209	18.611	1.00	0.21
ATOM	38	O	ASN	3	-14.478	14.235	18.461	1.00	0.29
ATOM	39	CB	ASN	3	-17.499	13.783	18.172	1.00	0.25
ATOM	40	CG	ASN	3	-18.879	13.944	18.814	1.00	0.28
ATOM	41	OD1	ASN	3	-19.878	13.516	18.270	1.00	1.09
ATOM	42	ND2	ASN	3	-18.984	14.560	19.961	1.00	1.16
ATOM	43	H	ASN	3	-16.007	14.953	20.385	1.00	0.26
ATOM	44	HA	ASN	3	-16.802	12.256	19.501	1.00	0.22
ATOM	45	HB	ASN	3	-17.163	14.742	17.812	1.00	0.27
ATOM	46	HB	ASN	3	-17.571	13.097	17.340	1.00	0.29
ATOM	47	HD2	ASN	3	-19.865	14.666	20.382	1.00	1.18
ATOM	48	HD2	ASN	3	-18.188	14.915	20.404	1.00	1.98
ATOM	49	N	ASP	4	-14.646	12.011	18.281	1.00	0.22
ATOM	50	CA	ASP	4	-13.290	11.823	17.688	1.00	0.23
ATOM	51	C	ASP	4	-13.353	10.783	16.560	1.00	0.26
ATOM	52	O	ASP	4	-13.923	9.723	16.723	1.00	0.37
ATOM	53	CB	ASP	4	-12.317	11.360	18.770	1.00	0.24
ATOM	54	CG	ASP	4	-12.487	9.860	19.000	1.00	0.34
ATOM	55	OD1	ASP	4	-13.592	9.399	18.774	1.00	0.30
ATOM	56	OD2	ASP	4	-11.499	9.262	19.390	1.00	0.57
ATOM	57	H	ASP	4	-15.232	11.245	18.441	1.00	0.25
ATOM	58	HA	ASP	4	-12.947	12.761	17.282	1.00	0.25
ATOM	59	HB	ASP	4	-11.302	11.560	18.460	1.00	0.28
ATOM	60	HB	ASP	4	-12.519	11.886	19.691	1.00	0.29
ATOM	61	N	CYS	5	-12.755	11.118	15.426	1.00	0.19
ATOM	62	CA	CYS	5	-12.735	10.212	14.247	1.00	0.18
ATOM	63	C	CYS	5	-11.387	10.282	13.528	1.00	0.17
ATOM	64	O	CYS	5	-10.854	11.350	13.300	1.00	0.22
ATOM	65	CB	CYS	5	-13.830	10.645	13.279	1.00	0.21
ATOM	66	SG	CYS	5	-13.702	12.314	12.591	1.00	0.48
ATOM	67	H	CYS	5	-12.320	11.996	15.387	1.00	0.23
ATOM	68	HA	CYS	5	-12.923	9.205	14.564	1.00	0.20
ATOM	69	HB	CYS	5	-13.843	9.950	12.454	1.00	0.29
ATOM	70	HB	CYS	5	-14.779	10.571	13.783	1.00	0.36
ATOM	71	HG	CYS	5	-14.465	12.816	12.884	1.00	1.05
ATOM	72	N	GLN	6	-10.853	9.121	13.180	1.00	0.36
ATOM	73	CA	GLN	6	-9.537	9.034	12.469	1.00	0.44
ATOM	74	C	GLN	6	-9.597	7.976	11.351	1.00	0.45
ATOM	75	O	GLN	6	-10.108	6.893	11.547	1.00	0.58
ATOM	76	CB	GLN	6	-8.455	8.664	13.479	1.00	0.54
ATOM	77	CG	GLN	6	-7.073	8.995	12.898	1.00	0.74
ATOM	78	CD	GLN	6	-6.557	10.290	13.531	1.00	1.23
ATOM	79	OE1	GLN	6	-6.781	11.372	13.028	1.00	1.93
ATOM	80	NE2	GLN	6	-5.860	10.221	14.633	1.00	1.76

ATOM	81	H	GLN	6	-11.351	8.307	13.403	1.00	0.44
ATOM	82	HA	GLN	6	-9.303	9.992	12.038	1.00	0.52
ATOM	83	HB	GLN	6	-8.606	9.223	14.392	1.00	0.62
ATOM	84	HB	GLN	6	-8.513	7.615	13.699	1.00	0.53
ATOM	85	HG	GLN	6	-6.384	8.193	13.114	1.00	1.07
ATOM	86	HG	GLN	6	-7.145	9.127	11.830	1.00	0.95
ATOM	87	HE2	GLN	6	-5.521	11.040	15.049	1.00	2.25
ATOM	88	HE2	GLN	6	-5.674	9.349	15.042	1.00	2.11
ATOM	89	N	GLU	7	-9.064	8.328	10.190	1.00	0.29
ATOM	90	CA	GLU	7	-9.049	7.403	9.010	1.00	0.28
ATOM	91	C	GLU	7	-7.686	7.419	8.299	1.00	0.26
ATOM	92	O	GLU	7	-7.148	8.467	8.000	1.00	0.35
ATOM	93	CB	GLU	7	-10.129	7.836	8.034	1.00	0.35
ATOM	94	CG	GLU	7	-11.459	7.206	8.446	1.00	0.41
ATOM	95	CD	GLU	7	-12.574	7.746	7.549	1.00	0.87
ATOM	96	OE1	GLU	7	-12.323	8.763	6.924	1.00	1.57
ATOM	97	OE2	GLU	7	-13.617	7.109	7.538	1.00	1.56
ATOM	98	H	GLU	7	-8.674	9.224	10.127	1.00	0.32
ATOM	99	HA	GLU	7	-9.262	6.412	9.338	1.00	0.30
ATOM	100	HB	GLU	7	-10.214	8.903	8.055	1.00	0.38
ATOM	101	HB	GLU	7	-9.865	7.519	7.035	1.00	0.38
ATOM	102	HG	GLU	7	-11.405	6.132	8.340	1.00	0.61
ATOM	103	HG	GLU	7	-11.679	7.452	9.475	1.00	0.66
ATOM	104	N	GLY	8	-7.151	6.234	8.041	1.00	0.56
ATOM	105	CA	GLY	8	-5.835	6.094	7.357	1.00	0.58
ATOM	106	C	GLY	8	-5.892	4.945	6.343	1.00	0.54
ATOM	107	O	GLY	8	-6.415	3.885	6.628	1.00	0.51
ATOM	108	H	GLY	8	-7.651	5.435	8.316	1.00	0.81
ATOM	109	HA	GLY	8	-5.598	7.013	6.848	1.00	0.65
ATOM	110	HA	GLY	8	-5.077	5.885	8.095	1.00	0.56
ATOM	111	N	HIS	9	-5.343	5.186	5.162	1.00	0.28
ATOM	112	CA	HIS	9	-5.323	4.163	4.075	1.00	0.29
ATOM	113	C	HIS	9	-3.961	4.180	3.378	1.00	0.30
ATOM	114	O	HIS	9	-3.437	5.233	3.066	1.00	0.50
ATOM	115	CB	HIS	9	-6.415	4.486	3.051	1.00	0.34
ATOM	116	CG	HIS	9	-7.790	4.408	3.717	1.00	0.36
ATOM	117	ND1	HIS	9	-8.354	5.354	4.314	1.00	0.43
ATOM	118	CD2	HIS	9	-8.677	3.349	3.788	1.00	0.46
ATOM	119	CE1	HIS	9	-9.496	5.008	4.752	1.00	0.50
ATOM	120	NE2	HIS	9	-9.788	3.742	4.463	1.00	0.50
ATOM	121	H	HIS	9	-4.942	6.069	5.014	1.00	0.33
ATOM	122	HA	HIS	9	-5.501	3.186	4.494	1.00	0.30
ATOM	123	HB	HIS	9	-6.264	5.483	2.663	1.00	0.36
ATOM	124	HB	HIS	9	-6.371	3.778	2.237	1.00	0.41
ATOM	125	HD1	HIS	9	-7.966	6.246	4.430	1.00	0.51
ATOM	126	HD2	HIS	9	-8.513	2.366	3.373	1.00	0.57
ATOM	127	HE1	HIS	9	-10.157	5.667	5.297	1.00	0.62
ATOM	128	N	ILE	10	-3.412	2.996	3.147	1.00	0.20
ATOM	129	CA	ILE	10	-2.084	2.856	2.475	1.00	0.22
ATOM	130	C	ILE	10	-2.133	1.649	1.498	1.00	0.19
ATOM	131	O	ILE	10	-2.638	0.603	1.845	1.00	0.19
ATOM	132	CB	ILE	10	-1.018	2.598	3.544	1.00	0.28

ATOM	133	CG1	ILE	10	-0.940	3.822	4.469	1.00	0.30
ATOM	134	CG2	ILE	10	0.340	2.380	2.864	1.00	0.36
ATOM	135	CD1	ILE	10	0.029	3.539	5.629	1.00	1.04
ATOM	136	H	ILE	10	-3.906	2.196	3.434	1.00	0.26
ATOM	137	HA	ILE	10	-1.841	3.758	1.955	1.00	0.22
ATOM	138	HB	ILE	10	-1.282	1.724	4.112	1.00	0.32
ATOM	139	HG1	ILE	10	-0.589	4.677	3.909	1.00	0.80
ATOM	140	HG1	ILE	10	-1.920	4.039	4.864	1.00	0.74
ATOM	141	HG2	ILE	10	0.263	2.610	1.812	1.00	0.89
ATOM	142	HG2	ILE	10	1.082	3.022	3.313	1.00	0.97
ATOM	143	HG2	ILE	10	0.644	1.352	2.980	1.00	1.01
ATOM	144	HD1	ILE	10	0.183	2.476	5.731	1.00	1.68
ATOM	145	HD1	ILE	10	0.977	4.018	5.436	1.00	1.64
ATOM	146	HD1	ILE	10	-0.382	3.927	6.549	1.00	1.58
ATOM	147	N	LEU	11	-1.600	1.848	0.301	1.00	0.27
ATOM	148	CA	LEU	11	-1.575	0.787	-0.735	1.00	0.30
ATOM	149	C	LEU	11	-0.233	0.783	-1.459	1.00	0.24
ATOM	150	O	LEU	11	0.238	1.809	-1.905	1.00	0.24
ATOM	151	CB	LEU	11	-2.698	1.086	-1.726	1.00	0.39
ATOM	152	CG	LEU	11	-3.390	-0.197	-2.223	1.00	0.46
ATOM	153	CD1	LEU	11	-4.099	-0.917	-1.040	1.00	1.23
ATOM	154	CD2	LEU	11	-4.415	0.243	-3.301	1.00	1.19
ATOM	155	H	LEU	11	-1.216	2.733	0.120	1.00	0.31
ATOM	156	HA	LEU	11	-1.737	-0.165	-0.277	1.00	0.33
ATOM	157	HB	LEU	11	-3.430	1.722	-1.245	1.00	0.53
ATOM	158	HB	LEU	11	-2.289	1.611	-2.571	1.00	0.41
ATOM	159	HG	LEU	11	-2.660	-0.865	-2.671	1.00	0.73
ATOM	160	HD1	LEU	11	-4.377	-0.194	-0.287	1.00	1.69
ATOM	161	HD1	LEU	11	-4.981	-1.432	-1.378	1.00	1.82
ATOM	162	HD1	LEU	11	-3.429	-1.642	-0.603	1.00	1.73
ATOM	163	HD2	LEU	11	-4.595	1.304	-3.213	1.00	1.64
ATOM	164	HD2	LEU	11	-4.012	0.040	-4.277	1.00	1.87
ATOM	165	HD2	LEU	11	-5.348	-0.275	-3.188	1.00	1.68
ATOM	166	N	LYS	12	0.367	-0.394	-1.564	1.00	0.32
ATOM	167	CA	LYS	12	1.689	-0.552	-2.249	1.00	0.29
ATOM	168	C	LYS	12	1.677	-1.816	-3.107	1.00	0.25
ATOM	169	O	LYS	12	1.277	-2.870	-2.658	1.00	0.31
ATOM	170	CB	LYS	12	2.797	-0.640	-1.216	1.00	0.30
ATOM	171	CG	LYS	12	2.708	0.582	-0.296	1.00	0.47
ATOM	172	CD	LYS	12	3.897	0.594	0.672	1.00	0.53
ATOM	173	CE	LYS	12	3.927	-0.710	1.470	1.00	0.73
ATOM	174	NZ	LYS	12	4.644	-0.514	2.761	1.00	1.37
ATOM	175	H	LYS	12	-0.089	-1.166	-1.174	1.00	0.48
ATOM	176	HA	LYS	12	1.862	0.302	-2.883	1.00	0.31
ATOM	177	HB	LYS	12	2.681	-1.544	-0.648	1.00	0.37
ATOM	178	HB	LYS	12	3.755	-0.654	-1.711	1.00	0.35
ATOM	179	HG	LYS	12	2.722	1.481	-0.893	1.00	0.73
ATOM	180	HG	LYS	12	1.789	0.548	0.259	1.00	0.64
ATOM	181	HD	LYS	12	4.815	0.701	0.117	1.00	1.09
ATOM	182	HD	LYS	12	3.798	1.427	1.352	1.00	1.00
ATOM	183	HE	LYS	12	2.918	-1.036	1.670	1.00	1.30
ATOM	184	HE	LYS	12	4.437	-1.473	0.898	1.00	1.42

ATOM	185	HZ	LYS	12	4.882	0.493	2.876	1.00	1.79
ATOM	186	HZ	LYS	12	4.031	-0.815	3.547	1.00	1.83
ATOM	187	HZ	LYS	12	5.514	-1.079	2.765	1.00	2.00
ATOM	188	N	MET	13	2.125	-1.681	-4.347	1.00	0.26
ATOM	189	CA	MET	13	2.172	-2.830	-5.301	1.00	0.28
ATOM	190	C	MET	13	3.485	-2.804	-6.097	1.00	0.30
ATOM	191	O	MET	13	3.901	-1.774	-6.591	1.00	0.37
ATOM	192	CB	MET	13	0.978	-2.757	-6.255	1.00	0.35
ATOM	193	CG	MET	13	0.987	-1.419	-6.993	1.00	1.15
ATOM	194	SD	MET	13	1.240	-1.464	-8.785	1.00	2.09
ATOM	195	CE	MET	13	0.185	-0.054	-9.200	1.00	2.25
ATOM	196	H	MET	13	2.429	-0.788	-4.624	1.00	0.28
ATOM	197	HA	MET	13	2.121	-3.749	-4.747	1.00	0.28
ATOM	198	HB	MET	13	1.038	-3.564	-6.970	1.00	0.94
ATOM	199	HB	MET	13	0.061	-2.853	-5.692	1.00	0.92
ATOM	200	HG	MET	13	0.043	-0.929	-6.809	1.00	1.89
ATOM	201	HG	MET	13	1.765	-0.802	-6.569	1.00	1.80
ATOM	202	HE	MET	13	1.045	0.456	-8.787	1.00	2.50
ATOM	203	HE	MET	13	0.330	0.718	-9.941	1.00	2.60
ATOM	204	HE	MET	13	0.101	-0.633	-10.106	1.00	2.53
ATOM	205	N	PHE	14	4.121	-3.961	-6.207	1.00	0.19
ATOM	206	CA	PHE	14	5.407	-4.089	-6.950	1.00	0.20
ATOM	207	C	PHE	14	5.422	-5.373	-7.776	1.00	0.21
ATOM	208	O	PHE	14	4.987	-6.413	-7.322	1.00	0.35
ATOM	209	CB	PHE	14	6.569	-4.128	-5.957	1.00	0.22
ATOM	210	CG	PHE	14	6.335	-3.110	-4.845	1.00	0.20
ATOM	211	CD1	PHE	14	5.580	-3.441	-3.732	1.00	0.18
ATOM	212	CD2	PHE	14	6.878	-1.848	-4.937	1.00	0.23
ATOM	213	CE1	PHE	14	5.371	-2.516	-2.732	1.00	0.17
ATOM	214	CE2	PHE	14	6.668	-0.922	-3.937	1.00	0.22
ATOM	215	CZ	PHE	14	5.916	-1.255	-2.835	1.00	0.18
ATOM	216	H	PHE	14	3.718	-4.745	-5.779	1.00	0.25
ATOM	217	HA	PHE	14	5.527	-3.242	-7.606	1.00	0.21
ATOM	218	HB	PHE	14	6.646	-5.107	-5.524	1.00	0.24
ATOM	219	HB	PHE	14	7.493	-3.890	-6.465	1.00	0.26
ATOM	220	HD1	PHE	14	5.159	-4.431	-3.641	1.00	0.19
ATOM	221	HD2	PHE	14	7.479	-1.590	-5.792	1.00	0.27
ATOM	222	HE1	PHE	14	4.783	-2.782	-1.868	1.00	0.18
ATOM	223	HE2	PHE	14	7.096	0.067	-4.018	1.00	0.26
ATOM	224	HZ	PHE	14	5.753	-0.532	-2.052	1.00	0.19
ATOM	225	N	PRO	15	5.933	-5.274	-8.995	1.00	1.08
ATOM	226	CA	PRO	15	6.013	-6.426	-9.902	1.00	1.04
ATOM	227	C	PRO	15	7.369	-6.432	-10.606	1.00	0.87
ATOM	228	O	PRO	15	7.811	-5.433	-11.141	1.00	1.05
ATOM	229	CB	PRO	15	4.874	-6.214	-10.911	1.00	1.27
ATOM	230	CG	PRO	15	4.304	-4.781	-10.660	1.00	1.32
ATOM	231	CD	PRO	15	5.070	-4.187	-9.461	1.00	1.26
ATOM	232	HA	PRO	15	5.866	-7.336	-9.362	1.00	1.16
ATOM	233	HB	PRO	15	5.246	-6.289	-11.920	1.00	1.35
ATOM	234	HB	PRO	15	4.101	-6.951	-10.754	1.00	1.44
ATOM	235	HG	PRO	15	4.452	-4.166	-11.535	1.00	1.40
ATOM	236	HG	PRO	15	3.251	-4.839	-10.433	1.00	1.46

ATOM	237	HD	PRO	15	5.672	-3.346	-9.780	1.00	1.32
ATOM	238	HD	PRO	15	4.391	-3.889	-8.685	1.00	1.45
ATOM	239	N	SER	16	8.025	-7.583	-10.595	1.00	0.29
ATOM	240	CA	SER	16	9.351	-7.738	-11.238	1.00	0.25
ATOM	241	C	SER	16	9.398	-9.094	-11.925	1.00	0.26
ATOM	242	O	SER	16	8.952	-10.084	-11.375	1.00	0.35
ATOM	243	CB	SER	16	10.444	-7.648	-10.188	1.00	0.27
ATOM	244	OG	SER	16	9.952	-6.700	-9.252	1.00	0.40
ATOM	245	H	SER	16	7.599	-8.341	-10.141	1.00	0.33
ATOM	246	HA	SER	16	9.488	-6.965	-11.965	1.00	0.24
ATOM	247	HB	SER	16	10.589	-8.595	-9.717	1.00	0.39
ATOM	248	HB	SER	16	11.367	-7.297	-10.625	1.00	0.35
ATOM	249	HG	SER	16	9.508	-6.002	-9.741	1.00	0.91
ATOM	250	N	THR	17	9.946	-9.116	-13.132	1.00	0.19
ATOM	251	CA	THR	17	10.061	-10.373	-13.925	1.00	0.18
ATOM	252	C	THR	17	11.385	-10.357	-14.678	1.00	0.17
ATOM	253	O	THR	17	11.715	-9.370	-15.313	1.00	0.29
ATOM	254	CB	THR	17	8.903	-10.454	-14.925	1.00	0.20
ATOM	255	OG1	THR	17	8.956	-9.225	-15.643	1.00	0.28
ATOM	256	CG2	THR	17	7.548	-10.450	-14.220	1.00	0.31
ATOM	257	H	THR	17	10.280	-8.267	-13.498	1.00	0.23
ATOM	258	HA	THR	17	10.030	-11.227	-13.265	1.00	0.19
ATOM	259	HB	THR	17	8.997	-11.297	-15.585	1.00	0.28
ATOM	260	HG1	THR	17	8.383	-8.597	-15.200	1.00	0.90
ATOM	261	HG2	THR	17	7.694	-10.468	-13.151	1.00	1.06
ATOM	262	HG2	THR	17	7.002	-9.558	-14.491	1.00	1.00
ATOM	263	HG2	THR	17	6.981	-11.319	-14.517	1.00	1.09
ATOM	264	N	TRP	18	12.117	-11.458	-14.590	1.00	0.22
ATOM	265	CA	TRP	18	13.442	-11.587	-15.278	1.00	0.20
ATOM	266	C	TRP	18	13.562	-12.996	-15.852	1.00	0.19
ATOM	267	O	TRP	18	13.196	-13.958	-15.204	1.00	0.22
ATOM	268	CB	TRP	18	14.571	-11.352	-14.277	1.00	0.19
ATOM	269	CG	TRP	18	14.582	-9.877	-13.861	1.00	0.23
ATOM	270	CD1	TRP	18	13.809	-9.376	-12.906	1.00	0.27
ATOM	271	CD2	TRP	18	15.346	-8.932	-14.394	1.00	0.25
ATOM	272	NE1	TRP	18	14.132	-8.075	-12.880	1.00	0.30
ATOM	273	CE2	TRP	18	15.096	-7.710	-13.787	1.00	0.29
ATOM	274	CE3	TRP	18	16.298	-9.007	-15.404	1.00	0.27
ATOM	275	CZ2	TRP	18	15.785	-6.583	-14.183	1.00	0.33
ATOM	276	CZ3	TRP	18	16.983	-7.874	-15.795	1.00	0.32
ATOM	277	CH2	TRP	18	16.726	-6.665	-15.186	1.00	0.35
ATOM	278	H	TRP	18	11.763	-12.202	-14.052	1.00	0.23
ATOM	279	HA	TRP	18	13.512	-10.868	-16.075	1.00	0.21
ATOM	280	HB	TRP	18	14.418	-11.963	-13.407	1.00	0.20
ATOM	281	HB	TRP	18	15.515	-11.613	-14.724	1.00	0.18
ATOM	282	HD1	TRP	18	13.087	-9.894	-12.294	1.00	0.29
ATOM	283	HE1	TRP	18	13.720	-7.439	-12.260	1.00	0.33
ATOM	284	HE3	TRP	18	16.506	-9.945	-15.887	1.00	0.25
ATOM	285	HZ2	TRP	18	15.584	-5.634	-13.708	1.00	0.36
ATOM	286	HZ3	TRP	18	17.723	-7.937	-16.576	1.00	0.35
ATOM	287	HH2	TRP	18	17.264	-5.781	-15.494	1.00	0.39
ATOM	288	N	TYR	19	14.078	-13.086	-17.069	1.00	0.41

ATOM	289	CA	TYR	19	14.257	-14.399	-17.759	1.00	0.33
ATOM	290	C	TYR	19	15.607	-14.436	-18.483	1.00	0.30
ATOM	291	O	TYR	19	15.983	-13.486	-19.139	1.00	0.32
ATOM	292	CB	TYR	19	13.133	-14.581	-18.781	1.00	0.36
ATOM	293	CG	TYR	19	11.787	-14.282	-18.118	1.00	0.38
ATOM	294	CD1	TYR	19	11.205	-15.200	-17.268	1.00	0.34
ATOM	295	CD2	TYR	19	11.135	-13.089	-18.359	1.00	0.47
ATOM	296	CE1	TYR	19	9.991	-14.931	-16.671	1.00	0.39
ATOM	297	CE2	TYR	19	9.922	-12.821	-17.761	1.00	0.51
ATOM	298	CZ	TYR	19	9.340	-13.739	-16.912	1.00	0.46
ATOM	299	OH	TYR	19	8.125	-13.470	-16.313	1.00	0.53
ATOM	300	H	TYR	19	14.344	-12.258	-17.512	1.00	0.45
ATOM	301	HA	TYR	19	14.215	-15.196	-17.040	1.00	0.33
ATOM	302	HB	TYR	19	13.280	-13.902	-19.610	1.00	0.43
ATOM	303	HB	TYR	19	13.133	-15.597	-19.148	1.00	0.36
ATOM	304	HD1	TYR	19	11.704	-16.139	-17.071	1.00	0.32
ATOM	305	HD2	TYR	19	11.580	-12.360	-19.021	1.00	0.54
ATOM	306	HE1	TYR	19	9.547	-15.660	-16.009	1.00	0.40
ATOM	307	HE2	TYR	19	9.423	-11.882	-17.958	1.00	0.60
ATOM	308	HH	TYR	19	7.495	-14.131	-16.609	1.00	1.09
ATOM	309	N	VAL	20	16.310	-15.550	-18.343	1.00	0.68
ATOM	310	CA	VAL	20	17.638	-15.729	-18.987	1.00	0.51
ATOM	311	C	VAL	20	17.763	-17.141	-19.547	1.00	0.46
ATOM	312	O	VAL	20	17.421	-18.106	-18.892	1.00	0.60
ATOM	313	CB	VAL	20	18.726	-15.508	-17.933	1.00	0.46
ATOM	314	CG1	VAL	20	19.513	-14.248	-18.276	1.00	1.11
ATOM	315	CG2	VAL	20	18.076	-15.336	-16.557	1.00	1.12
ATOM	316	H	VAL	20	15.933	-16.265	-17.799	1.00	0.81
ATOM	317	HA	VAL	20	17.760	-15.015	-19.781	1.00	0.57
ATOM	318	HB	VAL	20	19.388	-16.354	-17.912	1.00	0.67
ATOM	319	HG1	VAL	20	19.937	-14.338	-19.265	1.00	1.78
ATOM	320	HG1	VAL	20	18.857	-13.392	-18.246	1.00	1.49
ATOM	321	HG1	VAL	20	20.309	-14.115	-17.559	1.00	1.64
ATOM	322	HG2	VAL	20	17.459	-16.195	-16.333	1.00	1.59
ATOM	323	HG2	VAL	20	18.844	-15.246	-15.801	1.00	1.61
ATOM	324	HG2	VAL	20	17.465	-14.446	-16.548	1.00	1.71

DIS, DISCARD

NAME

DIS, DISCARD - discard the specified structure.

SYNOPSIS

DIS identifier
DIS ALL
DIS *
DISCARD identifier
DISCARD ALL
DISCARD *

DESCRIPTION

Discard the specified structure (macromolecular complex). The memory used to store the structure is freed. If keyword ALL is used (or asterisk, *), all structures will be discarded. Examples:

COMMAND	DESCRIPTION
dis 1	Discard the structure number 1.
dis 7	Discard the structure number 7.
dis *	Discard all. Nothing will be loaded after this command.

NOTES

(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure which should be discarded. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
PHE 192
CE2  1433  C
t.f.: 64.06
trans
phi:-120.71
psi:  72.93
phob:  1.19
selected
x:    -3.276
y:   -18.665
z:   -13.754
```

(2) If you discard everything, the indexing will be reset too. The first structure you load after discarding everything will be assigned index "1" (one).

(3) The command DISCARD resets the editing mode to default (no editing).

RELATED COMMANDS

LOAD (READ) loads the specified file.

DOC, DOCK

NAME
DOC, DOCK - prepare two structures for docking.

SYNOPSIS
DOC identifier_1 identifier_2
DOC OFF
DOCK identifier_1 identifier_2
DOCK OFF

DESCRIPTION
The command DOCK prepares two structures for docking. Before executing this command, two molecules (structures) have to be loaded. For each structure a region on the surface should be selected as a candidate region for interaction with another molecule. For example, if the first molecule is the substrate, the active site has to be identified as the region where the inhibitor should be placed. Assuming that another molecule is the inhibitor, the side which is expected to interact with the substrate should be identified.

When both molecules are ready for docking, the command DOCK should be executed. The identifiers of both molecules have to be issued as arguments. Both molecules will be translated and rotated to position and orientation suitable for docking. The first molecule will be moved to the bottom of the main window, with the selected region visible on the upper side. The second molecule will be placed atop the first molecule, with the selected region facing the first molecule.

Further, a special docking window will be opened, showing the orthogonal projections of polar side chains as symbols. The polar side chains of both molecules are projected to the plane associated with the first molecule. Cyan symbols belong to the bottom molecule (the first one) and red symbols belong to the top molecule. Hydrogen bond donors are shown as crosses, acceptors as circles, and side chains which are both hydrogen bond donors and acceptors are shown as crosses in circles.

The user might be able to combine two structures, using the information visible in both the main garlic window and in docking window. However, this routine is still quite naive, so don't expect too much. Docking is not an easy game. I hope that this command will be useful at least for educational purpose.

KEYWORDS
The keyword OFF is the only keyword which may be used with the command DOCK. DOCK OFF is used to hide docking window.

KEYWORD	DESCRIPTION
OFF	Hide docking window.

PARAMETERS
Except when used in combination with the keyword OFF, the command DOCK should be followed by two structure identifiers. If you have forgotten these numbers, just move the mouse pointer over the structure(s) and find the identifier(s) in the output window (the bottom right corner). The order is important: the first molecule will be placed to the bottom of the main window, while the second will be placed atop the first one.

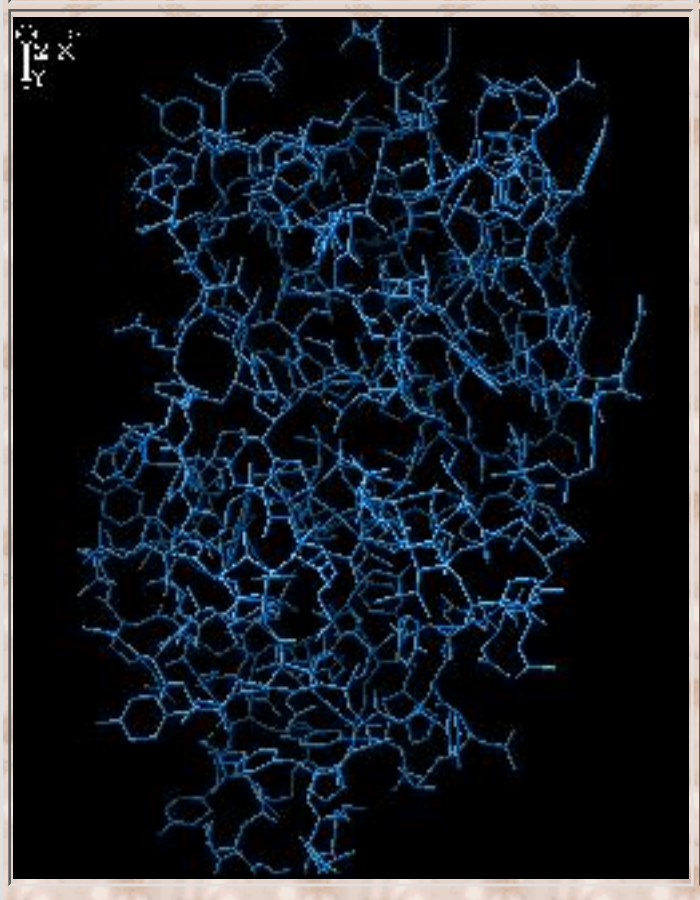
PARAMETER	DESCRIPTION

identifier_1	Identifier of the first molecule. (substrate, for example).
identifier_2	Identifier of the second molecule. (inhibitor, for example).

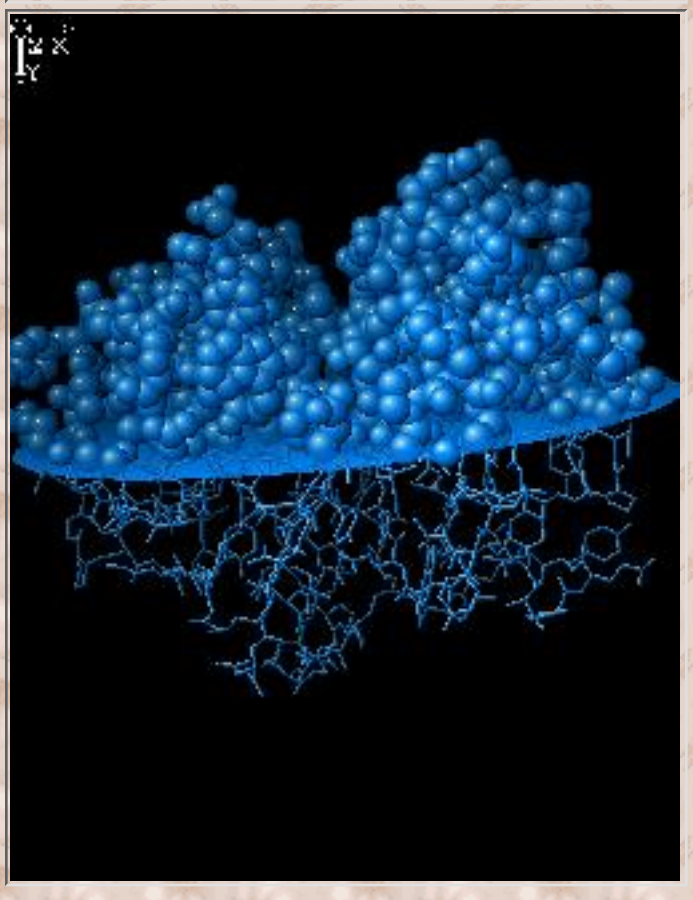
EXAMPLE

The example below shows how to prepare two structures for docking. In this example, the first structure is papain (reference 1) and the second structure is stefin (reference 2). The structure of the complex is known (PDB code 1STF).

STEP1:
Load the first structure:
load file1.pdb
Change the color. Cyan-blue might be a good choice:
color cyan-blue

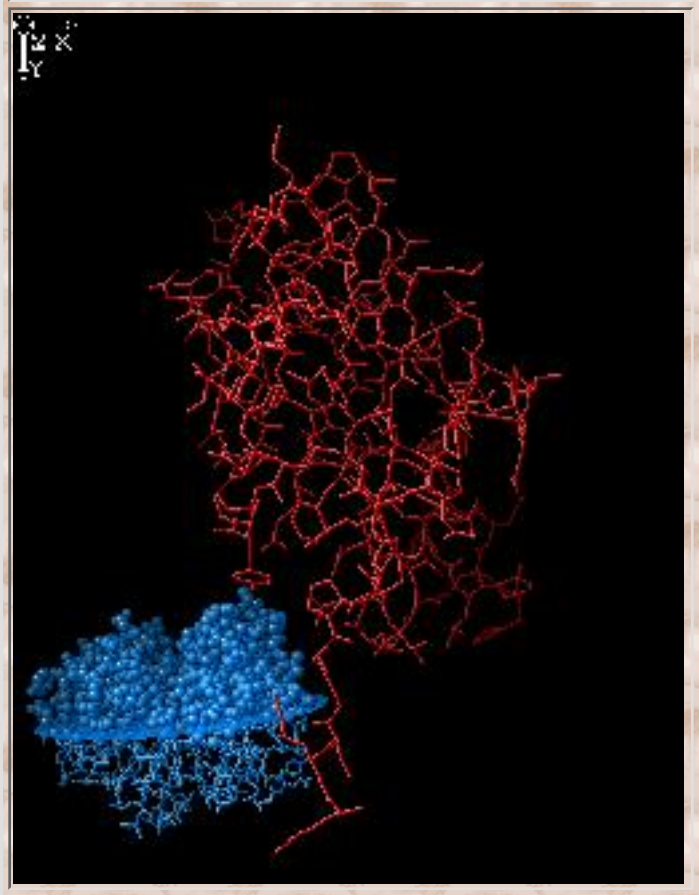


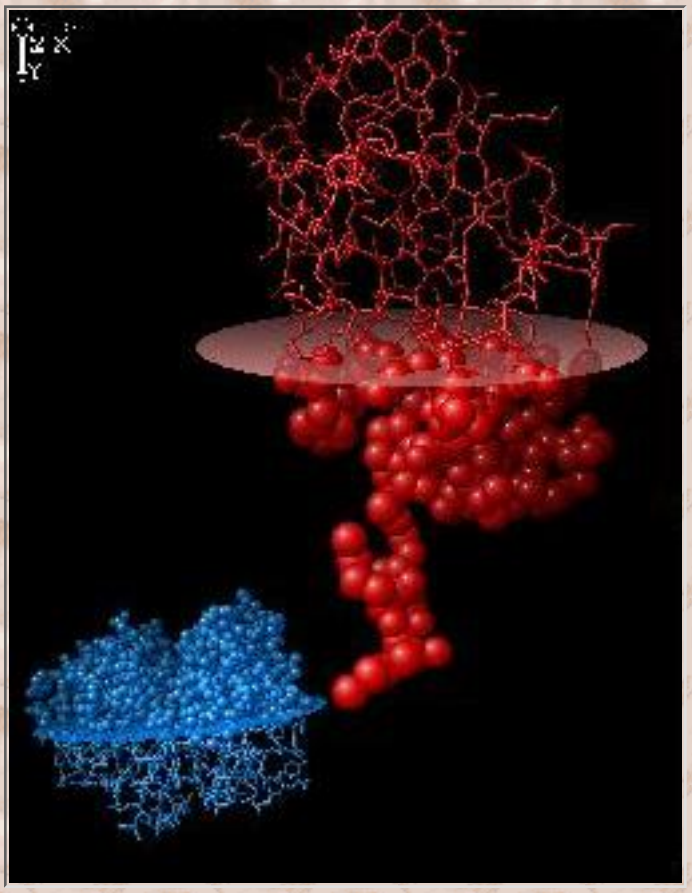
STEP 2:
Make the plane visible:
plane
Prepare to move the plane:
move plane
Use plane to divide structure in two parts.
The active site should be above the plane.
Change drawing style for atoms or bonds.
Here the spacefill style is used. This is bad idea if using slow machine.
sel above
atom sp2
Reset movement controls:
move all



STEP 3:
Push the first structure to the corner.
Load the second structure:
load file2.pdb
Change color. Red is recommended here:
color red

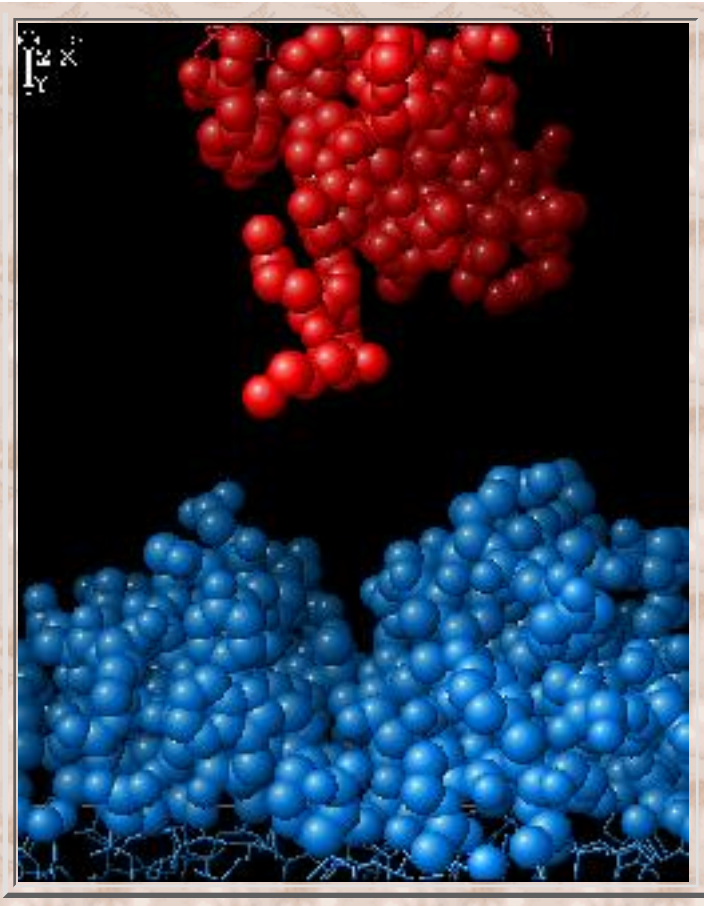
STEP 4:
Make the plane visible and divide the second structure in two parts. Change drawing style for atoms or bonds.
plane
move plane
(... now rotate and translate the plane)
sel above
atom sp2
Reset movement controls:
move all

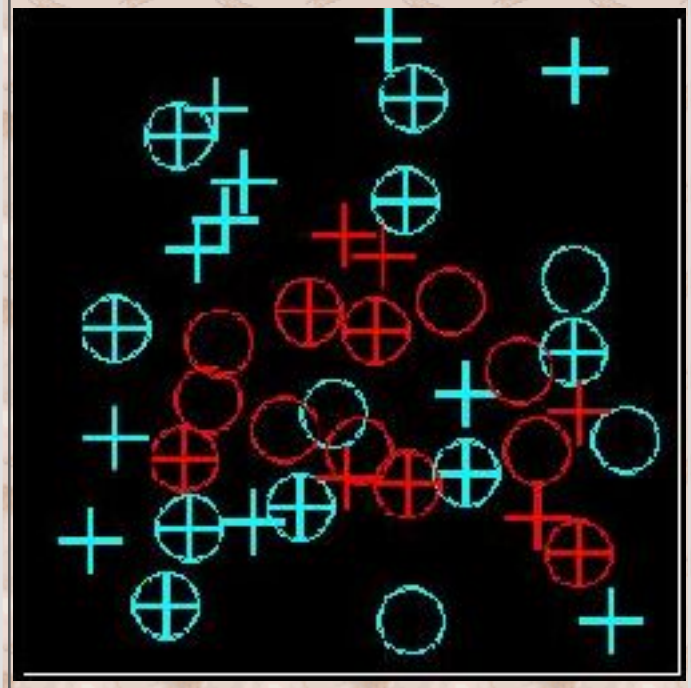




STEP 5:
Execute DOCK command:
dock 1 2

Rotate the second (top) structure. Check the relative arrangement of hydrogen bond donors and acceptors. The projections of these side chains are given in docking window.





NOTES

(1) If two structures are close, some important atoms might be unvisible (hidden by some closer atoms). Use slab to cut slices through structure(s).

(2) Don't forget to catch the right structure before applying some transformation. By default, after the command DOCK is executed, the movement controls are attached to the second (top) structure.

RELATED COMMANDS

LOAD is used to load the specified file (structure, molecule). MOVE is used to define which object should be moved (structure, plane or both). PLANE is used to manipulate the plane associated with the structure. CATCH is used to attach the movement controls to a chosen structure.

REFERENCES

(1) Kamphuis, I. G., Kalk, K. H., Swarte, M. B. A. and Drenth, J. (1984). J. Mol. Biol. 179, p. 233.

(2) Stubbs, M. T., Laber, B., Bode, W., Huber, R., Jerala, R., Lenarcic, B. and Turk, V. (1990). EMBO J. 9, p. 1939.

EDI, EDIT

NAME

EDI, EDIT - edit structure

SYNOPSIS

SHORT FORM	LONG FORM
EDI OFF	EDIT OFF
EDI ATO	EDIT ATOMS
EDI BON atom1 atom2	EDIT BOND atom1 atom2
EDI CLI	EDIT CLICK
EDI DIM	EDIT DIMENSIONS
EDI MAI	EDIT MAIN
EDI OME	EDIT OMEGA
EDI PHI	EDIT PHI
EDI PSI	EDIT PSI
EDI SID	EDIT SIDE

DESCRIPTION

The command EDI (EDIT), combined with one of associated keywords (except OFF), switches the program to editing mode. This will work for garlic version 1.2 or later. The keyword OFF may be used to switch the program to default mode (no editing). The command EDIT should always be combined with one of the keywords. The most comfortable keyword is CLI (CLICK): after executing the command EDI CLI (long form: EDIT CLICK), use the pointer (mouse) to pick one bond (torsion angle) for editing. Click the left mouse button.

The keywords ATO (ATOMS) and DIM (DIMENSIONS) are reserved for special purposes and should not be used to edit real molecular structures, unless you want to introduce (or to fix) some distortion. These keywords may be used to prepare some artificial structures, made from quarkonium and jellium atoms. An example of such structure is the model of the vascular system of human brain . Quarkonium and jellium are described here .

To avoid the accidental modification of the structure, a little sea creature will be visible at the position of the chosen bond or atom. If editing (moving) more than one bond (atom), the creature will be drawn at the position of the first bond (atom). If editing bonds (torsion angles), you will see a little seahorse. If editing atoms (keyword ATOMS) or dimensions (keyword DIMENSIONS) you will see a little squid. Why I have chosen these animals? Seahorse is a poor swimmer but has excellent maneuverability. Squid known hot to use jet propulsion for fast translation. These little creatures will warn you that you are working in editing mode. They will disappear after executing the command EDIT OFF.

The squid will be visible if using keywords DIMENSIONS or ATOMS and the seahorse will be visible if using keywords BOND, BOND, CLICK, MAIN, OMEGA, PHI, PSI or SIDE.

EDIT OFF

The keyword OFF may be used to switch the program to default mode (no editing, just viewing). The editing symbol (seahorse - if editing bonds or squid - if editing atoms) will disappear from the screen.

EDIT ATOMS

The command EDIT ATOMS (short form: EDI ATO) may be used to translate selected atoms. Normally, you will not use the keyword ATOMS if working with a real molecular structure. This keyword is intended for usage with artificial structures, consisting of polygonal lines. In rare cases, you may use this command to distort the molecular structure, for example to test your own molecular dynamics program. The model of the vascular system of human brain is an example of artificial structure, made from quarkonium and jellium atoms. Do not use this keyword unless you really know what you are doing!

The translation of atoms is done by using the keys /, *, +, -, 5 and 0 on numeric keypad.

EDIT BOND atom1 atom2

The command EDIT BOND (short form: EDI BON) should be followed by serial numbers of two atoms which form the bond. The keyword BOND may be used in scripts, to specify a single bond angle for editing. In interactive mode, the keyword CLICK is much more comfortable. Garlic will not allow the editing of the specified bond angle in two cases:
(1) If the specified two atoms do not form an ordinary covalent bond. Disulfide bonds are not counted as such.
(2) If these atoms form a covalent bond, but this bond in part of a closed structure (a ring).

The bond rotation may be done by using the keys 7 and 9 on numeric keypad. Garlic is capable to recognize the bond angle. For dihedral angles phi and psi, an auxiliary plot will be drawn to the bottom right corner of the main window. For dihedral angle omega, the auxiliary plot will be drawn to the bottom of the main window.

EDIT CLICK

The command EDIT CLICK (short form: EDI CLI) is the most comfortable way to chose a single bond angle for editing. Just execute this command and click a single bond. If this bond is as an ordinary covalent bond and if it is not part of some closed structure (a ring), the bond angle editing will be allowed. The seahorse will appear close to the place where the click occurred. Use the keys 7 and 9 on the numeric keypad to change the bond angle.

The keyword CLICK may be used to pick both the main chain bonds as well as side chain bonds. It may not replace the commands MAIN and SIDE, because these two keyword activate the simultaneous editing of two dihedral angles.

Be sure to select all atoms (residues) before using the command EDIT CLICK!

In some cases, a small auxiliary plot will appear in the main window. This means that you have chosen one of the main chain dihedral angles for editing. More details about these auxiliary plots may be found below (see EDIT MAIN).

EDIT DIMENSIONS

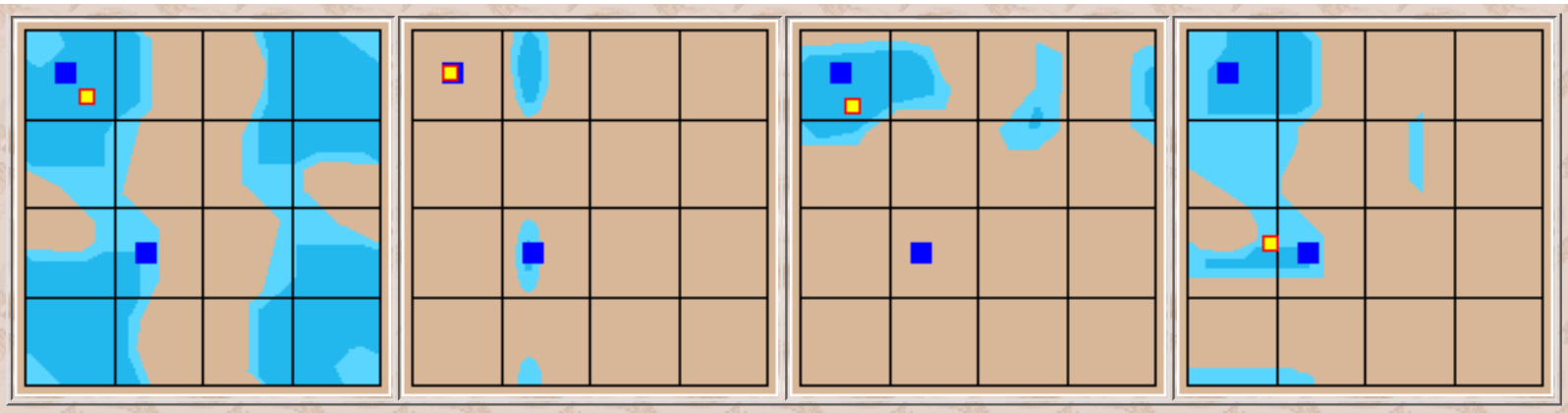
The command EDIT DIMENSIONS (short form: EDI DIM) may be used to resize the selected portion of the structure. Normally, you will not use the keyword DIMENSIONS if you are working with a real molecular structure. The translational controls should be used to change each of three dimensions independently: 0 and 5 may be used to change the depth of the structure, / and * to change the width and + and - to change the height of the structure. To resize the structure proportionally change all three dimensions consecutively. Be careful with the command EDIT DIMENSIONS!

EDIT MAIN

Change the main chain dihedral angles phi and psi, for all selected residues. A residue is treated as selected if the first atom of this residue is selected. The precise definitions of dihedral angles may be found at the page which describes the command RAM (RAMACHANDRAN) .

The current pair of values and the allowed regions for phi and psi will be visible in the auxiliary Ramachandran plot, in the bottom right corner of the main window. The current position in the Ramachandran plot may be recognized as the small, yellow square with red outline. The favorable regions are colored blue, with the more favorable regions colored dark blue. Two dark blue squares represent the positions of alpha helix and beta strand. Note that these conformations may be unfavorable in some cases (pre-proline in alpha helix, for example). There are four different types of auxiliary Ramachandran plot, describing residues with different steric constraints:

glycine	proline	pre-proline residues	all other residues



Be sure to read something about the revision of Ramachandran steric constrains: http://xray.bmc.uu.se/~gerard/rama/ramarev.html

EDIT OMEGA

Change the angle omega. The definition of this dihedral angle may also be found at the page which describes the command RAM (RAMACHANDRAN) . Most of residues in a protein are in trans conformation, with omega value of about 180 degrees. A small fraction of residues may be found in cis conformation, with omega value of about 0 degrees. The cis conformation is typical for proline. The auxiliary plot at the bottom of the main window shows the current omega value (yellow vertical line with red outline) and the statistical distribution of omega values, across the range between -180 degrees and +180 degrees. The blue peaks represent the most probable values. Note that -180 degrees is equivalent to +180 degrees; two prominent peaks in the auxiliary plot are actually two parts of the same (trans) peak. The central (cis) peak is almost invisible.

EDIT PHI

Change dihedral angle phi. The definition may be found at the page which describes the command RAM (RAMACHANDRAN) . The angle phi may be changed by using the keys 7 and 9 on numeric keypad. The operation will be done for every selected residue. A residue is treated as selected if the first atom of this residue is selected. An auxiliary Ramachandran plot (described above in EDIT MAIN section) will be visible in the bottom right corner.

EDIT PSI

Change dihedral angle psi. The definition may be found at the page which describes the command RAM (RAMACHANDRAN) . The angle psi may be changed by using the keys 7 and 9 on numeric keypad. The operation will be done for every selected residue. A residue is treated as selected if the first atom of this residue is selected. An auxiliary Ramachandran plot (described above in EDIT MAIN section) will be visible in the bottom right corner.

EDIT SIDE

Edit the side chain dihedral angles chi1 and chi2. Four numeric keys are used to change dihedral angles: 4 and 6 to change chi1 and 2 and 8 to change chi2. The command EDI SID (EDIT SIDE) is suitable for asparagine, aspartic acid, histidine, isoleucine, leucine, phenylalanine, proline, tyrosine and tryptophan.

NOTES

(1) The commands REPLACE, CREATE, LOAD, DISCARD, CATCH, SELECT, ADD and RESTRICT are switching program to default editing mode (no editing).

RELATED COMMANDS

The command SET may be used to set dihedral angles directly. It is more precise than the command EDIT. The commands ADD, RESTRICT and SELECT (short forms: ADD, RES and SEL) may be used to select one or more residues for editing. As it will be difficult to combine script execution and interactive rotational controls (numeric

keys), the command ROTATE (short form: ROT) may be used to change dihedral angles in scripts, after executing the command EDIT.

Jellium (J) and Quarkonium (Q)

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and "quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1. The interatomic distance is not important! Quarkonium is capable to form at most two bonds. To break the polygonal line, skip one serial index. For example, if three consecutive Q atoms in PDB file have serial numbers i-1, i and i+2, the atoms i-1 and i will be bound, but there will be no bond between atoms i and i+2. The same trick may be used to force Q atom to form no bonds: use indices i-2, i and i+2.

Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. Click here for an example.

By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. The term jellium is used is solid state physics (jellium model for electrons in solid). Note that symbols J and Q are not used in the periodic table of elements. For that reason these two terms were abused in garlic. If I should be thrown through the window at the next meeting of Croatian Physical Society, please note that my colleague Dario Faj deserves the same treatment, he was also involved in this dirty job.

RAM, RAMACHANDRAN

NAME

RAM, RAMACHANDRAN - draw Ramachandran plot.

SYNOPSIS

RAM
RAM SEL
RAM OFF
RAMACHANDRAN
RAMACHANDRAN SEL
RAMACHANDRAN OFF

DESCRIPTION

Draw Ramachandran plot (only for proteins). The main chain torsion angles, phi and psi, are used to prepare two-dimensional scatter plot. Residues for which both phi and psi angle may be calculated will be shown as small circles. The horizontal axis (abscisa) is used for phi values, while the vertical axis (ordinate) is used for psi values. Blue color is used for trans residues, magenta for cis residues and red for bad residues. Trans residues are drawn first, followed by cis residues. Bad residues are drawn last. A residue is treated as bad if peptide unit associated with this residue is not planar. Peptide unit is considered as non-planar if it is twisted for more than 20 degrees. Terminal residues will be missing, because at least one of dihedral angles is not defined for such residues.

The main chain dihedral angles are defined as follows:

(1) The phi angle is the angle of right-handed rotation around N-CA bond, the value being zero if CA-C bond is cis to C-N bond. Range: from -180 to 180 degrees.

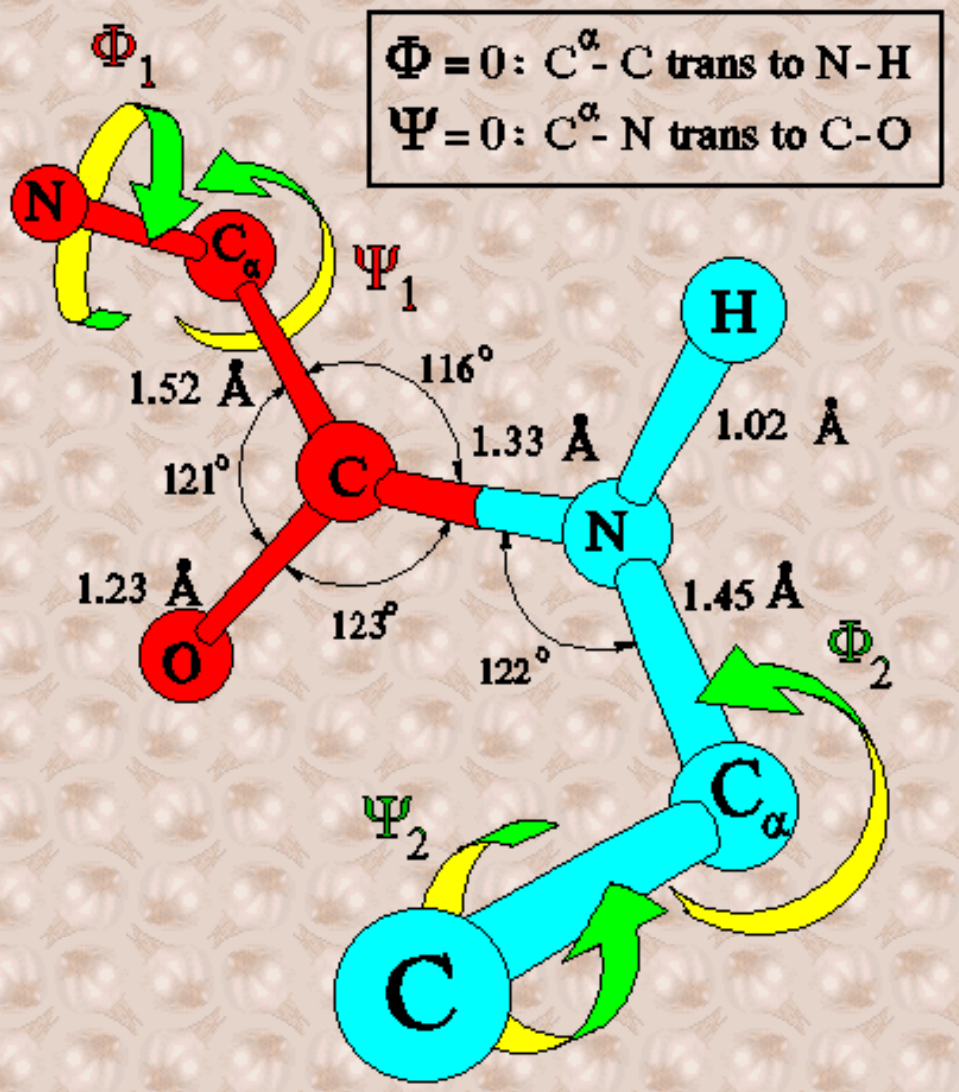
(2) The psi angle is the angle of right-handed rotation around CA-C bond, the value being zero if C-N bond is cis to N-CA bond. Range: from -180 to 180 degrees.

(3) The omega angle is the angle of right-handed rotation about C-N bond, the value being zero if CA-C bond of the preceding residue is cis to N-CA bond. Most residues in a typical protein are involved in the formation of two peptide bonds. The peptide bond formed by the residues I and I + 1 is assigned to the residue I + 1. The same applies to the omega angle. For that reason no omega angle is assigned to the first residue.

Since version 1.2, garlic uses the following procedure to calculate the main chain dihedral angles:

(1) In the first attempt, the coordinates of the main chain atoms are used to calculate the dihedral angles phi and psi. The phi angle will be missing for the first residue in each chain. The psi angle will be missing for the last residue in each chain.

(2) In the second attempt, the missing phi angles will be calculated using the coordinates of H (hydrogen) atoms, if available. The missing psi angles will be calculated using the coordinates of O (oxygen) atoms.



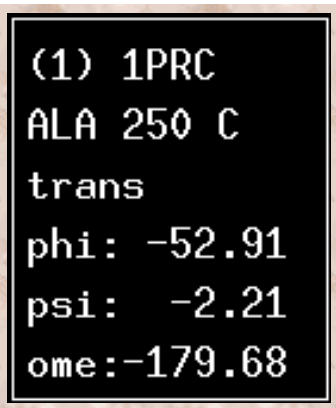
KEYWORDS

If used without any keyword, the command RAM will prepare the Ramachandran plot for protein structure(s) which are currently being handled ("caught"). Keyword OFF is used to switch off the Ramachandran plot, i.e. to return to the main drawing mode (atomic structure display). If keyword SEL (SELECTED) is used, only the residues which are currently selected will be visible in the Ramachandran plot. A residue is treated as selected if the first atom of this residue is selected. For proteins, this is usually N (nitrogen) atom. Here is the overview:

KEYWORD	DESCRIPTION
ram sel	Draw Ramachandran plot for selected residues.
ram off	Return to default drawing mode (atomic structure). Instead using this command, you can hit the ESCAPE key.

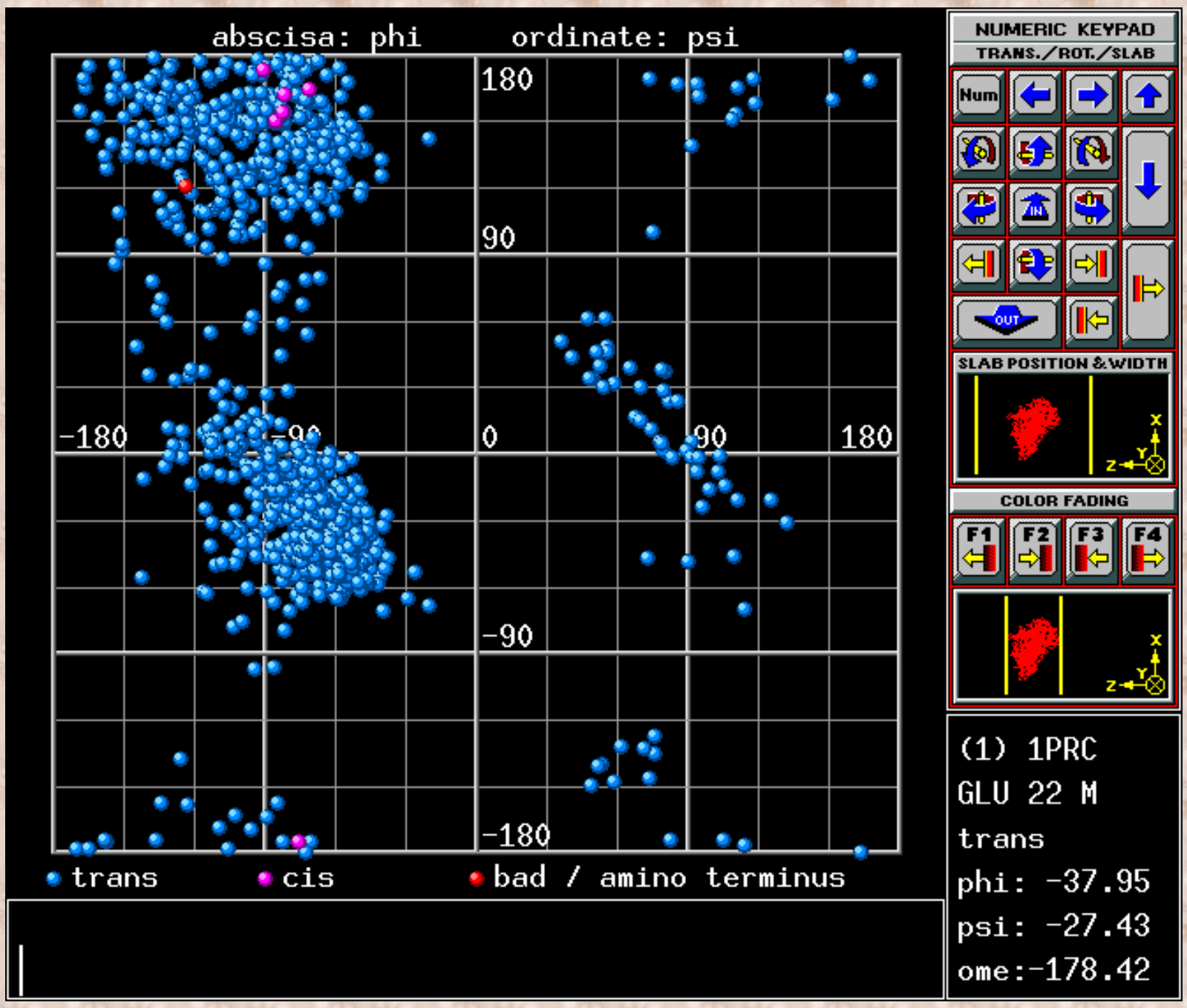
MOUSE USAGE

Pointing device (mouse) may be used to identify individual residues in Ramachandran plot. Just place the mouse pointer above the selected residue and the most important data for this residue will be shown in the output window. The output window will look like this:



EXAMPLE OF RAMACHANDRAN PLOT

The example below show the Ramachandran plot for photosynthetic reaction center from Rhodopseudomonas viridis.



EXAMPLES

COMMAND	DESCRIPTION
ram	Draw Ramachandran plot for all residues.
ram off	Return to default drawing mode (atomic structure).
ram sel	Draw Ramachandran plot for selected residues.
sel pro ram sel	Select all prolines and draw Ramachandran plot for prolines.
sel cis ram sel	Select all residues in cis conformation and draw Ramachandran plot for them.
sel bad ram sel	Select bad residues (peptide unit not planar) and draw Ramachandran plot.
sel tra ram sel	Select all residues in trans conformation and draw Ramachandran plot.

NOTES

(1) Instead using the command RAMA OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) G. N. Ramachandran devised in the late 1960's the steric constraints for amino acid residues in proteins. As the number of high resolution structures is increasing, it appears evident that these old constrains are becoming obsolete. If you are interested in this problem, read this article:

http://xray.bmc.uu.se/~gerard/rama/ramarev.html

RELATED COMMANDS

SEL may be used to select a portion of protein structure, to reduce the amount of data in Ramachandran plot.

SET

NAME
SET - set dihedral angle

SYNOPSIS
SET PHI value
SET PSI value
SET OME value
SET OMEGA value
SET CHI1 value
SET CHI2 value
SET CHI3 value
SET CHI4 value
SET CHI5 value

DESCRIPTION
The command SET may be used to set the chosen dihedral angle. The value of the angle should always be given in degrees. The keyword OMEGA may be abbreviated to OME. Do not abbreviate the keywords CHI1, CHI2, CHI3, CHI4 and CHI5.

EXAMPLES
set phi -179.0
set ome 0
set chi1 62
set chi2 178.50

RELATED COMMANDS
The command EDIT may be used to change dihedral angles by using rotational controls.

EXE, EXECUTE

NAME

EXE, EXECUTE - load and execute garlic script.

SYNOPSIS

EXE file_name
EXECUTE file_name

DESCRIPTION

Load and execute the specified garlic script. The garlic script file should contain garlic commands. There is only one command which is not executed if added into garlic script: the EXE command. This is done to avoid endless loops; the script which executes itself will generate an endless loop. If you don't like it, change to source file execute_command1.c (use the source, Luke!). Examples:

COMMAND	DESCRIPTION
exe tango.script	Execute the script which loads trp.pdb and forces this molecule to play something similar to Argentinian tango.

RELATED COMMANDS

LOG may be used to store commands used during a garlic session. The log file may be used later as a script.

EXI, EXIT, QUI, QUIT

NAME

EXI, EXIT, QUI, QUIT - quit garlic session (exit from garlic).

SYNOPSIS

EXI
EXIT
QUI
QUIT

DESCRIPTION

Quit garlic session, i.e. exit from garlic. The main garlic window will be closed, memory freed etc. At present, garlic is not capable to save any data (this will be changed, of course), so there are no warning messages.

FAD, FADING

NAME
FAD, FADING - change the color dependence on a distance from the observer.

SYNOPSIS
FAD keyword
FAD FRONT shift
FAD BACK shift
FADING keyword
FADING FRONT shift
FADING BACK shift

DESCRIPTION
Change the way color depends on distance. Distance is measured from the atom to the observer. This command comes in three versions:

(1) FADING FRONT shift ----> move the front color surface;
(2) FADING BACK shift ----> move the back color surface;
(3) FADING keyword ----> switch fading off or change the type of the surfaces.

FADING FRONT shift
This command moves the front fading surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys F1 and F2). The shift value should be given in angstroms. Positive shift moves the front color surface away from the observer. With most color schemes, the front (closer) portion of the structure will be brighter after the positive shift. FRONT may be abbreviated to FRO.

FADING BACK shift
This command moves the back fading surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys F3 and F4). The shift value should be given in angstroms. Positive shift moves the back color surface away from the observer. With most color schemes, the contrast will be reduced after the positive shift. Negative shift results in better contrast, i.e. distant atoms will become darker. BACK may be abbreviated to BAC.

FADING keyword
Some keywords may be used to change the type of color surfaces and to switch color fading off. Here is the list of keywords:

SHORT FORM	LONG FORM	DESCRIPTION
OFF	OFF	Switch fading off: colors should become distance independent
PLA	PLANE	Use planes as color surfaces
SPH	SPHERE	Use spheres as color surfaces
CYL	CYLINDER	Use cylinders as color surfaces
HALF-SPH	HALF-SPHERE	Use spheres as color surfaces, but apply only to the front half of the structure.
HALF-CYL	HALF-CYLINDER	Use cylinders as color surfaces, but apply only to the front half of the structure.

For most structures, the planar fading is the best choice. Spherical and semi-spherical fading may be useful when working with large globular proteins, while cylindrical and semi-cylindrical fading is useful when working with beta-barrel proteins (like porins). The cylinder axis is parallel to y axis (vertical from users standpoint).

EXAMPLES

COMMAND	DESCRIPTION
fading off	Switch color fading off
fading front 4.5	Move the front color surface 4.5 angstroms away from the observer
fading back -2.8	Move the back color surface 2.8 angstroms closer to the observer
fading half-sph	Change fading to semi-spherical

RELATED COMMANDS

COLOR defines the color for selected atoms.

FG, FOREG, FOREGROUND

NAME
FG, FOREG, FOREGROUND - change the main window foreground color.

SYNOPSIS
FG color
FOREG color
FOREGROUND color

DESCRIPTION
Change the main window foreground color. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted. This color is used to draw labels and titles. Note that this color is not used to draw atoms and bonds.

This command does not affect the main window in the sequence comparison mode. Check the command COMPARE .

Examples:

COMMAND	DESCRIPTION
fg white	White
fg DarkSlateGray	Dark dark slate gray
fg #3000a0007000	Kind of green
fg rgb:0/0/8	Dark blue
fg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
BG (BACKG, BACKGROUND) changes the main window background color.

FON, FONT

NAME

FON, FONT - change font.

SYNOPSIS

FON font_name
FONT font_name

DESCRIPTION

Change default font. At present, garlic uses only one font for input, output and main window. Try to execute xlsfonts on your system, to obtain a list of fonts. The initial font is set in .garlicrc file. Examples:

fon 10x20
fon olglyph-19

RELATED COMMANDS

FG changes the text color used to draw strings in the main window. TFG changes the text color used to draw strings in input and output window.

HID, HIDE

NAME
HID, HIDE - hide selected atoms.

SYNOPSIS
HID
HIDE

DESCRIPTION
Hide selected atoms and associated bonds.

RELATED COMMANDS
SHOW shows selected atoms and associated bonds.

HYB, HYBONDS

NAME

HYB, HYBONDS - generate hydrogen bonds.

SYNOPSIS

HYB
HYB style
HYB OFF
HYBONDS
HYBONDS style
HYBONDS OFF

DESCRIPTION

Generate hydrogen bonds for the entire structure. Show hydrogen bonds for visible atoms. At present, some very simple geometric restrains are used to generate hydrogen bonds. Check the configuration file (.garlicrc) and the source file gen_hybonds.c to learn more about these restrains.

Keyword OFF may be used to hide hydrogen bonds.

For hydrogen bonds, there is no proportional ("nice") style. The only available styles are 0, 1, 2, 3, 4 and 5.

Default style used to draw hydrogen bonds is 1 (a single line, fixed). You can change it by specifying the style. Examples:

hyb	Generate hydrogen bonds and show them using default style (1).
hyb 4	Generate hydrogen bonds and show them using style 4 (four lines).
hyb off	Hide hydrogen bonds

IGN, IGNORE

NAME

IGN, IGNORE - do nothing.

SYNOPSIS

IGN
IGNORE

DESCRIPTION

This command does nothing. It is absolutely useless. Do not use it to pause the program execution - PAUSE should be used for this purpose.

LAB, LABELS

NAME

LAB, LABELS - show or hide labels.

SYNOPSIS

LAB
LABELS
LAB OFF
LABELS OFF

DESCRIPTION

If used without keyword OFF, this command shows labels for selected atoms. If used with keyword OFF, this command hides labels. Each label contains:
(1) residue name;
(2) residue sequence number;
(3) chain identifier;
(4) atom name;
(5) alternate location indicator.

RELATED COMMANDS

TITLE adds the title to the main window. TAG assigns the specified tag to a structure. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

LOA, LOAD, REA, READ

NAME
LOA, LOAD, REA, READ - load the specified file.

SYNOPSIS
LOA file_name
LOAD file_name
REA file_name
READ file_name

DESCRIPTION
Load and display the specified file. The file content will be treated as a separate structure. The unique structure identifier (positive integer) will be assigned to this structure. The structure will be placed in the middle of the screen.

You can load any file more than once. A total number of structures which may be simultaneously loaded depends on the available memory. The hard-coded maximum is 1000, which should be more than enough.

The command LOAD may be written in uppercase, lowercase or mixed case, but the file name should be specified in correct case - unix file names are case sensitive.

SEARCH PATH
The file is searched in one or more directories, in the following order:

(1) the current working directory;
(2) directory specified in the environment variable MOL_DIR;
(3) all directories specified in the environment variable MOL_PATH.

The recommended environment variable is MOL_PATH.

NOTES
(1) The command LOAD resets the editing mode to default (no editing).

RELATED COMMANDS
DIS (DISCARD) discards the specified structure. SAV (SAVE) saves the atomic data to a file.

LOG

NAME

LOG - write interactive commands into the log file.

SYNOPSIS

LOG file_name
LOG OFF

DESCRIPTION

Use this command to log your garlic session into the specified file. The log file may be modified later and used as garlic script. LOG OFF closes the log file and stops logging.

NOTES

(1) If you logged the entire garlic session and want to use your log file as script, do not forget to remove the keyword QUIT (EXIT) which was used to end the garlic session!

(2) Lines which have # in the first column are treated as comments. Empty lines are ignored.

(3) Use PAUSE to pause the program execution. This is useful if preparing lecture or presentation, otherwise the script will run till the end without stopping.

(4) You can start and stop logging at any moment during your garlic session. Do not use the same log file name twice if you want to keep the old file - it will be overwritten.

RELATED COMMANDS

Exe executes the garlic script. PAUSE pauses the script execution.

MEM, MEMBRANE

NAME

MEM, MEMBRANE - generate and manipulate the membrane associated with the structure.

SYNOPSIS

SHORT FORM	LONG FORM
MEM	MEMBRANE
MEM RAD value	MEMBRANE RADIUS value
MEM THI value	MEMBRANE THICKNESS value
MEM TRA value	MEMBRANE TRANSPARENCY value
MEM OFF	MEMBRANE OFF

DESCRIPTION

The command MEM (MEMBRANE) may be used to associate the membrane with a protein structure. By default, no membrane is associated with the structure when it is loaded into memory. The membrane is initialized after the first execution of the command membrane. The membrane is useful when analysing some membrane protein, but it does not make much sense when working with a soluble protein.

The experimental determination of the structure of fluid lipid bilayers in The Stephen White Laboratory at UC Irvine has revealed a significant thermal motion of lipid molecules. This means that there is no clear edge of the biological membrane. However, the model used in garlic is just the opposite: the membrane is represented by two parralel planes, with clear external edges. The membrane thickness is also precisely defined. The idea was to give at least a bad model of the membrane, to allow selection of the transmembrane region. Please be sure to read those beatifull pages from Steven White Laboratory!

The planes used to simulate the membrane are represented as elliptical surfaces. The inner sides are colored orange-red, while the outer sides of the membrane are colored blue. The transparency of these planes may be adjusted, but not individually. The allowed range of transparency from 0 to 1. If the transparency is equal to zero both planes will be opaque. Default transparency is 0.4 (hard-coded).

In addition to the transparency, the membrane thickness and the radius of both planes may be adjusted (keywords THICKNESS and RADIUS, short forms THI and RAD). Default radius will be 50% larger than the membrane thickness. Default membrane thickness is 30 angstroms. It is not possible to change default membrane thickness through .garlicrc file. If you want to change it, modify the hard-coded value in the source file defines.h and recompile the program.

KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
OFF	OFF	Hide membrane.
RAD	RADIUS	Set the radius of both planes (use angstroms).
THI	THICKNESS	Set the membrane thickness (in angstroms).
TRA	TRANSPARENCY	Set the transparency of both planes (between 0 and 1).

EXAMPLES

COMMAND	DESCRIPTION
mem	Initialize the membrane and make it visible.
mem rad 20	Change the radius of both planes to 20 angstroms.
mem tra 0.3	Change the transparency of both planes (new value: 0.3).
mem off	Hide membrane.

NOTES

(1) By default, the membrane moves with the structure. If movement controls affect only the membrane, be sure to make it visible. Otherwise, you may push the membrane far away from the object to which this membrane belongs.

RELATED COMMANDS

LOAD is used to load the structure (PDB file). MOVE is used to define which object should be moved. POSITION is used to place the chosen object (structure, plane, membrane or all) to arbitrary position.

MON, MONO

NAME
MON, MONO - switch to mono mode.

SYNOPSIS
MON
MONO

DESCRIPTION
Switch to mono mode, i.e. switch stereo off.

RELATED COMMANDS
Use STEREO to switch to stereo mode. STEREO OFF does the same job as MONO.

MOV, MOVE

NAME

MOV, MOVE - define which object should be moved.

SYNOPSIS

MOV STR
MOV MEM
MOV PLA
MOV ALL
MOVE STRUCTURE
MOVE MEMBRANE
MOVE PLANE
MOVE ALL

DESCRIPTION

This command defines which object should be moved when rotation and translation controls or commands are used. When a PDB file is read, a new structure is stored into program memory. A single plane (initially invisible) is associated with each structure. On request (after the first execution of the command MEMBRANE), a single membrane may also be added to the structure. By default, the movement controls are affecting both the atomic structure and the associated objects (the plane and the membrane, if initialized). The command MOV (MOVE) may be used to change the action of the movement controls, to move only the choosen object.

The command MOVE affects only the molecule which is currently being handled (the structure which is "caught").

KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
STR	STRUCTURE	Move only the structure (atoms), leaving the plane and the membrane at the current position.
MEM	MEMBRANE	Move only the membrane, leaving the structure (atoms) and the plane at the current position.
PLA	PLANE	Move only the plane, leaving the structure (atoms) and the membrane at the current position.
ALL	ALL	Move all (atoms + plane + membrane).

EXAMPLES

COMMAND	DESCRIPTION
mov pla	Move the plane leaving the structure and the membrane at the current position.
mov all	Move structure, plane and membrane. This is default action.

NOTES

(1) The plane and the membrane are affected by rotation and translation controls and commands. Slab and color fading do not affect these objects.

(2) Never use two keywords with the command MOVE! If you want to move the plane and the membrane, for example, you should move it one by one!

RELATED COMMANDS

PLA (PLANE) is used to manipulate the plane associated with the molecular structure. MEM (MEMBRANE) is used to generate and manipulate the membrane. CATCH is used to catch the specified structure.

NEI, NEIGHBORHOOD

NAME
NEI, NEIGHBORHOOD - hide or show the sequence neighborhood.

SYNOPSIS
NEI
NEI OFF
NEIGHBORHOOD
NEIGHBORHOOD OFF

DESCRIPTION
Hide or show the sequence neighborhood of the residue covered by the pointer. When you cross an atom or bond with the mouse pointer, the output window will contain some useful information about this atom. In addition to this, the top portion of the main window will contain the list of the residues before and after the residue to which this atom belongs. The central residue will be enclosed in a small rectangle. The entire sequence neighborhood will be enclosed in a wide rectangle.

If you are not interested in the sequence neighborhood, execute the command:

nei off

If you want to remove the sequence neighborhood permanently, find this section in the configuration file .garlicrc and replace the keyword "yes" by "no":

```
# Sequence neighborhood of the residue under
# the pointer may be visible or hidden (yes/no):

show sequence neighborhood: yes
```

By default, the sequence neighborhood will be visible.

KEYWORDS
The only keyword is OFF. If used without any keyword, the command NEI will make the sequence neighborhood visible. If combined with the keyword OFF, the command will hide the sequence neighborhood.

EXAMPLES

COMMAND	DESCRIPTION
nei off	Hide the sequence neighborhood.
nei	Show the sequence neighborhood.

NOTES
(1) Residues in the sequence neighborhood are listed in direction from amino- to carboxyl-terminal residue.

(2) If the current residue is close to the polypeptide chain end, it will be displaced from the central position.

PAU, PAUSE

NAME

PAU, PAUSE - pause script execution.

SYNOPSIS

PAU
PAUSE

DESCRIPTION

Pause script execution. This may be useful if using garlic for lectures and conference presentations. The script execution will be paused until the return key is pressed.

RELATED COMMANDS

Use EXE (EXECUTE) to load and execute garlic script. Use LOG to log your garlic session. The log file may be modified into the script file later (or even left unchanged).

PLA, PLANE

NAME

PLA, PLANE - manipulate the plane associated with the structure.

SYNOPSIS

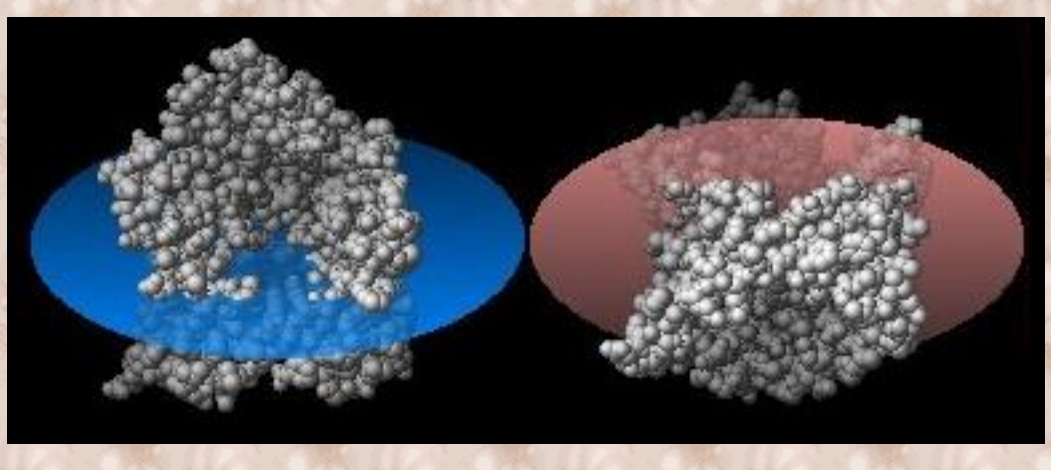
PLA
PLA RAD value
PLA TRA value
PLA OFF
PLANE
PLANE RADIUS value
PLANE TRANSPARENCY value
PLANE OFF

DESCRIPTION

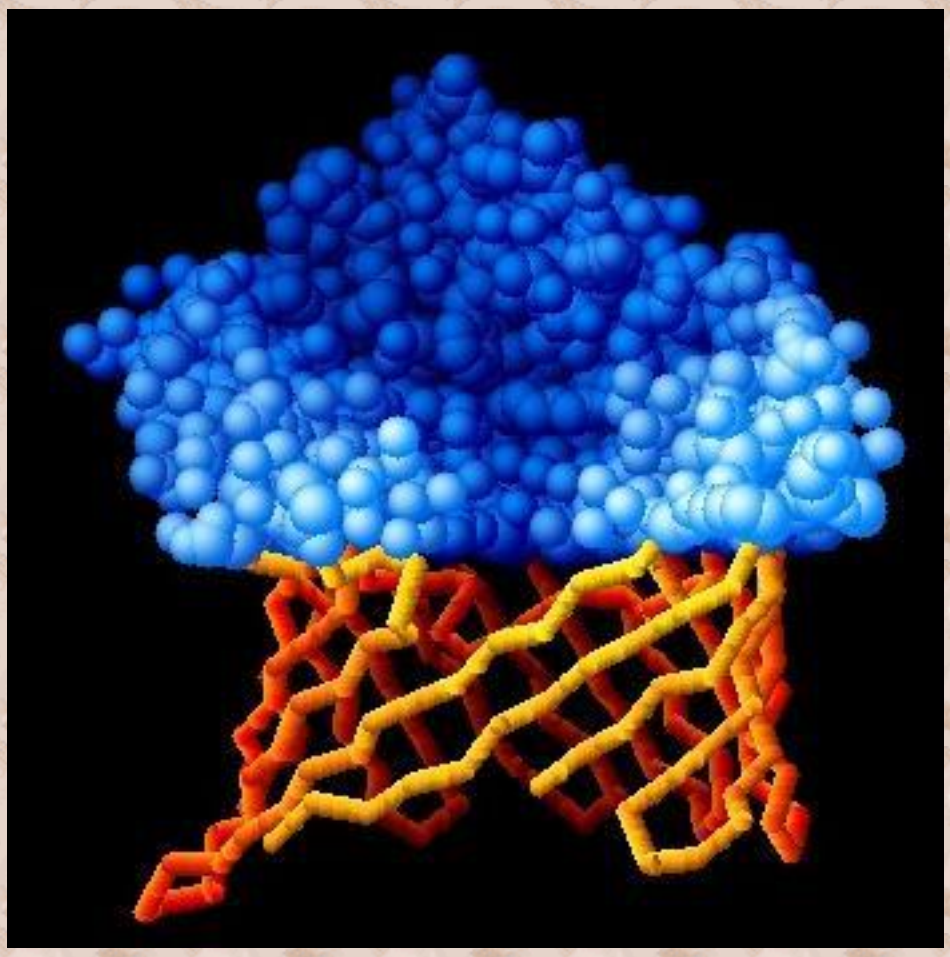
When a PDB file is read, a new structure is stored into program memory. A single plane is associated with this structure. By default, the plane is unvisible and movement controls are affecting both the structure and the associated plane. The command PLANE may be used to make the plane visible, to set the plane transparency or radius, or to hide the plane.

Plane is represented by an ellipse. One side of this ellipse will be colored blue and other side will be colored orange-red. Blue side is treated as top (upper) side, while orange-red side is treated as bottom side. Far side of the plane is dark.

The transparency value should be between 0 and 1. If the transparency is equal to zero the plane is opaque. Default plane transparency is 0.4 (hard-coded). The initial (default) plane radius is based on the spacial extent of the structure. The image below shows two semi-transparent planes: the left plane is seen from above, while the right plane is seen from below. The transparency is equal to 0.3 for both planes.



Plane may be used for different purposes:
(1) To distinguish protein domains. Many soluble proteins fold into two domains. Plane may be used to outline the border between these domains.
(2) Atoms may be selected according to their position with respect to plane. The command SEL ABO (SELECT ABOVE) selects atoms which are above the plane. The command SEL BEL (SELECT BELOW) selects atoms which are below the plane. The image below shows what may be achieved when applying different drawing styles to atoms on different sides of the plane.
(3) To represent the cellular membrane. Since version 1.2, garlic is capable to represent the membrane directly, so this usage of planes is obsolete.



KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
OFF	OFF	Hide plane.
RAD	RADIUS	Set plane radius (value should be given in angstroms).
TRA	TRANSPARENCY	Set plane transparency (between 0 and 1).

EXAMPLES

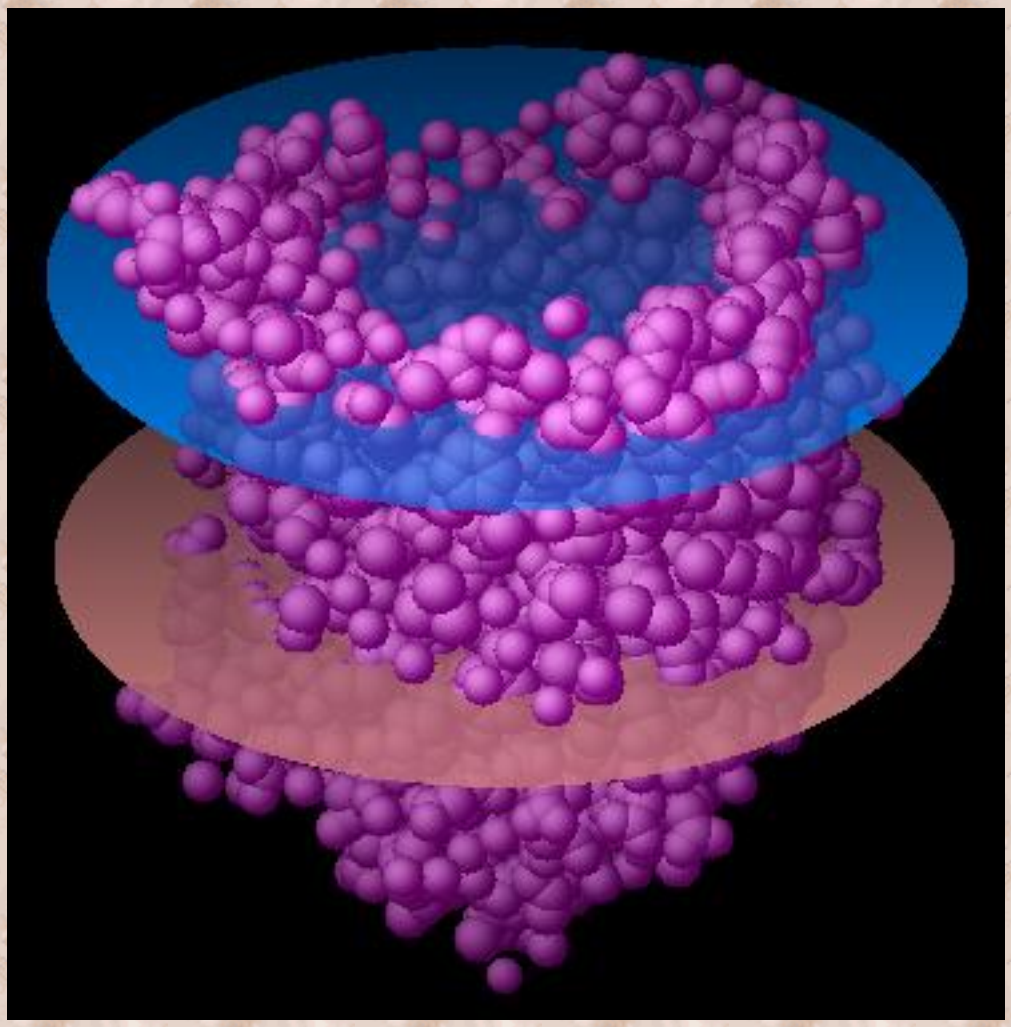
COMMAND	DESCRIPTION
plane	Make the plane visible.
pla rad 20	Change plane radius to 20 angstroms.
pla tra 0.3	Change plane transparency (new value: 0.3).
plane off	Hide plane.

NOTES

(1) By default, the plane moves with the structure. If movement controls affect only the plane, be sure to make it visible. Otherwise, you may push the plane far away from the object to which this plane belongs.

(2) In garlic source code, each plane is defined by the plane center (three coordinates) and by the normal vector (three-component vector).

(3) At present, garlic associates only one plane with each structure. If for some reason you need two planes (for example, to simulate the cellular membrane), use the following trick:
(3.1) Prepare the structure and its associated plane (the first plane).
(3.2) Load another structure (something small, like a single residue) and hide it.
(3.3) Make the plane (which is associated with this small structure) visible.
(3.4) Change radius and transparency for the second plane.
(3.5) Set the position and orientation of this plane.
If you learn this trick, you will be able to prepare images like this one:



RELATED COMMANDS

LOAD is used to load the structure (PDB file). MOVE is used to define which object should be moved. POSITION is used to place the chosen object (structure, plane, membrane or all) to arbitrary position. SELECT ABOVE selects atoms above the plane, while SELECT BELOW selects atoms below the plane.

PLO, PLOT

NAME

PLO, PLOT - draw averaged hydrophobicity and/or hydrophobic moment.

SYNOPSIS

PLO HYD
PLO HYD start_index end_index
PLO MOM
PLO MOM start_index end_index
PLO HYD MOM
PLO HYD MOM start_index end_index
PLO OFF
PLOT HYDROPHOBICITY
PLOT HYDROPHOBICITY start_index end_index
PLOT MOMENT
PLOT MOMENT start_index end_index
PLOT HYDROPHOBICITY MOMENT
PLOT HYDROPHOBICITY MOMENT start_index end_index
PLOT OFF

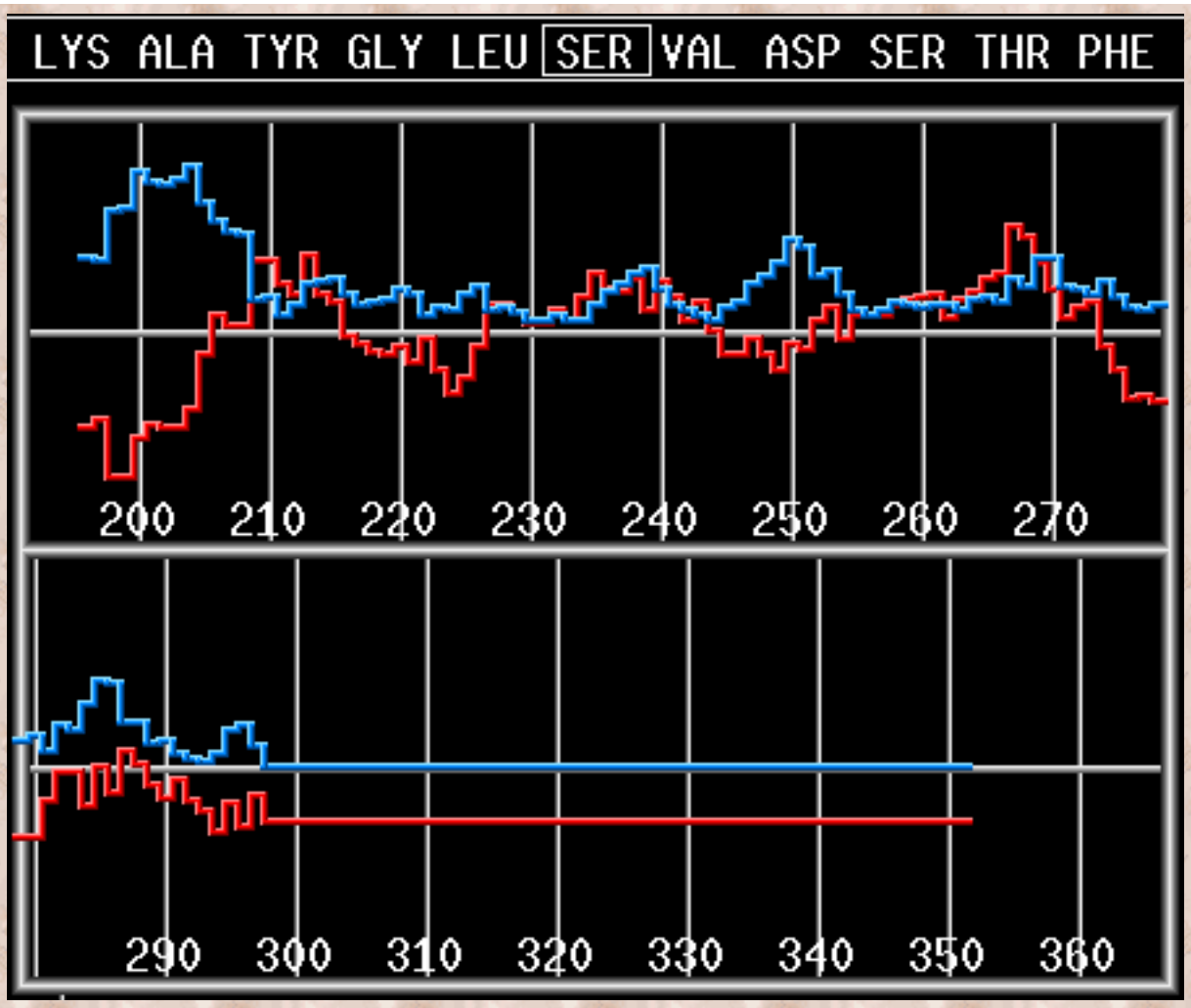
DESCRIPTION

Draw averaged hydrophobicity and/or hydrophobic moment. The averaged hydrophobicity and hydrophobic moment will be calculated using the sequence from the main sequence buffer, the current sliding window width and the current hydrophobicity scale. To calculate the hydrophobic moment one more parameter is required: the rotation angle between adjacent residues.

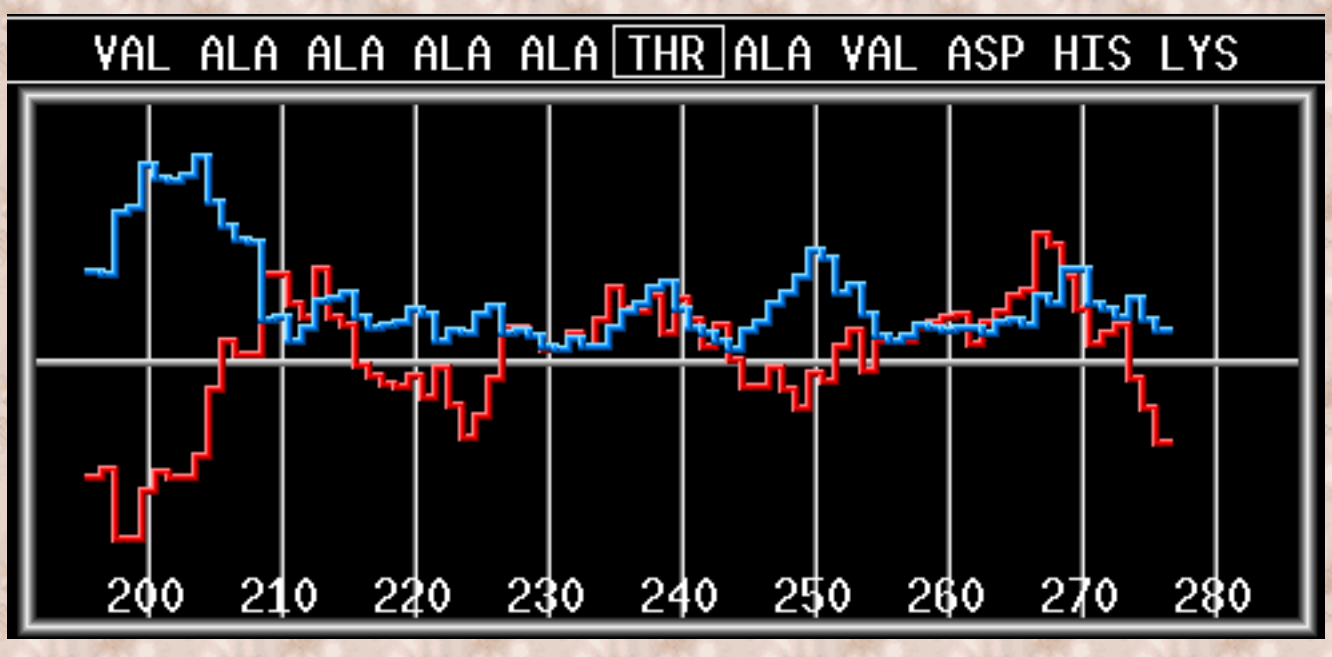
The averaged hydrophobicity will be shown as red line, while the hydrophobic moment will be shown as blue line. The information about the residue below or above the pointer (mouse) will be visible in the output window (bottom right corner of the main window), while the sequence neighborhood of the current residue will be visible above the plot (top of the main window).

If the entire sequence is used for calculation, there is a chance that plot will contain the straight line at the end. This portion of the plot refers to solvent molecules, which are typically stored to the end of PDB file. This trailing line may be easily removed by adjusting the residue range. Here are two examples:

The first image was prepared using all residues from 200 to the last one, including solvent molecules.



The second image was prepared using residues from 200 to 280, omitting the solvent molecules.



KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION

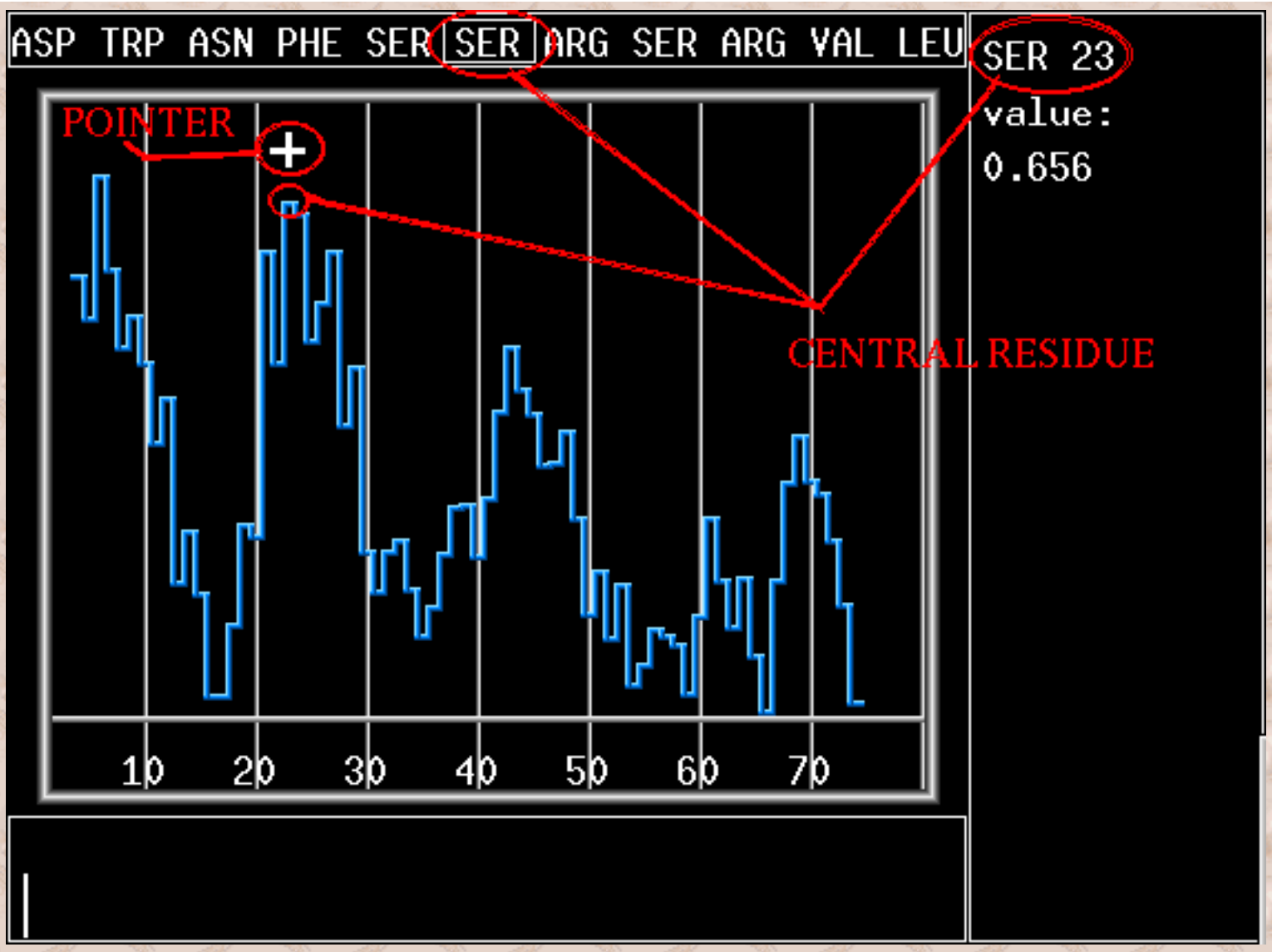
OFF	OFF	Return to the main drawing mode (draw atomic coordinates). Instead using this command, you can hit the ESCAPE key.
HYD	HYDROPHOBICITY	Draw averaged hydrophobicity.
MOM	MOMENT	Draw hydrophobic moment.

PARAMETERS

PARAMETER (SHORT)	DESCRIPTION
start_index	Serial index of the first residue.
end_index	Serial index of the last residue.

MOUSE USAGE

Mouse may be used to retrieve the information about averaged hydrophobicity and hydrophobic moment for a given residue. This residue is treated as the central residue of the current sliding window. The numerical data, along with residue name and serial number will be visible in the output window (bottom right corner). The sequence neighborhood of this residue will be visible above the plot. The information will be associated with the residue which has the same horizontal position (x coordinate) as the mouse pointer.



EXAMPLES

COMMAND	DESCRIPTION
load 2por.pdb seq from 1 scale eis win 7 angle 180 plot hyd mom 1-300	Load porin coordinates, copy sequence to the main sequence buffer, select Eisenberg hydrophobicity scale, set window width to 7 and set angle to 180 degrees. Draw averaged hydrophobicity and hydrophobic moment for residues from 1 to 300.
seq load sample.fasta scale eis angle 100 plot mom	Read the file sample.fasta, which contains the protein sequence in FASTA format (one letter code), select Eisenberg scale, set angle to 100 and draw hydrophobic moment.
plot off	Return to default drawing mode. Instead using this command, you can hit the ESCAPE key.

MATHEMATICAL BACKGROUND

Both the averaged hydrophobicity and the hydrophobic moment are calculated using a rectangular sliding window. If there are N residues in the sliding window, the averaged hydrophobicity is equal to:

$$\frac{1}{N}\sum_{i=0}^{N} h_i$$

Hydrophobic moment is equal to:

$$\frac{1}{N}\left\{\left[\sum_{i=1}^{N} h_i sin\,(i\alpha)\right]^2 + \left[\sum_{i=1}^{N} h_i cos\,(i\alpha)\right]^2\right\}^{\frac{1}{2}}$$

If you are searching for amphipatic alpha helices, set alpha to 100 degrees. To identify amphipatic beta strands, use 180 degrees. You can change alpha by using the command ANGLE.

NOTES

(1) Instead using the command PLOT OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) PLOT uses only the sequence stored to the main sequence buffer. Read description of the command SEQ (SEQUENCE) to learn how to initialize this buffer.

(3) If you plot both the averaged hydrophobicity and the hydrophobic moment, the output window (bottom right corner) will contain the hydrophobic moment of the central residue.

(3) Every time you change hydrophobicity scale, don't forget to refresh the plot (i.e., execute the command PLOT once more).

RELATED COMMANDS

SEQUENCE is used to copy, define or load the sequence. ANGLE defines the rotation angle between adjacent residues. SCALE is used to specify the hydrophobicity scale. WINDOW is used to set the sliding window width.

POS, POSITION

NAME

POS, POSITION - move the origin of the internal coordinate system to the specified position.

SYNOPSIS

POS x y z
POSITION x y z

DESCRIPTION

An internal coordinate system is assigned to each structure. The command POS (POSITION) sets the position of this origin. Three coordinates (x, y and z) should be specified.

Initially, the position of geometric center is used as the internal system origin for each structure. When loaded, this origin is set into the point (0, 0, 0).

RELATED COMMANDS

CEN (CENTER) redefines the internal system origin. MOV (MOVE) chooses the object which should be moved (structure, plane, membrane or all).

REF, REFRESH

NAME

REF, REFRESH - switch refreshing on or off.

SYNOPSIS

REF
REFRESH
REF OFF
REFRESH OFF

DESCRIPTION

Most of garlic commands require redrawing of the main window. This may slow down the execution of the program. To save some time, the refreshing may be switched off. Just execute the command:

ref off

(the long form is REFRESH OFF). After that, a number of time-consuming commands may be executed, and refreshing may be turned on again. To switch on refreshing, execute the command REF without the keyword OFF:

ref

This trick is very useful with scripts. Put the command REF OFF close to the top of the script and do not forget to put the command REF (without the keyword OFF!) to the bottom of the script. Try the sample scripts atoms.script , bonds.script and colors.script . The refreshing trick is used in these scripts.

If refreshing is switched off, you will see the message in the middle of the main garlic window (yellow text "Refreshing off" on red background).

Garlic Tutorial

Script 1 (atoms.script) - Drawing styles for atoms

This script shows the available drawing styles for atoms. Note that nothing is visible for style "0" (row one, column one)! The file trp.pdb is required as input. You can mark, copy and paste this script to your local host (create the file atoms.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe atoms.script

The sample image is at the bottom of this page.

```
# Show all drawing styles used to draw atoms. Bonds are hidden!
# This script requires garlic version 1.2!

# Atom style 0:
load trp.pdb
pos -24 -15 0
ato 0
bon 0
tag "0"

# Now inform user that refreshing is off:
title 1 50 50 "Please be patient ..."

# Switch refreshing off:
refresh off

# Atom style 1:
load trp.pdb
pos -12 -15 0
ato 1
bon 0
tag "1"

# Atom style 2:
load trp.pdb
pos 0 -15 0
ato 2
bon 0
```

```
tag "2"

# Atom style 3:
load trp.pdb
pos 12 -15 0
ato 3
bon 0
tag "3"

# Atom style 4:
load trp.pdb
pos 24 -15 0
ato 4
bon 0
tag "4"

# Atom style 5:
load trp.pdb
pos -24 -5 0
ato 5
bon 0
tag "5"

# Atom style 6:
load trp.pdb
pos -12 -5 0
ato 6
bon 0
tag "6"

# Atom style 7:
load trp.pdb
pos 0 -5 0
ato 7
bon 0
tag "7"

# Atom style bal:
load trp.pdb
pos 12 -5 0
ato bal
bon 0
tag "bal (ball)"

# Atom style ba2:
load trp.pdb
```

```
pos 24 -5 0
ato ba2
bon 0
tag "ba2"

#Atom style small:
load trp.pdb
pos -24 5 0
ato sma
bon 0
tag "sma (small)"

# Atom style sm2:
load trp.pdb
pos -12 5 0
ato sm2
bon 0
tag "sm2"

# Atom style covalent:
load trp.pdb
pos 0 5 0
ato cov
bon 0
tag "cov (covalent)"

#Atom style co2:
load trp.pdb
pos 12 5 0
ato co2
bon 0
tag "co2"

#Atom style spacefill:
load trp.pdb
pos -24 15 0
ato spa
bon 0
tag "spa (spacefill)"

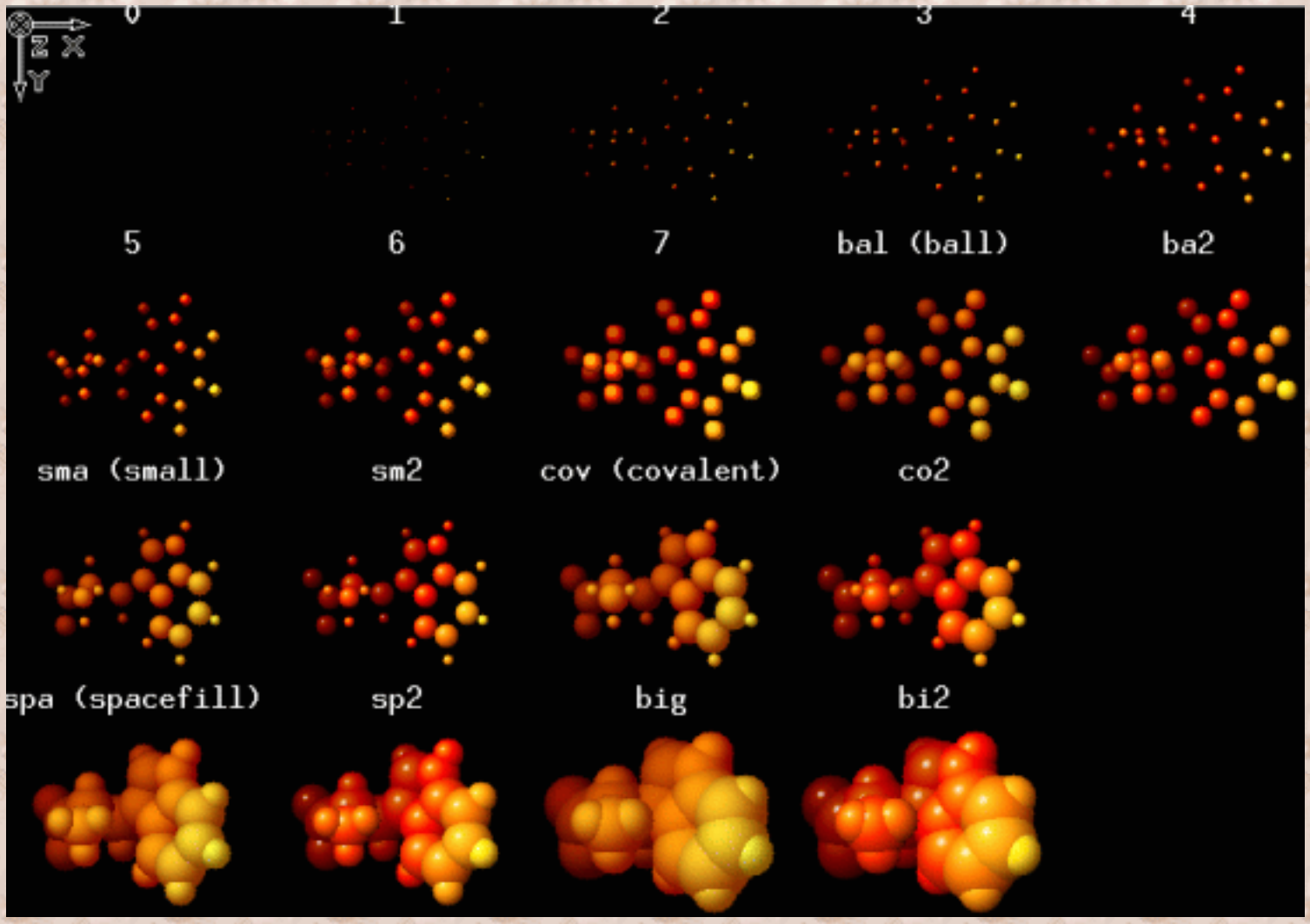
#Atom style sp2:
load trp.pdb
pos -12 15 0
ato sp2
bon 0
tag "sp2"
```

```
#Atom style big:
load trp.pdb
pos 0 15 0
ato big
bon 0
tag "big"

#Atom style bi2:
load trp.pdb
pos 12 15 0
ato bi2
bon 0
tag "bi2"

# Hide the title:
title 1 off

# Switch refreshing on:
refresh
```


0
1
2
3
4
Z X
Y
5
6
7
bal (ball)
ba2
sma (small)
sm2
cov (covalent)
co2
spa (spacefill)
sp2
big
bi2

Garlic Tutorial

Script 2 (bonds.script) - Drawing styles for bonds

This script shows the available drawing styles for bonds. The file trp.pdb is required as input. You can mark, copy and paste this script to your local host (create the file bonds.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe bonds.script

The sample image is at the bottom of this page.

```
# Show all drawing styles used to draw bonds. Atoms are hidden,
# except for nice bonds!
# This script will work if you use default .garlicrc script.
# This script requires garlic version 1.2!

# Bond style 1:
load trp.pdb
pos -12 -6 -40
ato 0
bon 1
tag "1"

# Now inform user that refreshing is off:
title 1 50 50 "Please be patient ..."

# Switch refreshing off:
refresh off

# Bond style 2:
load trp.pdb
pos 0 -6 -40
ato 0
bon 2
tag "2"

# Bond style 3:
load trp.pdb
pos 12 -6 -40
```

```
ato 0
bon 3
tag "3"

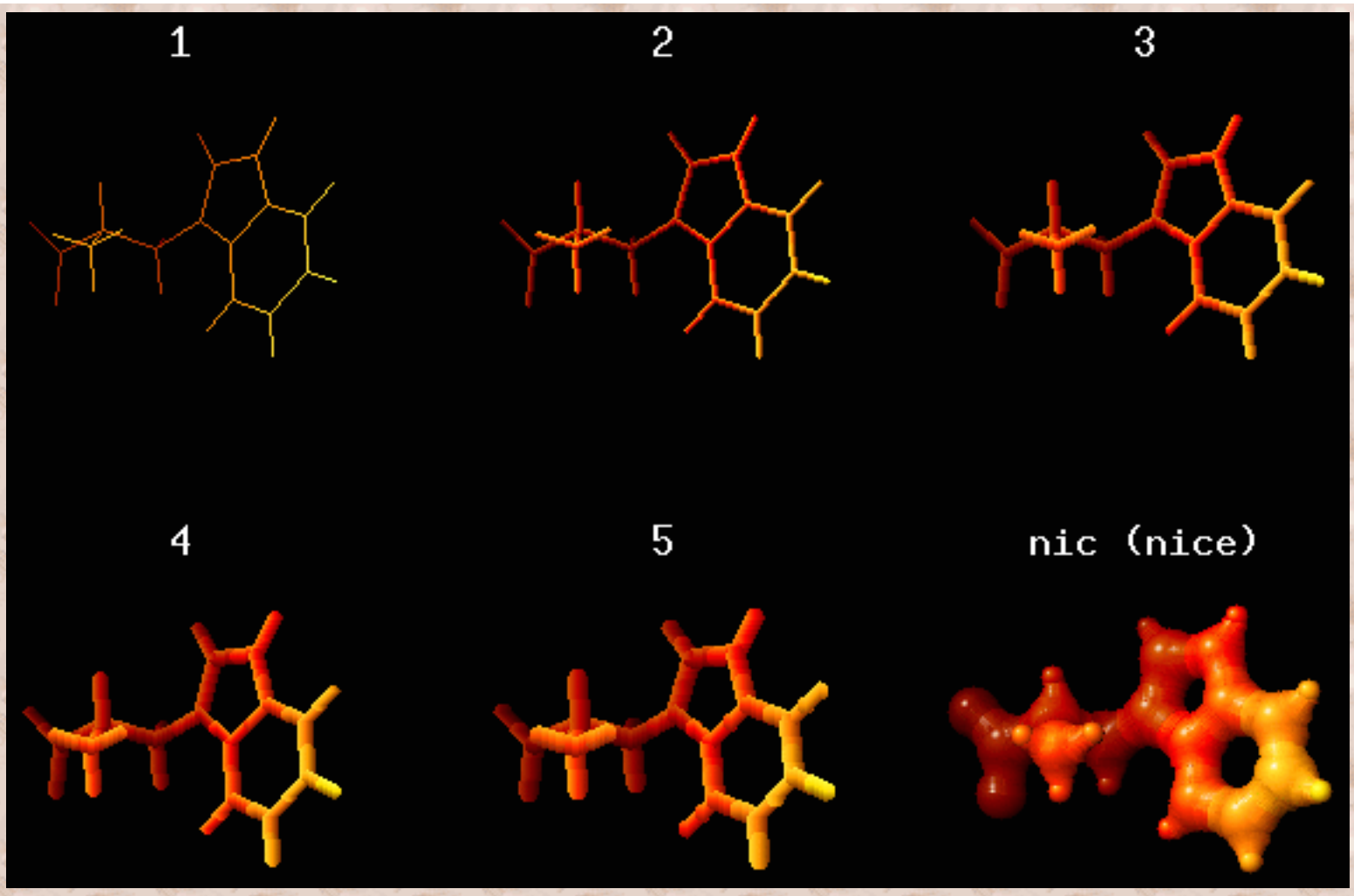
# Bond style 4:
load trp.pdb
pos -12 6 -40
ato 0
bon 4
tag "4"

# Bond style 5:
load trp.pdb
pos 0 6 -40
ato 0
bon 5
tag "5"

# Bond style nice:
load trp.pdb
pos 12 6 -40
ato co2
bon nice
tag "nic (nice)"

# Hide the title:
title 1 off

# Switch refreshing on:
refresh
```


1
2
3
4
5
nic (nice)

Garlic Tutorial

Script 3 (colors.script) - Predefined color schemes

This script shows some selected color schemes. All schemes shown here are hard-coded in the program. The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file colors.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe colors.script

The sample image is at the bottom of this page.

```
# Show predefined color schemes, version 1.2.
# This script will work if you use default .garlicrc script.
# This script requires garlic version 1.2!

load trp.pdb
pos -18 -15 0
ato sp2
bon nice
color red

# Now inform user that refreshing is off:
title 1 50 50 "Please be patient ..."

# Switch refreshing off:
refresh off

load trp.pdb
pos -6 -15 0
ato sp2
bon nice
color green

load trp.pdb
pos 6 -15 0
ato sp2
bon nice
color blue
```

```
load trp.pdb
pos 18 -15 0
ato sp2
bon nice
color yellow

load trp.pdb
pos -18 -5 0
ato sp2
bon nice
color cyan

load trp.pdb
pos -6 -5 0
ato sp2
bon nice
color magenta

load trp.pdb
pos 6 -5 0
ato sp2
bon nice
color white

load trp.pdb
pos 18 -5 0
ato sp2
bon nice
color yellow-green

load trp.pdb
pos -18 5 0
ato sp2
bon nice
color cyan-green

load trp.pdb
pos -6 5 0
ato sp2
bon nice
color cyan-blue

load trp.pdb
pos 6 5 0
ato sp2
bon nice
```

```
color magenta-blue

load trp.pdb
pos 18 5 0
ato sp2
bon nice
color magenta-red

load trp.pdb
pos -18 15 0
ato sp2
bon nice
color orange

load trp.pdb
pos -6 15 0
ato sp2
bon nice
color hot

load trp.pdb
pos 6 15 0
ato sp2
bon nice
color cold

load trp.pdb
pos 18 15 0
ato sp2
bon nice
color cpk

# Hide the title:
title 1 off

# Switch refreshing on:
refresh
```

REG, REGISTER

NAME
REG, REGISTER

SYNOPSIS
REG
REGISTER

DESCRIPTION
Register garlic: send a short e-mail to the author. This command will fail if your machine is not connected to the Internet. The only content of the message will be the word 'Hi!'. Your registration will not be abused, i.e. your e-mail address will not be given to spammers or anyone else. The registration will be used just to count garlic users.

If your machine is not connected to the Internet, send an e-mail from some other machine. Questions, comments and suggestions are welcome.

The author may be reached at:
zucic@garlic.mefos.hr
zucic@drava.etfos.hr
zucic@mia.os.carnet.hr

Author's home page:
http://garlic.mefos.hr/zucic

REGISTER GARLIC - by registering, you are supporting further development of this program!

REP, REPLACE

NAME
REP, REPLACE - replace selected residues

SYNOPSIS
REP
REPLACE

DESCRIPTION
Replace the selected residues, using the sequence from the main sequence buffer. At present (version 1.2), garlic is capable to replace protein residues only. Do not use this command to replace nucleic bases or hetero residues. After the replacement, the structure will need some refinement.

A residue is treated as selected if the first atom which belongs to this residue is selected. For proteins, this is typically N (nitrogen).

The main sequence buffer has to be initialized before issuing the command REPLACE. The number of residues in the main sequence buffer should be equal to the number of selected residues.

SINGLE RESIDUE REPLACEMENT
To replace a single residue, use the following commands:
select residue_sequence_number
sequence = new_residue_name
replace

Example:
sel 29
seq = ser
rep

REPLACING THE ENTIRE SEQUENCE
The command REPLACE may be used to prepare the model of some protein using the experimentally solved structure of the related protein. To replace the entire protein sequence follow these general instructions:
(1) Prepare the file with the sequence of the unsolved protein (use FASTA format).
(2) Find the related, experimentally solved protein structure.
(3) Fix insertions and deletions in the sequence of the unsolved protein.
(4) Start garlic and load the known structure.
(5) Exclude hetero residues from selection (first SEL HET, than SEL COM).
(6) If there is more than one chain restrict selection (RES chain_id/*/*/*).
(7) Load the new sequence (use the command SEQ LOAD).
(8) Replace the old sequence.

Don't forget that the number of selected residues should match the number of residues in the sequence of the unsolved protein.

TEMPLATE RESIDUES
The selected residues will be replaced with the residues from the template file. Default template file contains 20 standard residues. This file should be named residues.pdb and stored to at least one of the following directories (listed in the search order):
(1) The current working directory.
(2) $HOME/garlic (garlic subdirectory of user's home directory).

(3) /usr/local/lib/garlic (the system-wide template).

If you want to add some extra residues (like modified amino-acids) to the template file, make your own copy of the file residues.pdb and keep it either in $HOME/garlic subdirectory or in your favorite working directory. It is very easy to add residues to the template file: just copy and paste the chosen exotic residue from the PDB file where you have it to the end of garlic template file. Be sure to include hydrogen atoms! There is one more thing: be sure that your residue does not have the same residue serial number as the preceding residue. You don't have to worry about the position and the orientation of your residue.

If you don't have the file residues.pdb, click here for HTML version. It is very easy to convert this version to the plain PDB, just save it as the plain text.

NOTES

(1) The command REPLACE resets the editing mode to default (no editing).

RELATED COMMANDS

Use the command SELECT to define the residues which should be replaced and SEQUENCE to define the residues which will be used as replacement.

RES, RESTRICT

NAME

RES, RESTRICT - restrict the current selection.

SYNOPSIS

RES chain_identifiers/residue_serials/residue_names/atom_names
RES residue_ranges
RES residue_names
RES ATO atomic_ranges
RES keyword
RES ELE chemical_symbol
RESTRICT chain_identifiers/residue_serials/residue_names/atom_names
RESTRICT residue_ranges
RESTRICT residue_names
RESTRICT ATOMS atomic_ranges
RESTRICT keyword
RESTRICT ELEMENT chemical_symbol

DESCRIPTION

Restrict the current selection. Atoms which do not satisfy the specified cryteria are excluded from selection. Four types of restriction cryteria may be used:

(1) detailed selection;
(2) restriction by residue serial numbers;
(3) restriction by residue names;
(4) restriction selection (by keyword);
(5) restriction by chemical symbol;
(6) restriction by atom serial number.

DETAILED RESTRICTION

In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The string should contain exactly three slashes, separating different data types:

chain_identifiers/residue_serials/residue_names/atom_names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to specify all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from restriction.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from restriction.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from restriction. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical

symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to specify all atoms, while EXC may be used to exclude some atoms from this specification. Examples:

res a/*/*/*	Leave only atoms which belong to chain A.
res * exc m/*/*/ca	Leave only CA atoms which belong to chain M.
res */*/*/* exc ca,c,n,o	Remove CA, C, N and O atoms from the selection.
res a/* exc 72-112/*/ca	Leave only CA atoms which belong to chain A, but exclude residues 72-112.

RESTRICTION BY RESIDUE SERIAL NUMBERS

In this type of selection restriction, residue numbers, residue ranges or residue names may be specified. The restriction cryteria should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

res 1-100	Leave only atoms which belong to residues from 1 to 100.
res 1-100 exc 20-40	Leave only atoms which belong to residues 1-100, but exclude 20-40.
res 1, 4, 8, 11-48 exc 20-32	Leave atoms which belong to residues 1, 4, 8, 11-48 but exclude residues 20-32.

RESTRICTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

res phe,tyr,trp	Restrict selection to PHE, TYR and TRP.

RESTRICTION BY ATOMIC SERIAL NUMBERS

To restrict the current selection to a single atom by the atomic serial number, combine the command RES (RESTRICT) and the keyword ATO (ATOMS). For example, to restrict the selection to the atom number 102 type:

res ato 102

The same keyword may be used to restrict the current selection to a range of atoms or to two or more ranges. Examples:

res ato 1-100	Restrict the current selection to atoms which have serial numbers in the range between 1 and 100.
res 1-20 40-50	Restrict the current selection to atoms which have serial numbers between 1 and 20 and between 40 and 50.

Do not combine the keywords EXC (EXCLUDE) and ATO (ATOMS).

SPECIAL RESTRICTION KEYWORDS

Some special keywords may be combined with RES to specify residues or atoms according to some

properties. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted. COM (COMPLEMENT) may be specified, but restriction to complement means that nothing will be left in the selection. Examples:

res * res all	Leave the selection unchanged (trivial, useless).
res abo res above	Restrict to atoms above the plane.
res aci res acidic	Leave only acidic amino-acids in the selection (GLU and ASP).
res ali res aliphatic	Leave only aliphatic amino acids (ILE, LEU and VAL).
res alt	Restrict to atoms at alternate positions.
res bad	Restrict selection to bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
res bas res basic	Leave only basic amino acids (ARG, LYS and HIS).
res bel res below	Restrict to atoms below the plane.
res cha res charged	Leave only charged amino acids (ARG, LYS, HIS, GLU and ASP).
res cis	Restrict selection to cis residues.
res com res complement	Leave only atoms which were not select previously.
res het res hetero	Leave only hetero atoms (heme groups, water etc.).
res pho res hydrophobic	Leave only hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
res mai res main_chain	Leave only main chain atoms (CA, C, N and O).
res mod serial_number res model serial_number	Restrict to a model specified by serial_number. NMR structure is a set of models. Example: res mod 1
res neg res negative	Leave only negatively charged amino acids (GLU and ASP).
res pol res polar	Leave only polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
res seq res sequence	Restrict to sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
res pos res positive	Leave only positively charged amino acids (ARG, LYS and HIS).
res sid res side_chains	Leave only atoms which belong to side chains (all except CA, C, N and O).

res sma res small	Leave only small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
res sph res sphere	Restrict to the atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
res tin res tiny	Leave only tiny amino acids (GLY,ALA and SER).
res tra res trans	Restrict selection to trans residues.
sel tri sel triplet	If there are three (or more) positively charged residues in a fragment of up to five protein residues, restrict the current set of selected atoms to these three residues. Detailed explanation may found in the article: D. Juretic, L. Zoranic and D. Zucic, Basic charge clusters and predictions of membrane protein topology, Journal of Chemical Information and Computer Sciences 42, No. 3, 620-632 (2002).

RESTRICTING SELECTION TO THE SPECIFIED CHEMICAL ELEMENT

To restrict the selection to certain chemical element, use the keyword ELEMENT (short form: ELE) and the standard chemical symbol. To restrict your selection to iron atoms, for example, you should type the following command:

res ele fe

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and "quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1. The interatomic distance is not important! Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. Note that symbols J and Q are not used in the periodic table of elements.

NOTES

(1) The command RESTRICT resets the editing mode to default (no editing).

RELATED COMMANDS

SELECT overwrites the previous selection. ADD expands the previous selection.

ROT, ROTATE

NAME

ROT, ROTATE - rotate the structure for the given angle around the given axis.

SYNOPSIS

ROT axis angle

DESCRIPTION

Rotate the structure. The axis should be specified with one letter (x, y or z) and the angle should be given in degrees.

EXAMPLES

COMMAND	DESCRIPTION
rot z 90	Rotate around z for 90 degrees (counterclockwise).
rot x -0.5	Rotate around x for -0.5 degrees (clockwise).

SAV, SAVE

NAME

SAV, SAVE - save atomic data to the specified file.

SYNOPSIS

SAV file_name
SAV file_name SEL
SAVE file_name
SAVE file_name SEL

DESCRIPTION

Save atomic data to the specified file. By default, all atoms are saved. If keyword SEL is used, only selected atoms are saved. No header is written, just ATOM and HETATM records. You may copy and paste the header from the original (input) file. Coordinates will be expressed in the internal coordinate system (the geometric center used as the origin). Don't forget that unix (linux) file names are case sensitive. If the specified file exists already, it will be overwritten without warning!

RELATED COMMANDS

LOA (LOAD) loads the specified structure. DIS (DISCARD) discards the specified structure.

SCA, SCALE

NAME
SCA, SCALE - select hydrophobicity scale.

SYNOPSIS
SCA keyword
SCALE keyword

DESCRIPTION
The command SCALE selects the specified hydrophobicity scale. At present, three scales are available: Eisenberg normalized consensus scale, Kyte-Doolittle hydropathy scale and White octanol scale (experimental). The scale is assigned to the structure which is currently being handled (the structure which was caught using the command CATCH). It is also used as default hydrophobicity scale for the sequence in the main sequence buffer. The hydrophobicity scale is used to calculate the averaged hydrophobicity and hydrophobic moment. It may be also used to color the protein structure according to hydrophobicity.

Hard-coded program default is Eisenberg scale.

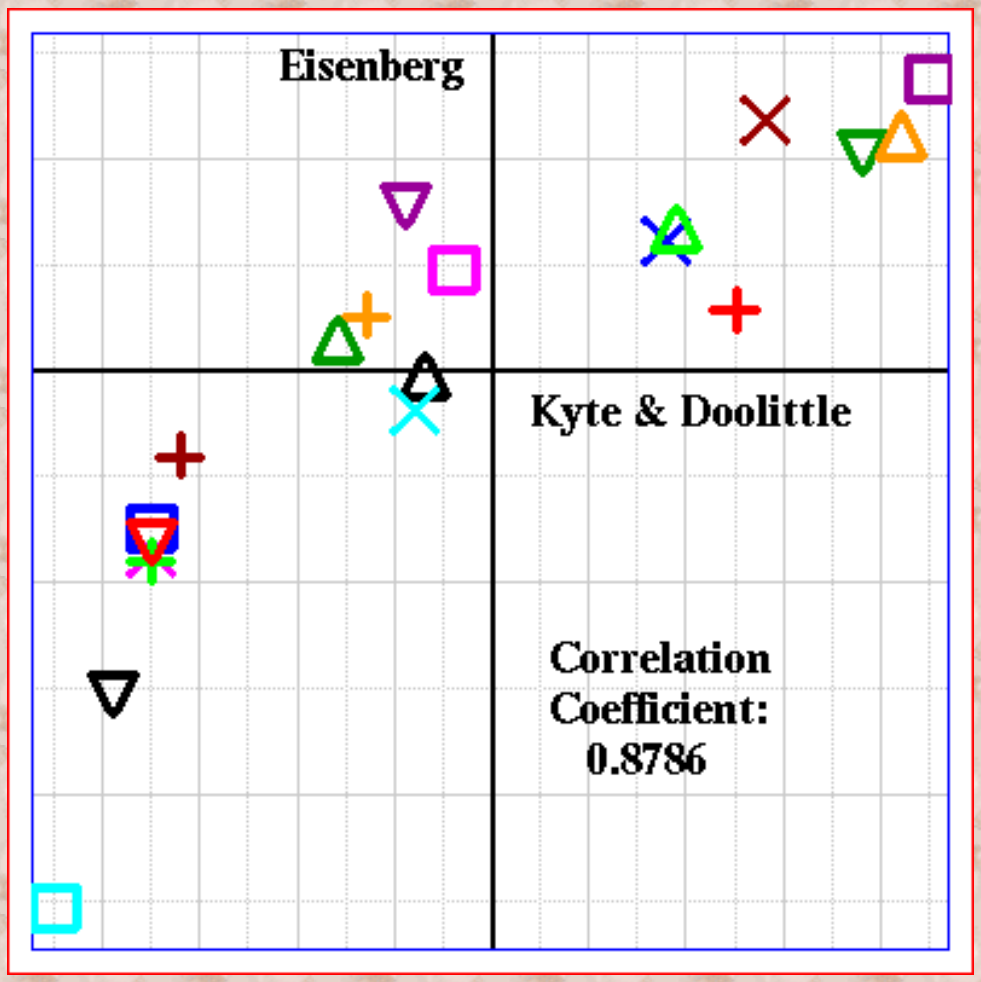
KEYWORDS

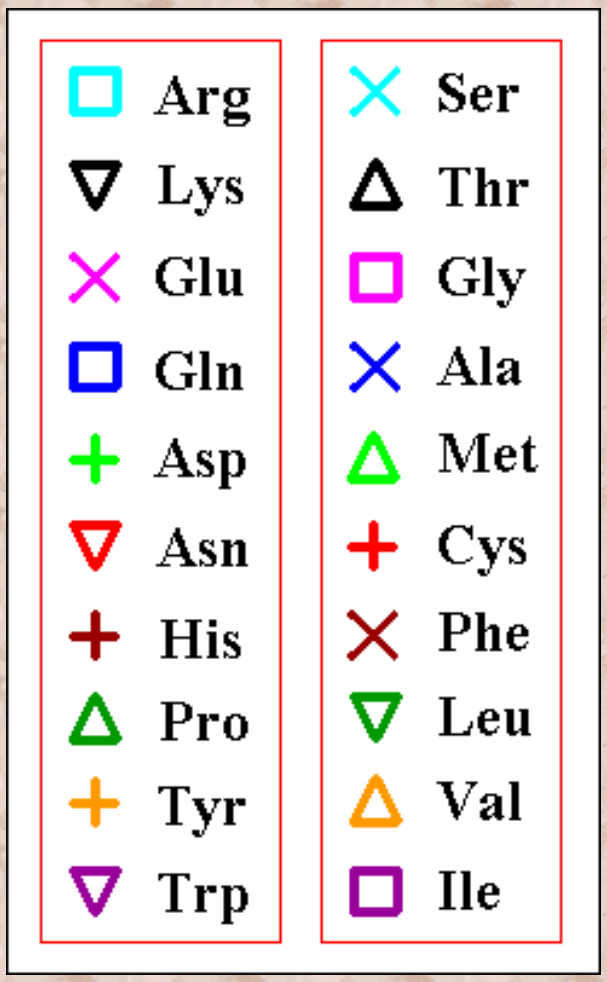
KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
EIS	EISENBERG	Use Eisenberg normalized consensus hydrophobicity scale.
KD	KD	Use Kyte-Doolittle hydropathicity scale.
WHI	WHITE	Use octanol scale (Steven White group, experimental data).

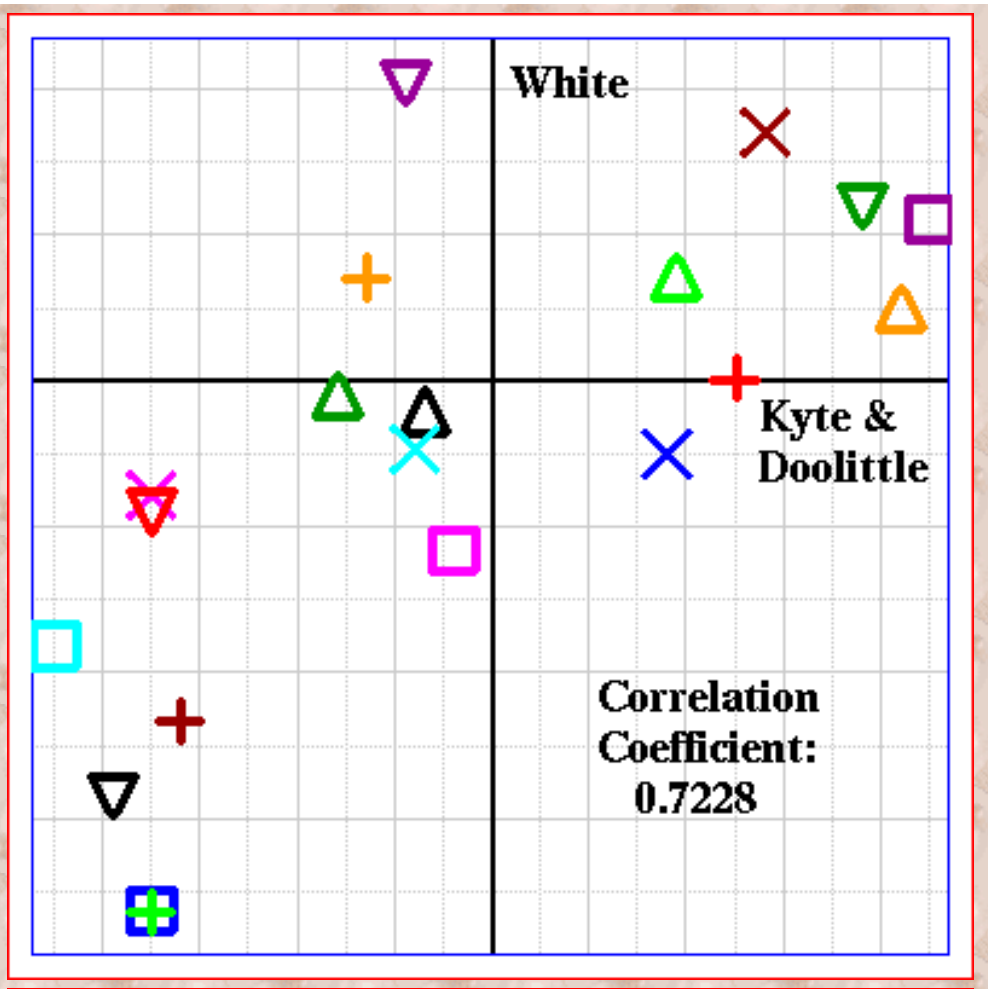
HYDROPHOBICITY SCALES
The table below contains numeric data for three hydrophobicity scales which are used in garlic. Correlation coefficients and plots are also given. The original White octanol scale contains free energy changes for a transfer of whole residues from water to octanol. In garlic, these free energy changes are multiplied by minus one and used as hydrophobicity values. The experimental values and nice theoretical explanations may be found at:
http://blanco.biomol.uci.edu/hydrophobicity_scales.html

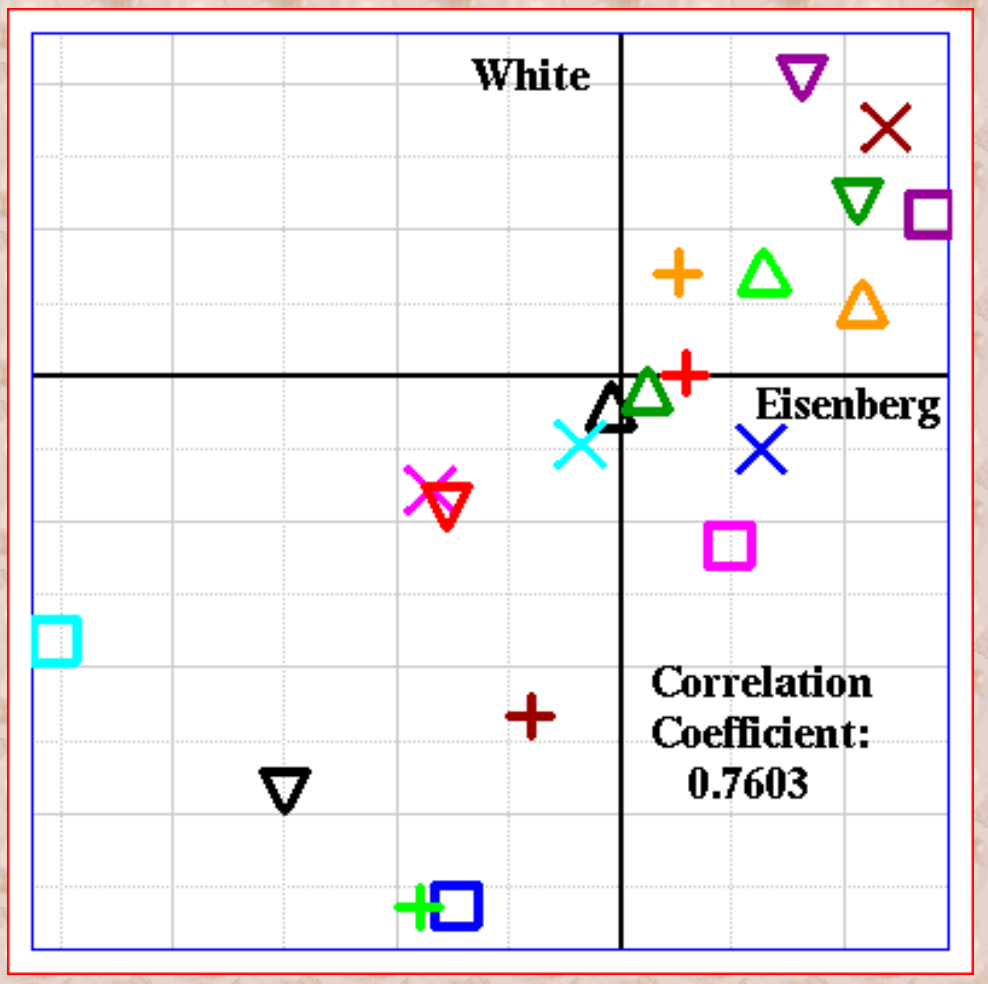
NAME	EIS	KD	WHI
ALA	0.62	1.80	-0.50
ARG	-2.53	-4.50	-1.81
ASN	-0.78	-3.50	-0.85
ASP	-0.90	-3.50	-3.64
CYS	0.29	2.50	0.02
GLN	-0.85	-3.50	-0.77
GLU	-0.74	-3.50	-3.63
GLY	0.48	-0.40	-1.15
HIS	-0.40	-3.20	-2.33
ILE	1.38	4.50	1.12
LEU	1.06	3.80	1.25
LYS	-1.50	-3.90	-2.80
MET	0.64	1.90	0.67
PHE	1.19	2.80	1.71
PRO	0.12	-1.60	-0.14

SER	-0.18	-0.80	-0.46
THR	-0.05	-0.70	-0.25
TRP	0.81	-0.90	2.09
TYR	0.26	-1.30	0.71
VAL	1.08	4.20	0.46
ASX	-0.84	-3.50	-2.25
GLX	-0.80	-3.50	-2.20
UNK	0.00	-0.49	-0.52






White
Kyte &
Doolittle
Correlation
Coefficient:
0.7228


White
Eisenberg
Correlation
Coefficient:
0.7603

EXAMPLES

COMMAND	DESCRIPTION
sca eis	Use the scale made by David Eisenberg.
sca whi	Use the experimental scale made by Steven White and coworkers.

NOTES

(1) Many hydrophobicity scales may be found in literature. However, most of these scales are mutually highly correlated.

RELATED COMMANDS

PLOT is used to draw averaged hydrophobicity and hydrophobic moment. COLOR HYPHOB is used to color the structure according to hydrophobicity of residues.

REFERENCES

(1) Kyte, J. and Doolittle, R. F. (1982). J. Mol. Biol. 157, p. 105.
(2) Eisenberg, D., Schwarz, E., Komaromy, M. and Wall, R. (1984). J. Mol. Biol. 179, p. 125.
(3) Wimley, W. C. and White, S. H. (1996). Nature Struct. Biol. 3, p. 842.
(4) Wimley, W. C., Creamer, T. P. and White, S. H. (1996). Biochemistry 35, p. 5109.
(5) White, S. H. and Wimley, W. C. (1998). Biochim. Biophys. Acta 1376, p 339.
(6) White, S. H. and Wimley, W. C. (1999). Annu. Rev. Biophys. Biomol. Struc. 28, p. 319.

SEL, SELECT

NAME

SEL, SELECT - select specified atoms. Overwrite the previous selection.

SYNOPSIS

SEL chain_identifiers/residue_serials/residue_names/atom_names
SEL residue_ranges
SEL residue_names
SEL ATO atomic_ranges
SEL keyword
SEL ELE chemical_symbol
SELECT chain_identifiers/residue_serials/residue_names/atom_names
SELECT residue_ranges
SELECT residue_names
SELECT ATOMS atomic_ranges
SELECT keyword
SELECT ELEMENT chemical_symbol

DESCRIPTION

Select specified atoms. Atoms are selected according to the specified cryteria. Six types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword);
(5) selection by chemical symbol;
(6) selection by atom serial number.

DETAILED SELECTION

In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain_identifiers/residue_serials/residue_names/atom_names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical

symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

sel a/*/*/*	Select all atoms from chain A.
sel * exc m/*/*/ca	Select CA atoms from all chains except chain M.
sel */*/*/* exc ca,c,n,o	Select all atoms except CA, C, N and O.
sel a/* exc 72-112/*/ca	Select CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

sel 1-100	Select residues from 1 to 100.
sel 1-100 exc 20-40	Select residues 1-100 but exclude 20-40.
sel 1, 4, 8, 11-48 exc 20-32	Select residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY ATOMIC SERIAL NUMBERS

To select a single atom by the atomic serial number, combine the command SEL (SELECT) and the keyword ATO (ATOMS). For example, to select the atom number 102 type:

sel ato 102

The same keyword may be used to select a range of atoms or two or more ranges. Examples:

sel ato 1-100	Select atoms which have serial numbers in the range between 1 and 100.
sel 1-20 40-50	Select atoms which have serial numbers between 1 and 20 and between 40 and 50.

Do not combine the keywords EXC (EXCLUDE) and ATO (ATOMS).

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

sel phe,tyr,trp	Select PHE, TYR and TRP.

SPECIAL SELECTION KEYWORDS

Some special keywords may be combined with SEL (SELECT) to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

sel * sel all	Select all atoms (select all).

sel abo sel above	Select atoms above the plane.
sel aci sel acidic	Select acidic amino acids (GLU and ASP).
sel ali sel aliphatic	Select aliphatic amino acids (ILE, LEU and VAL).
sel alt	Select atoms at alternate positions.
sel bad	Select bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
sel bas sel basic	Select basic amino acids (ARG, LYS and HIS).
sel bel sel below	Select atoms below the plane.
sel cha sel charged	Select charged amino acids (ARG, LYS, HIS, GLU and ASP).
sel cis	Select cis residues.
sel com sel complement	Select atoms which were not selected previously.
sel het sel hetero	Select hetero atoms (heme groups, water etc.).
sel pho sel hydrophobic	Select hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
sel mai sel main_chain	Select main chain atoms (CA, C, N and O).
sel mod serial_number sel model serial_number	Select model specified by serial_number. NMR structure is a set of models. Example: sel mod 1
sel neg sel negative	Select negatively charged amino acids (GLU and ASP).
sel pol sel polar	Select polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
sel pos sel positive	Select positively charged amino acids (ARG, LYS and HIS).
sel seq sel sequence	Select sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
sel sid sel side_chains	Select atoms which belong to side chains (all except CA, C, N and O).
sel sma sel small	Select small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
sel sph sel sphere	Select atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
sel tin sel tiny	Select tiny amino acids (GLY, ALA and SER).

sel tra sel trans	Select trans residues.
sel tri sel triplet	If there are three (or more) positively charged residues in a fragment of up to five protein residues, select them. Detailed explanation may found in the article: D. Juretic, L. Zoranic and D. Zucic, Basic charge clusters and predictions of membrane protein topology, Journal of Chemical Information and Computer Sciences 42, No. 3, 620-632 (2002).

SELECTING CHEMICAL ELEMENTS

To select certain chemical element, use the keyword ELEMENT (short form: ELE) and the standard chemical symbol. To select iron, for example, you should type the following command:

sel ele fe

In addition to real chemical elements, garlic accepts two imaginary elements: "jellium" (J) and "quarkonium" (Q). Jellium is inert and it never binds to neighboring atoms, no matter how close they are. Quarkonium binds to other quarkonium atoms which have adjacent atomic serial numbers. For example, if some quarkonium atom has serial number i, it may form bonds with quarkonium atoms i-1 and i+1. The interatomic distance is not important! Both elements were introduced to enable drawing of special objects. Quarkonium may be used to draw polygonal lines in three dimensions. The original idea was to adapt garlic for visualization of some medical data. For example, quarkonium may be used to represent blood vessels and jellium to represent retraction balls characteristic for broken axons in human brain. By the way, quarkonium is a serious thing in high energy physics, but there it looks quite different. Note that symbols J and Q are not used in the periodic table of elements.

NOTES

(1) The command SELECT resets the editing mode to default (no editing).

RELATED COMMANDS

ADD expands the previous selection. RESTRICT restrics the previous selection.

SEQ, SEQUENCE

NAME

SEQ, SEQUENCE - manipulate the content of the sequence buffer.

SYNOPSIS

SEQ = three_letters_code
SEQ LOAD filename
SEQ READ filename
SEQ FROM structure_identifier
SEQ COPY
SEQ SAVE filename
SEQ SWN filename
SEQ RESET

DESCRIPTION

The command SEQ (long form: SEQUENCE) manipulates the content of the main sequence buffer. Garlic mantains two sequence buffers: the main buffer and the reference buffer. The main sequence buffer is used to prepare the average hydrophobicity plot, the hydrophobic moment plot, helical wheel plot and for some other operations which require the sequence information. The reference sequence buffer is used for sequence comparison and other operations which require two sequences.

Both buffers store the following sequence information:
(1) The number of residues.
(2) The sequence in the form of three letters code. Uppercase letters are used.
(3) Disulfide bond flag, if information about disulfide bonds is available.
(4) Residue serial numbers.
(5) Raw hydrophobicity values (replaced by average value for exotic residues).

In addition, the main sequence buffer contains the following information:
(6) The average hydrophobicity. width.
(7) The hydrophobic moment.

As sequence information may be given independently from any structure, atomic coordinates are not required for most sequence manipulation routines. Thus, garlic may be used as the sequence analysing tool.

All version of the command SEQ, except one, are used to manipulate the content of the main sequence buffer. The only exception is SEQ COPY, which copies the content of the main sequence buffer to the reference buffer. This is the only way to store information to the reference buffer.

SEQ = three_letters_code

The command SEQ may be used with the keyword = (equal sign) to define sequence at garlic command prompt. This may be practical to define a short sequence fragment. This fragment may be used for helical wheel plot, or to locate the given sequence fragment in a structure which is being investigated. The syntax:

SEQ = three_letters_code

Example:

seq = ala phe tyr trp asn

The sequence fragment will be converted to uppercase. The sequence is not checked for exotic residues so you can use the non-standard codes. However, the routine which assigns the hydrophobicity values will fail to recognize them. The average hydrophobicity value (calculated for the current scale) will be assigned to these residues. At present, 23 codes are recognized:

```
ALA, CYS, LEU, MET, GLU, GLN, HIS, LYS, VAL, ILE,
PHE, TYR, TRP, THR, GLY, SER, ASP, ASN, PRO, ARG,
ASX, GLX, UNK.
```

SEQ LOAD filename

The keyword LOAD (or READ, short forms LOA and REA) may be used to read the sequence from the specified file. Garlic is capable to recognize two types of input file formats: FASTA files (one letter code) and files which contain three letters code in a free format.

If input file contains the symbol > (greater than) in the first column of the first useful line, the file is treated as one letter protein code in FASTA format. Empty lines are ignored. The lines beginning with the symbol # (numbersign) in the first column are treated as comments (ignored too). Thus, the lines which are not empty and do not contain the symbol # in the first column are treated as useful.

If input file is not recognized as FASTA file, it is expected to contain the three letters code in a free format. Empty lines and all lines which contain # in the first column are ignored. All other lines are treated as useful. Digits (serial numbers, for example) are ignored. The following characters are threated as separators:
(1) space
(2) tab
(3) comma (,)
(4) semicolon (;)
(5) newline (line feed)

If input file contains at least one bad code (a residue name which consists of four letters, for example) the reading will fail. The hard-coded maximal number of residues is 20000, but it may be easily changed (see MAXRESIDUES in the header file defines.h).

Example:
load sample.fasta

SEQ FROM structure_identifier

The keyword FROM (short form: FRO) may be used to copy the sequence from the specified structure to the main sequence buffer. Only selected residues are copied. Residue is treated as selected if the first atom is selected. For proteins, this is typically N (nitrogen). Residue insertion codes are ignored! Thus, the same residue serial index (number) may appear more than once in the array of residue serial numbers.

Example:
seq from 1

SEQ COPY

The command SEQ COPY (short form: SEQ COP) copies the sequence from the main sequence buffer to the reference buffer. This is the only way to initialize the reference buffer. This command must be executed (i.e., the keyword COPY must be used) before executing commands which require two sequences for proper operation. The main sequence buffer may be initialized prior to SEQ COPY by using one of the keywords described above (=, LOAD or FROM).

Example:
seq copy

SEQ SAVE filename

The command SEQ SAVE (short form: SEQ SAV) saves the sequence to the specified file. Ten codes (each consisting of up to three letters) are written per line, separated by space. Serial numbers are not included (but see the keyword SWN).

Example:
seq save 9pap.seq

SEQ SWN filename

The command SEQ SWN saves the sequence to the specified file. Both residue names and serial numbers are written to the output file. Insertion codes will be missing! Five serial numbers and residue names are written per line, separated by space.

Example:
seq swn 9pap.seq

SEQ RESET

Reset (clear) the main sequence buffer. The command SEQ RESET (short form: SEQ RES) sets the number of residues in the main sequence buffer to zero. The storage is not freed, so the buffer may be used again later.

Example:
seq reset

RELATED COMMANDS

PLOT prepares the average hydrophobicity and/or hydrophobic moment plot. COMPARE compares two sequences. VENN draws Venn diagram. WHEEL draws helical wheel plot. SEL SEQ selects portions of the structure which contain the sequence stored to the main sequence buffer. To use any of these commands, the main sequence buffer (to use COMPARE both buffers) must be initialized by using the command SEQ. STR defines the secondary structure and CREATE may be used to create a new peptide.

SHO, SHOW

NAME
SHO, SHOW - show selected atoms.

SYNOPSIS
SHO
SHOW

DESCRIPTION
Show selected atoms and associated bonds. Atoms and bonds drawn using style "0" will remain unvisible, but they are formally treated as visible.

RELATED COMMANDS
HIDE hides selected atoms and associated bonds.

SLA, SLAB

NAME
SLA, SLAB - change slab.

SYNOPSIS
SLA keyword
SLA FRONT shift
SLA BACK shift
SLAB keyword
SLAB FRONT shift
SLAB BACK shift

DESCRIPTION
Change the slab. Slab is used to cut the slice out from the structure and to hide the rest. Two slab surfaces are used: the front slab surface, which is the one closer to the observer and the back slab surface. There are three versions of this command:

(1) SLAB FRONT shift ----> move the front slab surface;
(2) SLAB BACK shift ----> move the back slab surface;
(3) SLAB keyword ----> switch slab off or change the type of the surfaces.

SLAB FRONT shift
This command moves the front slab surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys DEL and ENTER on numeric keypad). The shift value should be given in angstroms. Positive shift moves the front slab surface away from the observer. FRONT may be abbreviated to FRO.

SLAB BACK shift
This command moves the back slab surface. It is recommended to use this command in scripts - in interactive mode, use controls (keys 1 and 3 on the numeric keypad). The shift value should be given in angstroms. Positive shift moves the back slab surface away from the observer. BACK may be abbreviated to BAC.

SLAB keyword
Some keywords may be used to change the type of slab surfaces and to switch slab off. Here is the list of keywords:

SHORT FORM	LONG FORM	DESCRIPTION
OFF	OFF	Switch slab off: all parts of the structure should be visible.
PLA	PLANE	Use planes as slab surfaces
SPH	SPHERE	Use spheres as slab surfaces
CYL	CYLINDER	Use cylinders as slab surfaces
HALF-SPH	HALF-SPHERE	Use spheres as slab surfaces, but hide the back half of the structure.
HALF-CYL	HALF-CYLINDER	Use cylinders as slab surfaces, but hide the back half of the structure.

For most structures, the planar slab is the best choice. Spherical and semi-spherical slab may be useful when working with large globular proteins, while cylindrical and semi-cylindrical slab is useful when working with beta-barrel proteins (like porins). The cylinder axis is parallel to y axis (vertical from users standpoint).

EXAMPLES

COMMAND	DESCRIPTION
slab off	Switch slab off
slab front 4.5	Move the front slab surface 4.5 angstroms away from the observer
slab back -2.8	Move the back slab surface 2.8 angstroms closer to the observer
slab half-sph	Change slab to semi-spherical

SSB

NAME
SSB - change drawing style for disulfide bonds.

SYNOPSIS
SSB style

DESCRIPTION
Change drawing style for disulfide bonds. Disulfide bond style is defined separately from atom style. This command does not affect the ordinary covalent bonds: the command BONDS should be used for that purpose. Note that there is no separate keyword for curved bonds and sticks (nice style): the bond curvature is defined by the command PROBE .

STYLE	THICKNESS	TYPE
0	Unvisible bonds.	Fixed.
1	A single line.	Fixed.
2	Three lines.	Fixed.
3	Five lines.	Fixed.
4	Seven lines.	Fixed.
5	Nine lines.	Fixed.
nic nice	Curved bonds, conical sticks or cylindrical sticks, depending both on the probe radius and the atomic radii. This bond style is available for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2. Do not combine the nice bond style with atomic styles 0, 1, 2, 3, 4, 5, 6, 7, BALL and BA2.	Proportional.

NICE BONDS
Nice bonds may be curved or straight, cylindrical or conical, depending on probe radius. If this radius is small (like 0.8 angstroms), the bonds will be curved. Probe radius of 10 angstroms will give the straight bonds. If you want to draw the chemical bonds as cylindrical sticks, use the same atomic radius for all atoms and a relatively large probe. If your atoms are drawn using different radii, the bonds will appear conical. This is one of the things which make garlic different from most other programs: in garlic, sticks are just the special case of nice bonds. Most other programs are capable to draw just simple cylindrical sticks.

NOTES
(1) Unvisible disulfide bonds (style 0) are not treated as hidden - they are just invisible.

(2) The nice bond style is allowed for ordinary covalent bonds and for disulfide bonds, but not for hydrogen bonds.

(4) Remember that the nice disulfide bond style works only for the following atomic styles: SMALL, SM2, COVALENT, CO2, SPACEFILL, SP2, BIG and BI2.

RELATED COMMANDS

PRO (PROBE) is used to set the probe radius. ATO (ATOMS) is used to change the drawing style for atoms. BONDS is used to change the bond drawing style for the ordinary covalent bonds.

STE, STEREO

NAME

STE, STEREO - switch to stereo mode.

SYNOPSIS

STE
STEREO
STE OFF
STEREO OFF

DESCRIPTION

Switch to stereo mode. If keyword OFF is added, switch stereo off, i.e. switch to mono mode.

RELATED COMMANDS

Use MONO to switch to mono mode. It does exactly the same job as STEREO OFF.

STR, STRUCTURE

NAME
STR, STRUCTURE - manipulate the content of the secondary structure buffer.

SYNOPSIS
STR = one_letter_code
STR LOAD filename
STR READ filename
STR FROM structure_identifier
STR COPY
STR SAVE filename
STR RESET

DESCRIPTION
The command STR (long form: STRUCTURE) manipulates the content of the main secondary structure buffer. Garlic mantains two secondary structure buffers: the main buffer and the reference buffer. The main secondary structure buffer is used to create a new structure and to replace a portion of an existing structure.

Both buffers store the following secondary structure information:
(1) The length of the secondary structure.
(2) The secondary structure (one letter codes). The codes are:

C = coil,
E = strand,
G = 3-10 helix,
H = alpha helix,
T = turn.

As the secondary structure information may be defined independently from any structure, atomic coordinates are not required for most secondary structure manipulation routines.

All version of the command STR, except one, are used to manipulate the content of the main secondary structure buffer. The only exception is STR COPY, which copies the content of the main secondary structure buffer to the reference buffer. This is the only way to initialize the reference buffer.

STR = one_letter_code
The command STR may be used with the keyword = (equal sign) to define the secondary structure at garlic command prompt. This may be practical to define the secondary structure of a short peptide or a small protein. The syntax:

STR = one_letter_code

Example:

str = ccccccchhhhhhhctttteeeeeccccccccccccc

The secondary structure will be converted to uppercase. If at least one bad code is found, the command will fail and the main secondary structure buffer will be left empty. Space, comma and tab may be used as separators.

STR LOAD filename
The keyword LOAD (or READ, short forms LOA and REA) may be used to read the secondary structure from the specified file. The input file should be written in a format similar to FASTA. Empty lines and lines beginning with # will be ignored. The number of codes per line is arbitrary. Example:

```
 1xxx_  mol:protein length:103     Sample secondary structure
CCCCCCCCCCCEEEEEEEEEEEECCCCCCCCCCCHHHHHHHHHHHHHHHHHHHHCCCCCEEEEEEEEECCCCCCCCC
CCCCCCCCHHHHHHHHHHHCCCCCCCCC
```

The following characters are threated as separators:
(1) space
(2) tab
(3) comma (,)

If input file contains at least one bad code (a residue name which consists of four letters, for example) the reading will fail. The hard-coded maximal number of residues is 20000, but it may be easily changed (see MAXRESIDUES in the header file defines.h).

Example:

load secstr.fasta

STR FROM structure_identifier

The keyword FROM (short form: FRO) may be used to copy the secondary structure from the specified atomic structure to the main secondary structure buffer. Only the structure of selected residues is copied. Residue is treated as selected if the first atom is selected. For proteins, this is typically N (nitrogen).

Example:
str from 1

STR COPY

The command STR COPY (short form: STR COP) copies the secondary structure from the main secondary structure buffer to the reference buffer. This is the only way to initialize the reference buffer. This command must be executed (i.e., the keyword COPY must be used) before executing commands which require two secondary structures for proper operation. The main secondary structure buffer may be initialized prior to STR COPY by using one of the keywords described above (=, LOAD or FROM).

Example:
str copy

STR SAVE filename

The command STR SAVE (short form: STR SAV) saves the secondary structure to the specified file. The output file will be written in FASTA format.

Example:
str save 9pap.secstr

STR RESET

Reset (clear) the main secondary structure buffer. The short form is STR RES. The command STR RESET sets the number of codes in the main secondary structure buffer to zero. The storage is not freed, so the buffer may be used again later.

Example:
str reset

RELATED COMMANDS

SEQ may be used to define the sequence. CREATE may be used to create a new peptide.

TAG

NAME
TAG - assign tag (short text) to a structure.

SYNOPSIS
TAG "tag"
TAG OFF

DESCRIPTION
If used without keyword OFF, this command assigns the specified tag to the structure which is currently handled. If used with keyword OFF, this command hides tag. Tag may contain up to 128 characters.

EXAMPLES

COMMAND	DESCRIPTION
tag "PORIN"	Add the tag "PORIN" to a structure which is currently handled (caught)
tag off	Hide tag

RELATED COMMANDS
The command LABELS assigns labels to selected atoms. TITLE adds the title to the main window. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

TBG

NAME
TBG - change the background color used to draw input and output window.

SYNOPSIS
TBG color

DESCRIPTION
Change the background color used to draw input and output window. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted.

This command does not affect the output window in the sequence comparison mode. Check the command COMPARE .

Examples:

COMMAND	DESCRIPTION
tbg white	White
tbg DarkSlateGray	Dark dark slate gray
tbg #3000a0007000	Kind of green
tbg rgb:0/0/8	Dark blue
tbg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
TFG changes the foreground (text) color used in input and output window.

TFG

NAME
TFG - change the color used to draw text in input and output window.

SYNOPSIS
TFG color

DESCRIPTION
Change the color used to draw text in input and output window. The color should be specified in one of the formats recognized by your X server. Both color names and numerical specification are accepted.

This command does not affect the output window in the sequence comparison mode. Check the command COMPARE .

Examples:

COMMAND	DESCRIPTION
tfg white	White
tfg DarkSlateGray	Dark dark slate gray
tfg #3000a0007000	Kind of green
tfg rgb:0/0/8	Dark blue
tfg rgbi:0.0/0.0/0.5	The same dark blue as above

Read the file rgb.txt (in /lib/X11/ directory) and the man page with a general description of the X window system (man X), to learn other color specification standards.

RELATED COMMANDS
TBG changes the background color used to draw input and output window.

TIT, TITLE

NAME

TIT, TITLE - add, move or remove the specified title.

SYNOPSIS

TIT identifier OFF
TIT identifier screen_x screen_y
TIT identifier screen_x screen_y "title_string"
TITLE identifier OFF
TITLE identifier screen_x screen_y
TITLE identifier screen_x screen_y "title_string"

DESCRIPTION

The keyword TITLE may be used to add, move or remove the title to or from the main window. Up to 100 titles may be added to the main window, to explain the content. The title position may be specified through screen_x and screen_y. Each title has the unique identifier. The identifier is a number between 0 and 99 (these two values are allowed too). The title string should be included into quotes.

EXAMPLES

COMMAND	DESCRIPTION
tit 8 50 50 "This is porin"	Add the title number 8 to the main window, close to the top left corner
tit 8 100 400	Move the title number 8 to a new position
tit 8 off	Remove (hide) the title number 8

RELATED COMMANDS

The command LABELS assigns labels to selected atoms. TAG assigns the specified tag to a structure. Both labels and tag move along with the structure. Note that tag is assigned to the structure, labels to atoms and title is assigned to the main window.

TRA, TRANSLATE

NAME

TRA, TRANSLATE - translate the structure for the given shift in the given direction.

SYNOPSIS

TRA axis shift

DESCRIPTION

Translate the structure. The axis should be specified with one letter (x, y or z) and the shift should be given in angstroms.

EXAMPLES

COMMAND	DESCRIPTION
tra x 40	Move to the right, 40 angstroms.
tra y -0.5	Move up, 0.5 angstroms (y points down).

VEN, VENN

NAME

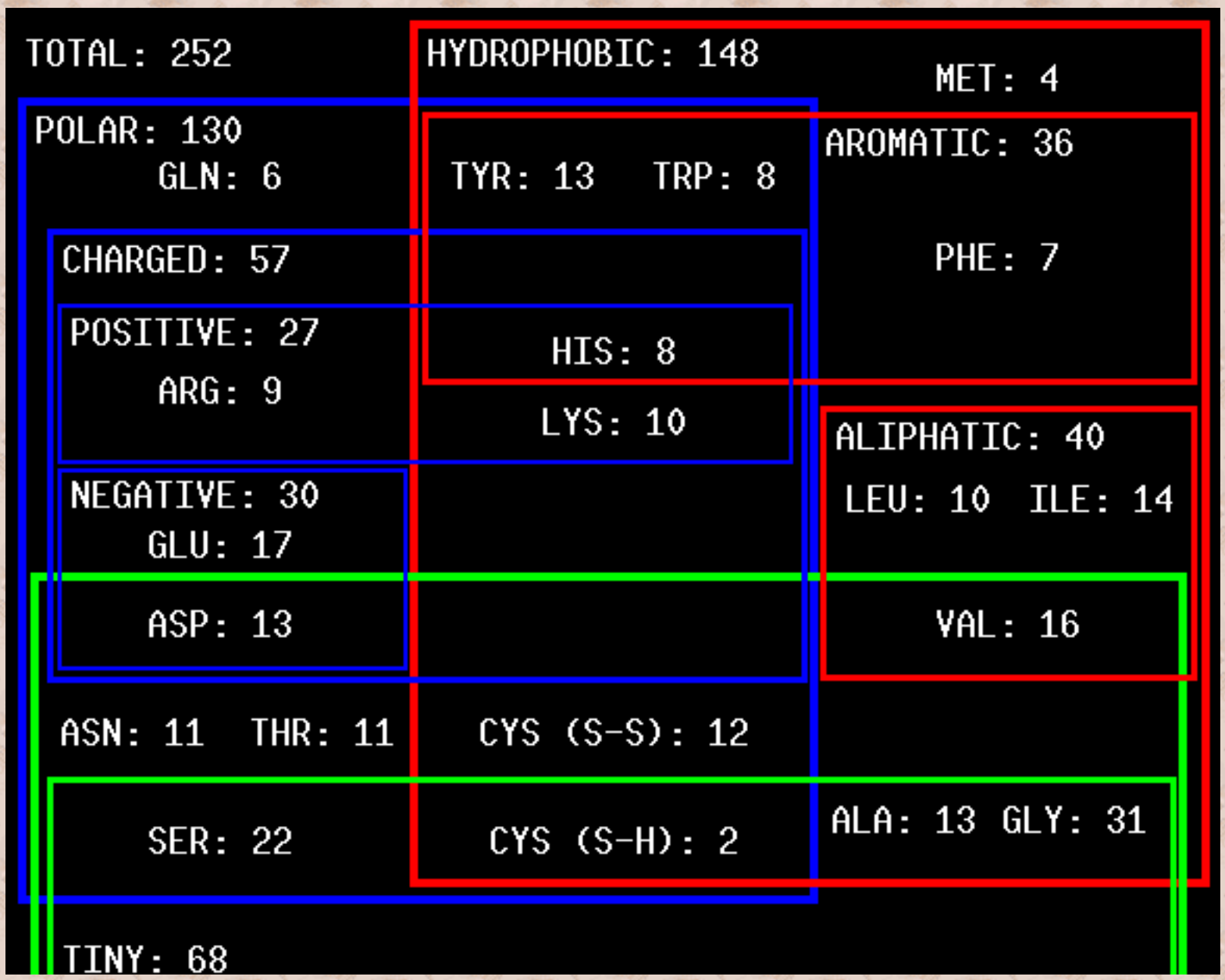
VEN, VENN - draw Venn diagram.

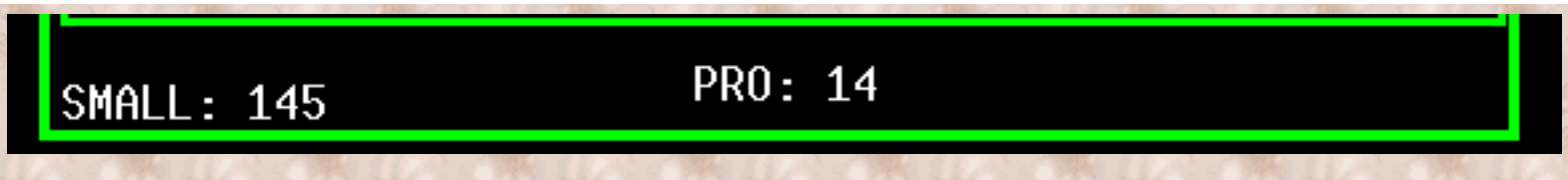
SYNOPSIS

VEN
VEN OFF
VEN start_index end_index
VENN
VENN OFF
VENN start_index end_index

DESCRIPTION

Draw Venn diagram for the given protein sequence or sequence fragment. Venn diagram gives the quick statistical overview of the protein sequence: count of residues and residue types. It is primarily intended for students. Experts will not find this routine very interesting.





KEYWORDS AND PARAMETERS

The command VENN may be used alone, combined with the keyword OFF or with two residue serial indices. If used alone, the Venn diagram will be drawn for the entire sequence stored in the main sequence buffer. Two residue serial indices may be used to specify the residue range. The keyword OFF is used to return to the main drawing mode (structure drawing mode).

EXAMPLES

COMMAND	DESCRIPTION
load 2por.pdb seq from 1 ven	Load the specified structure (porin), copy the sequence from this structure to the main sequence buffer and draw Venn diagram.
ven 1-100	Prepare Venn diagram with counts, but only for residues with serial numbers from 1 to 100.
ven off	Return to default drawing mode. Instead using this command, you can hit the ESCAPE key.

NOTES

(1) Instead using the command VENN OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) Ven diagram is a term from the set theory, which is part of mathematics. Different sorts of Venn diagrams may be found in different branches of science.

(3) If used without any parameters, Venn diagram will be drawn for the entire sequence, including solvent molecules, which are typically included to PDB file after the protein structure. However, these residues will not be included into individual residue counts. If you want to exclude the solvent molecules from Venn diagram, check the serial index of the last protein residue. After that, use the range from residue 1 to this residue (use the actual residue number in the place of last_residue):

ven 1 last_residue

RELATED COMMANDS

SEQUENCE is used to copy, define or load the sequence.

WHE, WHEEL

NAME

WHE, WHEEL - draw helical wheel plot.

SYNOPSIS

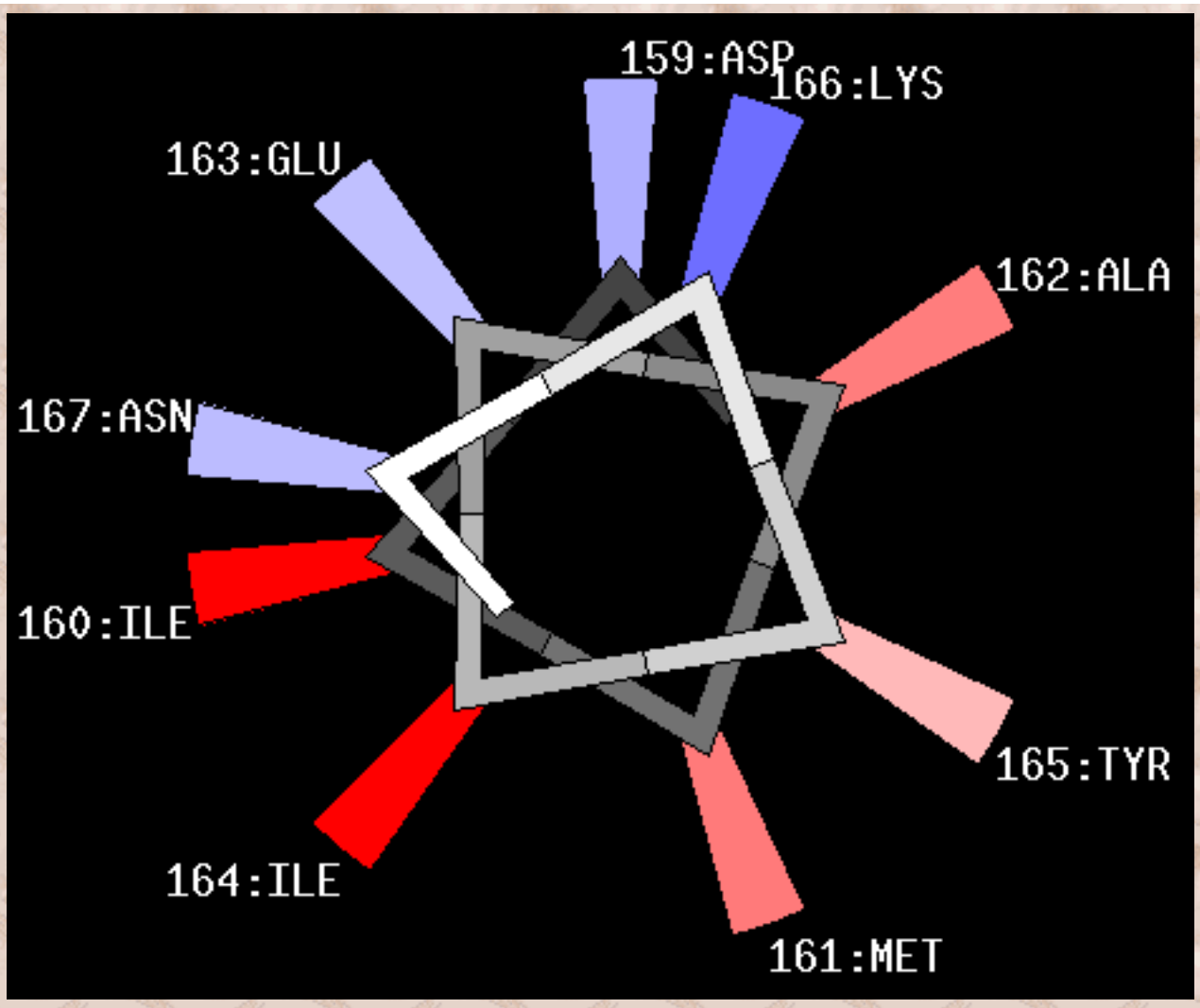
SHORT FORM	LONG FORM
WHE	WHEEL
WHE CLO	WHEEL CLOCKWISE
WHE start_index end_index	WHEEL start_index end_index
WHE start_index end_index CLO	WHEEL start_index end_index CLOCKWISE
WHE OFF	WHEEL OFF

DESCRIPTION

Draw helical wheel plot for the given sequence or sequence fragment. Helical wheel may be used to recognize the amphiphilic character of the specified sequence fragment. The sequence from the main sequence buffer (or part of it) is used as input. Additional input: the rotation angle between adjacent residues and hydrophobicity values. The angle should correspond to certain structural motif. Default (hard-coded) angle is 100 degrees, which corresponds to alpha helix, but this may be changed to some arbitrary value, using the command ANGLE. The value of 160 degrees is suitable for beta strand and 115 or 125 is suitable for 3-10 helix.

While helical wheel may be drawn for any sequence length, it makes sense only for short sequence fragments (up to about twenty residues). Hydrophobic residues will be colored in shades of red, while hydrophilic residues will be colored blue. Color intensity depends on the hydrophobicity: very hydrophobic residues will be intensely red and weakly hydrophobic residues will be almost white. Very hydrophilic residues will be intensely blue and weakly hydrophilic residues will be almost white. The command SCALE may be used to select the hydrophobicity scale.

The command WHEEL is usually used in combination with some other commands. See the examples below.



KEYWORDS AND PARAMETERS

The command WHEEL may be used alone, combined with one of two keywords (OFF and CLOCKWISE) or with two residue serial indices. If used alone, the helical wheel will be drawn for the entire sequence stored in the main sequence buffer. If this sequence is large the plot will be useless. Two residue serial indices may be used to specify the residue range.

By default, residues are drawn counterclockwise. This arrangement of residues gives the top view of a helix. The keyword CLO (long form: CLOCKWISE) may be used to force clockwise arrangement of residues (the bottom view of a helix).

The keyword OFF is used to return to the main drawing mode (the structure drawing mode).

EXAMPLES

COMMAND	DESCRIPTION
seq = asp ile met ala glu ile scale eis angle 100 wheel	Initialize the sequence fragment, select Eisenberg hydrophobicity scale, set angle to 100 degrees and draw helical wheel. It is assumed that that the specified sequence fragment belongs to alpha helix.

load 2por.pdb seq from 1 scale eis angle 160 wheel 2-10	Load porin coordinates, copy the sequence of this protein to the main sequence buffer, select Eisenberg hydrophobicity scale, set angle to 160 degrees and draw helical wheel for residues from 2 to 10. It is assumed that the specified sequence fragment belongs to beta strand.
whe clo	Draw residues clockwise. This gives the bottom view of a helix, which is more common in books.
whe off	Return to default drawing mode. Instead using this command, you can hit the ESCAPE key.

NOTES

(1) Instead using the command WHEEL OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) Don't forget that WHEEL uses only the sequence stored to the main sequence buffer. Read description of the command SEQ (SEQUENCE) to learn how to initialize this buffer.

RELATED COMMANDS

SEQUENCE is used to copy, define or load the sequence. ANGLE defines the rotation angle between adjacent residues. SCALE is used to specify the hydrophobicity scale.

WIN, WINDOW

NAME

WIN, WINDOW - set the sliding window width.

SYNOPSIS

WIN value
WINDOW value

DESCRIPTION

Set the sliding window width. The value is stored as an internal variable and used to calculate and draw average hydrophobicity and hydrophobic moment. The hard-coded default value is 11 residues. The minimal value is 1. The command PLOT may be used to plot the averaged hydrophobicity and/or hydrophobic moment.

EXAMPLES

COMMAND	DESCRIPTION
win 20	Set the sliding window width to 20.
win 8 plot mom	Set the sliding window width to 8 and draw hydrophobic moment.

RELATED COMMANDS

PLOT is used to draw averaged hydrophobicity and/or the hydrophobic moment. ANGLE is used to set the rotation angle between adjacent residues (important for hydrophobic moment, not for averaged hydrophobicity).

Mouse Usage

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

MOUSE USAGE IN DEFAULT MODE

Move the mouse pointer over the structure and you will see the textual information about the atom covered by the pointer. This information will be visible in the output window (the bottom right corner of the main window).

If viewing some large structure (like protein or DNA), the sequence neighborhood of the residue covered by the mouse pointer will be visible in the top portion of the main window (see the example below).

The structure drawing mode is not the only mode where this trick may be used: try also Ramachandran plot, hydrophobicity plots and sequence comparison. The examples below show the content of the output window for all four cases:

Structure display	Ramachandran plot	Averaged hydrophobicity	Sequence comparison
(1) 2POR PHE 192 C 1426 C t.f.: 55.22 phob: 1.19 selected phi: -120.71 psi: 68.12 ome: 178.15 chi1: -62.06 chi2: -42.35 chi3: - x: -5.550 y: -15.344 z: -18.352	(1) 1PRC ILE 145 H trans phi: -87.26 psi: 128.68 omeg: 174.92	GLY 62 value: 0.767	HORIZ. VERT. 23GLY GLY27 24SER SER28 25CYS CYS29 26TRP TRP30 27ALA ALA31 28PHE PHE32 29SER GLY33 30ALA ALA34 31VAL VAL35 32VAL GLU36 33THR ALA37

The image below is an example of the sequence neighborhood. Read the text about the command NEIGHBORHOOD for more information about sequence neighborhood.

USING MOUSE INSTEAD OF KEYBOARD CONTROLS

Mouse clicks may be used for rotations, translations, and for slab and color adjustment. If you want to rotate or translate the structure, or to change slab and color fading, click on a selected button in the control window (the top right corner of the main window). Shift, alt and control play the same role as if keyboard is used for the same job.

Some desktop environments (like KDE and Gnome) use function keys to launch pop-up menus or for some other purpose. This means that function keys F1, F2, F3 and F4 will not work properly with garlic. You can use mouse to click on dummy buttons in a control window. Another approach will be to change the desktop environment settings.

MOUSE USAGE IN EDITING MODE

After executing the EDIT CLICK command, the mouse may be used to pick a single bond for editing. Read the page about the command EDIT to learn how to pick a single bond.

Garlic Reference Card

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic reference card contains the list of commands and keywords, with short description of commands. Print this page and keep it at hand during your garlic sessions. Garlic reference card is not a learning tool, it is just a reminder. Newbies should start with garlic tutorial.

HTML version	**Recommended if your browser is properly configured for printing.**
StarOffice version	**Suitable for Sun StarOffice 5.2 (download via ftp).**
MS Word version	**MS Word 97/2000 format, created with StarOffice (ftp).**
PostScript version	**PostScript level 2 (ftp).**

Garlic Tutorial

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Lessons

These lessons should help you to learn how to use garlic. Command are given in lowercase, in a short form, but you can use the long form as well as the uppercase letters. File names should be specified in the correct case.

RECOMMENDED USAGE: Print lessons.

In addition, you should read the pages describing garlic commands and controls !

Lesson 1 - Get familiar with garlic
Lesson 2 - Load a small structure
Lesson 3 - Playing with two structures
Lesson 4 - Drawing styles and color schemes
Lesson 5 - How to select atoms
Lesson 6 - Ramachandran plot
Lesson 7 - Helical wheel plot
Lesson 8 - Plot averaged hydrophobicity and hydrophobic moment
Lesson 9 - Venn diagram
Lesson 10 - Semitransparent plane
Lesson 11 - Create small structure
Lesson 12 - Replace selected residues

Scripts

The scripts listed below may be used to demonstrate the available drawing styles for atoms and bonds, as well as some predefined color schemes. These scripts were included into the garlic source package 28. March 2000. If you have an older package, copy these scripts to your local host. There are two ways to copy scripts:
(1) Click here to download them via ftp.
(2) Go to the page which contains the script you selected. Mark and copy the script. Paste it into a local file. Recommended file names: 1: atoms.script, 2: bonds.script, 3: colors.script, 4: dance.script .

Script 1 - Drawing styles for atoms
Script 2 - Drawing styles for bonds
Script 3 - Predefined (hard-coded) color schemes
Script 4 - Dancing tryptophan

Garlic Tutorial

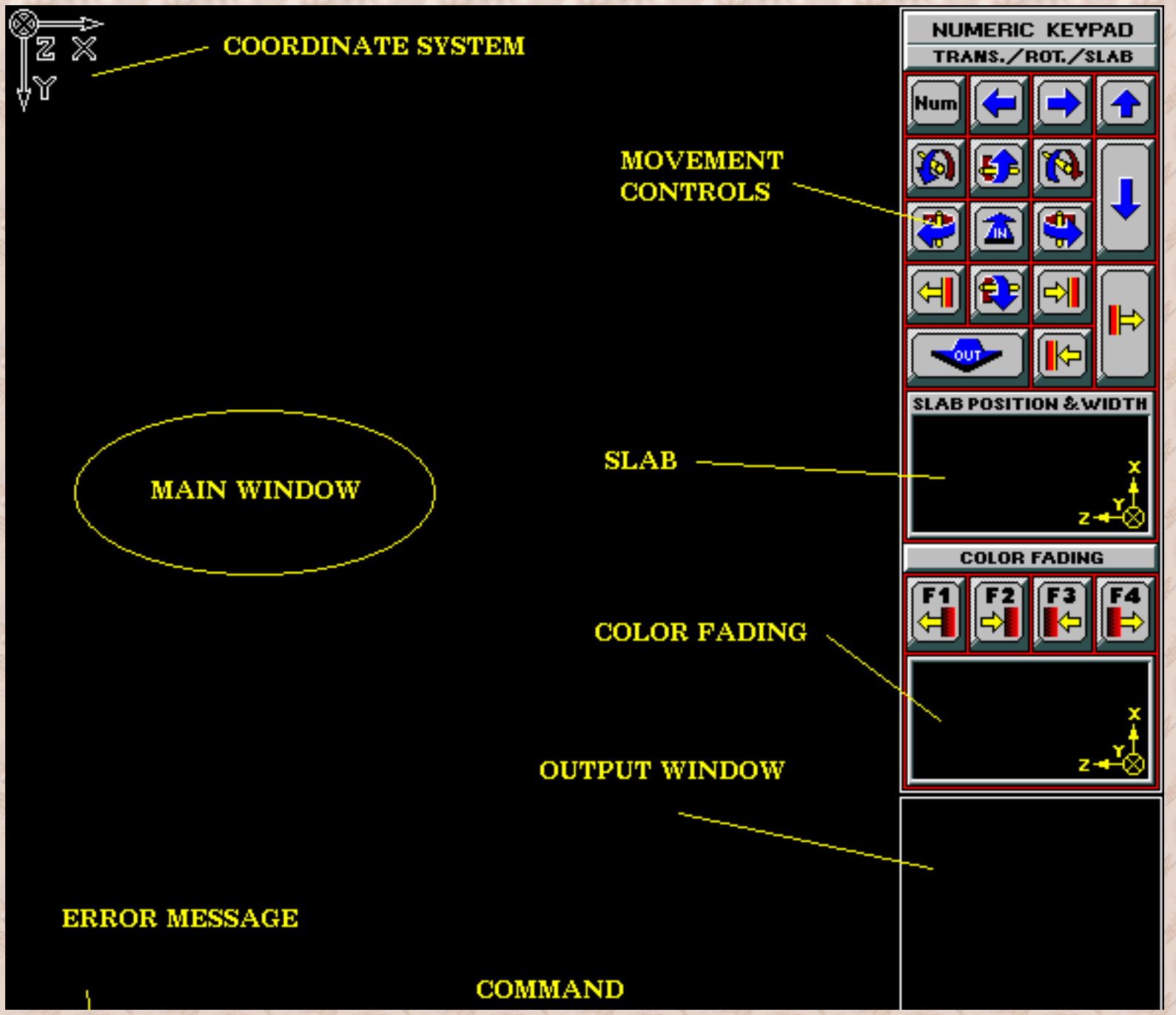
Lesson 1 - Get Familiar with Garlic

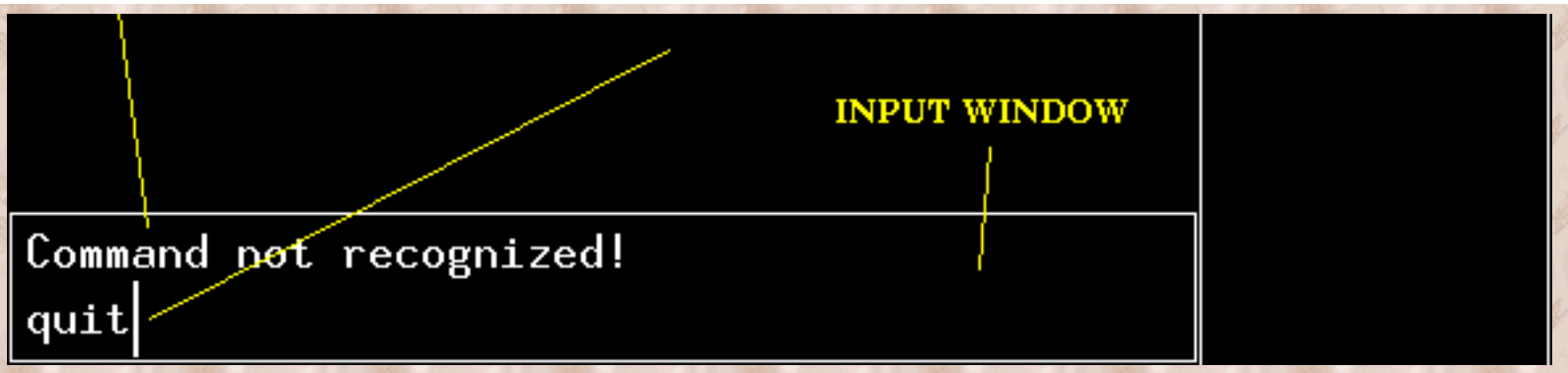
In this lesson, you will execute only one command at garlic prompt: exit, to quit the garlic session.

Start your X session. Use the terminal window to start garlic:

garlic

If garlic is in the path searched by your shell, the garlic window will appear on your screen. Try to remember what are the parts of the entire garlic window. The input window will be empty, but the image below is adapted to show the area reserved for error messages and the area reserved for commands.





When you have learned what are the main parts of the garlic window, quit your garlic session by typing exit or quit (exi or qui):

exit

Garlic Tutorial

Lesson 2 - Load a Small Structure

In this lesson, you will learn how to load a PDB file and how to move the structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load tryptophan (it should be included in the source package). This command should be executed at garlic prompt:

loa trp.pdb

Step 3 - how to use the pointing device (mouse):

Move the mouse pointer over atoms and bonds and read the text which appears in the output window (bottom right corner). Note that half of each bond is assigned to each of two atoms involved in bond formation.

Step 4 - use garlic controls (i.e. the keys on numeric keypad) to rotate the structure (just a single amino acid):

First play for a while with keys 4 and 6, then with 2 and 8, and finally with 7 and 9. Try the same while holding shift (alone), control (alone), alt and shift (simultaneously) and control and shift (simultaneously). Do not try control-alt combinations, unless you are very experienced with unix and X.

Step 5 - use garlic controls (numeric keypad) to translate the structure:

PC keyboard: use /, *, -, +, 5 and 0.
Terminal keyboard: use PF2, PF3, -, comma, 5 and 0.
Repeat while holding modifier keys (alone or in combination).

Step 6 - move the structure to the screen center again:

pos 0 0 0

Step 7 - rotate and translate the structure using commands instead of controls. Try the following set of commands:

rot x 90
tra x 4
tra y -4
tra z -50
rot y 180

Step 8 - move the color surfaces. As your structure is very small, be sure to hold the control key while pressing functions keys:

Hold control key and press F1.
Hold control key and press F4.
Note that color is changing.

Hold control key and play with F1, F2, F3 and F4 for a while.

Step 9 - move the slab surfaces. As your structure is very small, be sure to hold the control key:

Hold control key and 3 (numeric keypad). Repeat until some atoms and bonds disappear.
Hold control key and play with 1, 3, decimal separator (next to 0) and enter for a while. Note that (in control window) visible atoms are red and unvisible atoms are dark cyan.

Step 10 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 3 - Playing with Two Structures

In this lesson, you will learn how to work with two or more structures. The original source package contains two PDB files: trp.pdb and phe.pdb. Each contains a single amino acid: trp.pdb = tryptophan, phe.pdb = phenylalanine. In this lesson, tryptophan will be colored blue, while phenylalanine will be colored red. Note the role of the command cat (catch).

Step 1 - start garlic (if necessary):

garlic

Step 2 - load trypthophan:

loa trp.pdb

Step 3 - change TRP color to blue:

col blue

Step 4 - load phenylalanine:

loa phe.pdb

Step 5 - change PHE color to red:

col red

Two structures will be distinguished by color and by the identifier: tryptophan is treated as structure number 1, and phenylalanine is treated as structure number 2. Two structures are now overlapping.
Step 6 - move tryptophan to the left:

cat 1
pos -5 0 0

Step 7 - move phenylalanine to the right:

cat 2
pos 5 0 0

Step 8 etc. - use the command cat (catch) to rotate structures one by one:

Use cat 1 and cat 2 to catch and rotate structures, one by one.
Translate both structures to the position where they will be overlapped, but do not use keyword pos!

When finished, discard loaded structures:

dis all

Garlic Tutorial

Lesson 4 - Drawing Styles and Color Schemes

In this lesson, you will learn different drawing styles, used for atoms and bonds. Note that garlic uses separate styles for atoms and bonds. You will also try some predefined color schemes. Use the X server which offers 24 bits per pixel, if possible.

As you will often reuse some commands, just with a different argument, note that garlic has a history buffer, where commands which were previously used are stored. The arrow keys may be used to recall one of these commands.

Use the "UP" arrow to scan the history buffer backwards, "DOWN" arrow to scan it upwards, "LEFT" arrow to move the insertion mark left and "RIGHT" arrow to move the insertion mark to the right (if possible, of course). Backspace (or delete, if you have some unusual keyboard mapping) may be used to remove characters.

Step 1 - start garlic (if this wasn't done before):

```
garlic
```

Step 2 - load trypthophan and bring it closer to you:

```
loa trp.pdb
pos 0 0 -150
```

Step 3 - make bonds unvisible (i.e. set bond thickness to zero):

```
bon 0
```

Step 4 - learn which drawing styles are available for atoms.
Hint: use the arrow key "UP" to call the previous command.

```
ato 1
ato 2
ato 3
ato 4
ato 5
ato 6
ato 7
ato bal
ato ba2
ato big
ato bi2
ato spa
ato sp2
```

Step 5 - hide atoms:

```
ato 0
```

Step 6 - learn which drawing styles are available for bonds.
Hint: use the arrow key "UP" to call the previous command.

bon 1
bon 2
bon 3
bon 4
bon 5

Step 7 - learn how to draw balls and sticks:

bon 4
ato bal

Step 8 - try some predefined color schemes.
Hint: use the arrow key "UP" to call the previous command.
Warning: Always use the full color scheme name (do not abbreviate)!

col red
col green
col blue
col yellow
col cyan
col magenta
col white
col yellow-green
col cyan-green
col cyan-blue
col magenta-blue
col magenta-red
col orange
col hot
col cold
col cpk

Step 9 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 5 - How to Select Atoms

In this lesson, you will learn how to select atoms. The command select (or whatever command plays this role) is one of the most important commands in every molecular visualization program.

For this lesson, you will need a true protein structure, not just a single amino acid as in previous lessons.

Step 1 - obtain the protein structure:

Use you web browser to access The Protein Data Bank (www.rcsb.org) .
Type 1HUC into the small search field. Start the search and wait for the answer.
Choose the option "Download/Display File".
Finally, choose file format "PDB", compression "none" in the section "Download the Structure File" and wait.

Step 2 - start garlic (if necessary):

garlic

Step 3 - load the structure. You should have the file 1HUC.pdb somewhere in the path searched by garlic (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 4 - draw backbone, to simplify the picture:

bac

Step 5 - use different colors for different chains:

col chain

Step 6 - select chain A, draw balls and sticks and change color scheme to CPK:

sel a/*/*/*
bac off
bon 4
ato bal
col cpk

Step 7 - redefine the internal system origin (the rotation center) and move chain A to the screen center:

cen
pos 0 0 0

Step 8 - restrict the selection to aliphatic amino acids and change color to yellow (chain A):

res ali
col yellow

Step 9 - select all, make it visible, show only backbone but reduce the backbone thickness:

```
sel *
sho
bac 3
```

Step 10 - hide side chains:

Step 10 - select cysteine residues, but only for chains A and C; make them visible, use spacefill style:

```
sel a,c/*/cys/*
show
ato spa
```

Step 11 - discard loaded structure:

```
dis all
```

Garlic Tutorial

Lesson 6 - Draw Ramachandran Plot

In this lesson, you will learn how to prepare Ramachandran plot. This plot shows the pairs of dihedral angles phi and psi. You can find more details here .

You can use any protein structure for this lesson. Here we are going to use 1HUC.pdb, retrieved in the previous lesson.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure. You should have the file 1HUC.pdb somewhere in the path searched by garlic (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 3 - prepare Ramachandran plot.

rama

Step 4 - Identify some residues.

Use mouse (pointing device) to identify individual residues. Just move the pointer over the choosen residue symbol and you will see the residue name, serial number and dihedral angles in the output window.

Step 5 - draw Ramachandran plot for glycines.

sel gly
rama sel

Step 6 - return to the main drawing mode. You can either type the command rama off or hit the escape key.

rama off

Step 7 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 7 - Draw Helical Wheel

In this lesson, you will learn how to prepare the helical wheel plot. This plot may be used to identify amphipatic segments in a protein sequence, i.e. the amphipatic helices. In this lesson, the solved structure will be used for demonstration. For more details, read this (WHEEL command description).

You can use any protein structure for this lesson. In this example 1HUC.pdb is used, though you can use any protein structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure. You should have your PDB file (here 1HUC.pdb) somewhere in the search path (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 3 - select all atoms except hetero atoms. If this is not done the hetero "residues" (i.e., solvent molecules) will corrupt the helical wheel plot. The trick is to select hetero residues, and then to select complement. You don't have to hide hetero residues, so you can skip the command hide.

sel het
hide
sel com

Step 4 - check the number of chains in human cathepsin B. If there are two or more chains, the residue serial number should not be used as unique residue identifier.

color chain

Step 5 - there are obviously four chains. Hide all chains except B. Hide everything, after that select only the chain B and make it visible. Hetero residues will not be included into selection, so the step 3 was in fact unnecessary.

sel all
hide
sel b/*/*/*
show

Step 6 - try to find one helix at the chain B surface. Helices may be easily recognized if using backbone representation of the protein. It is also practical to use the geometric center of the chain B as the rotation center, and to move it to the screen center.

bac
cen
pos 0 0 0

Step 7 - play with the chain B to find this helix:

76 77 78 79 80 81 82 83 84 85 86

PRO ALA GLU ALA TRP ASN PHE TRP THR ARG LYS

Step 8 - copy the sequence of the chain B to the main sequence buffer. Note that the helical wheel plot uses the sequence which is stored in the main sequence buffer. Right now this buffer is empty!

seq from 1

Step 9 - draw helical wheel for residues from 76 to 86:

wheel 76-86

Step 10 - return to the main drawing mode. Hit the escape key or type the following command:

whe off

Step 11 - discard loaded structure:

dis all

Step 12 - clear the main sequence buffer:

seq reset

Do not forget that for helical wheel plot, the main sequence buffer should be initialized!

Garlic Tutorial

Lesson 8 - Draw Averaged Hydrophobicity and Hydrophobic Moment

---

In this lesson, you will learn how to draw the averaged hydrophobicity and hydrophobic moment for the sequence which is stored in the main sequence buffer.

In this lesson no atomic coordinates will be used. The only information available will be the sample protein sequence stored in FASTA format. The sample sequence may be found in the original garlic package or downloaded via ftp . Save this sequence as ASCII text, not as HTML.

In this example, mouse may be used to identify residues and their imminent sequence neighborhood. The residue information will be visible in the output window (bottom right corner), while the neighboring residues will be listed in the upper part of the main window. The central residue (the one choosen by the mouse) will be enclosed in a small rectangle.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the sequence.

seq load sample.fasta

Step 3 - plot the averaged hydrophobicity. Use mouse to identify the residues in the plot. The residue information will be visible in the output window (bottom right corner).

plot hyd

Step 4 - plot the hydrophobic moment. Use mouse to identify residues.

plot mom

Step 5 - plot both averaged hydrophobicity and hydrophobic moment. Note that the numeric value in the output window will be equal to the hydrophobic moment in this case!

plot hyd mom

Step 6 - return to the main drawing mode. You can either type the command plot off or hit the escape key.

plot off

Step 7 - clear the sequence buffer. You can skip this step, it is not very important.

seq reset

Garlic Tutorial

Lesson 9 - Venn Diagram

In this simple lesson, you will learn how to prepare the Venn diagram with some residue counts. There is nothing special in this routine and experts will not find it very useful. It is primarily intended for students and other newbies, which are interested in the residue composition of the given protein.

The only information required to prepare the Venn diagram is the protein sequence. In this example, the sequence will be extracted from PDB data. Another approach will be to load the sequence from some FASTA file. The PDB file used here is 1HUC.pdb, but you can replace it with any PDB file which contains the protein structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure.

load 1HUC.pdb

Step 3 - discard all hetero atoms:

sel het
sel com

Step 4 - restrict your selection to chains A and B:

res a,b/*/*/*

Step 5 - extract sequence:

seq from 1

Step 6 - draw Venn diagram with residue counts:

venn

Step 7 - discard the structure:

dis all

Step 8 - clear the sequence buffer. You can omit this command.

seq reset

Garlic Tutorial

Lesson 10 - The Semitransparent Plane

This lesson explains how to control the plane associated with the structure. More precisely, you will learn how to show, hide or move the plane and how to change the plane properties. The plane may be used to divide the structure in two parts, for selection and to model the cellular membrane.

It might be good idea to read the text about the command PLANE before you start with this lesson.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load some the structure. In this lesson the papain structure is used, but you can use any other structure.

load 9PAP.pdb

Step 3 - make the plane visible:

pla

Now you should see an ellipsa which represents the plane. If you have not rotated the structure before making the plane visible, the ellipsa will be blue. The near edge will be bright, while the far edge will be dark.

Step 4 - rotate both the structure and the plane about x axis:

Hold the [shift] key and press 8 on numeric keypad.

Note the change of the ellipsa color: now you see another face of the plane. The blue face is treated as the upper side, while the orange-red face is treated as bottom side.

Step 5 - change the plane radius.

pla rad 20

Step 6 - Change the plane transparency (make it opaque):

pla tra 0

Step 7 - select all atoms above the plane:

sel above

Step 8 - change color for the current selection:

color cold

Step 9 - attach movement controls to the plane:

mov pla

Step 10 - rotate the plane, leaving the structure in its current orientation:

Use numeric keypad (keys 2, 8, 4 and 6) and modifier keys (shift, alt, control) to rotate the plane.

Step 11 - attach controls to both structure and plane:

mov all

Step 12 - hide the plane:

pla off

Step 13 - discard the structure:

dis all

Garlic Tutorial

Lesson 11 - Creating Small Structure

In this lesson you will learn how to create a short alpha helix. The structure created using the method described here may be saved as any other structure.

Before starting with this lesson, read something about the command CREATE .

Step 1 - start garlic (if not started already):

garlic

Step 2 - prepare a short sequence (polyalanine, eight residues):

seq = ala ala ala ala ala ala ala ala

Step 3 - initialize the secondary structure (let's play with an alpha helix):

str = hhhh hhhh

Step 4 - create a short alpha helix:

create

Step 5 - save your structure:

save test.pdb

Step 6 - discard the structure:

dis all

That's all!

Garlic Tutorial

Lesson 12 - Replace Selected Residues

In this lesson you will learn how to replace selected residues. The structure used in this example will be 1HUC.pdb, but you can use any other protein structure.

Before starting with this lesson, read something about the command REPLACE .

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure:

load 1HUC.pdb

Step 3 - change color:

color cold

Step 4 - select the residue 26 in the chain A:

sel a/26/*/*

Step 5 - define the replacement for this residue:

seq = ser

Step 6 - replace CYS 26 by SER:

replace

Move the residue 26 closer to check the replacement (use numeric keys).

Step 7 - discard structure:

dis all

Garlic Tutorial

Script 4 - Dancing tryphophan

Just try it!

Type the following command at garlic prompt:

exe dance.script

```
load trp.pdb
bon 4
pos 0 0 1000
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
```

```
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
tra z -50
rot y -20
tra z -50
rot y 20
```

COM.	ARGUMENTS	APPLIES TO	DESCRIPTION
ADD	the same as for SEL	structure	Add to selection
ANG	angle (degrees)	helical wheel, hydrophobic moment	Angle for helical wheel and hydrophobic moment calculation
ATO	0, 1, 2, 3, 4, 5, 6, 7, BAL, BA2, SMA, SM2, COV, CO2, SPA, SP2, BIG, BI2	selection	Set drawing style for atoms
BAC	0, 1, 2, 3, 4, 5, OFF	selection	Draw backbone
BG	color_specification	main window	Change background color
BON	0, 1, 2, 3, 4, 5, NICE	selection	Set drawing style for bonds
CAT	structure_identifier	structure	Catch structure
CEN	none	structure, selection	Redefine system origin
COL	detailed_color_specification, red, green, blue, yellow, cyan, magenta, white, yellow-green, cyan-green, cyan-blue, magenta-blue, magenta-red, orange, hot, cold, monochrome, cpk, zebra, chain, hyphob	selection	Assign color; do not abbreviate color scheme name!
COM	none, OFF, minimal_score segment_width, CORNER serial1 serial2, ZOOM zoom_factor	both sequence buffers	Compare two sequences
CRE	none	main sequence buffer, main structure buffer	Create new structure
DIS	structure_identifier *, all	structure	Discard structure
DOC	identifier_1 identifier_2 OFF	Two structures	Prepare two structures for docking
EDI	OFF, ATO, BON atom1 atom2, CLI, DIM, MAI, OME, PHI, PSI, SID	structure	Edit structure
EXE	file_name	script file	Execute script
EXI	none	garlic session	Quit garlic session
FAD	FRO shift, BAC shift, OFF, PLA, SPH, CYL, HALF-SPH, HALF-CYL	structure	Change color fading
FG	color_specification	main window	Change text color
FON	font_name	all windows	Change font
HID	none	selection	Hide atoms and bonds
HYB	none, OFF	structure	Generate hydrogen bonds
LAB	none, OFF	selection	Show labels
LOA	file_name	structure_file	Load structure (file)
LOG	file_name, OFF	commands	Log garlic commands
MEM	none, OFF, RAD radius, THI thickness, TRA transparency	membrane	Show or hide membrane, set properties
MON	none	main window	Switch to mono mode

MOV	**ALL, MEM, PLA, STR**	**struct., memb., plane**	**Attach controls to given object**
NEI	**none, OFF**	**main window**	**Show or hide seq. neighborhood**
PAU	**none**	**garlic script**	**Pause script execution**
PLA	**none, OFF, RAD radius, TRA transparency**	**plane**	**Show or hide plane, set properties**
PLO	**HYD, MOM, OFF, HYD start_residue end_residue, MOM_start_residue end_residue**	**sequence buffer**	**Plot hydrophobicity and/or hydrophobic moment**
POS	**x, y, z**	**structure**	**Move to (x, y, z)**
PRO	**radius (angstroms)**	**structure**	**Set probe radius**
QUI	**none**	**garlic session**	**Quit garlic session**
RAD	**radius (angstroms)**	**Selection sphere**	**Change selection sphere radius**
RAM	**none, SEL, OFF**	**structure**	**Draw Ramachandran plot**
REF	**none, OFF**	**main window**	**Refreshing on/off**
REG	**none**	**mail**	**Register garlic**
REP	**none**	**structure main sequence buffer,**	**Replace selected residues**
RES	**the same as for SEL**	**selection**	**Restrict selection**
ROT	**axis angle (degrees)**	**structure**	**Rotate**
SAV	**file_name file_name SEL**	**structure, selection**	**Save atomic data to file (SEL = selection only)**
SCA	**EIS, KD, WHI**	**hydrophobicity scale**	**Choose hydrophobicity scale: Eisenberg, Kyte-Doolittle, White**
SEL	**chains/res_nums/res_names/atom_names, residue_numbers, residue_names, *, ALL, ABO, ACI, ALI, ALT, BAD, BAS, BEL, CHA, CIS, COM, HET, PHO, MAI, MOD model_number, NEG, POL, POS, SEQ, SID, SMA, SPH, TIN, TRA, TRI**	**structure, selection**	**Define new selection (overwrite previous)**
SEQ	**= three_letters_code, LOAD filename, FROM structure_identifier, COPY, SAVE filename, SWN filename, RESET**	**sequence buffer, reference seq. buffer**	**Manipulate sequence buffer**
SET	**PHI, PSI, OME, CHI1, CHI2, CHI3, CHI4, CHI5 (angle required, degrees)**	**structure**	**Set the specified dihedral angle**
SHO	**none**	**selection**	**Show atoms and bonds**
SLA	**FRO shift, BAC shift, OFF, PLA, SPH, CYL, HALF-SPH, HALF-CYL**	**structure**	**Change slab**
SSB	**0, 1, 2, 3, 4, 5, NICE**	**disulfide bonds**	**Set draw. style for disulf. bonds**
STE	**none, OFF**	**main window**	**Switch to stereo mode**
STR	**= one_letter_code, LOAD filename, FROM structure_identifier, COPY, SAVE filename, RESET**	**sec. struct. buffer, ref. sec. struct. buffer**	**Manipulate sec. structure buffer**

TAG	**"string" OFF**	**structure**	**Assign or remove tag**
TBG	**color_specification**	**input&output window**	**Change text background**
TFG	**color_specification**	**input&output window**	**Change text color**
TIT	**identifier x y "string" identifier x y identifier OFF**	**main window**	**Add, move or remove title**
TRA	**axis shift**	**structure**	**Translate**
VEN	**none, OFF, start_residue end_residue**	**sequence buffer**	**Draw Venn diagram with statistics**
WHE	**none, OFF, CLOCKWISE, start_index end_index, start_index end_index CLOCKWISE**	**sequence buffer**	**Draw helical wheel**
WIN	**number_of_residues**	**sliding window**	**Set sliding window width**

Garlic Command Line Options

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page explains the command line options. To see this list, type one of the following commands:

garlic -h
garlic -h | less

```
==============================================================================
                Garlic - free molecular viewer and editor
==============================================================================

Garlic was written by  Damir Zucic  (zucic@garlic.mefos.hr) as a complement
to other molecular visualization  programs, like rasmol (by Roger Sayle).
It was written to simplify  the analysis of membrane proteins, but it can
be used as general purpose molecular visualization program, provided that
molecular coordinates are available in  PDB format, version 2.1 or older.
Garlic may also be used to analyze protein sequences.

Some of the  features, which  distinguish this program from  others, are:
(1) Coordinates, labels and  other data are  automatically displayed  for
    the atom nearest to the current pointer (mouse) position.
(2) Additional numeric data,  like  hydrophobicity, may be associated  to
    each amino acid. The  whole  structure  may be  colored  according to
    these values.
(3) Selection mechanism is different.
(4) Two bonds at different distance from  observer have different colors.
------------------------------------------------------------------------------
Usage:              garlic [true_garlic_options] [X11_options] [filename]
------------------------------------------------------------------------------
Command line options may be divided in two groups: true (specific) garlic
options and X11 options.  Options may be given in any order.  All options
and hard-coded  default values are listed  in the table  below.  For each
parameter, the value defined through command line is used,  if available.
If not, the value defined in .garlicrc file is used. If .garlicrc file is
not  available,  or there is  no corresponding  entry in  this file,  the
hard-coded default value is used.  The sample  .garlicrc file included in
the original package contains  the values equal to  hard-coded  defaults.
------------------------------------------------------------------------------
garlic option:        Description:
------------------------------------------------------------------------------
-h, --help            Print help and exit.
-v, --version         Print version and exit.
-r, --register        Register garlic:  inform author that  your site has
```

```
                        garlic installed and that someone is going to use
                        this program. By registering, you are encouraging
                        author to continue development of garlic. You can
                        also help  author to  ensure support  for further
                        development. This option sends an e-mail message,
                        containing only the e-mail message header and the
                        word 'Hi!',to zucic@garlic.mefos.hr. Please execute
                        garlic -r   if you are going to use this program.
                        If your system is  not connected to the Internet,
                        you can send short e-mail from some other system.
-nosys                  Hide the coordinate system icon  (top left corner).
-no-control             Hide the control window (upper right corner).
-stereo                 Display stereo image.
-slab mode              Default slab mode.  Available slab modes are:  off,
                        planar (default),  sphere, half-sphere,  cylinder
                        and half cylinder.
-fading mode            Default color fading mode.  Available  modes:  off,
                        planar (default),  sphere, half-sphere,  cylinder
                        and half cylinder.
-as number              Default atom drawing style (hard-coded default: 2).
-bs number              Default bond drawing style (hard-coded default: 3).
-fs number              Default number of  color fading surfaces.  Parallel
                        planes, concentric spheres or conc. cylinders may
                        be used as  fading surfaces.  Three  RGB triplets
                        are assigned to each surface. Surfaces are evenly
                        spaced;  at least one and at most eight should be
                        defined. At least three colors  (left, middle and
                        right) are assigned to  each visible atom.  These
                        three colors are based on the position of a given
                        atom  relative to  the nearest  fading surface(s)
                        and on colors assigned to these surfaces.  Colors
                        are combined using linear weighting.
-lc[i] color            Left color at the  i-th surface;  i is between zero
                        and seven.  The color string should be  compliant
                        with X11R5.  Blue, for example,  may be specified
                        as blue or as RGB:0000/0000/FFFF etc. For example
                        -lc4 RGB:BBBB/8888/4444  defines  the left  color
                        at the surface whose index is equal to four.
-mc[i] color            Middle color at the i-th surface.
-rc[i] color            Right color at the i-th surface.
-pc, --print-config     Print configuration data and exit.
-pcn                    Print cursor names to stdout and exit.
-log logfile            Write commands and messages to  log file.  The file
                        will be created in the current working directory.
                        If this is not possible, log file will be created
                        in users home directory.
-----------------------------------------------------------------------------
X11 option:             Description:
```

```
-----------------------------------------------------------------------
-display displayname  X server to contact.
-geometry geom        Window geometry (default: almost the whole screen).
-bg color             Main window background color (default is black).
-fg color             Main window foreground color (default: white).
-fn fontname          Text font; (default is 10x20).
-tbg color            Text background color (default is black).
-tfg color            Text color (default is white).
-cursor cursorname    Cursor name; see  /usr/include/X11/cursorfont.h for
                         names; remove the XC_ prefix.
-----------------------------------------------------------------------
filename:             The input file name.  Full pathname may be used. If
                      filename does not contain the path, garlic will try
                      to find  the specified file in  the current working
                      directory.  If the first attempt  to open  the file
                      fails,  the filename  is appended to the content of
                      the environment  variable  MOL_DIR  for  the second
                      attempt.  If this fails too, garlic will search all
                      directories  specified in  the environment variable
                      MOL_PATH.
-----------------------------------------------------------------------
Personal initializations may be written to .garlicrc file. Normally, this
file should be kept in users home directory.  Note that this is  not  the
first directory to be searched for  .garlicrc file!  Up to six  pathnames
are tryed in the following order:

.garlicrc                       .garlicrc  in current  working directory.
$HOME/.garlicrc                 .garlicrc in home directory.  This is the
                                   recommended location.
$HOME/garlic/.garlicrc          ./garlicrc,  subdirectory garlic of users
                                   home directory.
/etc/garlicrc                   garlicrc in /etc, Debian linux; note that
                                   file name is garlicrc in this case!
/usr/local/lib/garlic/.garlicrc .garlicrc  in  /usr/local/lib/garlic dir.
/usr/lib/garlic/.garlicrc       .garlicrc in /usr/lib/garlic; this is the
                                   last attempt; if it failes, hard-coded
                                   default values will be used.
-----------------------------------------------------------------------
Environment variables:
-----------------------------------------------------------------------
MOL_DIR               Defines where to look for the specified file if not
                         found in the current working directory.
MOL_PATH              The list of directories to be searched.  It is used
                         if attempt with MOL_DIR failes  or if MOL_DIR is
                         not defined. Use space  or colon (:) to separate
                         directory names. MOL_PATH is quite useful; it is
                         recommended to define  this environment variable
                         through  .login,  .bashrc or  some other script.
```

```
                    MOL_PATH  is more useful  than  MOL_DIR so it is
                    recommended  to define only  MOL_PATH  variable.
DISPLAY             X server to which  the program should be connected.
-----------------------------------------------------------------------
garlic home page:                          http://garlic.mefos.hr/garlic
Damir Zucic home page:                     http://garlic.mefos.hr/zucic
E-mail:                                    zucic@garlic.mefos.hr
=======================================================================
```

Support Garlic!

---

garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

You can support garlic development in different ways. Some options are listed here, sorted by complexity (the simplest one is the first). Though garlic is a free software, someone has to pay for it. The author will need strong arguments to ensure support for a program which makes no money. If you like garlic, support it!

REGISTER GARLIC

The fact that you use garlic doesn't help much if I don't know that there is one more user. The easiest way to register is to execute the command:
reg
at garlic prompt. This requires that your machine is connected to the Internet. A short message will be send to zucic@garlic.mefos.hr; the only content of this message will be the word 'Hi!'. I will use the header of this message to extract your address. The address will be added to the list. Your address will not be abused, it will be kept secret and used only to count garlic users.

You can also send a more verbose message to zucic@garlic.mefos.hr with comments and suggestions.

There is one more way to register garlic: at your shell (terminal) prompt, type:
garlic -r
(if connected to the Internet, of course).

SEND A POSTCARD

You can also register by sending a postcard. I like stamps!
Here is the address:

Damir Zucic
ETF Osijek
Kneza Trpimira 2B
31000 Osijek
Croatia
Europe

INFORM OTHERS

Inform your colleagues and friends about garlic. Many potential users do not read Usenet news, so it is difficult to reach all those who might be interested to use garlic. I don't like spam and other aggressive forms of communication so I wouldn't use such methods to attract users.

ADD LINK TO YOUR WEB PAGES

Add link to your personal web page(s), pointing to garlic.

MIRROR GARLIC

If you like garlic and you can set aside few megabytes of disk space, you can establish a mirror site with garlic sources and related material. This should not be very complicated - there is only one source

package and few dozens of web pages. The national academic network (CARNet) here in Croatia is pretty good, but communication lines to some countries (like U.K. and Germany) are overcrowded most of the time.

USE IT FOR LECTURES AND PRESENTATIONS

An experienced user may use garlic for lectures and presentations. There is a command pau (pause) which makes it easy to control script execution.

MAKE A DONATION

Donations are welcome, of course. Contact the author for technical details (zucic@garlic.mefos.hr).

What is Garlic?

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic is a free molecular visualization program written for unix and unix clones.

Garlic was born September 30, 1998. At that time I needed a good molecular visualization program and almost the only thing at hand was RasMol. I had some hard time with RasMol so I tryed to adapt it to my needs. However, I realized that it is very hard to read and change RasMol source code, so I decided to write my own molecular visualization program.

Further, I decided to learn programming for the X window system, and this is my first serious program written for X11.

Since 1997 I use GNU/Linux software, so I concluded that it would be fair to add something useful and modern to the existing collection of free software because this software significantly improved my working conditions.

Garlic was forgotten few times, for months, as I had some other things to do, but now it is finaly operative.

Thoug the version number of the current version (1.1) is not very high, the program is very stable and robust, at least on systems which were available for testing here at University of Osijek, Croatia.

The name garlic was choosen because my original intention was to write a modular program, which will be capable to call a number of modules via system calls. In fact, I did the opposite thing: garlic now consists of a single unit which integrates all functions. Anyway, back in 1998 I thought that this program will be similar to garlic - a small core with a number of units packed around this core. I also like garlic.

Later, I reallized that program name may be reinterpreted as follows:
G stands for GNU (license),
AR for analysis and rendering,
LI for linux,
C for C (the computer language).

Who might be interested to use this program?

Students
As garlic is free and open, students may find it interesting as a learning tool. Garlic may be installed on a cheap, no-name PC (running a free linux distribution) or even on a laptop (very handy!).

University assistents and professors
It is somewhat delicate to use a commercial software for lectures and seminars (assignments). In their later carrier students may be boosted toward the software which they used during their study just because they have some experience with it. Universities should not influence the software market by choosing certain commercial product just because it is cheap or for some other reason suitable for university assignments.
Garlic may also be used for lectures, presentations and for scientific work.

Professionals

Many professionals would like to use some molecular visualization program at home or on a portable computer. Some others may be interested to adapt the program to their own needs. Software makers are unwilling to give the source code and to allow modification of their product. They also try to drain as much money as possible for additional (home) copies. Anyone wishing to cut the rope is invited to use and modify garlic, but the final product has to remain free and open, in agreement with GNU General Public License .

Others

Anyone interested to learn something about proteins and DNA may find garlic useful.

Download garlic

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garlic, free molecular viewer and editor, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

If your browser failes to recognize what should be done with the choosen file, please try the following:

(1) Click the right mouse button while pointing at the choosen file.

(2) Select the option "Save Link As ..." (from the pop-up menu).

(3) A dialog box will be opened - change directory and file name if necessary.

HTTP DOWNLOAD

Croatia: http://garlic.mefos.hr/sources/garlic-1.1

DEBIAN PACKAGES

Program: http://packages.debian.org/stable/science/garlic.html

Documentation: http://packages.debian.org/stable/doc/garlic-doc.html

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RPM PACKAGES

The RPM package may be found at at.rpmfind.net . Use the search engine (at this site) to find the appropriate RPM package.

At least two RPM-based linux distributions contain garlic:

[Mandrake] [SuSE]

Garlic Installation

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic is the most portable molecular visualization program in the unix world, because the only libraries required by this program are the standard C library (libc), the standard math library (libm) and the standard X library (libX11). All other molecular visualization programs require some additional libraries.

Before starting the installation, you might be interested to check the technical requirements . Most contemporary unix and unix-like systems (like linux) meet these requirements without need to change the configuration, so you can skip this text if you are impatient.

If you have Apple McIntosh running Xtools from Tenon, please read these hints , contributed by Chris from Macinchem.

To compile and install garlic, follow these instructions:

(1)	Put garlic package (garlic-1.1.tar.gz) into some empty directory.
(2)	Uncompress and unpack the package: gzip -d garlic-1.1.tar.gz tar xf garlic-1.1.tar
(3)	Change your working directory: cd garlic-1.1
(4)	Check which C compiler is available on your system. If you don't know how to find this information, try this: man -k compiler to obtain the list of available compilers.
(5)	If gcc (GNU C) compiler is not available on your system, use your favorite editor to edit Makefile. Replace gcc in: CC = gcc line with the name of your compiler (this may be cc, for example). If gcc is available on your system, do not change the CC line.
(6)	Find a directory which contains the Xlib library. Try this: cd / find . -name libX11* Check where is the file libX11.so (sharable library - prefered) or libX11.a (static library - reserve option). If your directory is different from /usr/X11R6/lib, modify the line: LIBPATH = -L/usr/X11R6/lib in Makefile. For example, if libX11.so is stored in /usr/shlib directory on your system, the LIBPATH should be changed to: LIBPATH = -L/usr/shlib
(7)	Compile the package - just type: make and wait some time.

(8)	If everything worked fine, copy the executable to a choosen directory. /usr/local/bin may be a good choice. This job should be done by root (system administrator): cp garlic /usr/local/bin If you don't have root privileges, ask your local administrator to install garlic, or just leave it in one of your directories.
(9)	Now the .garlicrc configuration file should be copied to a directory where it will be accessible to everyone as the public configuration script. If this is not done, garlic will work anyway, using hard-coded defaults. The recommended directory is /usr/local/lib/garlic but if /usr/local/lib does not exist on your system, /usr/lib/garlic may be used. This should be done by root (system administrator): mkdir /usr/local/lib/garlic cp .garlicrc /usr/local/lib/garlic
(10)	It may be good idea to copy the configuration file to your home directory. If you do this, you can personalize your garlic sessions, because your private configuration file overrides the system-wide defaults. Of course, you don't need root privileges for this: cp .garlicrc $HOME
(11)	It is recommended to set the environment variable MOL_PATH, so garlic will search all directories listed in this variable to find the specified file. Click here for detailed instructions.
(12)	Clean up the mess (sources and .o files). Be sure to leave trp.pdb for later practice (this is the only PDB file included in the original garlic package). Do not delete files with extension .script (tutorial scripts).

If garlic refuses to work because it fails to get the TrueColor visual, try to execute xdpyinfo and xwininfo (click into root window); check the list of supported visuals and the current color depth. Choose the color depth for which the TrueColor visual is available. If you have the SGI Octane workstation, please read this text , contributed by Randal R. Ketchem.

Protein and DNA coordinates may be found at The Protein Data Bank .

If you can't compile, install or run garlic, write to me (Damir Zucic), my address is zucic@garlic.mefos.hr .

Technical Requirements

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic tends to be POSIX compliant. It is also ANSI C compliant, to the maximum possible extent. Xlib functions are the only non-ANSI functions used by this program.

OPERATING SYSTEM
Unix or unix clone and the X window system. Linux and XFree86 recommended.

SUPPORTED HARDWARE PLATFORMS
Desktop PC, laptop, notebook, unix workstation equipped with a color monitor with a color depth of at least 8 bits per pixel. Garlic may also be used on Apple MacIntosh running Xtools from Tenon . Click here for instructions if you have such system. No dials are required. Some X servers do not support TrueColor visual at 8 bits per pixel: try to switch to higher color depth (12, 15, 24, ...)! If you have the SGI Octane workstation, you might be interested to read this text.

CPU
Intel, Digital Alpha, HP, SUN MIPS, SGI and some others. This program has no special hardware requirements.

GRAPHICS INTERFACE
Garlic requires the X window system. The recommended version is X11R6, but older versions may work too.
THE X SERVER SHOULD BE CAPABLE TO SUPPORT TrueColor VISUAL!
Some older servers may be unable to support the TrueColor visual; if you have such X server, garlic will refuse to work. Some modern X servers do not support the TrueColor visual at 8 bits per pixel, but these are usually running on a hardware which may offer 12 or more bits per pixel.

COMPILER
GNU C compiler is recommended, but other compilers compliant with ANSI C standard should work too.

REQUIRED LIBRARIES
The only required libraries are libc (C), libm (mathematical) and libX11 (the standard X11 library).

KEYBOARD
The standard PC 101/102 keyboard should work fine. The laptop keyboard may be used too. If you have some kind of unix workstation with terminal keyboard, this may work too.

MOUSE
Any mouse should serve well.

THE LIST OF COMPATIBLE SYSTEMS
Up to now, it is confirmed that garlic may be compiled and used on these systems:
Intel (486, Pentium MMX) and compatible processors;
Digital Alpha;
Sun Solaris;
SGI (Silicon Graphics);
HPUX (Hewlett-Packard).

Please inform me (zucic@garlic.mefos.hr) if you successfully compiled and used garlic on a system which is not listed here.

Compiling Garlic on Apple McIntosh

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Here you can read how to compile garlic for Apple MacIntosh running Xtools from Tenon . I would like to thank Chris from Macinchem for this contribution. Chris is also porting other chemistry related programs to Apple MaxIntosh. Please visit his Macinchem site: http://www.macinchem.fsnet.co.uk/macosx.htm

---

If you don't have access to Chris site, here is the important part:

```
... This was my first port, it requires X-Tools from Tenon.
Minor modifications of the Makefile (highlighted in red below) allow
compilation ...

        CC = gcc

        CCOPT = -O -I/usr/X11R6/include

        #CCOPT = -O3

        #CCOPT = -ansi -pedantic -O -Wall -Wstrict-prototypes -g3

        HEADERS = defines.h typedefs.h

        LIBPATH = -L/usr/X11R6/lib

        LINKOPT = -lX11 -lm
```

Setting the Color Depth on SGI Octane

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Some people are using SGI Octane in 8 bits per pixel mode. The TrueColor visual is not available at this color depth on this system. If you have such system, think of using it at its full power. I have no access to SGI Octane, so I had no idea how to change the color depth. I would like to thank Mr. Randal R. Ketchem for contributing the answer to this question.

Edit /usr/lib/X11/xdm/Xservers and change the argument list passed to /usr/bin/X11/X.

e.g.
To change the default configuration from the 8-bit pseudomap visual to the 24-bit TrueColor visual, change the single line:
:0 secure /usr/bin/X11/X -bs -nobitscale -c -pseudomap 4sight -solidroot sgilightblue -cursorFG red -cursorBG white

to a single line with:
:0 secure /usr/bin/X11/X -bs -nobitscale -c -class TrueColor -depth 24 -solidroot sgilightblue -cursorFG red -cursorBG white

---

Environment Varible MOL_PATH

---

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The environment varible MOL_PATH may be used to define the list of directories which should be searched when you are trying to load certain PDB file. It is not mandatory to define this environment variable, but it is very practical.

MOL_PATH is not the only environment variable recognized by garlic. There is also MOL_DIR, but it is capable to specify only one directory, so it is not recommended.

The exact procedure which should be used to define the environment variable MOL_PATH depends on the shell you use. The procedure is described here for some commonly used shells.

If you don't know what is you shell, execute these commands:

```
echo $shell
echo $SHELL
```

Bourne Shell

If you are using the Bourne shell (sh) or the GNU clone called Bourne-again shell (bash), use the example bellow to create your own MOL_PATH variable. Use colon (:) to separate directories. It is important to export the variable! You should define this variable through your .bash_profile or .bashrc resource file in your home directory. Don't forget to replace the user name and directories.

```
MOL_PATH="/home/zucic/pdb:/home/zucic/glob:/home/zucic/memb"
export MOL_PATH
```

C Shell

If you are using the C shell (csh) or it's clone tcsh, use the command setenv to define the environment variable MOL_PATH. Use colon (:) to separate directories. You should define this variable through your .cshrc, .tcshrc or .login resource file in your home directory. The user name and directories should be replaced, of course.

```
setenv MOL_PATH /home/zucic/pdb:/home/zucic/glob:/home/zucic/memb
```

Other Shells

For other shells, read the manual page to learn how to define the environment variable MOL_PATH. In most cases, the method is similar to one of the methods described above.

Garlic Documentation

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic documentation is written in HTML format. The sections are listed below, with a brief description. Newbies are recommended to read at least parts of each section.

Garlic Features	**An overview of garlic features.**
Controls	**Reserved keys: rotations, translations, slab and color.**
Commands	**Detailed description of garlic commands.**
Mouse Usage	**Mouse tricks specific for garlic.**
Reference Card	**A quick reminder, both for newbies and experienced users.**
Tutorial	**A collection of lessons and demonstration scripts.**
Options	**Command line options which may be specified when starting garlic.**
Configuration File	**Configuration file for garlic, called .garlicrc (for experts).**
Environment Variables	**The variable which specifies the search path for PDB files.**
Molecular Structures	**Proteins, nucleic acids and hetero compounds.**

Garlic Features

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Features which are already implemented are marked DONE.
Features which are still unavailable are marked TODO.
Partially available features are marked PARTIAL.

DONE	Garlic is free. The source code is available to everyone.
DONE	Five types of slab are available: planar, spherical, semi-spherical, cylindrical and semi-cylindrical.
DONE	The slab position and thickness are visible in a small window.
DONE	Atomic bonds as well as atoms are treated as independent drawable objects.
DONE	The atomic and bond colors depend on position. Five mapping modes are available (as for slab).
DONE	Garlic is capable to display stereo image.
DONE	Garlic will be capable to display other geometric objects, like membrane, for example.
DONE	Atomic information is available for atom covered by the mouse pointer. No click required, just move the mouse pointer over the structure!
DONE	Garlic is capable to load more than one structure.
TODO	It will be possible to replace the original residues by some others. Torsion angles will be adjustable. This is planned for version 1.2.
PARTIAL	It will be possible to color the residues according to hydrophobicity and other properties.
DONE	Garlic is capable to draw Ramachandran plot, helical wheel, Venn diagram, averaged hydrophobicity and hydrophobic moment plot.
DONE	The command prompt is available at the bottom of the main window. It is capable to display one error message and one command string.

Garlic Controls

---

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The image in the main window is controled by CONTROLS and by COMMANDS . This page contains description of garlic controls.

Garlic controls are reserved keys, which may be used to rotate and translate the structure, to change the position of slab surfaces and to change the way color depends on distance from the observer. At present, the reserved keys are numeric keypad keys and four function keys (F1, F2, F3 and F4).

Some desktop environments are reserving function keys for some special purposes. This means that function keys will fail to work properly with garlic. To avoid this problem, you can use mouse to click on dummy buttons in control window. Another solution will be to change desktop environment settings.

Numeric keypad	Function keys

For each control, five steps are available: normal, large, very large, small and very small. If you press the control without holding a modifier key (shift, alt or control), the normal step will be used.

Modifier keys may be used in combination with reserved keys to select large, very large, small or very small step. Here is the table of modifier keys:

MODIFIER KEYS	STEP	EXAMPLE
none	Normal	
shift	Large	
alt_shift	Very large	
control	Small	
shift_control	Very small	

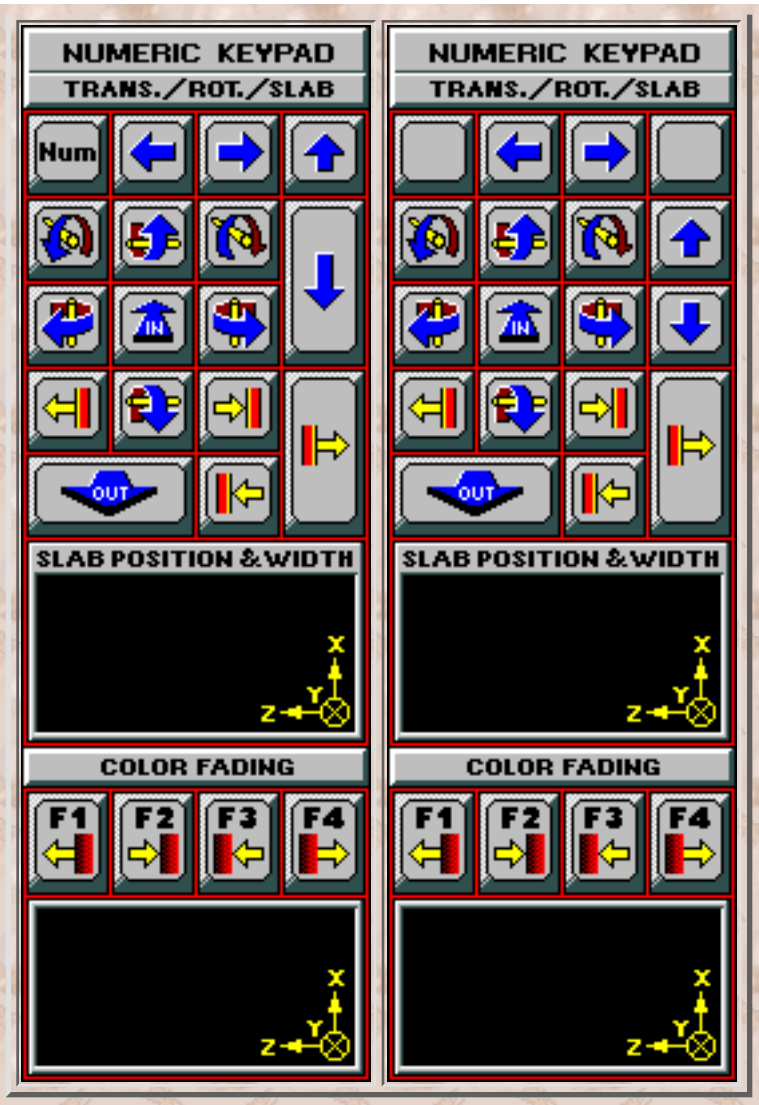
Be sure to avoid ctrl_alt combinations, because some of these combinations may have a very interesting effect (try, for example, ctrl_alt_del or ctrl_alt_F1).

The table below contains the list of controls and corresponding action upon the structure which is currently handled (held, catched). The table refers to PC (101/102) keyboard. There are slight differences between PC and terminal keyboard; three terminal keys are listed in the table (KP_F2, KP_F3, KP_Separator). If you have some exotic keyboard, use the program xshowkey to check the mapping of keys and send this list to the author: zucic@garlic.mefos.hr

KEY	LOCATION	ACTION
0	Numeric keypad	Translate structure along z in negative direction.
1	Numeric keypad	Move back (distant) slab surface along z in positive direction.
2	Numeric keypad	Rotate structure clockwise around x.
3	Numeric keypad	Move back (distant) slab surface along z in negative direction.
4	Numeric keypad	Rotate structure clockwise around y.
5	Numeric keypad	Translate structure along z in positive direction.
6	Numeric keypad	Rotate structure counterclockwise around y.
7	Numeric keypad	Rotate structure counterclockwise around z.
8	Numeric keypad	Rotate structure counterclockwise around x.
9	Numeric keypad	Rotate structure clockwise around z.
delete	Numeric keypad	Move front (close) slab surface along z in positive direction.
enter	Numeric keypad	Move front (close) slab surface along z in negative direction.
/ (slash) KP_F2	Numeric keypad	Translate structure left.
* (asterisk) KP_F3	Numeric keypad	Translate structure right.
- (minus)	Numeric keypad	Translate structure up.
+ (plus) KP_Separator	Numeric keypad	Translate structure down.
F1	Function keys	Move back (distant) color surface along z in positive direction.
F2	Function keys	Move back (distant) color surface along z in negative direction.
F3	Function keys	Move front (close) color surface along z in positive direction.
F4	Function keys	Move front (close) color surface along z in negative direction.
Num Lock	Numeric keypad	Unused key.
Escape	Top left corner	Return to the main drawing mode (display structure).

Here are the illustrations:

PC keyboard	Terminal keyboard


NUMERIC KEYPAD
TRANS./ROT./SLAB
Num
IN
OUT
SLAB POSITION & WIDTH
X
Y
Z
COLOR FADING
F1
F2
F3
F4
NUMERIC KEYPAD
TRANS./ROT./SLAB
IN
OUT
SLAB POSITION & WIDTH
X
Y
Z
COLOR FADING
F1
F2
F3
F4

Garlic Commands

---

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The image in the main window is controled by CONTROLS and by COMMANDS. This page contains the list of garlic commands.

Garlic commands are strings, consisting of one or more words. A command is executed when you press the RETURN key (this key is labeled ENTER on some keyboards). Note that ENTER key on the numeric keypad (the one in the bottom right corner of your keyboard) is NOT the right key! Commands will be displayed in the area called "input window".

Input window is placed at the bottom of the main garlic window, left justified. You don't have to the click into this area to enter the command string - just type it. The input window is capable to display a single error message (top) and a single command (bottom).

You can access previously executed commands by using arrow keys on your keyboard (the UP arrow scans the history buffer backwards and DOWN arrow in the opposite direction).

This page contains the alphabetic list of garlic commands with a short description and with link to detailed description.

Commands are generally case insensitive, but file names are case sensitive because unix (linux) is case sensitive.

SHORT FORM	LONG FORM	SHORT DESCRIPTION
ADD	ADD	Expand current selection.
ANG	ANGLE	Define angle.
ATO	ATOMS	Change atom drawing style.
BAC	BACKBONE	Draw backbone.
BACKG	BACKGROUND	The same as BG.
BG	BACKGROUND	Change main window background color.
BON	BONDS	Change bond drawing style.
CAT	CATCH	Catch the specified structure.
CEN	CENTER	Change the internal coordinate system origin.
COL	COLOR	Set color.
COM	COMPARE	Compare two sequences.
DIS	DISCARD	Discard structure.
DOC	DOCK	Prepare two structures for docking.
EXE	EXECUTE	Execute garlic script.

EXI	EXIT	Quit garlic session.
EXP	EXPAND	The same as ADD.
FAD	FADING	Change color fading style or parameter(s).
FG	FOREGROUND	Change main window foreground color.
FON	FONT	Change font.
FOREG	FOREGROUND	The same as FG.
HID	HIDE	Hide selected atoms.
HYB	HYBONDS	Generate hydrogen bonds.
IGN	IGNORE	Ignore (this command does nothing).
LAB	LABELS	Show labels.
LOA	LOAD	Load the specified file.
LOG	LOG	Write commands to log file.
MON	MONO	Switch to mono mode.
MOV	MOVE	Define which object should be moved.
NEI	NEIGHBORHOOD	Show or hide the sequence neighborhood.
PAU	PAUSE	Pause execution (useful in scripts).
PLA	PLANE	Plane manipulation.
PLO	PLOT	Plot averaged hydrophob. and/or hydrophobic moment.
POS	POSITION	Move structure to specified position.
QUI	QUIT	The same as exit.
RAD	RADIUS	Define sphere radius (used for selection).
RAM	RAMACHANDRAN	Draw Ramachandran plot.
REA	READ	The same as LOAD.
REG	REGISTER	Register garlic.
RES	RESTRICT	Restrict current selection.
ROT	ROTATE	Rotate structure.
SAV	SAVE	Save atomic data to file.
SCA	SCALE	Select hydrophobicity scale.
SEL	SELECT	Select atoms.
SEQ	SEQUENCE	Sequence buffer manipulation.
SHO	SHOW	Show selected atoms.
SLA	SLAB	Change slab style or parameter(s).
SSB	SSB	Change drawing style for disulfide bonds.
STE	STEREO	Switch to stereo mode.
TAG	TAG	Assign tag (short text) to structure.

TAK	TAKE	The same as CATCH.
TBG	TEXT_BACKGROUND	Change text background color.
TFG	TEXT_FOREGROUND	Check text foreground color.
TIT	TITLE	Add title to the main window.
TRA	TRANSLATE	Translate structure.
VEN	VENN	Draw Venn diagram.
WHE	WHEEL	Draw helical wheel.
WIN	WINDOW	Set sliding window width.

ADD, EXP, EXPAND

NAME
ADD, EXP, EXPAND - add specified atoms to current selection.

SYNOPSIS
ADD chain identifiers/residue serials/residue names/atom names
ADD residue_ranges
ADD residue_names
ADD keyword

DESCRIPTION
Add specified atoms to current selection. Atoms are added according to the specified cryteria. The command EXPAND does exactly the same job as ADD. The essential difference between ADD and SELECT is that ADD does not overwrite the previous selection. Four types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword).

DETAILED SELECTION
In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain identifiers/residue serials/residue names/atom names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

add a/*/*/*	Add all atoms from chain A to current selection.
add * exc m/*/*/ca	Add CA atoms from all chains except chain M.
add */*/*/* exc ca,c,n,o	Add all atoms except CA, C, N and O.

add a/* exc 72-112/*/ca	Add CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

add 1-100	Add residues from 1 to 100 to current selection.
add 1-100 exc 20-40	Add residues 1-100 but exclude 20-40.
add 1, 4, 8, 11-48 exc 20-32	Add residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

add phe,tyr,trp	Add PHE, TYR and TRP to current selection.

SPECIAL SELECTION KEYWORDS

Some special keywords may be combined with ADD to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

add * add all	Add all atoms to current selection, i.e. select all.
add abo add above	Add atoms above the plane.
add aci add acidic	Add acidic amino acids (GLU and ASP).
add ali add aliphatic	Add aliphatic amino acids (ILE, LEU and VAL).
add alt	Add atoms at alternate positions.
add bad	Add bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
add bas add basic	Add basic amino acids (ARG, LYS and HIS).
add bel add below	Add atoms below the plane.
add cha add charged	Add charged amino acids (ARG, LYS, HIS, GLU and ASP).
add cis	Add cis residues.
add com add complement	Add atoms which were not select previously.

add het add hetero	Add hetero atoms (heme groups, water etc.).
add pho add hydrophobic	Add hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
add mai add main_chain	Add main chain atoms (CA, C, N and O).
add mod serial_number add model serial_number	Add model specified by serial_number. NMR structure is a set of models. Example: add mod 1
add neg add negative	Add negatively charged amino acids (GLU and ASP).
add pol add polar	Add polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
add pos add positive	Add positively charged amino acids (ARG, LYS and HIS).
add seq add sequence	Add sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
add sid add side_chains	Add atoms which belong to side chains (all except CA, C, N and O).
add sma add small	Add small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
add sph add sphere	Add atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
add tin add tiny	Add tiny amino acids (GLY,ALA and SER).
add tra add trans	Add trans residues.

RELATED COMMANDS

EXPAND does exactly the same job as ADD. SELECT overwrites the previous selection. RESTRICT restrics the previous selection.

ATO, ATOMS

NAME
ATO, ATOMS - change drawing style for atoms.

SYNOPSIS
ATO style
ATOMS style

DESCRIPTION
Change drawing style for atoms. Atom style is defined separately from bond style. For BALLS, BIG and SPACEFILL style, atom sizes are read from .garlicrc file. If this file is not available, hard-coded defaults are used.

STYLE	DESCRIPTION	SIZE
0	Unvisible atoms	Fixed
1	A single pixel	Fixed
2	3x3 cross (5 pixels)	Fixed
3	3x3 square (9 pixels)	Fixed
4	5x5 circle (21 pixel)	Fixed
5	7x7 square (37 pixels)	Fixed
6	9x9 circle (61 pixel)	Fixed
7	11x11 circle (109 pixels)	Fixed
bal balls	Balls (suitable to draw balls and sticks)	Proportional
ba2	Balls with enhanced contrast	Proportional
big	Big (oversized atoms)	Proportional
bi2	Big with enhanced contrast	Proportional
spa spacefill	Spacefill style; the size of atom depends on atom type	Proportional
sp2	Spacefill style with enhanced contrast; the size of atom depends on atom type	Proportional

NOTES
(1) Unvisible atoms (style 0) are not treated as hidden - they are just invisible.

(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

RELATED COMMANDS
BON (BONDS) changes drawing style for bonds.

BON, BONDS

NAME
BON, BONDS - change drawing style for bonds.

SYNOPSIS
BON style
BONDS style

DESCRIPTION
Change drawing style for bonds. Bond style is defined separately from atom style. At present, proportionally sized styles are not available. This command does not affect disulfide bonds: the command SSB should be used for that purpose.

STYLE	THICKNESS	TYPE
0	Unvisible bonds	Fixed
1	A single line	Fixed
2	Three lines	Fixed
3	Five lines	Fixed
4	Seven lines	Fixed
5	Nine lines	Fixed

NOTES
(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.

(2) A good performance and fairly good contrast may be achieved choosing atom drawing style 0 (no pixels) and bond drawing style 2 (line width of three pixels).

RELATED COMMANDS
ATO (ATOMS) changes drawing style for atoms. SSB changes bond drawing style for disulfide bonds.

CAT, CATCH

NAME

CAT, CATCH - catch the specified macromolecular complex.

SYNOPSIS

CAT identifier
CATCH identifier

DESCRIPTION

Catch the specified structure (macromolecular complex). The structure is a set of atoms read from a single file. Thus, every file is treated as a separate structure. The structure identifier is positive integer. The value zero is not used; structures are numbered 1, 2, 3, etc. When you catch a single structure, all transformations (rotations, translations etc.) are applied to this structure, leaving other structures intact. Selection (commands SELECT, ADD, RESTRICT) are also applied only to this structure. The command CATCH is used when working with more than one structure - for example, when docking an inhibitor to a substrate. When only one structure (file) is loaded, this command has no purpose. Examples:

COMMAND	DESCRIPTION
cat 1	Catch the structure number 1.
cat 7	Catch the structure number 7.

NOTES

(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure you want to catch. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
PHE 192
CE2  1433  C
t.f.: 64.06
trans
phi:-120.71
psi:  72.93
phob:  1.19
selected
x:    -3.276
y:   -18.665
z:   -13.754
```

RELATED COMMANDS

TAK (TAKE) does exactly the same job as CATCH.

COL, COLOR

NAME
COL, COLOR - change the color of selected atoms and their corresponding bonds.

SYNOPSIS
COL color_scheme_name
COL left_1 middle_1 right_1 ... ... left_N, middle_N, right_N

DESCRIPTION
Change the color used to draw selected atoms and their corresponding bonds. Half of each bond belongs to one atom, while half of the same bond belongs to another atom. The easy way to specify color is to use the predefined color scheme. The powerfull (but more complicated) way to specify color is to issue detailed color specification.

COLOR USAGE
In garlic, colors are used to create 3D illusions. In most color schemes, the atoms close to the observer have bright colors, while distant atoms have dark colors. Atoms and bonds look like three-dimensional objects because one side is brighter than the other. Here are some technical details about color usage:

At least one and at most eight surfaces are assigned to each structure. These surfaces are equidistant planes, spheres or cylinders. The surface which is nearest to the observer is called "front surface", while the most distant surface is called "back surface". To each surface, three colors are assigned: left, middle and right color. In most color schemes, left color is bright and right color is dark. Atoms may be divided in three groups:

(1) Atoms which are in front of the front surface;
(2) Atoms which are behind the back surface;
(3) All other atoms, positioned in the sandwich between two surfaces.

All atoms which are in front of the front surface are drawn using the same set of three colors which assigned to front surface. Atoms behind the back surface are colored using three colors assigned to back surface. Colors for atoms laying between two surfaces are prepared by linear interpolation of colors assigned to these two surfaces. This is what I call color fading (this term was not the best choice I could make, sorry).

In a special case, when only one surface is used, color does not depend on distance.

Almost all predefined color schemes typically define two surfaces, i.e. a total of six colors. There are some exceptions: color schemes HOT and COLD use three surfaces, while MONOCHROME uses only one.

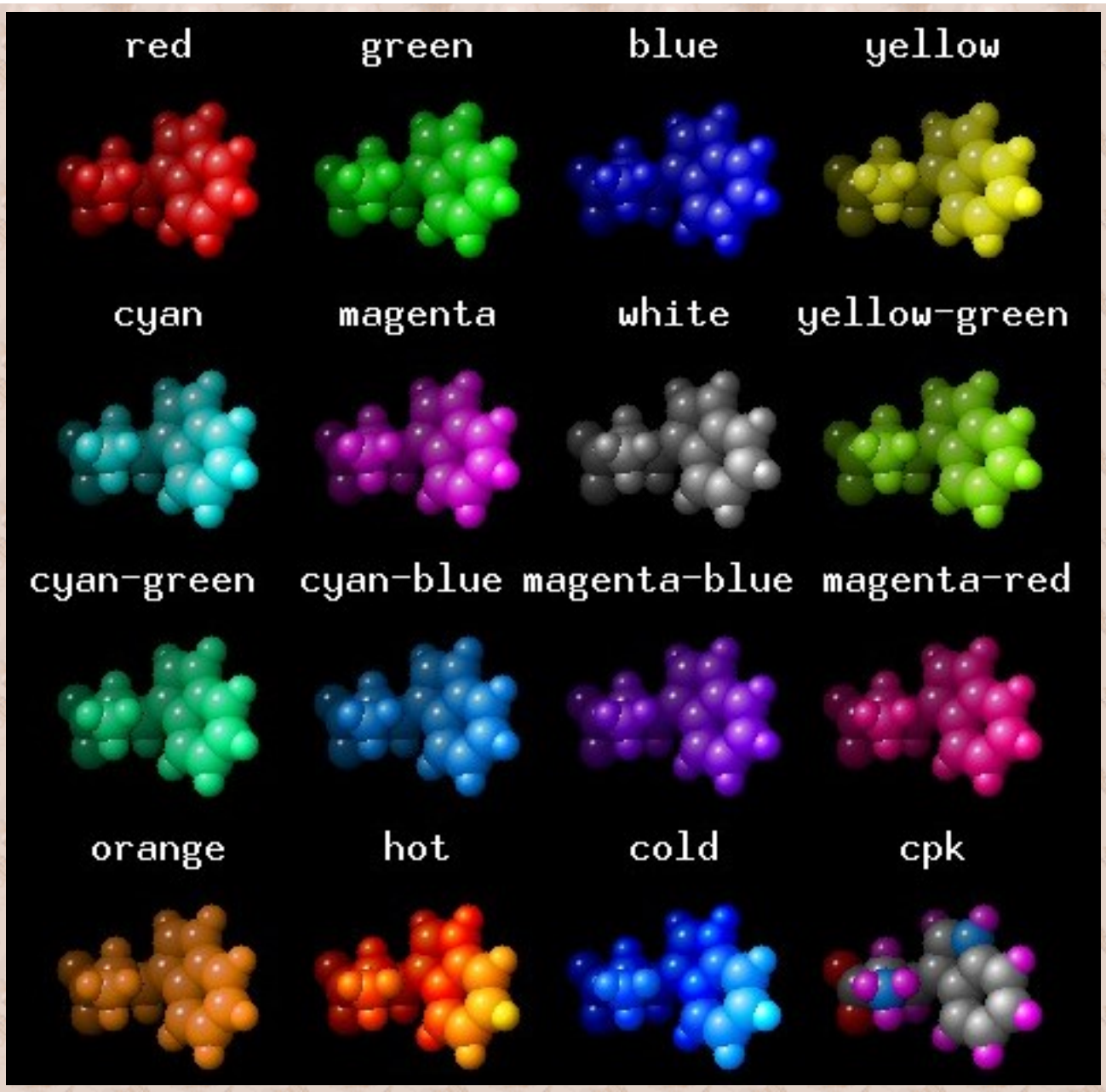
Planes, spheres and cylinders
For most proteins and other molecules, planar fading is the best choice. In this case, a set of planes, perpendicular to z axis is used. Concentric spheres may be used when working with large globular proteins, while cylinders may be used for beta-barrel proteins, like porins. The axis of concentric cylinders is parallel to y.

USING PREDEFINED COLOR SCHEMES
Twenty predefined color schemes are available:

SCHEME NAME	DESCRIPTION

RED	**Red color scheme; distant atoms are dark**
GREEN	**Green, distant atoms are dark**
BLUE	**BLUE (deep sea), distant atoms are dark**
YELLOW	**Yellow, distant atoms are dark**
CYAN	**Cyan (cloudless sky), distant atoms are dark**
MAGENTA	**Magenta, distant atoms are dark**
WHITE	**Shades of gray, distant atoms almost black**
YELLOW-GREEN	**Somewhere between yellow and green, distant atoms dark**
CYAN-GREEN	**Somewhere between green and blue-green, distant atoms dark**
CYAN-BLUE	**Somewhere between blue and blue-green, distant atoms dark**
MAGENTA-BLUE	**Somewhere between blue and magenta, distant atoms are dark**
MAGENTA-RED	**Somewhere between red and magenta, distant atoms are dark**
ORANGE	**Orange, distant atoms are dark**
HOT	**The nearest atoms are yellow, atoms in the middle are orange and distant atoms are dark red**
COLD	**The nearest atoms are cyan, atoms in the middle are cyan-blue and distant atoms are dark blue**
MODEL	**Use different colors for different NMR models**
MONOCHROME	**Edge black, central region white, distance independent**
CPK	**Modified Corey-Pauling-Kultun color scheme, distant atoms are dark**
ZEBRA	**Residues with even serial number are red, odd residues cyan-blue, distant atoms are dark**
CHAIN	**Use color to distinguish chains; distant atoms are should be dark**
HYPHOB	**Assign color according to hydrophobicity; distant atoms are dark**

Do not abbreviate the color scheme name! Case is not important. Some selected schemes are shown below. The atom drawing style SP2 was used to prepare this image, but the image quality was later reduced by JPEG compression. Execute colors2.script for better reproduction.



DETAILED COLOR SPECIFICATION

Most users should be satisfied with predefined color schemes. Anyway, it is fairly easy to use colors which are not available through predefined schemes. To define N color planes (up to eight), you have to define 3 * N colors. The keyword OLD may be used to leave the previous value unchanged. Here are some examples:

col yellow orange red red DarkRed black	**Define two color surfaces with six colors.**
col rgb:ffff/ffff/4444 rgb:ffff/dddd/0000 DarkRed	**One color surface, three colors.**
col old old old black black black	**Leave the front colors unchanged, set all back colors to black.**

Be careful with the keyword OLD - it may be used only if the currently used color scheme has at least as many colors as a new one.

RELATED COMMANDS

FADING may be used to change the position of outer color surfaces and to switch color fading on and off.

COM, COMPARE

NAME
COM, COMPARE - compare two sequences.

SYNOPSIS
COM
COM minimal_score segment_width
COM OFF
COM COR serial1 serial2
COM ZOO zoom_factor
COMPARE
COMPARE minimal_score segment_width
COMPARE OFF
COMPARE CORNER serial1 serial2
COMPARE ZOOM zoom_factor

DESCRIPTION
Compare two sequences. Garlic mantains two sequence buffers: the main sequence buffer and the reference sequence buffer. After initializing both buffers, the command COMPARE may be used to prepare the plot with comparison of these two sequences. Matching residues will be marked by dots or squares, depending on the zoom factor. Dots or squares which represent residue pairs which match exactly will be colored yellow, while residues which are different but have similar properties will be colored red. The reference sequence will be assigned to the horizontal (x) axis, while another (investigated) sequence will be assigned to the vertical (y) axis.

The plot will contain only residues which belong to the segments for which the score of matching residues is equal to or larger than minimal score. The minimal score (the number of matching pairs) and the width of the segment used for comparison may be specified by the user. Hard-coded defaults are SEGMENT_WIDTH and MINIMAL_SCORE, defined in defines.h file. The values used in the original garlic package: SEGMENT_WIDTH=5, MINIMAL_SCORE=5.

SCORING
Two sequences are compared using fixed width segments. The matrix shown below is used to identify matching residues. It was inspired by Dayhoff PAM250 matrix. However, while PAM250 matrix contains a range of values, both positive and negative, the only values used in the substitution matrix below are zero and one. One is used to identify matching residue pairs and zero for pairs which do not match.

		A	B	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	Z	X
ALA	A	1	0	0	0	0	0	1	0	0	0	0	0	0	1	0	0	1	1	0	0	0	0	0
ASX	B	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	0	0	0	0	0	0	1	0
CYS	C	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASP	D	0	1	0	1	1	0	1	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
GLU	E	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
PHE	F	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0	0
GLY	G	1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0
HIS	H	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	1	0	0	0	0	0	1	0
ILE	I	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
LYS	K	0	1	0	0	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	0
LEU	L	0	0	0	0	0	1	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
MET	M	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
ASN	N	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	0	1	0	0	0	0	1	0
PRO	P	1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0
GLN	Q	0	1	0	1	1	0	0	1	0	1	0	0	1	0	1	1	0	0	0	0	0	1	0
ARG	R	0	0	0	0	0	0	0	1	0	1	0	0	0	0	1	1	0	0	0	1	0	0	0
SER	S	1	0	0	0	0	0	1	0	0	0	0	0	1	1	0	0	1	1	0	0	0	0	0
THR	T	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0
VAL	V	0	0	0	0	0	0	0	0	1	0	1	1	0	0	0	0	0	0	1	0	0	0	0
TRP	W	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0
TYR	Y	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
GLX	Z	0	1	0	1	1	0	0	1	0	0	0	0	1	0	1	0	0	0	0	0	0	1	0
UNK	X	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

The scoring scheme used in garlic is much simpler than the elaborate schemes used in advanced programs for sequence alignments. However, this scheme is still quite useful and I believe that many users will like to play with the various segment widths and scores.

KEYWORDS AND PARAMETERS

All keywords and associated parameters are explained in the table below. Note that the minimal score may not exceed the segment width.

KEYWORD AND/OR PARAMETERS	DESCRIPTION
None	Draw sequence comparison, using default segment width and default minimal score.
OFF	Return to the main drawing mode. The same may be achieved by hiting the ESCAPE key.

minimal_score segment_width	Draw sequence comparison, using the specified segment width and the specified minimal score. Both parameters should be positive.
CORNER ref_offset main_offset	Draw sequence comparison, but skip some leading residues. Skip (ref_offset - 1) residues of the reference sequence and (main_offset - 1) residues of the main sequence.

MOUSE USAGE

The pointing device (mouse) may be used to find the residue serial numbers and names for matching pairs and residues which follow after them. After a choosen pair is reached with the pointer, the information about this pair and residues which follow them will be available in the output window (the bottom right corner). Color codes: yellow is used for residues which are equal, magenta for acceptable substitutions and red for mismatching residues.

HORIZ.	VERT.
27ALA	ALA31
28PHE	PHE32
29SER	GLY33
30ALA	ALA34
31VAL	VAL35
32VAL	GLU36
33THR	ALA37
34ILE	ILE38
35GLU	SER39
36GLY	ASP40
37ILE	ARG41

EXAMPLES

COMMAND	DESCRIPTION
load 9PAP.pdb sel het sel com seq from 1 seq copy	Load the structure of papain, select all hetero atoms and then select the complement of this selection. The purpose of this trick is to exclude all hetero atoms from selection. Extract the sequence and copy it to the reference buffer.
load 1HUC.pdb sel a,b/*/*/* seq from 2 compare 8 10	After that, load the structure of human cathepsin B, select chains A and B (one molecules consists of two chains), extract the sequence and compare it with the content of the reference buffer. The minimal score is 8 and the segment width is 10.

load 9PAP.pdb **sel het** **sel com** **seq from 1** **seq copy** **seq load sample.fasta** **compare 6 7**	**Load the structure of papain and copy the sequence to the reference buffer using the same method as in the previous example. Read the second sequence from the specified FASTA file (one letter codes). Compare two sequences, using the specified minimal score and segment width (5/7).** **This is the typical usage of sequence comparison: compare a fresh sequence with the sequence of a solved structure.**
com zoom 4	**Change zoom factor to 4.**
com cor 100 100	**Skip the first hundred residues of both sequences.**

NOTES

(1) You don't need protein 3D structures to compare two sequences. The minimal information required for protein comparison is the primary structure, i.e. the protein sequence.

RELATED COMMANDS

The command SEQ (SEQUENCE) is used to manipulate the content of the main sequence buffer and of the reference sequence buffer. LOAD is used to load the PDB file. SELECT, ADD and RESTRICT are used for selection.

DIS, DISCARD

NAME
DIS, DISCARD - discard the specified structure.

SYNOPSIS
DIS identifier
DIS ALL
DIS *
DISCARD identifier
DISCARD ALL
DISCARD *

DESCRIPTION
Discard the specified structure (macromolecular complex). The memory used to store the structure is freed. If keyword ALL is used (or asterisk, *), all structures will be discarded. Examples:

COMMAND	DESCRIPTION
dis 1	Discard the structure number 1.
dis 7	Discard the structure number 7.
dis *	Discard all. Nothing will be loaded after this command.

NOTES
(1) Sometimes you will forget the identifiers, especially when working with many structures. Move the mouse pointer over the structure which should be discarded. The identifier will be displayed in the output window (bottom right corner of the garlic window). The number in parentheses is the identifier you need. In the example below, the identifier is equal to one.

```
(1) 2POR
PHE 192
CE2  1433  C
t.f.: 64.06
trans
phi:-120.71
psi:  72.93
phob:  1.19
selected
x:    -3.276
y:   -18.665
z:   -13.754
```

(2) If you discard everything, the indexing will be reset too. The first structure you load after discarding everything will be assigned index "1" (one).

RELATED COMMANDS

LOAD (READ) loads the specified file.

DOC, DOCK

NAME
DOC, DOCK - prepare two structures for docking.

SYNOPSIS
DOC identifier_1 identifier_2
DOC OFF
DOCK identifier_1 identifier_2
DOCK OFF

DESCRIPTION
The command DOCK prepares two structures for docking. Before executing this command, two molecules (structures) have to be loaded. For each structure a region on the surface should be selected as a candidate region for interaction with another molecule. For example, if the first molecule is the substrate, the active site has to be identified as the region where the inhibitor should be placed. Assuming that another molecule is the inhibitor, the side which is expected to interact with the substrate should be identified.

When both molecules are ready for docking, the command DOCK should be executed. The identifiers of both molecules have to be issued as arguments. Both molecules will be translated and rotated to position and orientation suitable for docking. The first molecule will be moved to the bottom of the main window, with the selected region visible on the upper side. The second molecule will be placed atop the first molecule, with the selected region facing the first molecule.

Further, a special docking window will be opened, showing the orthogonal projections of polar side chains as symbols. The polar side chains of both molecules are projected to the plane associated with the first molecule. Cyan symbols belong to the bottom molecule (the first one) and red symbols belong to the top molecule. Hydrogen bond donors are shown as crosses, acceptors as circles, and side chains which are both hydrogen bond donors and acceptors are shown as crosses in circles.

The user might be able to combine two structures, using the information visible in both the main garlic window and in docking window. However, this routine is still quite naive, so don't expect too much. Docking is not an easy game. I hope that this command will be useful at least for educational purpose.

KEYWORDS
The keyword OFF is the only keyword which may be used with the command DOCK. DOCK OFF is used to hide docking window.

KEYWORD	DESCRIPTION
OFF	Hide docking window.

PARAMETERS
Except when used in combination with the keyword OFF, the command DOCK should be followed by two structure identifiers. If you have forgotten these numbers, just move the mouse pointer over the structure(s) and find the identifier(s) in the output window (the bottom right corner). The order is important: the first molecule will be placed to the bottom of the main window, while the second will be placed atop the first one.

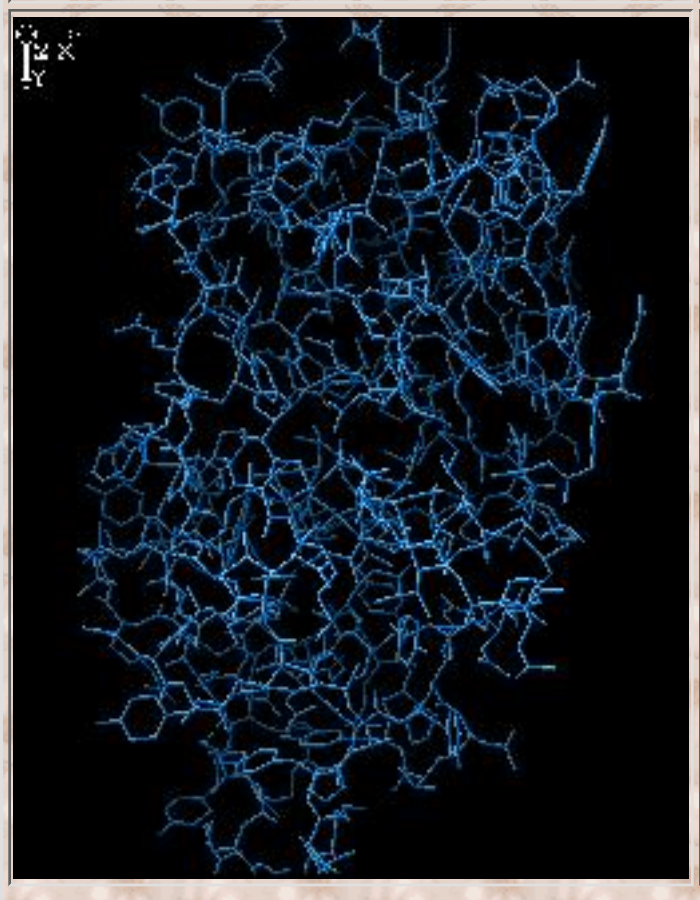
PARAMETER	DESCRIPTION

identifier_1	Identifier of the first molecule. (substrate, for example).
identifier_2	Identifier of the second molecule. (inhibitor, for example).

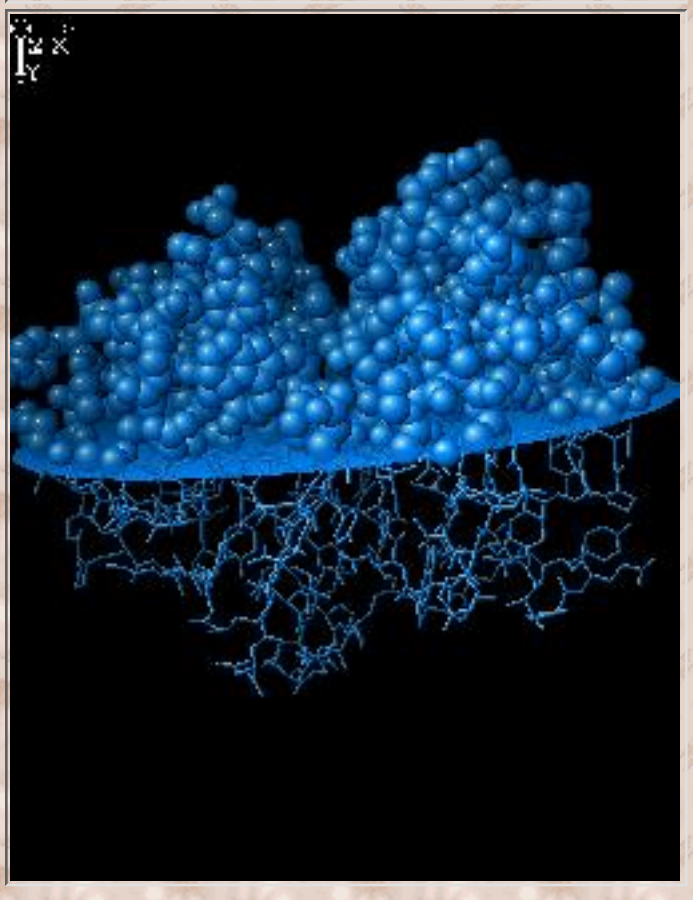
EXAMPLE

The example below shows how to prepare two structures for docking. In this example, the first structure is papain (reference 1) and the second structure is stefin (reference 2). The structure of the complex is known (PDB code 1STF).

STEP1:
Load the first structure:
load file1.pdb
Change the color. Cyan-blue might be a good choice:
color cyan-blue

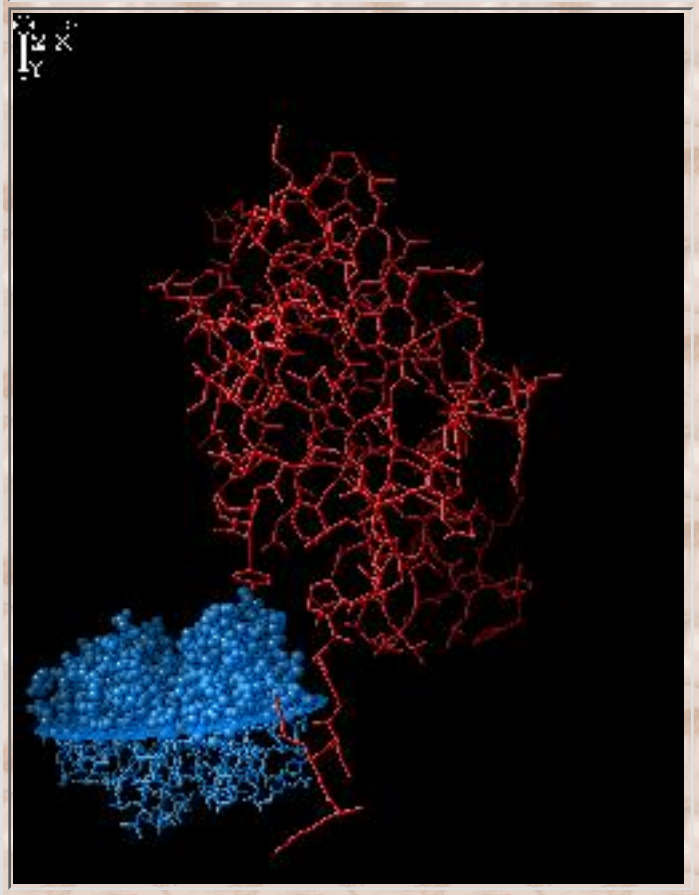


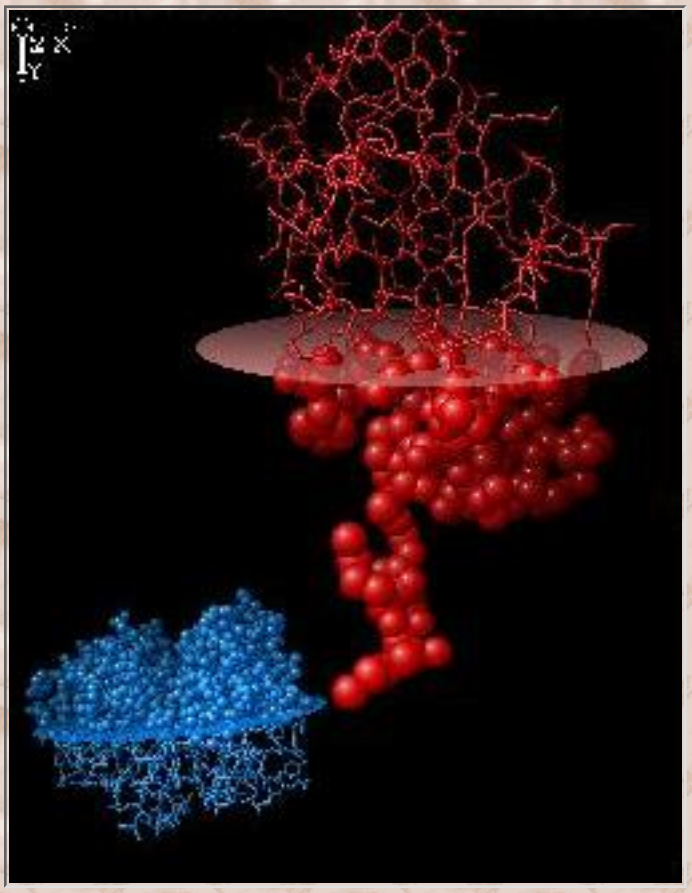
STEP 2:
Make the plane visible:
plane
Prepare to move the plane:
move plane
Use plane to divide structure in two parts.
The active site should be above the plane.
Change drawing style for atoms or bonds.
Here the spacefill style is used. This is bad idea if using slow machine.
sel above
atom sp2
Reset movement controls:
move all



STEP 3:
Push the first structure to the corner.
Load the second structure:
load file2.pdb
Change color. Red is recommended here:
color red

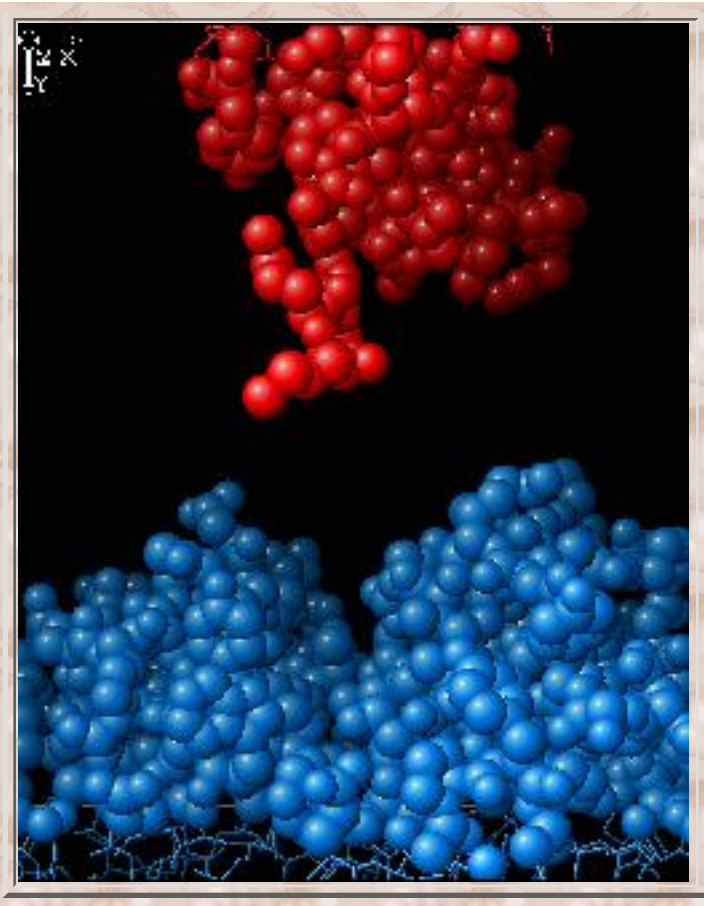
STEP 4:
Make the plane visible and divide the second structure in two parts. Change drawing style for atoms or bonds.
plane
move plane
(... now rotate and translate the plane)
sel above
atom sp2
Reset movement controls:
move all

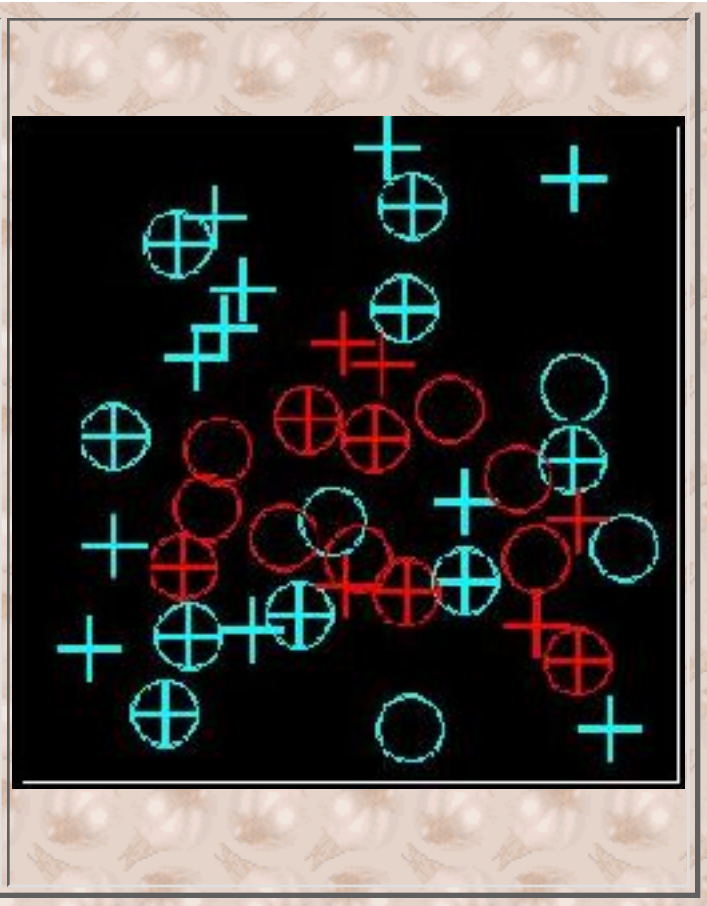




STEP 5:
Execute DOCK command:
dock 1 2

Rotate the second (top) structure. Check the relative arrangement of hydrogen bond donors and acceptors. The projections of these side chains are given in docking window.





NOTES

(1) If two structures are close, some important atoms might be unvisible (hidden by some closer atoms). Use slab to cut slices through structure(s).

(2) Don't forget to catch the right structure before applying some transformation. By default, after the command DOCK is executed, the movement controls are attached to the second (top) structure.

RELATED COMMANDS

LOAD is used to load the specified file (structure, molecule). MOVE is used to define which object should be moved (structure, plane or both). PLANE is used to manipulate the plane associated with the structure. CATCH is used to attach the movement controls to a choosen structure.

REFERENCES

(1) Kamphuis, I. G., Kalk, K. H., Swarte, M. B. A. and Drenth, J. (1984). J. Mol. Biol. 179, p. 233.

(2) Stubbs, M. T., Laber, B., Bode, W., Huber, R., Jerala, R., Lenarcic, B. and Turk, V. (1990). EMBO J. 9, p. 1939.

FON, FONT

NAME

FON, FONT - change font.

SYNOPSIS

FON font_name
FONT font_name

DESCRIPTION

Change font. At present, garlic uses only one font for input, output and main window. Try to execute xlsfonts on your system, to obtain a list of fonts. Default font is set in .garlicrc file. Examples:

fon 10x20
fon olglyph-19

RELATED COMMANDS

FG changes the text color used to draw strings in the main window. TFG changes the text color used to draw strings in input and output window.

HYB, HYBONDS

NAME

HYB, HYBONDS - generate hydrogen bonds.

SYNOPSIS

HYB
HYB style
HYB OFF
HYBONDS
HYBONDS style
HYBONDS OFF

DESCRIPTION

Generate hydrogen bonds for the entire structure. Show hydrogen bonds for visible atoms. At present, some very simple geometric restrains are used to generate hydrogen bonds. Check the configuration file (.garlicrc) and the source file gen_hybonds.c to learn more about these restrains.

Keyword OFF may be used to hide hydrogen bonds.

Default style used to draw hydrogen bonds is 1 (a single line, fixed). You can change it by specifying the style. Examples:

hyb	**Generate hydrogen bonds and show them using default style (1).**
hyb 4	**Generate hydrogen bonds and show them using style 4 (four lines).**
hyb off	**Hide hydrogen bonds**

LOA, LOAD, REA, READ

NAME
LOA, LOAD, REA, READ - load the specified file.

SYNOPSIS
LOA file_name
LOAD file_name
REA file_name
READ file_name

DESCRIPTION
Load and display the specified file. The file content will be treated as a separate structure. The unique structure identifier (positive integer) will be assigned to this structure. The structure will be placed in the middle of the screen.

You can load any file more than once. A total number of structures which may be simultaneously loaded depends on the available memory. The hard-coded maximum is 1000, which should be more than enough.

The command LOAD may be written in uppercase, lowercase or mixed case, but the file name should be specified in correct case - unix file names are case sensitive.

SEARCH PATH
The file is searched in one or more directories, in the following order:

(1) the current working directory;
(2) directory specified in the environment variable MOL_DIR;
(3) all directories specified in the environment variable MOL_PATH.

The recommended environment variable is MOL_PATH.

RELATED COMMANDS
DIS (DISCARD) discards the specified structure. SAV (SAVE) saves the atomic data to a file.

MOV, MOVE

NAME
MOV, MOVE - define which object should be moved.

SYNOPSIS
MOV PLA
MOV STR
MOV ALL
MOVE PLANE
MOVE STRUCTURE
MOVE ALL

DESCRIPTION
This command defines which object should be moved when rotation and translation controls or commands are used. When a PDB file is read, a new structure is stored into program memory. A single plane is associated with each structure. By default, this plane is unvisible and movement controls are affecting both the structure and the associated plane. The command PLANE may be used to make the plane visible. In that case, it will be represented by an ellipse. One side of this ellipse will be colored blue and other side will be colored orange-red.

The command MOVE affects only the structure which is currently being handled (the structure which is "caught").

KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
STR	STRUCTURE	Move structure leaving plane at the current position.
PLA	PLANE	Move plane leaving structure at the current position.
ALL	ALL	Move both structure and plane.

EXAMPLES

COMMAND	DESCRIPTION
mov pla	Move the plane leaving the structure at the current position.
mov all	Move both plane and structure.

NOTES
(1) Plane is affected by rotation and translation controls and commands. Slab and color fading do not affect plane.

(2) Do not use two keywords with command MOVE. If you want to move both the structure and the associated plane use keyword ALL.

RELATED COMMANDS

PLANE is used to show or hide the plane associated with the molecular structure. CATCH is used to catch the specified structure.

NEI, NEIGHBORHOOD

NAME
NEI, NEIGHBORHOOD - hide or show the sequence neighborhood.

SYNOPSIS
NEI
NEI OFF
NEIGHBORHOOD
NEIGHBORHOOD OFF

DESCRIPTION
Hide or show the sequence neighborhood of the current residue. The current residue is the residue to which the atom covered by the mouse pointer belongs. When you cross an atom or bond with the mouse pointer, the output window will contain some useful information about this atom. The top portion of the main window will contain the list of the residues around this atom. The central residue (called also "the current residue") will be enclosed in a small rectangle. The entire sequence neighborhood will be enclosed in a wide rectangle.

If you are not interested in the sequence neighborhood of the current residue, execute the command:

nei off

If you want to remove the sequence neighborhood permanently, find this section in the configuration file .garlicrc and replace the keyword "yes" by "no":

```
# Sequence neighborhood of the residue under
# the pointer may be visible or hidden (yes/no):

show sequence neighborhood: yes
```

By default, the sequence neighborhood will be visible.

KEYWORDS
The only keyword is OFF. If used without any keyword, the command NEI will make the sequence neighborhood visible. If combined with the keyword OFF, the command will hide the sequence neighborhood.

EXAMPLES

COMMAND	DESCRIPTION
nei off	Hide the sequence neighborhood.
nei	Show the sequence neighborhood.

NOTES
(1) Residues in the sequence neighborhood are listed in direction from amino- to carboxyl-terminal residue, left to right.

(2) If the current residue is close to polypeptide chain end, it will be displaced from the central position.

(3) The output window is visible in the bottom right corner of the main window.

PLA, PLANE

NAME

PLA, PLANE - manipulate the plane associated with the structure.

SYNOPSIS

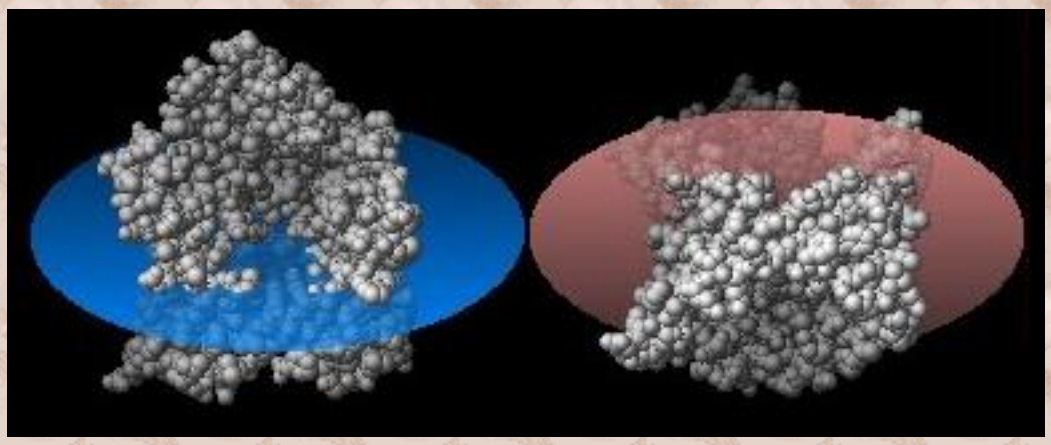
PLA
PLA RAD value
PLA TRA value
PLA OFF
PLANE
PLANE RADIUS value
PLANE TRANSPARENCY value
PLANE OFF

DESCRIPTION

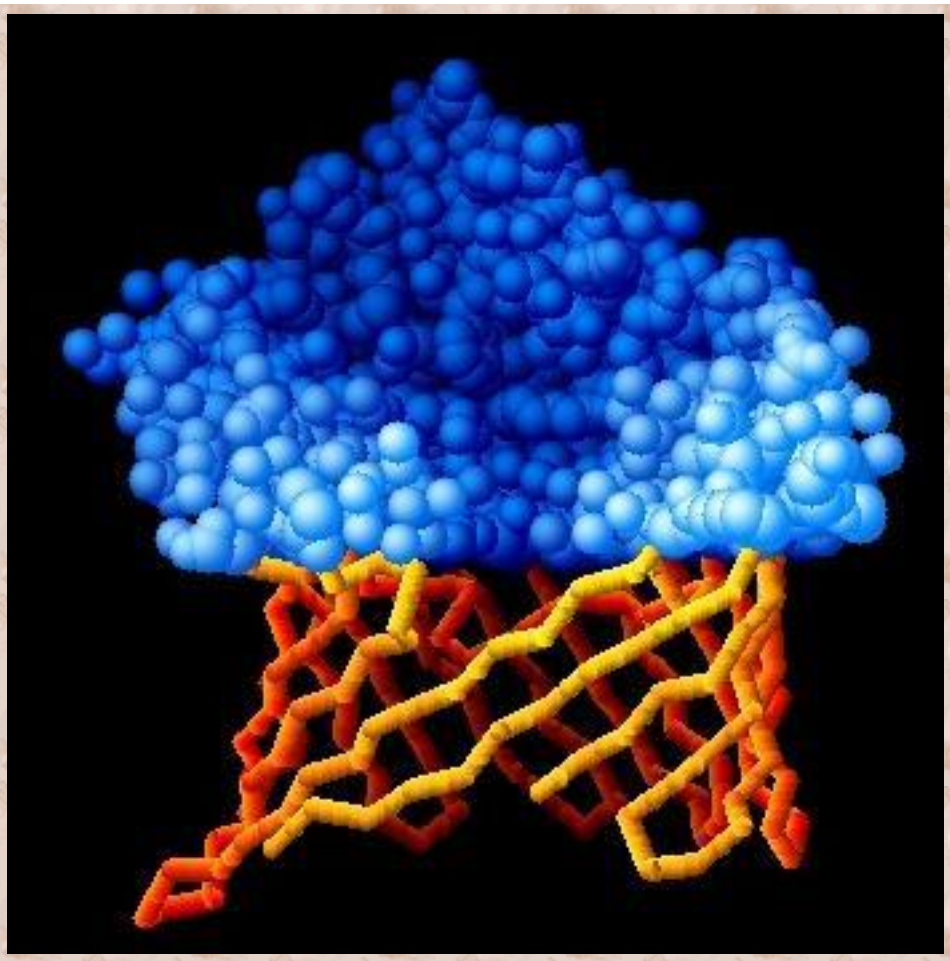
When a PDB file is read, a new structure is stored into program memory. A single plane is associated with this structure. By default, the plane is unvisible and movement controls are affecting both the structure and the associated plane. The command PLANE may be used to make the plane visible, to set the plane transparency or radius, or to hide the plane.

Plane is represented by an ellipse. One side of this ellipse will be colored blue and other side will be colored orange-red. Blue side is treated as top (upper) side, while orange-red side is treated as bottom side. Far side of the plane is dark.

The transparency value should be between 0 and 1. If transparency is equal to zero the plane is opaque. Default plane transparency is 0.4 (hard-coded). The initial (default) plane radius is based on the spacial extent of the structure. The image below shows two semi-transparent planes: the left plane is seen from above, while the right plane is seen from below. Transparency is equal to 0.3 for both planes.



Plane may be used for different purposes:
(1) To represent the cellular membrane. This is interesting for visualization of membrane proteins (like in the image above).
(2) To distinguish protein domains. Many soluble proteins fold into two domains. Plane may be used to outline the border between these domains.
(3) Atoms may be selected according to their position with respect to plane. The command SEL ABO (SELECT ABOVE) selects atoms which are above the plane. The command SEL BEL (SELECT BELOW) selects atoms which are below the plane. The image below shows what may be achieved when applying different drawing styles to atoms on different sides of the plane.



KEYWORDS

KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
OFF	OFF	Hide plane.
RAD	RADIUS	Set plane radius (value should be given in angstroms).
TRA	TRANSPARENCY	Set plane transparency (between 0 and 1).

EXAMPLES

COMMAND	DESCRIPTION
plane	Make the plane visible.
pla rad 20	Change plane radius to 20 angstroms.
pla tra 0.3	Change plane transparency (new value: 0.3).
plane off	Hide plane.

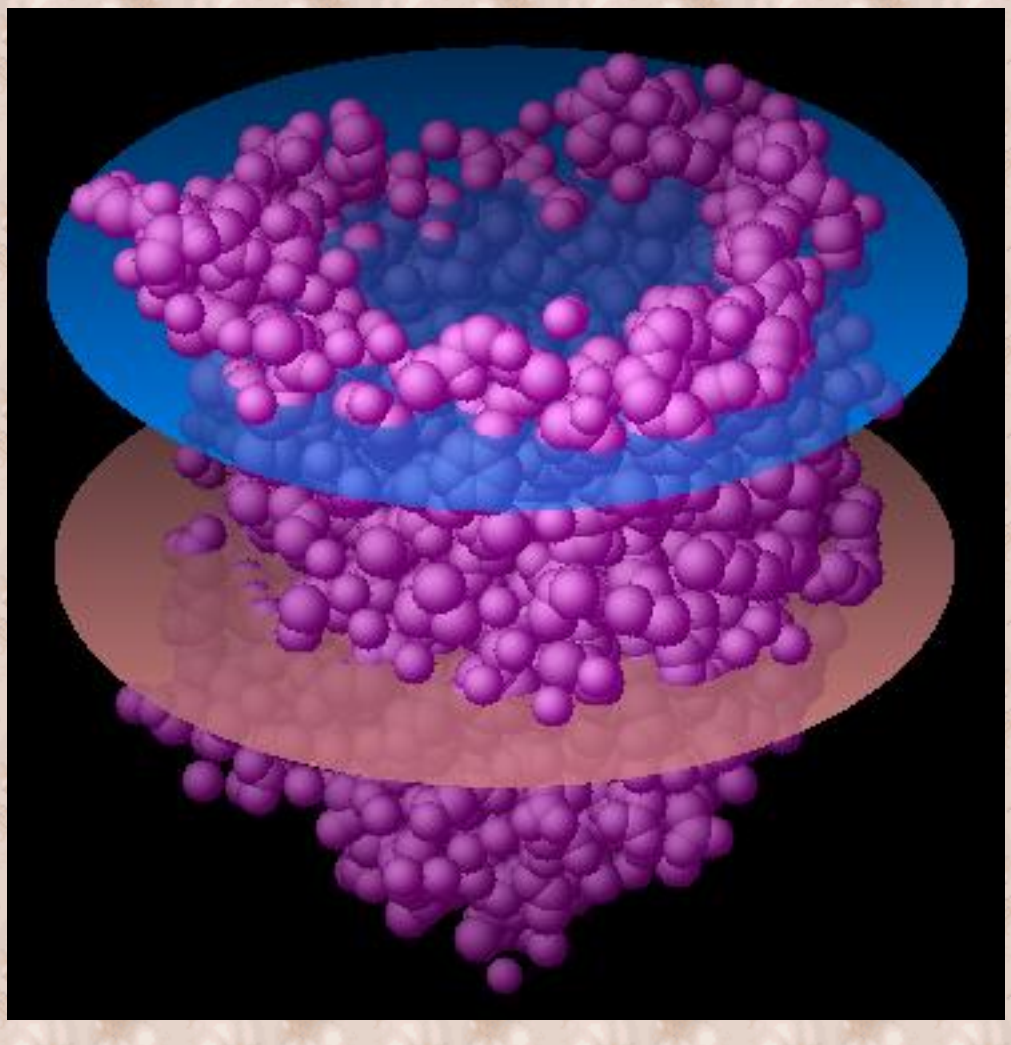
NOTES

(1) By default, the plane moves with the structure. If movement controls affect only the plane, be sure to make it visible. Otherwise, you may push the plane far away from the object to which this plane belongs.

(2) In garlic source code, each plane is defined by the plane center (three coordinates) and by the

normal vector (three-component vector).

(3) At present, garlic associates only one plane with each structure. If for some reason you need two planes (for example, to simulate the cellular membrane), use the following trick:
(3.1) Prepare the structure and its associated plane (the first plane).
(3.2) Load another structure (something small, like a single residue) and hide it.
(3.3) Make the plane (which is associated with this small structure) visible.
(3.4) Change radius and transparency for the second plane.
(3.5) Set the position and orientation of this plane.
If you learn this trick, you will be able to prepare images like this one:



RELATED COMMANDS

LOAD is used to load the structure (PDB file). MOVE is used to define which object should be moved. POSITION is used to place the choosen object (structure, plane or both) to arbitrary position. SELECT ABOVE selects atoms above the plane, while SELECT BELOW selects atoms below the plane.

POS, POSITION

NAME

POS, POSITION - move the origin of the internal coordinate system to the specified position.

SYNOPSIS

POS x y z
POSITION x y z

DESCRIPTION

An internal coordinate system is assigned to each structure. The command POS (POSITION) sets the position of this origin. Three coordinates (x, y and z) should be specified.

Initially, the position of geometric center is used as the internal system origin for each structure. When loaded, this origin is set into the point (0, 0, 0).

RELATED COMMANDS

CEN redefines the internal system origin.

RAM, RAMACHANDRAN

NAME

RAM, RAMACHANDRAN - draw Ramachandran plot.

SYNOPSIS

RAM
RAM SEL
RAM OFF
RAMACHANDRAN
RAMACHANDRAN SEL
RAMACHANDRAN OFF

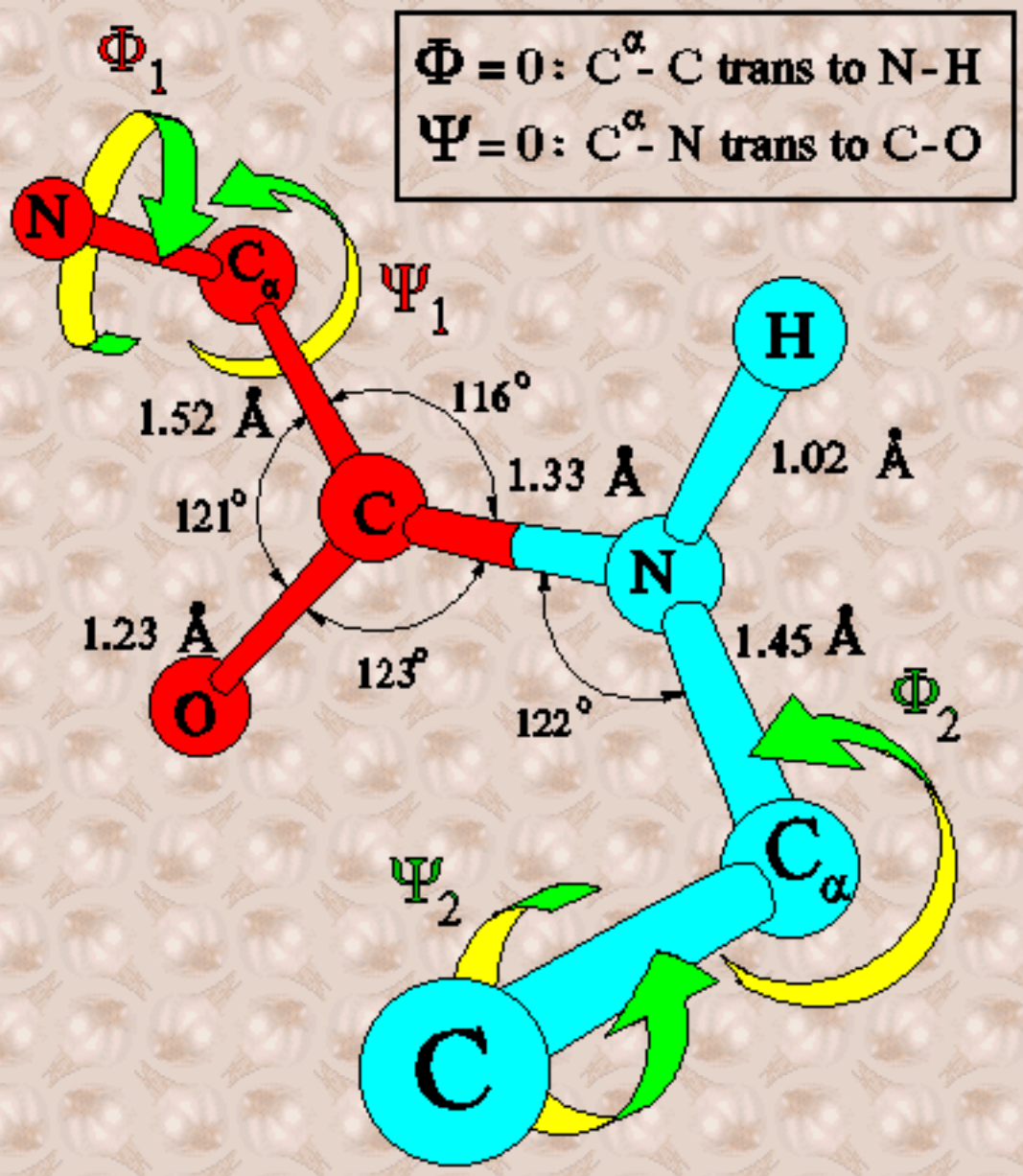
DESCRIPTION

Draw Ramachandran plot (only for proteins). The main chain torsion angles, phi and psi, are used to prepare two-dimensional scatter plot. Residues for which both phi and psi angle may be calculated will be shown as small circles. The horizontal axis (abscisa) is used for phi values, while the vertical axis (ordinate) is used for psi values. Blue color is used for trans residues, magenta for cis residues and red for bad residues. Trans residues are drawn first, followed by cis residues. Bad residues are drawn last. A residue is treated as bad if peptide unit associated with this residue is not planar. Peptide unit is considered as non-planar if it is twisted for more than 20 degrees. Terminal residues will be missing, because at least one of dihedral angles is not defined for such residues.

Dihedral angles are defined as follows:

(1) The phi angle is the angle of right-handed rotation around N-CA bond, the value being zero if CA-C bond is trans to N-H bond. Range: from -180 to 180 degrees.

(2) The psi angle is the angle of right-handed rotation around CA-C bond, the value being zero if N-CA bond is trans to C-O bond. Range: from -180 to 180 degrees.



KEYWORDS

If used without any keyword, the command RAM will prepare the Ramachandran plot for protein structure(s) which are currently being handled ("caught"). Keyword OFF is used to switch Ramachandran plot, i.e. to return to the main drawing mode (atomic structure display). If keyword SEL (SELECTED) is used, only the residues which are currently selected will be included in Ramachandran plot. A residue is treated as selected if the first atom of this residue is selected. For proteins, this is usually N (nitrogen) atom. Here is the overview:

KEYWORD	DESCRIPTION
ram sel	Draw Ramachandran plot for selected residues.
ram off	Return to default drawing mode (atomic structure). Instead using this command, you can hit the ESCAPE key.

MOUSE USAGE

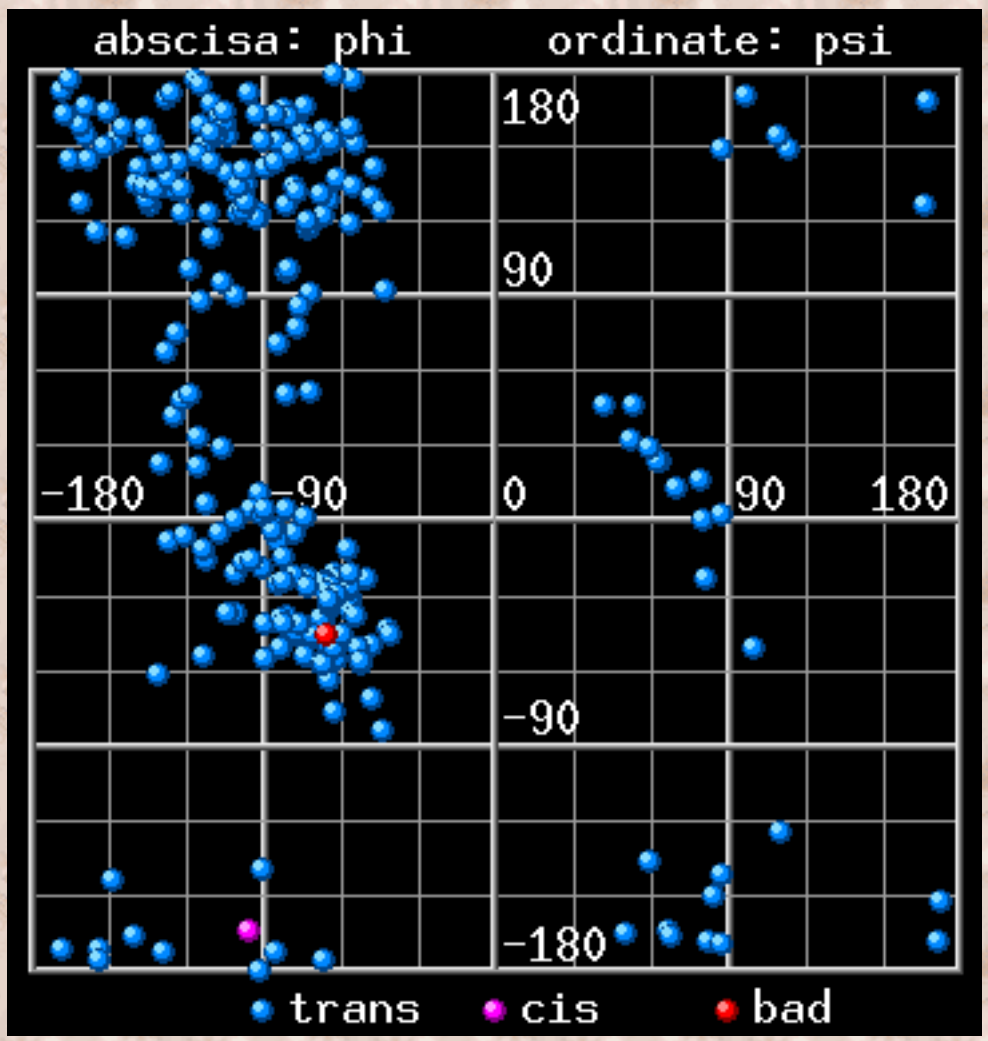
Pointing device (mouse) may be used to identify individual residues in Ramachandran plot. Just place

the mouse pointer above the selected residue and the most important data for this residue will be shown in the output window. The output window will look like this:

```
(1) 2POR
ALA 194
trans
phi: -73.31
psi:  -7.17
```

EXAMPLE OF RAMACHANDRAN PLOT

The example below show the Ramachandran plot for one typical globular protein, consisting of 250 residues. Only the essential part of the main garlic window is shown.



EXAMPLES

COMMAND	DESCRIPTION
ram	Draw Ramachandran plot for all residues.
ram off	Return to default drawing mode (atomic structure).

ram sel	Draw Ramachandran plot for selected residues.
sel pro ram sel	Select all prolines and draw Ramachandran plot for prolines.
sel cis ram sel	Select all residues in cis conformation and draw Ramachandran plot for them.
sel bad ram sel	Select bad residues (peptide unit not planar) and draw Ramachandran plot.
sel tra ram sel	Select all residues in trans conformation and draw Ramachandran plot.

NOTES

(1) Instead using the command RAMA OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) G. N. Ramachandran devised in the late 1960's the steric constrains for amino acid residues in proteins. As the number of high resolution structures is increasing, it appears evident that these old constrains are becoming obsolete. If you are interested in this problem, read this article:

alpha2.bmc.uu.se/~gerard/rama/rama.html

RELATED COMMANDS

SEL may be used to select a portion of protein structure, to reduce the amount of data in Ramachandran plot.

RES, RESTRICT

NAME

RES, RESTRICT - restrict the current selection.

SYNOPSIS

RES chain identifiers/residue serials/residue names/atom names
RES residue_ranges
RES residue_names
RES keyword

DESCRIPTION

Restrict the current selection. Atoms which do not satisfy the specified cryteria are excluded from selection. Four types of restriction cryteria may be used:

(1) detailed restriction;
(2) restriction by residue serial numbers;
(3) restriction by residue names;
(4) special restriction (by keyword).

DETAILED RESTRICTION

In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The string should contain exactly three slashes, separating different data types:

chain identifiers/residue serials/residue names/atom names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to specify all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from restriction.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from restriction.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from restriction. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to specify all atoms, while EXC may be used to exclude some atoms from this specification. Examples:

res a/*/*/*	**Leave only atoms which belong to chain A.**
res * exc m/*/*/ca	**Leave only CA atoms which belong to chain M.**
res */*/*/* exc ca,c,n,o	**Remove CA, C, N and O atoms from the selection.**
res a/* exc 72-112/*/ca	**Leave only CA atoms which belong to chain A, but exclude residues 72-112.**

RESTRICTION BY RESIDUE SERIAL NUMBERS

In this type of selection restriction, residue numbers, residue ranges or residue names may be specified. The restriction cryteria should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

res 1-100	Leave only atoms which belong to residues from 1 to 100.
res 1-100 exc 20-40	Leave only atoms which belong to residues 1-100, but exclude 20-40.
res 1, 4, 8, 11-48 exc 20-32	Leave atoms which belong to residues 1, 4, 8, 11-48 but exclude residues 20-32.

RESTRICTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

res phe,tyr,trp	Restrict selection to PHE, TYR and TRP.

SPECIAL RESTRICTION KEYWORDS

Some special keywords may be combined with RES to specify residues or atoms according to some properties. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted. COM (COMPLEMENT) may be specified, but restriction to complement means that nothing will be left in the selection. Examples:

res * res all	Leave the selection unchanged (trivial, useless).
res abo res above	Restrict to atoms above the plane.
res aci res acidic	Leave only acidic amino-acids in the selection (GLU and ASP).
res ali res aliphatic	Leave only aliphatic amino acids (ILE, LEU and VAL).
res alt	Restrict to atoms at alternate positions.
res bad	Restrict selection to bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
res bas res basic	Leave only basic amino acids (ARG, LYS and HIS).
res bel res below	Restrict to atoms below the plane.
res cha res charged	Leave only charged amino acids (ARG, LYS, HIS, GLU and ASP).
res cis	Restrict selection to cis residues.

res com res complement	Leave only atoms which were not select previously.
res het res hetero	Leave only hetero atoms (heme groups, water etc.).
res pho res hydrophobic	Leave only hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
res mai res main_chain	Leave only main chain atoms (CA, C, N and O).
res mod serial_number res model serial_number	Restrict to a model specified by serial_number. NMR structure is a set of models. Example: res mod 1
res neg res negative	Leave only negatively charged amino acids (GLU and ASP).
res pol res polar	Leave only polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
res seq res sequence	Restrict to sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
res pos res positive	Leave only positively charged amino acids (ARG, LYS and HIS).
res sid res side_chains	Leave only atoms which belong to side chains (all except CA, C, N and O).
res sma res small	Leave only small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
res sph res sphere	Restrict to the atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
res tin res tiny	Leave only tiny amino acids (GLY,ALA and SER).
res tra res trans	Restrict selection to trans residues.

RELATED COMMANDS

SELECT overwrites the previous selection. ADD expands the previous selection.

SCA, SCALE

NAME
SCA, SCALE - select hydrophobicity scale.

SYNOPSIS
SCA keyword
SCALE keyword

DESCRIPTION
The command SCALE selects the specified hydrophobicity scale. At present, three scales are available: Eisenberg normalized consensus scale, Kyte-Doolittle hydropathy scale and White octanol scale (experimental). The scale is assigned to the structure which is currently being handled (the structure which was caught using the command CATCH). It is also used as default hydrophobicity scale for the sequence in the main sequence buffer. The hydrophobicity scale is used to calculate the averaged hydrophobicity and hydrophobic moment. It may be also used to color the protein structure according to hydrophobicity.

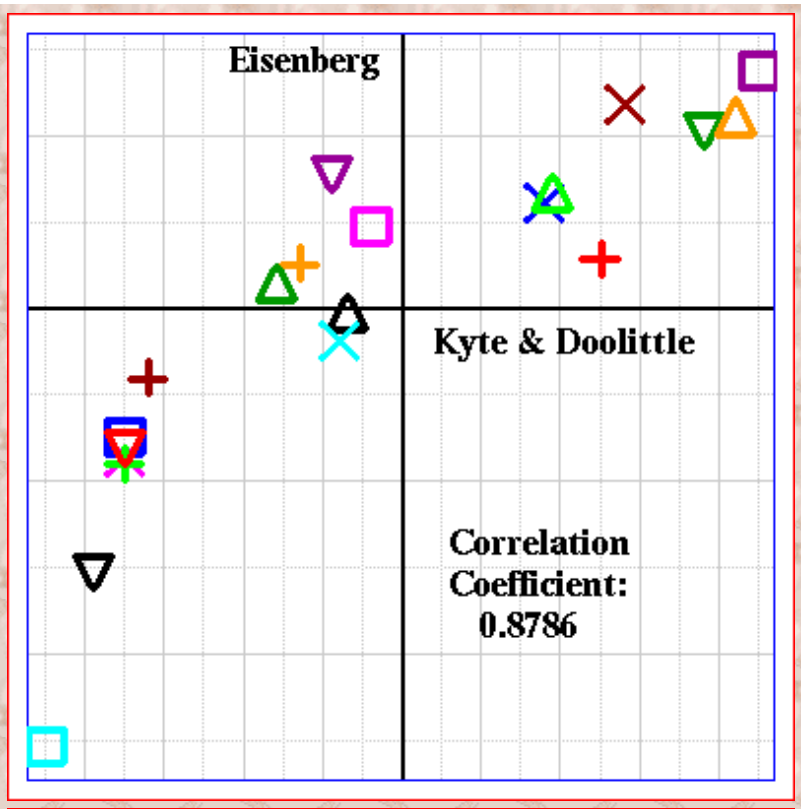
Hard-coded program default is Eisenberg scale.

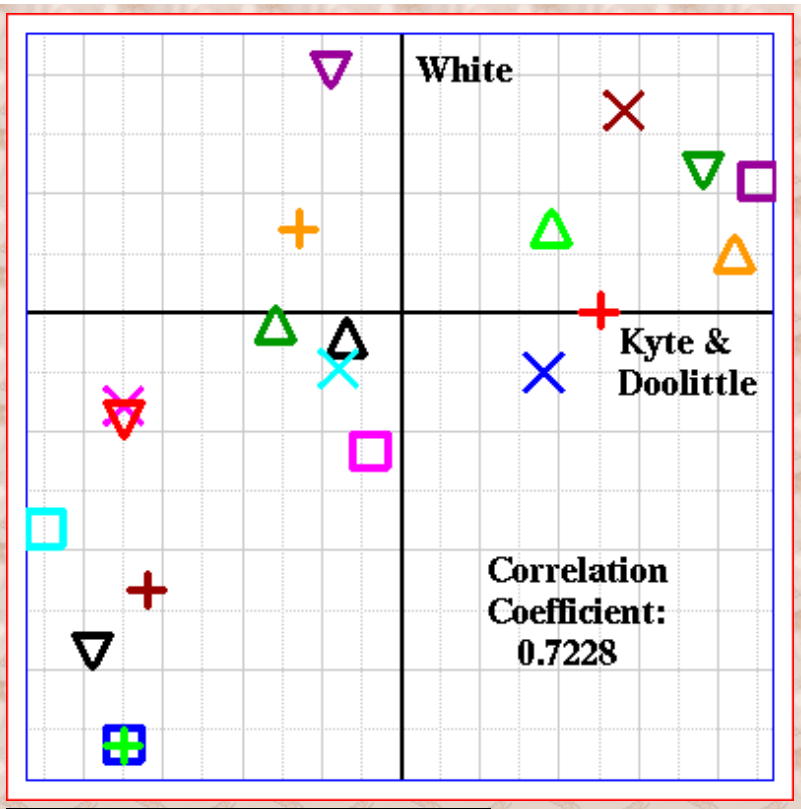
KEYWORDS

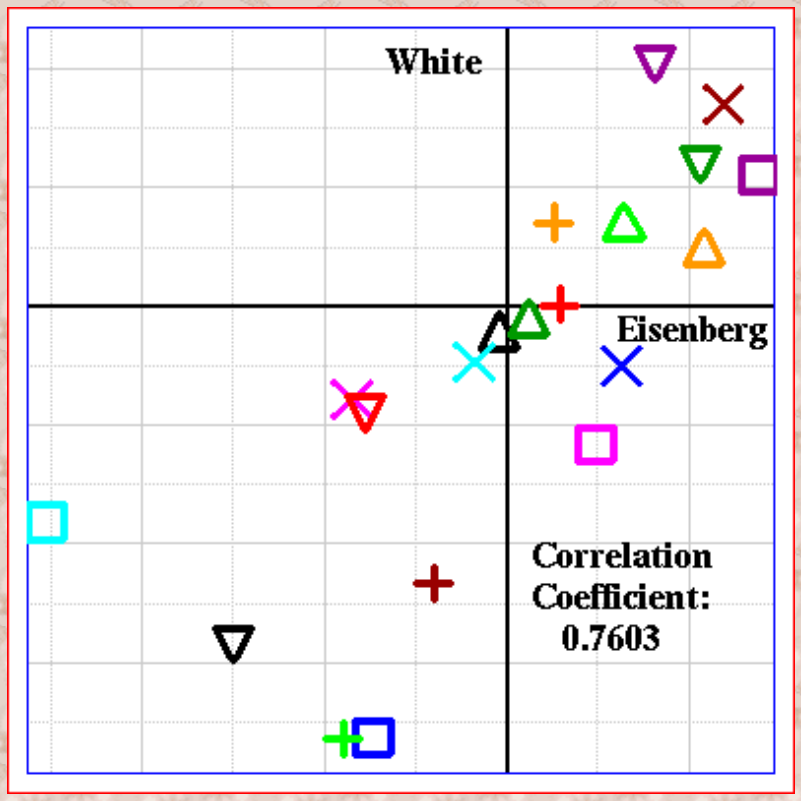
KEYWORD (SHORT)	KEYWORD (LONG)	DESCRIPTION
EIS	EISENBERG	Use Eisenberg normalized consensus hydrophobicity scale.
KD	KD	Use Kyte-Doolittle hydropathicity scale.
WHI	WHITE	Use octanol scale (Steven White group, experimental data).

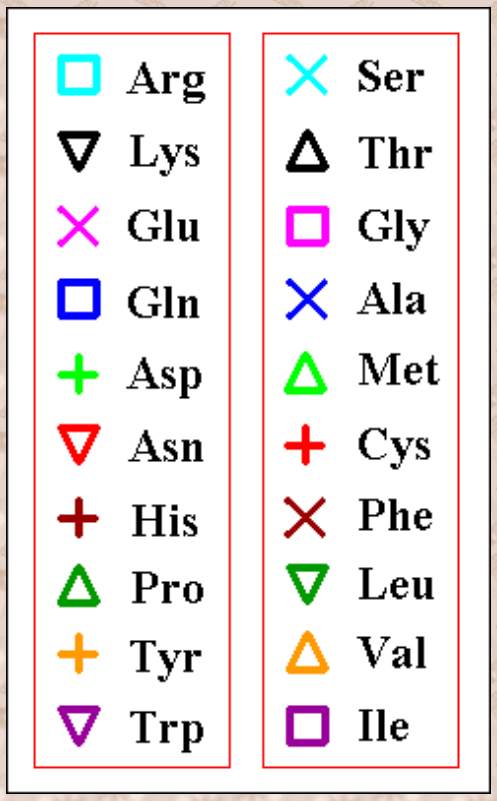
HYDROPHOBICITY SCALES
The table below contains numeric data for three hydrophobicity scales which are used in garlic. Correlation coefficients and plots are also given. The original White octanol scale contains free energy changes for a transfer of whole residues from water to octanol. In garlic, these free energy changes are multiplied by minus one and used as hydrophobicity values. The experimental values and nice theoretical explanations may be found at:
http://blanco.biomol.uci.edu/hydrophobicity_scales.html

NAME	EIS	KD	WHI
ALA	0.62	1.80	-0.50
ARG	-2.53	-4.50	-1.81
ASN	-0.78	-3.50	-0.85
ASP	-0.90	-3.50	-3.64
CYS	0.29	2.50	0.02
GLN	-0.85	-3.50	-0.77
GLU	-0.74	-3.50	-3.63
GLY	0.48	-0.40	-1.15
HIS	-0.40	-3.20	-2.33
ILE	1.38	4.50	1.12
LEU	1.06	3.80	1.25
LYS	-1.50	-3.90	-2.80
MET	0.64	1.90	0.67
PHE	1.19	2.80	1.71
PRO	0.12	-1.60	-0.14
SER	-0.18	-0.80	-0.46
THR	-0.05	-0.70	-0.25
TRP	0.81	-0.90	2.09
TYR	0.26	-1.30	0.71
VAL	1.08	4.20	0.46
ASX	-0.84	-3.50	-2.25
GLX	-0.80	-3.50	-2.20
UNK	0.00	-0.49	-0.52









EXAMPLES

COMMAND	DESCRIPTION
sca eis	Use the scale made by David Eisenberg.
sca whi	Use the experimental scale made by Steven White and coworkers.

NOTES

(1) Many hydrophobicity scales may be found in literature. However, most of these scales are mutually highly correlated. If you are interested in these correlations, try the web server SCACOR . All you have to do is to select two scales for comparison. The web server will calculate the

correlation factor and prepare the scatter plot.

RELATED COMMANDS

PLOT is used to draw averaged hydrophobicity and hydrophobic moment. COLOR HYPHOB is used to color the structure according to hydrophobicity of residues.

REFERENCES

(1) Kyte, J. and Doolittle, R. F. (1982). J. Mol. Biol. 157, p. 105.
(2) Eisenberg, D., Schwarz, E., Komaromy, M. and Wall, R. (1984). J. Mol. Biol. 179, p. 125.
(3) Wimley, W. C. and White, S. H. (1996). Nature Struct. Biol. 3, p. 842.
(4) Wimley, W. C., Creamer, T. P. and White, S. H. (1996). Biochemistry 35, p. 5109.
(5) White, S. H. and Wimley, W. C. (1998). Biochim. Biophys. Acta 1376, p 339.
(6) White, S. H. and Wimley, W. C. (1999). Annu. Rev. Biophys. Biomol. Struc. 28, p. 319.

SEL, SELECT

NAME

SEL, SELECT - select specified atoms. Overwrite the previous selection.

SYNOPSIS

SEL chain identifiers/residue serials/residue names/atom names
SEL residue_ranges
SEL residue_names
SEL keyword

DESCRIPTION

Select specified atoms. Atoms are selected according to the specified cryteria. Four types of selection are available:

(1) detailed selection;
(2) selection by residue serial numbers;
(3) selection by residue names;
(4) special selection (by keyword).

DETAILED SELECTION

In this case four data types are specified simultaneously: chain identifiers, residue serial numbers, residue names and atom names. It is not possible to specify atomic serial numbers. The selection string should contain exactly three slashes, separating different data types:

chain identifiers/residue serials/residue names/atom names.

Both uppercase and lowercase characters are accepted. Space ( ), comma (,) and semicolon (;) may be used as separators.

Chain identifiers are single alphabetic characters. Asterisk (*) may be used to select all chains. The keyword EXC (EXCEPT) may be used to exclude one or more chains from selection.

Residue serial numbers consist of digits. Minus may be used to specify a range of residue serial numbers. For example, 1-100 specifyes residues from 1 to 100, including these two. Asterisk (*) may be used to specify all residue serials. The keyword EXC (EXCEPT) may be used to exclude serial numbers or ranges from selection.

Residue names are expected in three letters code. Asterisk (*) may be used to specify all residue names. The keyword EXC (EXCEPT) may be used to exclude one or more names from selection. Non-standard names are accepted.

The names of atoms are expected as used in the input file; do not replace them with pure chemical symbols. C alpha, for example, should be specified as CA or ca (case is not important), if coordinates are read from PDB file. Asterisk (*) may be used to select all atoms, while EXC may be used to exclude some atoms from selection. Examples:

sel a/*/*/*	Select all atoms from chain A.
sel * exc m/*/*/ca	Select CA atoms from all chains except chain M.
sel */*/*/* exc ca,c,n,o	Select all atoms except CA, C, N and O.
sel a/* exc 72-112/*/ca	Select CA atoms from chain A, but exclude residues from 72 to 112.

SELECTION BY RESIDUE SERIAL NUMBERS

To select all atoms in a single residue, a residue range or in a number of residues and residue ranges, a simple syntax may be used. The selection string should contain no slashes. Keyword EXC (EXCEPT) is accepted, but asterisk (*) will be missintepreted. Minus may be used to specify residue ranges. Comma (,), semicolon (;) and space ( ) may be used as separators. Examples:

sel 1-100	Select residues from 1 to 100.
sel 1-100 exc 20-40	Select residues 1-100 but exclude 20-40.
sel 1, 4, 8, 11-48 exc 20-32	Select residues 1, 4, 8 and 11-48 but exclude 20-32.

SELECTION BY RESIDUE NAMES

Three letters code should be used. Asterisk (*) and keyword EXC (EXCEPT) are not accepted. Example:

sel phe,tyr,trp	Select PHE, TYR and TRP.

SPECIAL SELECTION KEYWORDS

Some special keywords may be combined with SEL (SELECT) to select residues or atoms according to some properties. It is also possible to select the complement, i.e. all atoms which were not selected previously. A single keyword should be used; asterisk (*) and keyword EXC (EXCEPT) are not accepted.

sel * sel all	Select all atoms (select all).
sel abo sel above	Select atoms above the plane.
sel aci sel acidic	Select acidic amino acids (GLU and ASP).
sel ali sel aliphatic	Select aliphatic amino acids (ILE, LEU and VAL).
sel alt	Select atoms at alternate positions.
sel bad	Select bad residues. A residue is treated as bad if the peptide bond assigned to this residue is non-planar. The peptide bond is non-planar if the omega angle is different for 20 or more degrees from 0 or 180 degrees.
sel bas sel basic	Select basic amino acids (ARG, LYS and HIS).
sel bel sel below	Select atoms below the plane.
sel cha sel charged	Select charged amino acids (ARG, LYS, HIS, GLU and ASP).
sel cis	Select cis residues.
sel com sel complement	Select atoms which were not selected previously.

sel het sel hetero	Select hetero atoms (heme groups, water etc.).
sel pho sel hydrophobic	Select hydrophobic amino acids (ALA, ILE, LEU, MET, PHE, TRP, VAL, TYR, CYS, GLY and HIS).
sel mai sel main_chain	Select main chain atoms (CA, C, N and O).
sel mod serial_number sel model serial_number	Select model specified by serial_number. NMR structure is a set of models. Example: sel mod 1
sel neg sel negative	Select negatively charged amino acids (GLU and ASP).
sel pol sel polar	Select polar amino acids (ARG, LYS, HIS, ASP, GLU, ASN, GLN, SER, THR, TRP and TYR).
sel pos sel positive	Select positively charged amino acids (ARG, LYS and HIS).
sel seq sel sequence	Select sequence fragments which match the sequence stored to the sequence buffer. The sequence buffer should be initialized before executing this command.
sel sid sel side_chains	Select atoms which belong to side chains (all except CA, C, N and O).
sel sma sel small	Select small amino acids (GLY, ALA, SER, THR, CYS, VAL, PRO, ASP and ASN).
sel sph sel sphere	Select atoms inside the sphere. Use the command RAD (RADIUS) to set the sphere radius.
sel tin sel tiny	Select tiny amino acids (GLY, ALA and SER).
sel tra sel trans	Select trans residues.

RELATED COMMANDS

ADD expands the previous selection. RESTRICT restrics the previous selection.

SEQ, SEQUENCE

NAME
SEQ, SEQUENCE - manipulate the content of the sequence buffer.

SYNOPSIS
SEQ = three_letters_code
SEQ LOAD filename
SEQ READ filename
SEQ FROM structure_identifier
SEQ COPY
SEQ SAVE filename
SEQ SWN filename
SEQ RESET

DESCRIPTION
The command SEQ (long form: SEQUENCE) manipulates the content of the main sequence buffer. Garlic mantains two sequence buffers: the main buffer and the reference buffer. The main sequence buffer is used to prepare the average hydrophobicity plot, the hydrophobic moment plot, helical wheel plot and for some other operations which require the sequence information. The reference sequence buffer is used for sequence comparison and other operations which require two sequences.

Both buffers store the following sequence information:
(1) The number of residues.
(2) The sequence in the form of three letters code. Uppercase letters are used.
(3) Disulfide bond flag, if information about disulfide bonds is available.
(4) Residue serial numbers.
(5) Raw hydrophobicity values (replaced by average value for exotic residues).

In addition, the main sequence buffer contains the following information:
(6) The average hydrophobicity. width.
(7) The hydrophobic moment.

As sequence information may be given independently from any structure, atomic coordinates are not required for most sequence manipulation routines. Thus, garlic may be used as a sequence analysing tool.

All version of the command SEQ, except one, are used to manipulate the content of the main sequence buffer. The only exception is SEQ COPY, which copies the content of the main sequence buffer to the reference buffer. This is the only way to store information to the reference buffer.

SEQ = three_letters_code
The command SEQ may be used with the keyword = (equal sign) to define sequence at garlic command prompt. This may be practical to define a short sequence fragment. This fragment may be used for helical wheel plot, or to locate the given sequence fragment in a structure which is being investigated. The syntax:

SEQ = three_letters_code

Example:
seq = ala phe tyr trp asn

The sequence fragment will be converted to uppercase. The sequence is not checked for exotic

residues so you can use the non-standard codes. However, the routine which assigns the hydrophobicity values will fail to recognize them. The average hydrophobicity value (calculated for the current scale) will be assigned to these residues. At present, 23 codes are recognized:

```
ALA, CYS, LEU, MET, GLU, GLN, HIS, LYS, VAL, ILE,
PHE, TYR, TRP, THR, GLY, SER, ASP, ASN, PRO, ARG,
ASX, GLX, UNK.
```

SEQ LOA filename
SEQ LOAD filename
SEQ REA filename
SEQ READ filename

The keyword LOAD (or READ) may be used to read a sequence from the specified file. Garlic is capable to recognize two types of input file formats: FASTA files (one letter code) and files which contain three letters code in a free format.

If input file contains the symbol > (greater than) in the first column of the first useful line, the file is treated as one letter protein code in FASTA format. Empty lines are ignored. The lines beginning with the symbol # (numbersign) in the first column are treated as comments (ignored too). Thus, the lines which are not empty and do not contain the symbol # in the first column are treated as useful.

If input file is not recognized as FASTA file, it is expected to contain the three letters code in a free format. Empty lines and all lines which contain # in the first column are ignored. All other lines are treated as useful. Digits (serial numbers, for example) are ignored. The following characters are threated as separators:
(1) space
(2) tab
(3) comma (,)
(4) semicolon (;)
(5) newline (line feed)

If input file contains at least one bad code (a residue name which consists of four letters, for example) the reading will fail. The hard-coded maximal number of residues is 50000, but it may be easily changed (see MAXRESIDUES in the header file defines.h).

Example:
load sample.fasta

SEQ FRO structure_identifier
SEQ FROM structure_identifier

The keyword FROM may be used to copy the sequence from the specified structure to the main sequence buffer. Only selected residues are copied. Residue is treated as selected if the first atom is selected. For proteins, this is typically N (nitrogen). Residue insertion codes are ignored! Thus, the same residue serial index (number) may appear more than once in the array of residue serial numbers.

Example:
seq from 1

SEQ COP
SEQ COPY

The command SEQ COPY copies the sequence from the main sequence buffer to the reference buffer. This is the only way to initialize the reference buffer. This command must be executed (i.e., the keyword COPY must be used) before executing commands which require two sequences for proper operation. The main sequence buffer may be initialized prior to SEQ COPY by using one of the keywords

described above (=, LOAD or FROM).

Example:
seq copy

SEQ SAV filename
SEQ SAVE filename

The command SEQ SAVE saves the sequence to the specified file. Ten codes (each consisting of up to three letters) are written per line, separated by space. Serial numbers are not included (see SWN keyword).

Example:
seq save 9pap.seq

SEQ SWN filename

The command SEQ SWN saves the sequence to the specified file. Both residue names and serial numbers are written to the output file. Insertion codes will be missing! Five serial numbers and residue names are written per line, separated by space.

Example:
seq swn 9pap.seq

SEQ RES
SEQ RESET

Reset (clear) the main sequence buffer. The command SEQ RESET sets the number of residues in the main sequence buffer to zero. The storage is not freed, so the buffer may be used again later.

Example:
seq reset

RELATED COMMANDS

PLOT prepares the average hydrophobicity and/or hydrophobic moment plot. COMPARE compares two sequences. VENN draws Venn diagram. WHEEL draws helical wheel plot. SEL SEQ selects portions of the structure which contain the sequence stored to the main sequence buffer. To use any of these commands, the main sequence buffer (to use COMPARE both buffers) must be initialized by using the command SEQ.

SSB

NAME
SSB - change drawing style for disulfide bonds.

SYNOPSIS
SSB style

DESCRIPTION
Change drawing style for disulfide bonds. This command is very similar to BONDS, except that it affects only disulfide bonds. Bond style is defined separately from atom style. At present, proportionally sized styles are not available.

STYLE	THICKNESS	TYPE
0	Unvisible disulfide bonds	Fixed
1	A single line	Fixed
2	Three lines	Fixed
3	Five lines	Fixed
4	Seven lines	Fixed
5	Nine lines	Fixed

NOTES
(1) Unvisible bonds (style 0) are not treated as hidden - they are just invisible.

RELATED COMMANDS
ATO (ATOMS) changes drawing style for atoms. BON (BONDS) changes drawing style for all except disulfide bonds.

TRA, TRANSLATE

NAME

TRA, TRANSLATE - translate the structure for the given shift in the given direction.

SYNOPSIS

TRA axis shift

DESCRIPTION

Translate the structure. The axis should be specified with one letter (x, y or z) and the shift should be given in angstroms.

EXAMPLES

COMMAND	DESCRIPTION
tra x 40	Move to the right, 40 angstroms.
tra y -0.5	Move up, 0.5 angstroms (y points down).

WHE, WHEEL

NAME

WHE, WHEEL - draw helical wheel plot.

SYNOPSIS

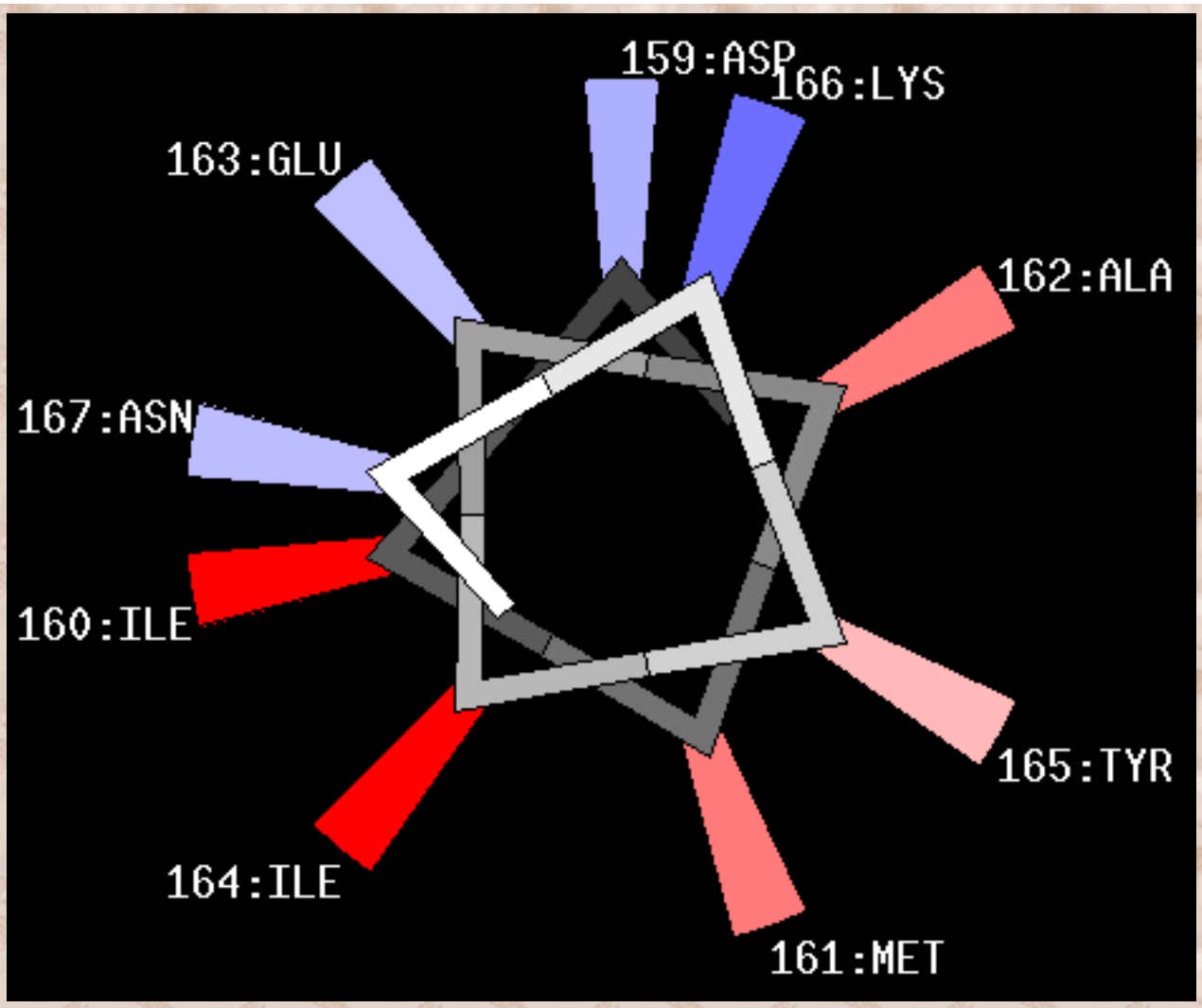
WHE
WHE OFF
WHE start_index end_index
WHEEL
WHEEL OFF
WHEEL start_index end_index

DESCRIPTION

Draw helical wheel plot for the given sequence or sequence fragment. Helical wheel may be used to recognize the amphiphilic character of the specified sequence fragment. The sequence from the main sequence buffer (or part of it) is used as input. Additional input: the rotation angle between adjacent residues and hydrophobicity values. The angle should correspond to certain structural motif. Default (hard-coded) angle is 100 degrees, which corresponds to alpha helix, but this may be changed to some arbitrary value, using the command ANGLE. The value of 160 degrees is suitable for beta strand and 115 or 125 is suitable for 3-10 helix.

While helical wheel may be drawn for any sequence length, it makes sense only for short sequence fragments (up to about twenty residues). Hydrophobic residues will be colored in shades of red, while hydrophilic residues will be colored blue. Color intensity depends on the hydrophobicity: very hydrophobic residues will be intensely red and weakly hydrophobic residues will be almost white. Very hydrophilic residues will be intensely blue and weakly hydrophilic residues will be almost white. The command SCALE may be used to select the hydrophobicity scale.

The command WHEEL is usually used in combination with some other commands. See the examples below.



KEYWORDS AND PARAMETERS

The command WHEEL may be used alone, combined with the keyword OFF or with two residue serial indices. If used alone, the helical wheel will be drawn for the entire sequence stored in the main sequence buffer. If this sequence is large the plot will be useless. Two residue serial indices may be used to specify the residue range. The keyword OFF is used to return to the main drawing mode (structure drawing mode).

EXAMPLES

COMMAND	DESCRIPTION
seq = asp ile met ala glu ile scale eis angle 100 wheel	Initialize the sequence fragment, select Eisenberg hydrophobicity scale, set angle to 100 degrees and draw helical wheel. It is assumed that that the specified sequence fragment belongs to alpha helix.
load 2por.pdb seq from 1 scale eis angle 160 wheel 2-10	Load porin coordinates, copy the sequence of this protein to the main sequence buffer, select Eisenberg hydrophobicity scale, set angle to 160 degrees and draw helical wheel for residues from 2 to 10. It is assumed that the specified sequence fragment belongs to beta strand.

whe off	**Return to default drawing mode. Instead using this command, you can hit the ESCAPE key.**

NOTES

(1) Instead using the command WHEEL OFF, the ESCAPE key may be pressed to return to the main drawing mode.

(2) Don't forget that WHEEL uses only the sequence stored to the main sequence buffer. Read description of the command SEQ (SEQUENCE) to learn how to initialize this buffer.

RELATED COMMANDS

SEQUENCE is used to copy, define or load the sequence. ANGLE defines the rotation angle between adjacent residues. SCALE is used to specify the hydrophobicity scale.

Mouse Usage

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Move the mouse pointer over the structure and you will see the textual information about the atom covered by the pointer. This information will be visible in the output window (the bottom right corner of the main window).

The structure drawing mode is not the only mode where this trick may be used: try also Ramachandran plot, hydrophobicity plots and sequence comparison. The examples below show the content of the output window for all four cases:

Structure display	Ramachandran plot	Averaged hydrophobicity	Sequence comparison
(1) 2POR TYR 161 OH 1202 0 t.f.: 85.47 trans phi:-107.10 psi: 137.98 phob: 0.26 selected x: 2.333 y: -20.365 z: -15.514	(1) 9PAP GLN 114 trans phi: -50.56 psi: 116.21	ALA 211 value: 0.658	HORIZ. VERT. 27ALA ALA31 28PHE PHE32 29SER GLY33 30ALA ALA34 31VAL VAL35 32VAL GLU36 33THR ALA37 34ILE ILE38 35GLU SER39 36GLY ASP40 37ILE ARG41

Since April 10. 2000 (garlic version 1.0 and later), mouse clicks may be used for rotations and translations and also for slab and color adjustment. Click on a selected button in a control window (top right corner of the main window). Shift, alt and control play the same role as if keyboard is used for the same job.

Some desktop environments (like KDE and Gnome) use function keys to launch popup menus or for some other purpose. This means that function keys F1, F2, F3 and F4 will not work properly with garlic. You can use mouse to click on dummy buttons in a control window. Another approach will be to change desktop environment settings.

Perhaps it will be good idea to use right mouse button for some kind of menu and left mouse button for

selection. If you have some ideas, write to me. The address is: zucic@garlic.mefos.hr .

Garlic Reference Card

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Garlic reference card contains the list of commands and keywords, with short description of commands. Print this page and keep it at hand during your garlic sessions. Garlic reference card is not a learning tool, it is just a reminder. Newbies should start with garlic tutorial.

HTML version	**Recommended if your browser is properly configured for printing.**
StarOffice version	**Suitable for Sun StarOffice 5.2 (download via ftp).**
MS Word version	**MS Word 97/2000 format, created with StarOffice (ftp).**
PostScript version	**PostScript level 2 (ftp).**

Garlic Tutorial

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garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

Lessons

These lessons should help you to learn how to use garlic. Command are given in lowercase, in a short form, but you can use the long form as well as the uppercase letters. File names should be specified in the correct case.

RECOMMENDED USAGE: Print lessons.

In addition, you should read the pages describing garlic commands and controls !

Lesson 1 - Get familiar with garlic
Lesson 2 - Load a small structure
Lesson 3 - Playing with two structures
Lesson 4 - Drawing styles and color schemes
Lesson 5 - How to select atoms
Lesson 6 - Ramachandran plot
Lesson 7 - Helical wheel plot
Lesson 8 - Plot averaged hydrophobicity and hydrophobic moment
Lesson 9 - Venn diagram
Lesson 10 - Semitransparent plane

Scripts

The scripts listed below may be used to demonstrate the available drawing styles for atoms and bonds, as well as some predefined color schemes. These scripts were included into the garlic source package 28. March 2000. If you have an older package, copy these scripts to your local host. There are two ways to copy scripts:
(1) Click here to download them via ftp.
(2) Go to the page which contains the script you selected. Mark and copy the script. Paste it into a local file. Recommended file names: 1: atoms.script, 2: bonds.script, 3: colors.script, 4: dance.script .

Script 1 - Drawing styles for atoms
Script 2 - Drawing styles for bonds
Script 3 - Predefined (hard-coded) color schemes
Script 4 - Dancing tryptophan

Garlic Tutorial

Lesson 2 - Load a Small Structure

In this lesson, you will learn how to load a PDB file and how to move the structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load tryptophan (it should be included in the source package). This command should be executed at garlic prompt:

loa trp.pdb

Step 3 - how to use the pointing device (mouse):

Move the mouse pointer over atoms and bonds and read the text which appears in the output window (bottom right corner). Note that half of each bond is assigned to each of two atoms involved in bond formation.

Step 4 - use garlic controls (i.e. the keys on numeric keypad) to rotate the structure (just a single amino acid):

First play for a while with keys 4 and 6, then with 2 and 8, and finally with 7 and 9. Try the same while holding shift (alone), control (alone), alt and shift (simultaneously) and control and shift (simultaneously). Do not try control-alt combinations, unless you are very experienced with unix and X.

Step 5 - use garlic controls (numeric keypad) to translate the structure:

PC keyboard: use /, *, -, +, 5 and 0.
Terminal keyboard: use PF2, PF3, -, comma, 5 and 0.
Repeat while holding modifier keys (alone or in combination).

Step 6 - move the structure to the screen center again:

pos 0 0 0

Step 7 - rotate and translate the structure using commands instead of controls. Try the following set of commands:

rot x 90
tra x 4
tra y -4
tra z -50
rot y 180

Step 8 - move the color surfaces. As your structure is very small, be sure to hold the control key while pressing functions keys:

Hold control key and press F1.
Hold control key and press F4.
Note that color is changing.

Hold control key and play with F1, F2, F3 and F4 for a while.

Step 9 - move the slab surfaces. As your structure is very small, be sure to hold the control key:

Hold control key and 3 (numeric keypad). Repeat until some atoms and bonds disappear.
Hold control key and play with 1, 3, decimal separator (next to 0) and enter for a while. Note that (in control window) visible atoms are red and unvisible atoms are dark cyan.

Step 10 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 3 - Playing with Two Structures

In this lesson, you will learn how to work with two or more structures. The original source package contains two PDB files: trp.pdb and phe.pdb. Each contains a single amino acid: trp.pdb = tryptophan, phe.pdb = phenylalanine. In this lesson, tryptophan will be colored blue, while phenylalanine will be colored red. Note the role of the command cat (catch).

Step 1 - start garlic (if necessary):

garlic

Step 2 - load trypthophan:

loa trp.pdb

Step 3 - change TRP color to blue:

col blue

Step 4 - load phenylalanine:

loa phe.pdb

Step 5 - change PHE color to red:

col red

Two structures will be distinguished by color and by the identifier: tryptophan is treated as structure number 1, and phenylalanine is treated as structure number 2. Two structures are now overlapping.
Step 6 - move tryptophan to the left:

cat 1
pos -5 0 0

Step 7 - move phenylalanine to the right:

cat 2
pos 5 0 0

Step 8 etc. - use the command cat (catch) to rotate structures one by one:

Use cat 1 and cat 2 to catch and rotate structures, one by one.
Translate both structures to the position where they will be overlapped, but do not use keyword pos!

When finished, discard loaded structures:

dis all

Garlic Tutorial

Lesson 4 - Drawing Styles and Color Schemes

In this lesson, you will learn different drawing styles, used for atoms and bonds. Note that garlic uses separate styles for atoms and bonds. You will also try some predefined color schemes. Use the X server which offers 24 bits per pixel, if possible.

As you will often reuse some commands, just with a different argument, note that garlic has a history buffer, where commands which were previously used are stored. The arrow keys may be used to recall one of these commands.

Use the "UP" arrow to scan the history buffer backwards, "DOWN" arrow to scan it upwards, "LEFT" arrow to move the insertion mark left and "RIGHT" arrow to move the insertion mark to the right (if possible, of course). Backspace (or delete, if you have some unusual keyboard mapping) may be used to remove characters.

Step 1 - start garlic (if this wasn't done before):

```
garlic
```

Step 2 - load trypthophan and bring it closer to you:

```
loa trp.pdb
pos 0 0 -150
```

Step 3 - make bonds unvisible (i.e. set bond thickness to zero):

```
bon 0
```

Step 4 - learn which drawing styles are available for atoms.
Hint: use the arrow key "UP" to call the previous command.

```
ato 1
ato 2
ato 3
ato 4
ato 5
ato 6
ato 7
ato bal
ato ba2
ato big
ato bi2
ato spa
ato sp2
```

Step 5 - hide atoms:

```
ato 0
```

Step 6 - learn which drawing styles are available for bonds.
Hint: use the arrow key "UP" to call the previous command.

bon 1
bon 2
bon 3
bon 4
bon 5

Step 7 - learn how to draw balls and sticks:

bon 4
ato bal

Step 8 - try some predefined color schemes.
Hint: use the arrow key "UP" to call the previous command.
Warning: Always use the full color scheme name (do not abbreviate)!

col red
col green
col blue
col yellow
col cyan
col magenta
col white
col yellow-green
col cyan-green
col cyan-blue
col magenta-blue
col magenta-red
col orange
col hot
col cold
col cpk

Step 9 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 5 - How to Select Atoms

In this lesson, you will learn how to select atoms. The command select (or whatever command plays this role) is one of the most important commands in every molecular visualization program.

For this lesson, you will need a true protein structure, not just a single amino acid as in previous lessons.

Step 1 - obtain the protein structure:

Use you web browser to access The Protein Data Bank (www.rcsb.org) .
Type 1HUC into the small search field. Start the search and wait for the answer.
Choose the option "Download/Display File".
Finally, choose file format "PDB", compression "none" in the section "Download the Structure File" and wait.

Step 2 - start garlic (if necessary):

garlic

Step 3 - load the structure. You should have the file 1HUC.pdb somewhere in the path searched by garlic (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 4 - draw backbone, to simplify the picture:

bac

Step 5 - use different colors for different chains:

col chain

Step 6 - select chain A, draw balls and sticks and change color scheme to CPK:

sel a/*/*/*
bac off
bon 4
ato bal
col cpk

Step 7 - redefine the internal system origin (the rotation center) and move chain A to the screen center:

cen
pos 0 0 0

Step 8 - restrict the selection to aliphatic amino acids and change color to yellow (chain A):

res ali
col yellow

Step 9 - select all, make it visible, show only backbone but reduce the backbone thickness:

```
sel *
sho
bac 3
```

Step 10 - hide side chains:

Step 10 - select cysteine residues, but only for chains A and C; make them visible, use spacefill style:

```
sel a,c/*/cys/*
show
ato spa
```

Step 11 - discard loaded structure:

```
dis all
```

Garlic Tutorial

Lesson 6 - Draw Ramachandran Plot

In this lesson, you will learn how to prepare Ramachandran plot. This plot shows the pairs of dihedral angles phi and psi. You can find more details here .

You can use any protein structure for this lesson. Here we are going to use 1HUC.pdb, retrieved in the previous lesson.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure. You should have the file 1HUC.pdb somewhere in the path searched by garlic (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 3 - prepare Ramachandran plot.

rama

Step 4 - Identify some residues.

Use mouse (pointing device) to identify individual residues. Just move the pointer over the choosen residue symbol and you will see the residue name, serial number and dihedral angles in the output window.

Step 5 - draw Ramachandran plot for glycines.

sel gly
rama sel

Step 6 - return to the main drawing mode. You can either type the command rama off or hit the escape key.

rama off

Step 7 - discard loaded structure:

dis all

Garlic Tutorial

Lesson 7 - Draw Helical Wheel

In this lesson, you will learn how to prepare the helical wheel plot. This plot may be used to identify amphipatic segments in a protein sequence, i.e. the amphipatic helices. In this lesson, the solved structure will be used for demonstration. For more details, read this (WHEEL command description).

You can use any protein structure for this lesson. In this example 1HUC.pdb is used, though you can use any protein structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure. You should have your PDB file (here 1HUC.pdb) somewhere in the search path (if you defined the environment variable MOL_PATH), or in your current working directory.

loa 1HUC.pdb

Step 3 - select all atoms except hetero atoms. If this is not done the hetero "residues" (i.e., solvent molecules) will corrupt the helical wheel plot. The trick is to select hetero residues, and then to select complement. You don't have to hide hetero residues, so you can skip the command hide.

sel het
hide
sel com

Step 4 - check the number of chains in human cathepsin B. If there are two or more chains, the residue serial number should not be used as unique residue identifier.

color chain

Step 5 - there are obviously four chains. Hide all chains except B. Hide everything, after that select only the chain B and make it visible. Hetero residues will not be included into selection, so the step 3 was in fact unnecessary.

sel all
hide
sel b/*/*/*
show

Step 6 - try to find one helix at the chain B surface. Helices may be easily recognized if using backbone representation of the protein. It is also practical to use the geometric center of the chain B as the rotation center, and to move it to the screen center.

bac
cen
pos 0 0 0

Step 7 - play with the chain B to find this helix:

76 77 78 79 80 81 82 83 84 85 86

PRO ALA GLU ALA TRP ASN PHE TRP THR ARG LYS

Step 8 - copy the sequence of the chain B to the main sequence buffer. Note that the helical wheel plot uses the sequence which is stored in the main sequence buffer. Right now this buffer is empty!

seq from 1

Step 9 - draw helical wheel for residues from 76 to 86:

wheel 76-86

Step 10 - return to the main drawing mode. Hit the escape key or type the following command:

whe off

Step 11 - discard loaded structure:

dis all

Step 12 - clear the main sequence buffer:

seq reset

Do not forget that for helical wheel plot, the main sequence buffer should be initialized!

Garlic Tutorial

Lesson 8 - Draw Averaged Hydrophobicity and Hydrophobic Moment

---

In this lesson, you will learn how to draw the averaged hydrophobicity and hydrophobic moment for the sequence which is stored in the main sequence buffer.

In this lesson no atomic coordinates will be used. The only information available will be the sample protein sequence stored in FASTA format. The sample sequence may be found in the original garlic package or downloaded via ftp . Save this sequence as ASCII text, not as HTML.

In this example, mouse may be used to identify residues and their imminent sequence neighborhood. The residue information will be visible in the output window (bottom right corner), while the neighboring residues will be listed in the upper part of the main window. The central residue (the one choosen by the mouse) will be enclosed in a small rectangle.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the sequence.

seq load sample.fasta

Step 3 - plot the averaged hydrophobicity. Use mouse to identify the residues in the plot. The residue information will be visible in the output window (bottom right corner).

plot hyd

Step 4 - plot the hydrophobic moment. Use mouse to identify residues.

plot mom

Step 5 - plot both averaged hydrophobicity and hydrophobic moment. Note that the numeric value in the output window will be equal to the hydrophobic moment in this case!

plot hyd mom

Step 6 - return to the main drawing mode. You can either type the command plot off or hit the escape key.

plot off

Step 7 - clear the sequence buffer. You can skip this step, it is not very important.

seq reset

Garlic Tutorial

Lesson 9 - Venn Diagram

In this simple lesson, you will learn how to prepare the Venn diagram with some residue counts. There is nothing special in this routine and experts will not find it very useful. It is primarily intended for students and other newbies, which are interested in the residue composition of the given protein.

The only information required to prepare the Venn diagram is the protein sequence. In this example, the sequence will be extracted from PDB data. Another approach will be to load the sequence from some FASTA file. The PDB file used here is 1HUC.pdb, but you can replace it with any PDB file which contains the protein structure.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load the structure.

load 1HUC.pdb

Step 3 - discard all hetero atoms:

sel het
sel com

Step 4 - restrict your selection to chains A and B:

res a,b/*/*/*

Step 5 - extract sequence:

seq from 1

Step 6 - draw Venn diagram with residue counts:

venn

Step 7 - discard the structure:

dis all

Step 8 - clear the sequence buffer. You can omit this command.

seq reset

Garlic Tutorial

Lesson 10 - The Semitransparent Plane

This lesson explains how to control the plane associated with the structure. More precisely, you will learn how to show, hide or move the plane and how to change the plane properties. The plane may be used to divide the structure in two parts, for selection and to model the cellular membrane.

It might be good idea to read the text about the command PLANE before you start with this lesson.

Step 1 - start garlic (if not started already):

garlic

Step 2 - load some the structure. In this lesson the papain structure is used, but you can use any other structure.

load 9PAP.pdb

Step 3 - make the plane visible:

pla

Now you should see an ellipsa which represents the plane. If you have not rotated the structure before making the plane visible, the ellipsa will be blue. The near edge will be bright, while the far edge will be dark.

Step 4 - rotate both the structure and the plane about x axis:

Hold the [shift] key and press 8 on numeric keypad.

Note the change of the ellipsa color: now you see another face of the plane. The blue face is treated as the upper side, while the orange-red face is treated as bottom side.

Step 5 - change the plane radius.

pla rad 20

Step 6 - Change the plane transparency (make it opaque):

pla tra 0

Step 7 - select all atoms above the plane:

sel above

Step 8 - change color for the current selection:

color cold

Step 9 - attach movement controls to the plane:

mov pla

Step 10 - rotate the plane, leaving the structure in its current orientation:

Use numeric keypad (keys 2, 8, 4 and 6) and modifier keys (shift, alt, control) to rotate the plane.

Step 11 - attach controls to both structure and plane:

mov all

Step 12 - hide the plane:

pla off

Step 13 - discard the structure:

dis all

Garlic Tutorial

Script 1 - Drawing styles for atoms

This script shows the available drawing styles for atoms. Note that nothing is visible for style "0" (first row, first column)! The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file atoms.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe atoms.script

The sample image is at the bottom of this page. Note that the quality of this image is reduced by high compression.

```
# Show all drawing styles used to draw atoms. Bonds are hidden!

# Atom style 1:
load trp.pdb
pos -21 -15 0
ato 1
bon 0
tag "1"

# Atom style 2:
load trp.pdb
pos -7 -15 0
ato 2
bon 0
tag "2"

# Atom style 3:
load trp.pdb
pos 7 -15 0
ato 3
bon 0
tag "3"

# Atom style 4:
load trp.pdb
pos 21 -15 0
ato 4
bon 0
tag "4"

# Atom style 5:
load trp.pdb
pos -21 -5 0
ato 5
bon 0
```

```
tag "5"

# Atom style 6:
load trp.pdb
pos -7 -5 0
ato 6
bon 0
tag "6"

# Atom style 7:
load trp.pdb
pos 7 -5 0
ato 7
bon 0
tag "7"

# Atom style spa:
load trp.pdb
pos -21 5 0
ato spa
bon 0
tag "spa (spacefill)"

#Atom style sp2:
load trp.pdb
pos -7 5 0
ato sp2
bon 0
tag "sp2"

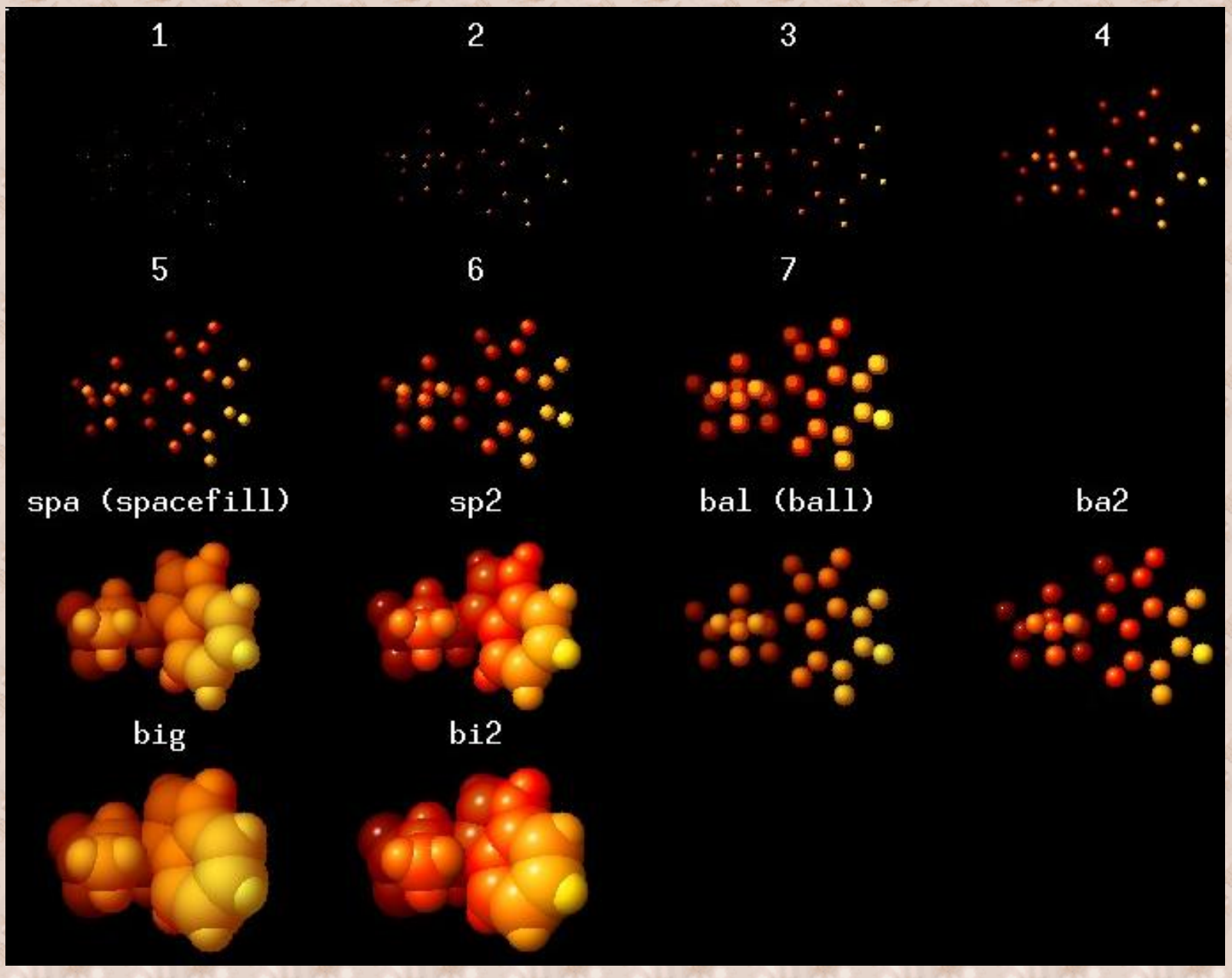
# Atom style bal:
load trp.pdb
pos 7 5 0
ato bal
bon 0
tag "bal (ball)"

# Atom style ba2:
load trp.pdb
pos 21 5 0
ato ba2
bon 0
tag "ba2"

#Atom style big:
load trp.pdb
pos -21 15 0
ato big
bon 0
tag "big"

#Atom style bi2:
load trp.pdb
```

```
pos -7 15 0
ato bi2
bon 0
tag "bi2"
```



Garlic Tutorial

Script 2 - Drawing styles for bonds

This script shows the available drawing styles for bonds. Note that nothing is visible for style "0" (first row, first column)! The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file bonds.script). Or, click here to download the script.

Type the following command at garlic prompt:

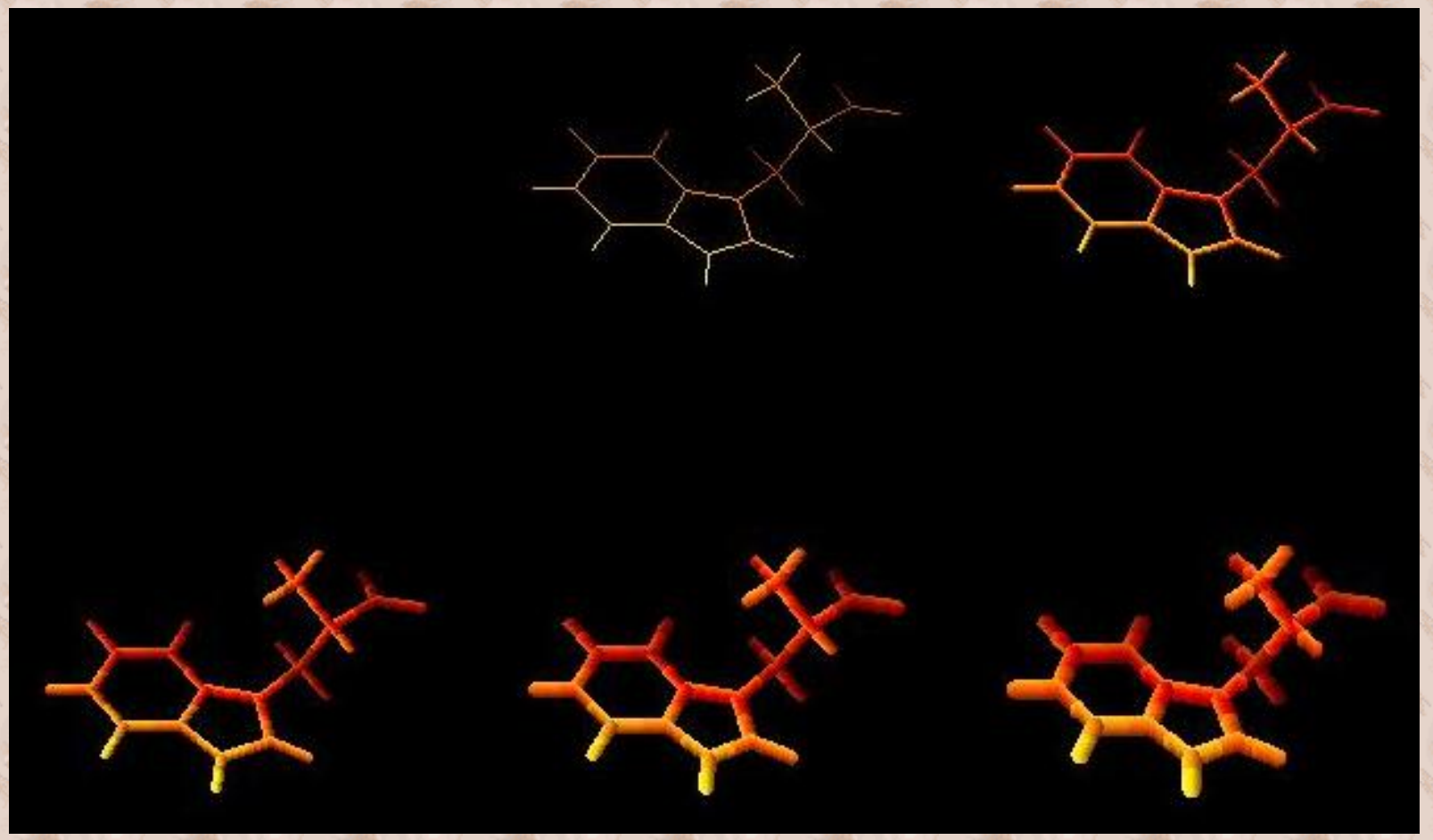
exe bonds.script

The sample image is at the bottom of this page.

```
# Show all drawing styles used to draw bonds. Atoms are hidden!
# This scripts will work if you use default .garlicrc script.

# Bond style 0:
load trp.pdb
pos -12 -6 -100
ato 0
bon 0
# Bond style 1:
load trp.pdb
pos 0 -6 -100
ato 0
bon 1
# Bond style 2:
load trp.pdb
pos 12 -6 -100
ato 0
bon 2
# Bond style 3:
load trp.pdb
pos -12 6 -100
ato 0
bon 3
# Bond style 4:
load trp.pdb
pos 0 6 -100
ato 0
bon 4
# Bond style 5:
load trp.pdb
pos 12 6 -100
```

```
ato 0
bon 5
```



Garlic Tutorial

Script 3 - Predefined color schemes

This script shows some selected color schemes. All schemes shown here are hard-coded in the program. The file trp.pdb is used. You can mark, copy and paste this script to your local host (create the file colors.script). Or, click here to download the script.

Type the following command at garlic prompt:

exe colors.script

The sample image is at the bottom of this page.

```
# Show predefined color schemes.
# This scripts will work if you use default .garlicrc script.

load trp.pdb
pos -18 -18 0
bon 0
ato sp2
color red

load trp.pdb
pos -6 -18 0
bon 0
ato sp2
color green

load trp.pdb
pos 6 -18 0
bon 0
ato sp2
color blue

load trp.pdb
pos 18 -18 0
bon 0
ato sp2
color yellow

load trp.pdb
```

```
pos -18 -6 0
bon 0
ato sp2
color cyan

load trp.pdb
pos -6 -6 0
bon 0
ato sp2
color magenta

load trp.pdb
pos 6 -6 0
bon 0
ato sp2
color white

load trp.pdb
pos 18 -6 0
bon 0
ato sp2
color yellow-green

load trp.pdb
pos -18 6 0
bon 0
ato sp2
color cyan-green

load trp.pdb
pos -6 6 0
bon 0
ato sp2
color cyan-blue

load trp.pdb
pos 6 6 0
bon 0
ato sp2
color magenta-blue

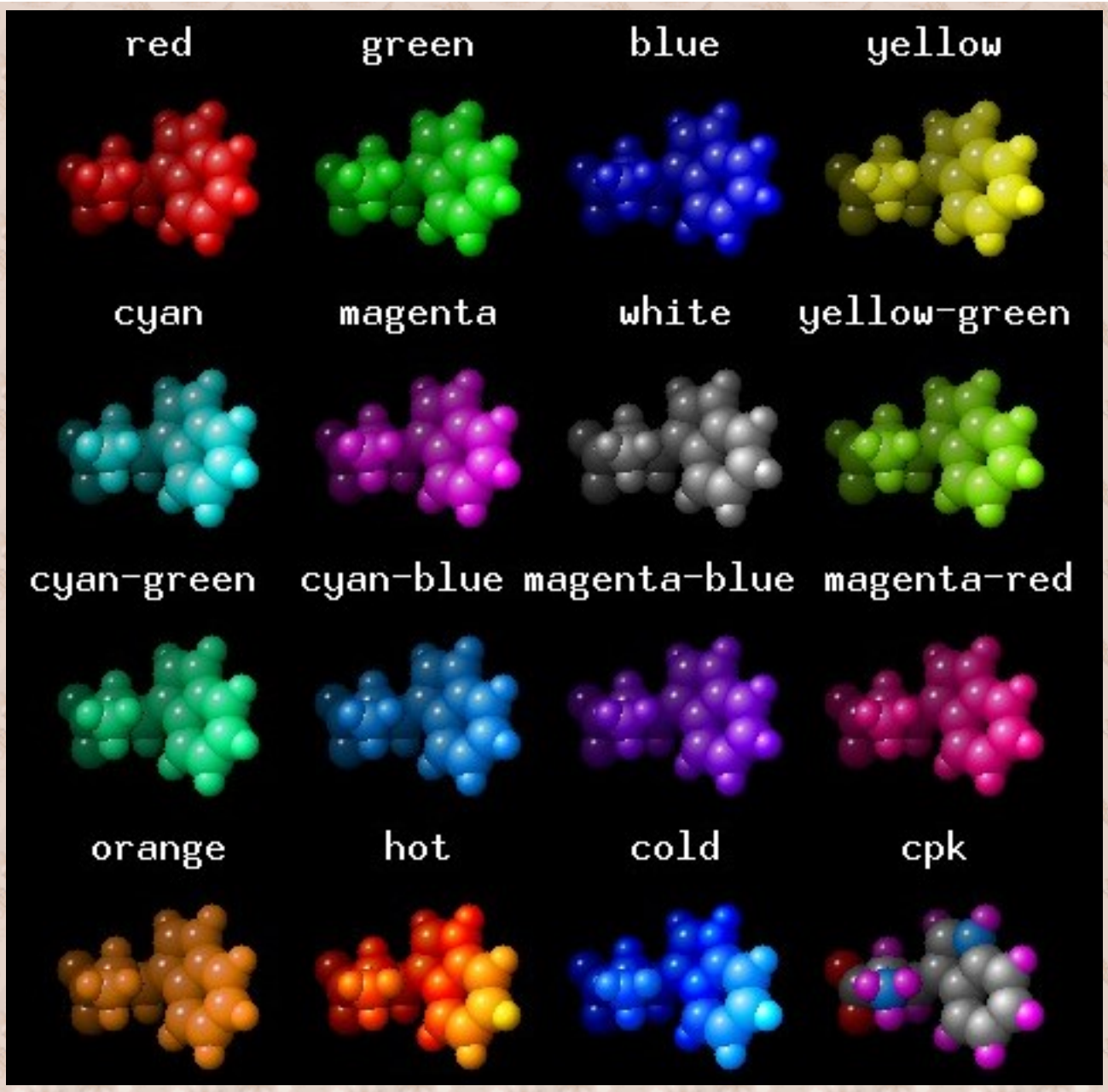
load trp.pdb
pos 18 6 0
bon 0
ato sp2
color magenta-red
```

```
load trp.pdb
pos -18 18 0
bon 0
ato sp2
color orange

load trp.pdb
pos -6 18 0
bon 0
ato sp2
color hot

load trp.pdb
pos 6 18 0
bon 0
ato sp2
color cold

load trp.pdb
pos 18 18 0
bon 0
ato sp2
color cpk
```


red
green
blue
yellow
cyan
magenta
white
yellow-green
cyan-green
cyan-blue
magenta-blue
magenta-red
orange
hot
cold
cpk

COM.	ARGUMENTS	APPL. TO	DESCRIPTION
ADD	the same as for SEL	structure	Add to selection
ANG	angle (degrees)	helical wheel, hydrophobic moment	Angle for helical wheel and hydrophobic moment calculation
ATO	0, 1, 2, 3, 4, 5, 6, 7, BAL, BIG, SPA	selection	Drawing style for atoms
BAC	0, 1, 2, 3, 4, 5, OFF	selection	Draw backbone
BG	color_specification	main window	Change background color
BON	0, 1, 2, 3, 4, 5	selection	Drawing style for bonds
CAT	structure_identifier	structure	Catch structure
CEN	none	structure, selection	Redefine system origin
COL	detailed_color_specification, red, green, blue, yellow, cyan, magenta, white, yellow-green, cyan-green, cyan-blue, magenta-blue, magenta-red, orange, hot, cold, monochrome, cpk, zebra, chain, hyphob	selection	Assign color; do not abbreviate color scheme name!
COM	none, OFF, minimal_score segment_width, CORNER serial1 serial2, ZOOM zoom_factor	both sequence buffers	Compare two sequences
DIS	structure_identifier *, all	structure	Discard structure
DOC	identifier_1 identifier_2 OFF	Two structures	Prepare two structures for docking
EXE	file_name	script file	Execute script
EXI	none	garlic session	Quit garlic session
FAD	FRO shift, BAC shift, OFF, PLA, SPH, CYL, HALF-SPH, HALF-CYL	structure	Change color fading
FG	color_specification	main window	Change text color
FON	font_name	all windows	Change font
HID	none	selection	Hide atoms and bonds
HYB	none, OFF	structure	Generate hydrogen bonds
LAB	none, OFF	selection	Show labels
LOA	file_name	structure_file	Load structure (file)
LOG	file_name, OFF	commands	Log garlic commands
MON	none	main window	Switch to mono mode
MOV	PLANE, STRUCTURE, ALL	structure and plane	Attach controls to struct. or plane
NEI	none, OFF	main window	Show or hide seq. neighborhood
PAU	none	garlic script	Pause script execution
PLA	none, RADIUS, TRANSPARENCY, OFF	plane	Show or hide plane, set properties
PLO	HYD, MOM, OFF, HYD start_residue end_residue, MOM_start_residue end_residue	sequence buffer	Plot hydrophobicity or hyd. moment
POS	x, y, z	structure	Move to (x, y, z)
QUI	none	garlic session	Quit garlic session
RAD	radius (angstroms)	Selection sphere	Change selection sphere radius
RAM	none, SEL, OFF	structure	Draw Ramachandran plot

REG	**none**	**mail**	**Register garlic**
RES	**the same as for SEL**	**selection**	**Restrict selection**
ROT	**axis angle (degrees)**	**structure**	**Rotate**
SAV	**file_name** **file_name SEL**	**structure, selection**	**Save atomic data to file** **(SEL = selection only)**
SCA	**EIS, KD, WHI**	**hydrophobicity scale**	**Choose hydrophobicity scale:** **Eisenberg, Kyte-Doolittle, White**
SEL	**chains/res_nums/res_names/atom_names** **residue_numbers** **residue_names** ***, all, aci, bas, cha, com, het, pho,** **mai, neg, pol, pos, sid, sma, tin**	**structure,** **selection**	**Define new selection** **(overwrite previous)**
SEQ	**= three_letters_code, LOAD,** **FROM, COPY, SAVE, SWN, RESET**	**sequence buffer,** **reference seq. buffer**	**Manipulate sequence buffer**
SHO	**none**	**selection**	**Show atoms and bonds**
SLA	**FRO shift, BAC shift, OFF, PLA,** **SPH, CYL, HALF-SPH, HALF-CYL**	**structure**	**Change slab**
SSB	**0, 1, 2, 3, 4, 5**	**disulfide bonds**	**Drawing style for disulfide bonds**
STE	**none, OFF**	**main window**	**Switch to stereo mode**
TAG	**"string"** **OFF**	**structure**	**Assign or remove tag**
TBG	**color_specification**	**input&output window**	**Change text background**
TFG	**color_specification**	**input&output window**	**Change text color**
TIT	**identifier x y "string"** **identifier x y** **identifier OFF**	**main window**	**Add, move or** **remove title**
TRA	**axis shift**	**structure**	**Translate**
VEN	**none, OFF,** **start_residue end_residue**	**sequence buffer**	**Draw Venn diagram with statistics**
WHE	**none, OFF,** **start_residue end_residue**	**sequence buffer**	**Draw helical wheel**
WIN	**number_of_residues**	**sliding window**	**Set sliding window width**

Garlic Command Line Options

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page explains the command line options. To see this list, type one of the following commands:

garlic -h
garlic -h | less

```
==============================================================================
                Garlic - free molecular visualization program
==============================================================================

Garlic was written by  Damir Zucic  (zucic@garlic.mefos.hr) as a complement
to other molecular visualization  programs, like rasmol (by Roger Sayle).
It was written to simplify  the analysis of membrane proteins, but it can
be used as general purpose molecular visualization program, provided that
molecular coordinates are available in  PDB format, version 2.1 or older.
Garlic may also be used to analyze protein sequences.

Some of the  features, which  distinguish this program from  others, are:
(1) Coordinates, labels and  other data are  automatically displayed  for
    the atom nearest to the current pointer (mouse) position.
(2) Additional numeric data,  like  hydrophobicity, may be associated  to
    each amino acid. The  whole  structure  may be  colored  according to
    these values.
(3) Selection mechanism is different.
(4) Two bonds at different distance from  observer have different colors.
------------------------------------------------------------------------------
Usage:              garlic [true_garlic_options] [X11_options] [filename]
------------------------------------------------------------------------------
Command line options may be divided in two groups: true (specific) garlic
options and X11 options.  Options may be given in any order.  All options
and hard-coded  default values are listed  in the table  below.  For each
parameter, the value defined through command line is used,  if available.
If not, the value defined in .garlicrc file is used. If .garlicrc file is
not  available,  or there is  no corresponding  entry in  this file,  the
hard-coded default value is used.  The sample  .garlicrc file included in
the original package contains  the values equal to  hard-coded  defaults.
------------------------------------------------------------------------------
garlic option:        Description:
------------------------------------------------------------------------------
-h, --help            Print help and exit.
-v, --version         Print version and exit.
-r, --register        Register garlic:  inform author that  your site has
                        garlic installed and that someone is going to use
```

```
                        this program. By registering, you are encouraging
                        author to continue development of garlic. You can
                        also help  author to  ensure support  for further
                        development. This option sends an e-mail message,
                        containing only the e-mail message header and the
                        word 'Hi!',to zucic@garlic.mefos.hr. Please execute
                        garlic -r   if you are going to use this program.
                        If your system is  not connected to the Internet,
                        you can send short e-mail from some other system.
-nosys                  Hide the coordinate system icon  (top left corner).
no-control              Hide the control window (upper right corner).
-stereo                 Display stereo image.
-slab mode              Default slab mode.  Available slab modes are:  off,
                        planar (default),  sphere, half-sphere,  cylinder
                        and half cylinder.
-fading mode            Default color fading mode.  Available  modes:  off,
                        planar (default),  sphere, half-sphere,  cylinder
                        and half cylinder.
-as number              Default atom drawing style (hard-coded default: 2).
-bs number              Default bond drawing style (hard-coded default: 2).
-fs number              Default number of  color fading surfaces.  Parallel
                        planes, concentric spheres or conc. cylinders may
                        be used as  fading surfaces.  Three  RGB triplets
                        are assigned to each surface. Surfaces are evenly
                        spaced;  at least one and at most eight should be
                        defined. At least three colors  (left, middle and
                        right) are assigned to  each visible atom.  These
                        three colors are based on the position of a given
                        atom  relative to  the nearest  fading surface(s)
                        and on colors assigned to these surfaces.  Colors
                        are combined using linear weighting.
-lc(i) color            Left color at the  i-th surface;  i is between zero
                        and seven.  The color string should be  compliant
                        with X11R5.  Blue, for example,  may be specified
                        as blue or as RGB:0000/0000/FFFF etc. For example
                        -lc4 RGB:BBBB/8888/4444    defines the left color
                        at the surface whose index is equal to four.
-mc(i) color            Middle color at the i-th surface.
-rc(i) color            Right color at the i-th surface.
-pc, --print-config     Print configuration data and exit.
-pcn                    Print cursor names to stdout and exit.
-log logfile            Write commands and messages to  log file.  The file
                        will be created in the current working directory.
                        If this is not possible, log file will be created
                        in users home directory.
-----------------------------------------------------------------------------
X11 option:             Description:
-----------------------------------------------------------------------------
```

```
-display displayname  X server to contact.
-geometry geom        Window geometry (default: almost the whole screen).
-bg color             Main window background color (default is black).
-fg color             Main window foreground color (default: white).
-fn fontname          Text font; (default is 10x20).
-tbg color            Text background color (default is black).
-tfg color            Text color (default is white).
-cursor cursorname    Cursor name; see  /usr/include/X11/cursorfont.h for
                        names; remove the XC_ prefix.
-----------------------------------------------------------------------
filename:             The input file name.  Full pathname may be used. If
                      filename does not contain the path, garlic will try
                      to find  the specified file in  the current working
                      directory.  If the first attempt  to open  the file
                      fails,  the filename  is appended to the content of
                      the environment  variable  MOL_DIR  for  the second
                      attempt.  If this fails too, garlic will search all
                      directories  specified in  the environment variable
                      MOL_PATH.
-----------------------------------------------------------------------
Personal initializations may be written to .garlicrc file. Normally, this
file should be kept in users home directory.  Note that this is  not  the
first directory to be searched for .garlicrc file! Up to five directories
are searched in the following order:

.                        Current working directory.
$HOME                    Users home directory (recommended).
$HOME/garlic             Subdirectory garlic (of users home directory).
/usr/local/lib/garlic    Public  initialization file  should be  there.
/usr/lib/garlic          The last  attempt;  if this fails,  hard-coded
                           default values are used.
-----------------------------------------------------------------------
Environment variables:
-----------------------------------------------------------------------
MOL_DIR               Defines where to look for the specified file if not
                        found in the current working directory.
MOL_PATH              The list of directories to be searched.  It is used
                        if attempt with  MOL_DIR failes or if  MOL_DIR is
                        not defined.  Use space  or colon (:) to separate
                        directory names. MOL_PATH is quite useful;  it is
                        recommended to define  this environment  variable
                        through .login or some other login script.
DISPLAY               X server to which  the program should be connected.
-----------------------------------------------------------------------
garlic home page:                        http://garlic.mefos.hr/garlic
Damir Zucic home page:                   http://garlic.mefos.hr/zucic
E-mail:                                  zucic@garlic.mefos.hr
=======================================================================
```

Garlic Configuration File - Version 1.1

.garlicrc

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

This page contains the sample configuration file for garlic. When started, garlic will try to find the configuration file called .garlicrc in the following directories:

(1) the current working directory;
(2) users home directory ($HOME);
(3) garlic subdirectory of user's home directory ($HOME/garlic);
(4) /usr/local/lib/garlic ;
(5) /usr/lib/garlic .

The recommended directories are:

/usr/local/lib/garlic (system-wide configuration file),
$HOME (private configuration file).

If all attempts fail, the hard-coded defaults will be used. The configuration file .garlicrc should be included in the original garlic package. Most parameters are explained below (read the comments). Anyway, if you have some questions, send an e-mail to me:
zucic@garlic.mefos.hr

```
# Personal initialization file for garlic (molecular visualization program).
# Version 1.1.
# Last modification: February 07, 2001.


# Geometry of the main window. Use the keyword default, or specify the
# geometry string (for example 780x560+10+10).

main window geometry: default


# Margins; used only if geometry string is not given. Geometry string may be
# given through command line arguments.

main window left margin: 50 pixels
main window right margin: 50 pixels
main window top margin: 50 pixels
main window bottom margin: 70 pixels


# Main font:

main font: 10x20


# Main window cursor. If you don't like default cursor, replace it; read
```

```
# the file /usr/include/X11/cursorfont.h ; remove the XC_ prefix to obtain
# the cursor name.

main window cursor: default


# A small coordinate system may be displayed in the top left corner (yes/no):

show coordinate system: yes


# Control window (top right corner) may be visible or hidden (yes/no):

show control window: yes


# Sequence neighborhood of the residue under
# the pointer may be visible or hidden (yes/no):

show sequence neighborhood: yes


# Stereo flag (yes/no):

display stereo image: no


# Parameters for stereo image:

stereo internal margin (screen units): 10 pixels
stereo angle: 5.0 degrees


# Light source theta and phi angle (theta is defined with respect to z axis,
# phi with respect to x axis:

light source theta angle: 150 degrees
light source phi angle:   225 degrees


# Default slab mode (possible modes are off, planar, sphere, half-sphere,
# cylinder and half-cylinder):

default slab mode: planar


# Default color fading mode (off, planar, sphere, half-sphere, cylinder and
# half-cylinder):

default color fading mode: planar
```

```
# Default drawing style for atoms:

default atom drawing style: 2


# Default drawing style for bonds:

default bond drawing style: 2


# Default drawing style for backbone:

default backbone drawing style: 5


# Window colors:

main window background color: black
main window foreground color: white
text background color: black
text foreground color: white


# The number of color fading surfaces:

number of color fading surfaces: 3


# Colors at given fading surface(s). The surface index is given in brackets.
# The largest surface index is (number of color fading surfaces) - 1.

left   color 0: RGB:FFFF/FFFF/4444
middle color 0: RGB:FFFF/DDDD/0000
right  color 0: RGB:8888/5555/0000

left   color 1: RGB:FFFF/8888/0000
middle color 1: RGB:FFFF/0000/0000
right  color 1: RGB:8888/0000/0000

left   color 2: RGB:8888/0000/0000
middle color 2: RGB:4444/0000/0000
right  color 2: RGB:2222/0000/0000


# Rotation steps. Normal steps is used if numeric key is pressed without
# any modifier. Large step is selected by holding [shift] while pressing
# the key, and very large step is selected by using both [alt] and [shift].
# Small step is selected by holding [control] while pressing the key, and
# very small step by using both [alt] and [control].
```

```
rotations steps: 0.2 1.0 5.0 30.0 90.0


# Five translation steps (very small, small, normal, large and very large).
# Use angstrom units.

translation steps: 0.2 1.0 5.0 25.0 100.0


# Five slab steps (very small, small, normal, large and very large).
# Use angstrom units.

slab steps: 0.2 1.0 5.0 20.0 80.0


# Five fading steps (very small, small, normal, large and very large).
# Use angstrom units.

fading steps: 0.2 1.0 5.0 20.0 80.0


# Window size limits: used only if screen width and/or height are larger
# than values specified here. By default, screen width and height are used.

maximal main window width: 3000 pixels
maximal main window height: 2500 pixels


# The nearest line (bond) thickness; used only if drawing bonds as lines
# and line thickness is used for perspective.

the nearest line thickness: 5 pixels


# Screen dimensions and position of garlic user in real world. Use realistic
# values. Do not change units (mm). Strange values may cause image distortions.

screen width in real world: 270 millimeters
screen height in real world: 195 millimeters
distance between user and screen in real world: 500 millimeters


# Scaling information: used to scale user and screen down to atomic scale.
# Only screen width is required, in angstrom units.

screen width in atomic world: 1.0 angstroms


# User z coordinate in atomic coordinate system. It must be negative
# and absolute value should be quite large. The x axis points to the right,
# y axis downward and z axis in direction opposite to observers direction.
```

```
user position in atomic coordinate system: -150.0 angstroms


# Maximal bond length is used to check which atoms and bonds are invisible.
# It is assumed that there are no atoms with radius larger than this length.

maximal bond length: 2.2 angstroms


# Crude limits for bond lengths. No distinction between N-CA and C-N is made.
# Use angstrom units. Be tolerant, there are many bad structures around.
# Generic bond length is used for atomic pairs which are not recognized.

approximate C-C bond length: from 1.3 to 1.8 angstroms
approximate C-N bond length: from 1.0 to 1.7 angstroms
approximate C-O bond length: from 1.0 to 1.5 angstroms
approximate C-S bond length: from 1.4 to 2.1 angstroms
approximate C-H bond length: from 0.8 to 1.2 angstroms
approximate N-H bond length: from 0.9 to 1.3 angstroms
approximate O-H bond length: from 0.7 to 1.3 angstroms
approximate S-H bond length: from 0.9 to 1.6 angstroms
approximate O-P bond length: from 1.2 to 1.8 angstroms
approximate S-S bond length: from 1.8 to 2.3 angstroms
generic bond length:         from 0.8 to 2.0 angstroms
hydrogen bond length:        from 2.4 to 4.1 angstroms


# Hydrogen bond C-O...N angle range:

hydrogen bond C-O...N angle: from 125 to 180 degrees


# The upper limit for CA-CA distance for neighbouring residues. Used to
# draw backbone, connection neighbouring CA atoms.

maximal CA-CA distance: 4.1 angstroms


# Atomic radii, used for spacefill style. 70% of van der Waals radius may be
# a good choice.

hydrogen radius:   0.70 angstroms
carbon radius:     1.20 angstroms
nitrogen radius:   1.05 angstroms
oxygen radius:     1.00 angstroms
sulfur radius:     1.25 angstroms
phosphorus radius: 1.25 angstroms
generic radius:    1.40 angstroms
```

```
# Van der Waals radii.

hydrogen van der Waals radius:   1.00 angstroms
carbon van der Waals radius:     1.70 angstroms
nitrogen van der Waals radius:   1.50 angstroms
oxygen van der Waals radius:     1.40 angstroms
sulfur van der Waals radius:     1.80 angstroms
phosphorus van der Waals radius: 1.80 angstroms
generic van der Waals radius:    2.00 angstroms


# Ball radius, used to draw balls and sticks:

ball radius: 0.45 angstroms


# For a given atom, the chemical bonds are identified by inspecting
# distances to the neighboring atoms. The array with atomic data should
# be scanned in forward and backward direction (with respect to the given atom)
# to find which atoms are bound to a given atom. The following parameters
# define how many neighboring atoms should be checked in each direction.

number of bond candidates: 50 before and 50 after the given atom
```

Molecular Structures

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

DATA	LINK	REFERENCE
Proteins and nucleic acids	The Protein Data Bank, http://www.rcsb.org/pdb/	H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov, P.E.Bourne, The Protein Data Bank, Nucleic Acids Research, 28 pp. 235-242 (2000)
Hetero compounds	Hetero-compound Information Centre - Uppsala http://xray.bmc.uu.se/hicup/	Kleywegt, G.J. and Jones, T.A. (1998). Databases in protein crystallography. Acta Cryst D54, 1119-1131 (CCP4 Proceedings).

Support Garlic!

---

garlic, free molecular visualization program, protein structure, DNA structure, PDB, molecular rendering, biological macromolecule, unix, linux, free software download, open source software, Damir Zucic.

You can support garlic development in different ways. Some options are listed here, sorted by complexity (the simplest one is the first). Though garlic is a free software, someone has to pay for it. The author will need strong arguments to ensure support for a program which makes no money. If you like garlic, support it!

REGISTER GARLIC

The fact that you use garlic doesn't help much if I don't know that there is one more user. The easiest way to register is to execute the command:
reg
at garlic prompt. This requires that your machine is connected to the Internet. A short message will be send to zucic@garlic.mefos.hr; the only content of this message will be the word 'Hi!'. I will use the header of this message to extract your address. The address will be added to the list. Your address will not be abused, it will be kept secret and used only to count garlic users.

You can also send a more verbose message to zucic@garlic.mefos.hr with comments and suggestions.

There is one more way to register garlic: at your shell (terminal) prompt, type:
garlic -r
(if connected to the Internet, of course).

SEND A POSTCARD

You can also register by sending a postcard. I like stamps!
Here is the address:

Damir Zucic
ETF Osijek
Kneza Trpimira 2B
31000 Osijek
Croatia
Europe

INFORM OTHERS

Inform your colleagues and friends about garlic. Many potential users do not read Usenet news, so it is difficult to reach all those who might be interested to use garlic. I don't like spam and other aggressive forms of communication so I wouldn't use such methods to attract users.

ADD LINK TO YOUR WEB PAGES

Add link to your personal web page(s), pointing to garlic.

MIRROR GARLIC

If you like garlic and you can set aside few megabytes of disk space, you can establish a mirror site with garlic sources and related material. This should not be very complicated - there is only one source

package and few dozens of web pages. The national academic network (CARNet) here in Croatia is pretty good, but communication lines to some countries (like U.K. and Germany) are overcrowded most of the time.

USE IT FOR LECTURES AND PRESENTATIONS

An experienced user may use garlic for lectures and presentations. There is a command pau (pause) which makes it easy to control script execution.

MAKE A DONATION

Donations are welcome, of course. Contact the author for technical details (zucic@garlic.mefos.hr).