# MidasPlus Index

## NAME

unmtrix − expand MTRIX records in PDB files

## SYNOPSIS

**unmtrix** [**−i** *original_PDB_file*] [**−o** *new_PDB_file*] [**−m** *MTRIX_serial_id*]

## DESCRIPTION

*Unmtrix* reads a Protein Data Bank file and generates coordinates for sub-units specified by MTRIX records. The **−i** argument specifies the input PDB file. If no input file is given, *unmtrix* will read from standard input. The **−o** argument specified the output PDB file. If no output file is given, *unmtrix* will write to standard output. Normally, *unmtrix* will generate coordinates for all MTRIX records which do not have atoms associated with them. When given the **−m** argument, *unmtrix* will generate coordinates only for the MTRIX records that match the given *MTRIX_serial_id*.

## SEE ALSO

Protein Data Bank, Atomic Coordinate and Bibliographic Entry Format Description, March 1989.

## AUTHOR

Conrad Huang
Computer Graphics Laboratory
University of California, San Francisco

**NEON ( 1 )**

**AUTHOR**

Thomas R. Hynes
Protein Engineering Department, Genentech Inc.
Department of Pharmaceutical Chemistry, UCSF

Controls the distance in Angstroms between the center of atoms and the ends of the dashed lines so that dashes do not bump into the model.

Dash/space ratio

Controls the relative proportions of dash and intervening space. A value of 0.0 gives dots, 0.4 is good for dashed lines, 1.0 gives solid line.

CA connect distance

Cutoff distance in Angstroms for determining if the backbone tube will be drawn between subsequent $\alpha$-carbons of each model. For example if you displayed residues 1-10 and 30-40 of your model, the program uses the cutoff to find the break between residues 10 and 30 and will not connect them. If unwanted breaks occur, this value should be increased.

**RUNNING NEON**

A copy of the **/usr/local/lib/neon.dat** file should be present in your current working directory. Default values will be used if the file is not found.

To create an image, set the desired parameters in **neon.dat**. In the interactive window of *midas*, display, orient and color the model or models of interest. Enter the command **neon -p** to preview the image. After a short pause a small *conic* window will open displaying the image. Option flags following the **neon** command correspond to options of *conic*, which control the appearance of the image and whether the image is saved in a file for later use.

**PRENEON**

To create a complex image, multiple outputs of *neon* can be saved, combined, and then sent to *conic* to draw the final image. The Midas command **preneon** runs only *neon*, and the output must be directed to a file. If the output of **preneon** is not directed to a file it is returned by default to *midas*, which will have to work its way through many lines of invalid commands. The **preneon** command does not accept any command line flags.

**EXAMPLES**

1) To have a quick look at an image
*Command:* **neon -p**

2) To save a full screen image in the file **figure.i**
*Command:* **neon -f -ofigure.i**

3) To create a complex image with a ligand shown with stick bonds and the binding site shown with space filling atoms, set **neon.dat** for stick atoms, display just the ligand and save the output of *neon* in the file **site**.
*Command:* **preneon > site**

Turn on the CPK flag in **neon.dat** and display just the binding site atoms. Append the output of *neon* to the file **site**.
*Command:* **preneon >> site**

Send the combined information in the file **site** to *conic* using Conic parameters from the file **param**, and save the full screen image in the file **figure.i**.
*Command:* **conic -cparam -f -ofigure.i site**

**SEE ALSO**

conic(1), ilabel(1), ipaste(1), livemap(1), midas(1)
Midas User's Guide

**FILES**

/usr/local/lib/neon.dat

**BUGS**

The *livemap* program has not been released yet.

Dash flag
: Set to 1 to draw lines between between atoms connected by the distance command in Midas. The type of line is under control of dash parameters listed below.

Object flag
: Set to 1 to include Midas objects. Move (**.m**) and draw (**.d**) commands are supported to draw lines. Dot (**.dot**) and marker (**.marker**) commands cause a single sphere to be placed. See the Midas User's Guide for details on objects. Display of electron density created by *livemap*(1) is also controlled by the object flag.

CPK Flag
: Set to 1 to get the same space filling representation of atoms obtained with Conic with the addition of depth cueing, coloring by temperature factor and the inclusion of objects when the corresponding parameters are set.

Stick thickness
: Radius in Angstroms of sticks connecting atoms.

Tube thickness
: Radius in Angstroms of tubes connecting $\alpha$-carbons.

Dash thickness
: Radius in Angstroms of dashed lines.

Object thickness
: Radius in Angstroms of lines and dots of objects. This also controls the thickness of electron density created by *livemap*(1).

Density thickness
: Radius in Angstroms of electron density lines.

Atom rendering
: Controls whether atoms are represented as sticks or balls & sticks.

Atom size
: Radius of balls in ball & stick mode as a percent of the van der Waals radius specified by *midas*.

Depthcue, percent
: First value turns depth cue on or off. Second value is the percent intensity of atoms at the back of the image.

B-factor, range
: Control of coloring by temperature factor. First value controls the coloring type. Type 0 turns option off, model colored with displayed color. Type 1 creates a gradient of color starting with the B-factor color specified below for atoms with lowest temperature factor to the displayed color for atoms with highest temperature factor. Type 2 creates a gradient of color (blue, magenta, red, orange, yellow) from lowest to highest temperature factor value. Second and third value specify the minimum and maximum temperature factors over which the gradient of color is calculated. Atoms with temperature factors above and below the values are colored yellow and blue respectively. If both values are 0.0, the minimum and maximum values are determined from the displayed atoms.

B-factor color
: The RGB (red, green, blue) color of atoms with lowest temperature factor. Used with B-factor coloring type 1.

Number of dashes
: Controls the number of dashes drawn between pairs of atoms.

Dash color
: The RGB (red, green, blue) color of dashed lines.

Dash offset

**NAME**

neon − generate a molecular model with solid stick bonds and shadows

**SYNOPSIS**

**neon** [ *conic options* ]
**preneon**

**DESCRIPTION**

*Neon* works with the Midas package to create solid ball and stick representations of molecular models. The currently displayed atoms, their orientation, position and colors are taken from the interactive display of *midas*(1) using the **pdbrun** Midas command and are sent to *neon*. *Neon* processes the information under the control of parameters set in the **neon.dat** file (in the current directory) and the output is sent to the Midas utility *conic*(1) to create the final image. See *conic*(1) for a detailed description of its command line options. *Neon* has three parameters for the depiction of a simplified backbone; a 'smooth' tube connecting α-carbons, an intermediate 'bent' tube, and a 'straight' tube with straight segments connecting α-carbons. *Neon* has two parameters which create a smooth gradient of color over the the model based on the temperature factors of the atoms. Dashed or solid lines can be drawn between atoms joined by the **distance** command in *midas* to illustrate hydrogen bonds and other interactions. *Neon* handles Midas objects, allowing arrows and lines to be displayed. Electron density generated with *livemap*(1) can also be included in the image.

**EXAMPLE OF THE NEON.DAT CONTROL FILE**

This file, **neon.dat**, is read from the current working directory of *midas*. The example below lists the default control parameters for when the **neon.dat** file is missing. Input is free format, one control parameter per line.

```
0           |Tubetype           |0=all atoms, 1=smooth, 2=bent, 3=straight|
3           |Sphere density     |1=rough, 5=high resolution               |
1           |Dash    flag       |0=no dashes,  1=draw dashes              |
1           |Object  flag       |0=no objects, 1=draw objects             |
0           |CPK     flag       |0=normal Render output, 1=CPK output     |
0.25        |Stick   thickness  |Angstroms                                |
0.50        |Tube    thickness  |Angstroms                                |
0.10        |Dash    thickness  |Angstroms                                |
0.10        |Object  thickness  |Angstroms                                |
0.04        |Density thickness  |Angstroms                                |
0           |Atom rendering     |0=stick, 1=ball & stick                  |
0.25        |Atom size          |Percent of vdw radius (ball & stick mode)|
0 0.50      |Depthcue,Percent   |0=n, 1=y; percent aft intensity          |
0 0.0 0.0   |B-factor,Range     |0=n, 1=shade to color, 2=rainbow; min-max|
1.0 1.0 1.0 |B-factor color     |RGB (red, green, blue)                   |
5           |Number of dashes   |Number drawn between each pair of atoms  |
1.0 1.0 0.0 |Dash color         |RGB (red, green, blue)                   |
0.30        |Dash offset        |Dist. from atom to first dash, Angstroms |
0.40        |Dash/space ratio   |0.0=dots, 0.4=dashes, 1.0=solid line     |
4.00        |CA conect distance |Angstroms                                |
```

**CONTROL CARDS**

Tubetype

Backbone atom representation; all atoms, smooth tube, bent tube, straight tube. The color of the tube representation corresponds to the color of the α-carbon.

Sphere density

Density of spheres drawn to create sticks, tubes, dashes and objects. A value of 3 is good for most work, 4 is recommended for final full screen image so that individual spheres are not resolved, 5 is best when focused on a small number of residues. Increasing the number slows the calculation.

**LIMITATIONS**

Six thousand atoms. Also, there cannot be more than 8000 waters involved in overlapping reentrant surface removal. This is generally not a problem, unless you have a large protein with many internal cavities and you have not used the **-d** flag to reduce the density.

**FILES**

| | |
|---|---|
| r?????? | intermediate file of reentrant surface points - binary |
| a?????? | intermediate file of reentrant surface points - ascii |
| s?????? | intermediate file of reentrant surface points - sorted |
| c?????? | intermediate file of contact surface points - ascii |
| o?????? | intermediate file of all surface points |
| k?????? | intermediate file from getcoord |
| e?????? | intermediate file of atoms inside ellipsoid |
| b?????? | binary file of coordinates for buffering |

**DIAGNOSTICS**

Many and varied. Be sure to examine the **-g** file and ‘‘submit.out’’ before you leave a background job running overnight.

statement and the residue name, sequence number, and atom name (if specified) must match those of the input file exactly. The residue name must be left justified, and the sequence number must be right justified. The sequence number may contain letters. Up to one hundred such records may be used. The **-e** and **-i** flags are compatible. The surface generated using the **-i** flag is not always the same as the surface generated by running the entire molecule and afterwards selecting out the desired atoms. The first surface will not include reentrant surface lying between an atom in the **-i** file and atoms not in the file. (The QCPE version of *ms* does not have this bug.)

**-s** Use the supplied file argument to specify the atomic radii. The format of the file is an atomic symbol followed by its radius, one per line. */usr/local/lib/midas/connect.tpl* uses this format.

**-n** Include the unit normals to the surface with each surface point record.

**-o** The output is written to *file.* This flag is not optional.

**-r** Only residues numbered *b* through *e* inclusive are used in the calculation. This is quite different from the **-i** flag. Residue sequence numbers involving letters may cause problems.

**-w** Change the water probe radius from the default radius of 1.4 Angstroms. This parameter must be between 1.0 and 2.0.

The output consists of a series of atom and surface point records, with the same format for the first 6 fields. Each atom is followed by the surface points (if any) which belong to it. These first 6 fields are in the following format: residue name, sequence number, atom name, x coordinate, y coordinate, z coordinate. For an atom record, the seventh field is ‘‘A’’. For a surface point record, the seventh field begins with an ‘‘S’’, followed by a ‘‘C’’ or ‘‘R’’ according to whether the point is part of contact or reentrant surface. This is followed a digit used for depicting different density levels. The eighth field is the molecular surface area associated with the point in square Angstroms. If the **-n** flag is specified, the next three fields are the unit normal vector pointing outward from the surface. Informative messages and errors are written to the standard error output unless a **-g** file is specified. The calculation takes about 5 seconds per atom for molecules of fewer than 1000 atoms and 7 seconds per atom for larger molecules (timings are for a VAX780).

The chemical elements that the program can currently handle are those which the author has found to occur in molecules of interest *and* whose van der Waals radii could be located in the literature. The atoms currently recognized are:

| Element | Radius |
|---|---|
| H | 1.20 |
| C | 1.90 |
| N | 1.50 |
| O | 1.40 |
| F | 1.35 |
| P | 1.90 |
| S | 1.85 |
| Cl | 1.8 |
| Fe | 0.64 |
| Cu | 1.28 |
| Zn | 1.38 |
| Br | 1.95 |
| I | 2.15 |

**BUGS**

Atoms must be consecutively numbered in the PDB file for correct results.

**AUTHOR**

Michael Connolly
University of California, San Francisco

**NAME**

ms − calculate a solvent accessible molecular surface

**SYNOPSIS**

**ms** file [ **-a** ] [ **-d** density] [ **-e** file] [ **-g** file] [ **-i** file] [**-s** file] [**-n**] [**-r** b-e] [**-w** radius] **-o** file

**NOTE**

**The *ms* command has been obsoleted by the *dms* command and in the future will no longer be distributed with the MidasPlus distribution. It is recommended that *dms*(1L) be used instead of *ms.* *Dms* alleviates many of the shortcomings of *ms* such as handling of chain identifiers, recognition of uncommon atom types, etc. See the *dms*(1L) manual page for further details.**

**DESCRIPTION**

*Ms* calculates the molecular surface of a molecule. The molecular surface resembles the van der Waals surface of a molecule, except that crevices between atoms are smoothed over and interstices too small to accommodate the probe are eliminated. The surface includes cavities in the interior of the molecule, even if they are not accessible to a solvent molecule coming from the outside.

The molecular surface calculated is that defined by F. M. Richards (1977, *Ann. Rev. Biophys. Bioeng.* ). According to Richards' definition the molecular surface consists of two parts: *contact surface* and *reentrant surface.* The contact surface is made up of ''those parts of the molecular van der Waals surface that can actually be in contact with the surface of the probe.'' The reentrant surface is defined by ''the interior-facing part of the probe when it is simultaneously in contact with more than one atom.''

*File* is an input file of coordinates. The input file must be in the Protein Data Bank format. The first letter or first two letters of the atom name is used to determine the element type. Implicit hydrogens are always included for carbon, nitrogen and oxygen atoms, thus aromatic carbons and nitrogens will have van der Waals radii that are somewhat too big. Note that only amino acid residues will be included unless **-a** is also specified. Because coordinates are multiplied by 100 and stored as integers, coordinates must have absolute values smaller than 327.67.

The flags may be in any order. The meanings of the flags are described below:

**-a** Include all atoms, not just those in amino acid residues.

**-d** Change the density of points on the surface. *Density* is a factor affecting the density of points on the surface: the default of 1.0 produces about 5 points per square Angstrom. Only values between 0.1 and 1.0 are permitted. For large proteins, a density of 0.5 is recommended.

**-e** Calculate only the surface lying within the ellipsoid specified in *file. File* consists of 5 lines which define an ellipsoid. The five lines are: the ellipsoid center (line 1), an orthogonal matrix representing the orientation of the ellipsoid (lines 2-4), and the lengths of the three semiaxes (line 5). The normalized vectors of the semiaxes form the columns of the orthogonal matrix. It is recommended that you use a sphere so the matrix will be a unit matrix and all three lengths will just be the sphere radius.

**-g** Write all the informative messages to *file,* instead of the standard error output. Genuine errors still go to the standard error output. This file is not rewound at any time, so messages from several runs may be accumulated.

**-i** Calculate the molecular surface only for those residues and atoms specified in *file,* but keeping the rest of the molecule for collision checks. This is equivalent to calculating the molecular surface for the entire molecule and then selecting out the surface belonging to the specified residues and atoms. The file consists of a series of lines such as the following:

```
ASP  205 CA
TYR   13 *
GLY  116 FRM
HIS  178 TO
```

The asterisk means all atoms of the residue and the ''FRM'' and ''TO'' mean all residues from 116 to 178 inclusive. These records are read with a FORTRAN ''a3,1x,a4,1x,a3'' format

**NAME**

midas.tty – terminal based version of MidasPlus display program

**SYNOPSIS**

**midas.tty** [–**b**] [–**s** *script*] [–**d** *delegate_name*] [*session_file|model_file(s)*] [ *file...* ]

**DESCRIPTION**

*Midas.tty* is a version of MidasPlus that runs on any CRT terminal. *Midas.tty* does everything that the *midas* interactive display program does except generate a three dimensional image of the molecular model. In particular, it accepts all normal MidasPlus commands (*e.g.* open, chain, label, distance, copy, save...). This is useful for editing an annotated PDB file or setting up session files without requiring access to the graphics display on a workstation.

If either standard input or standard output is redirected (*i.e.* is not a terminal), then *midas.tty* runs in a line-oriented batch mode. Thus it can be called from within a shell script for mass processing of MIDAS sessions.

**OPTIONS**

The –**b** option puts *midas.tty* into a batch mode regardless.

The –**s** *script* option lets you specify a command script to be sourced at start up time.

The –**d** *delegate_name* option treats standard input and output as a delegate with the given name.

**SEE ALSO**

midas(1), MidasPlus User's Manual

**AUTHOR**

Greg Couch, UCSF Computer Graphics Laboratory

**BUGS**

Interactive distances/angles are not shown in batch mode.

The aspect ratio of the terminal emulation window affects the size and orientation of hardcopy images generated with the **copy** command. Use the –**C** *columns* and –**R** *rows* command line options to change the aspect ratio by changing the number of rows and columns.

| | |
|---|---|
| rot 0 #1:248a@ca,cb | establish a bond rotation about the **ca**->**cb** bond of residue **248a** in model **1** |
| ˜rot 0 | remove the above rotation |
| ˜dist 1 | disable the above distance calculation |

**SEE ALSO**

MidasPlus User's Manual

**AUTHORS**

Conrad Huang and Thomas Ferrin, UCSF Computer Graphics Laboratory
Paul Bash contributed vdw style surfaces and the **addaa**, **addgrp**, **swapaa** and **swapna** commands.

**NAME**

midas − MidasPlus molecular interactive display program

**SYNOPSIS**

**midas** [−**f**] [−**F**] [−**s** *script*] [−**d** *delegate_name*] [*session_file*|*model_file(s)*]

**DESCRIPTION**

*Midas*, or MidasPlus as the second generation program is called, is an interactive molecular modeling system for 3D graphics displays. The system is designed to generate easily manipulated views of large molecules, primarily proteins and nucleic acids. *Midas* normally starts up in a window, but if the −**f** flag is used, then *midas* will use the entire graphics display on start up.

On the Silicon Graphics IRISes, the −**F** flag forces *midas* to start running on the console even though you aren't logged in on the console. This overrides the safety feature of not starting of midas when you are remotely logged in and not physically at the console.

The −**s** *script* option lets you specify a command script to be sourced at start up time.

The −**d** *delegate_name* option treats standard input and output as a delegate with the given name.

If there is more than one filename specified on the command line, *midas* opens then first file as model 0, the second as model 1, etc. (see **open** in the Command Reference Guide section of the MidasPlus User's Manual). If only one argument is given on the command line, then *midas* will try to read it as a session file first, and then open it as a model if it isn't a session.

*Midas* commands consist of a command word followed by 0 or more command arguments. The command arguments typically form a hierarchical specification for an area of interest within a molecule. The following symbols are part of the specification hierarchy:

| | |
|---|---|
| *#n* or *#name* | indicates a particular model; *n* is a digit indicating the model number (assigned when model was first opened), or, alternatively, the 3 or 4 alphanumeric abbreviation for the molecule (*e.g.*, **cpa** for carboxypeptidase). This part of the command argument is optional; if it is omitted, all models are processed. |
| *:n* or *:name* | indicates a particular residue (*e.g.*, **102**) or a particular group of residues (*e.g.*, **tyr**). |
| *@name* | indicates a particular atom (*e.g.*, **ca** for alpha-carbon) |

Note that space characters between arguments are ignored and may be freely inserted (if desired) for readability. Omitting a portion of an argument is the same as specifying ''∗'' (matches anything). In addition to these symbols, the following symbols may be used to modify command arguments:

| | |
|---|---|
| %*n* | specifies a skip count (*n* is a digit) |
| − | used to specify an inclusive range of items |
| ∗ | matches anything |
| ? | matches a single alpha-numeric character |
| , | used for grouping |
| ˜ | logical complement of command |
| ; | separator for multiple commands on the same line |
| <RETURN> | separator for commands |

**EXAMPLES**

| | |
|---|---|
| label #2:248a@∗ | label all atoms in residue **248a** of model **2** |
| label #2:248a | same as above |
| dist 1 #1:248a@oh#2:1b@n | establish a distance calculation between atom **oh** of residue **248a** in model **1** and atom **n** of residue **1b** of model **2** |

**NAME**

itops − convert an Iris image file to Color PostScript

**SYNOPSIS**

**itops** [−**a**] [−**b** *bits-per-color*] [−**g** *gamma-factor*] [−**i**] [−**l**] [−**p** *page-type*] [−**q**] [−**r**] [−**s** *scale-factor*] [−**z**] [−**8**] image-file

**DESCRIPTION**

*itops* converts a Silicon Graphics Iris image file to Color PostScript. The output appears on standard output and would normally be piped directly to the *lpr*(1) or *lp*(1) command.

**OPTIONS**

The −**l** option lists all known page types.

The −**p** option sets the page type, the default is **Letter**.

The −**r** option rotates the image so it's in landscape mode instead of portrait mode.

The −**g** option gamma corrects the image data by the given amount. Depending on the printer, this value should range from from 0.9 to 1.8; the default is 1.5.

The −**s** option scales the image by the given amount.

The −**a** option overrides the −**s** option and automatically scales the image to fit the page type. If the −**r** option is given as well, then the image is optionally rotated for the best fit.

The −**i** option makes one pixel match one square PostScript unit. Otherwise, a pixel is normally shrunk to give the PostScript image the same size as the screen image.

The −**b** option sets the number of bits per color to download. 8 is equivalent to 24 bit RGB; other possible values are 1, 2, or 4. Since the printer's color gamut is smaller than the screen's, the default is 4.

The −**q** option suppresses all informational and error messages (quiet).

The −**z** option will remove (zap) the image file after it's opened.

**SEE ALSO**

icut(1), scrsave(1), "Graphics Library User's Guide", 4Dgifts/iristools

**DIAGNOSTICS**

The amount of time to download the image at 9600 baud is reported.

The program refuses to generate output if the image won't fit on the page.

**BUGS**

Only works with RGB image files.

The image library does not allow one to pipe images from one program to another.

Doesn't do any color correction.

For autoscaling to the imageable area to work properly, *itops* needs a spooling system that understands the PostScript document structuring comment: **%%BeginFeature: ∗ImageableArea** *page-type*.

**AUTHOR**

Greg Couch, UCSF Computer Graphics Lab.

**NAME**

ilabel – label an IRIS image with arbitrary text

**SYNOPSIS**

**ilabel** [ **–f** ] [ **–i** file ] [ **–o** file ] image_file

**DESCRIPTION**

*ilabel* displays the given Silicon Graphics Iris *image_file* and lets the user put labels over the image. The IRIS image file may be generated by *scrsave*(1), *imgsnap*(1), or some other program, such as *conic*(1L), that use the IRIS image library. The labels are drawn using the IRIS Font Manager, which supports many fonts in arbitrary sizes. Labels may be saved to a file for reuse via the **–o** flag. The stored attributes of labels include color, vertical and horizontal justification, font, size, and position relative to the image. The saved label files may be displayed again using the **–i** flag. There may be several **–i** files but at most one **–o** file. The output file is created when the user selects **Exit** from the pop-up menu. If the file already exists, the user is asked whether the file should be overwritten (unless the **-f** flag was specified, in which case no question is asked).

To add a new label, simply click the left mouse button, which should make a triangular cursor appear, and type in the label. Labels containing multiple lines may be created by typing either **RETURN** or **LINEFEED** at the appropriate place. The left button is also used to select other labels so that they may be edited. The middle button is used to select and move labels. The right button displays a menu which contains options to show and hide the defaults panel (see below), redraw the images and labels, turn the mouse cursor on and off, and quit.

The default display attributes for labels are as follows:

| | |
|---|---|
| font | Times Roman |
| size | 14 |
| color | white |
| justification | bottom left |

All these values may be changed via the defaults panel, which is shown when the user selects the **Show Defaults** option from the right-button menu. When the mouse cursor is over the defaults panel, the left mouse button is used to select the justification mode and label color; the font size may be entered via the keyboard; and new fonts may be selected from the right-button menu. Also, colors may be selected from anywhere on the screen. If the mouse button is depressed over the color selection area, the mouse may be moved anywhere and a color will not be selected until the button is *released.*

**SEE ALSO**

conic(1L), icut(1), scrsave(1)

**BUGS**

Cannot display arrows.

**AUTHOR**

Conrad Huang
UCSF Computer Graphics Laboratory

**NAME**

gentpl − generate a MIDAS template from a Protein Data Bank coordinate file

**SYNOPSIS:**

**gentpl -r** *residue* [**–i** *infile*] [**–c** *radiifile*]

**DESCRIPTION:**

*Gentpl* is a utility program for generating a MIDAS template from a Protein Data Bank coordinate file. Standard input is assumed unless otherwise specified. One file is produced: the ASCII instruction file, *residue*.ins, where ‘‘*residue*’’ is the residue name specified on the command line. These files are placed in the directory defined by the MODELS variable in the user’s program environment (see part II of the MidasPlus User’s Manual).

**-r** *residue* specifies the *residue* name. This name must correspond to the residue name as it appears in the Protein Data Bank input file.

**-i** *infile* specifies an input file. The input *must* be in standard Brookhaven Protein Data Bank format. The file may contain data other than the coordinate data for the specified residue, but these extraneous records are ignored.

**-c** *radiifile* specifies a file containing the radii of the atoms used to calculate the connectivity. If no file specified, the program uses as default */usr/local/lib/connect.tpl*. The format of the radii file is a series of records containing the atom name followed by the atom radius in angstroms. At least one space must appear between the atom name and the radius.

**-v** indicates verbose mode and is useful for tracking down errors.

**BUGS**

The radii file must be ordered such that in the case of overlapping atoms names, longest names appear before shorter ones. For example, if the file contains the radius for both B and BR, BR must appear before B in file.

**SEE ALSO**

midas(1), midas.in(1)
Protein Data Bank File Record Formats, December 1981

**AUTHOR**

Laurie Jarvis
UCSF Computer Graphics Laboratory

**NAME**

fixatname − correct AMBER pseudo-PDB files so they are in standard PDB format

**SYNOPSIS:**

**fixatname** [ file1 ... ]

**DESCRIPTION:**

Versions of AMBER prior to version 3.0 revision A produced PDB files that had atom names aligned in the wrong columns (see MidasPlus User's Manual, Part I, *Protein Data Bank Format* for details of PDB format). *Fixatname* corrects this mis-alignment. AMBER PDB files have their atom names left-adjusted in columns 13-16 of each line. *Fixatname* left-adjusts the atom name in columns 14-16, with the former contents of column 16 being placed in column 13. This results in atom names that conform to the PDB standard with the rather infrequent exception of atom names with a two character atomic symbol (such as iron, *FE*). Such cases can be corrected by hand after processing by *fixatname*.

*Fixatname* reads from standard input if no file names are specified. *Fixatname* prints the corrected PDB file on standard output.

**BUGS**

Atoms with two character atomic symbols are mis-aligned, as mentioned above.

**SEE ALSO**

MidasPlus User's Guide

**AUTHOR**

Conrad Huang
UCSF Computer Graphics Laboratory

**NAME**

esp − calculate electrostatic potential

**SYNOPSIS:**

**esp** −**i** *dms_file* [−**o** *esp_file*] [−**q** *file*] −**a** *pdb_file* [−**r**] [−**n**] [−**c** *cutoff*] [−**e** *epsilon*] [−**p** *len*] [−**v**] [−**w**]

**DESCRIPTION:**

*Esp* calculates the electrostatic potential of a solvent accessible surface and stores it in an annotated *ms* surface file. This information can then be used by MIDAS to selectively color molecular surfaces based on electrostatic charge. *Esp* prints out a summary of the conditions used to calculate the potential.

−**i** *dms_file* — specifies a *dms* surface input file. The electrostatic potential is calculated for all points of this surface. Use the *dms(1)* program with the **-n** flag (to calculate normals) to generate *dms_file*. If the −**p** flag (see below) is given a value of 0, the normals need not be calculated by *dms*(1).

−**o** *esp_file* — indicates the annotated *dms* surface file to which the calculated electrostatic surface is output.

−**q** *charge_file* — The option −**q** *charge_file* supplies an alternate charge file for residue types. The default file used is */usr/local/lib/charges.esp*. Instructions for constructing alternate charge values are contained in the default file. The −**q** flag must *precede* the name of the Protein Data Bank format file (−**a** flag) to which the alternate charge file is applied. Thus, a series of command line parameters, −**q** *file1* −**a** *db1* −**q** *file2* −**a** *db2* may be used to associate alternate charge files with specific models.

−**a** *pdb_file* — is the name of the Protein Data Bank format file containing the coordinates for the associated *ms* surface file and any other atoms which should be included in the electrostatic calculation. The potential is calculated *only* for those surface points in *dms_file*, but *all* atoms in *pdb_file* are used in the calculation.

−**r** — indicates that the dielectric constant is dependent on the distance from the atom or charge to each surface point.

−**n** — specifies neutral spheres. Charges are summed within the *cutoff* radius defining the sphere, and an equal and opposite charge is spread uniformly across the sphere surface.

−**c** *cutoff* — indicates the cut off radius in angstroms. The default value is 10.0.

−**e** *epsilon* — indicates the value of epsilon. The default value is 1.0.

−**p** *len* — calculates the potential at a distance *len* angstroms from the surface. Positive values of *len* lie outside of the surface, while negative values lie within the surface. The default value of *len* is 1.4 angstroms.

−**w** — indicates that the electrostatic potential of each point should be appended to the corresponding line in the input *dms_file*.

−**v** — indicates verbose mode. Auxiliary information (*e.g.*, the number of points found for each atom) is reported.

**SEE ALSO**

dms(1), midas(1) MidasPlus User’s Manual

**AUTHOR**

Conrad Huang
UCSF Computer Graphics Laboratory

The idea of neutral spheres came from Paul Weiner while a graduate student in the Department of Pharmaceutical Chemistry, UCSF.

The output consists of a series of atom and surface point records, with the same format for the first 6 fields. Each atom is followed by the surface points (if any) which belong to it. These first 6 fields are in the following format: residue name, sequence number, atom name, x coordinate, y coordinate, z coordinate. For an atom record, the seventh field is ‘‘A’’. For a surface point record, the seventh field begins with an ‘‘S’’, followed by a ‘‘C’’ or ‘‘R’’ according to whether the point is part of contact or reentrant surface. This is followed a digit used for depicting different density levels. The eighth field is the molecular surface area associated with the point in square Angstroms. If the **-n** flag is specified, the next three fields are the unit normal vector pointing outward from the surface. Informative messages and errors are written to the standard error output unless a **-g** file is specified.

The chemical elements and radii that the program handles are detailed in the table below. The program gets these values from the file */usr/local/lib/dms/radii*. If there is a file in the current directory called *radii*, then *dms* will use that file instead. So in order to add uncommon elements or use different radii, one should copy the default file and modify it. The file format is documented in the file itself.

| Element | Radius |
|---|---|
| H | 1.20 |
| C | 1.90 |
| N | 1.50 |
| O | 1.40 |
| F | 1.35 |
| P | 1.90 |
| S | 1.85 |
| Cl | 1.8 |
| Fe | 0.64 |
| Cu | 1.28 |
| Zn | 1.38 |
| Br | 1.95 |
| I | 2.15 |
| Other | 1.90 |

**AUTHOR**

Conrad Huang
University of California, San Francisco

**FILES**

/usr/local/lib/dms/radiidefault atomic radii

**DIAGNOSTICS**

Many and varied. Be sure to examine the **-g** file and ‘‘submit.out’’ before you leave a background job running overnight.

**NAME**

dms − calculate a solvent accessible molecular surface

**SYNOPSIS**

**dms** file [ **-a** ] [ **-d** density] [ **-g** file] [ **-i** file] [**-s** file] [**-n**] [**-w** radius] **-o** file

**DESCRIPTION**

*Dms* calculates the molecular surface of a molecule. The molecular surface resembles the van der Waals surface of a molecule, except that crevices between atoms are smoothed over and interstices too small to accommodate the probe are eliminated. The surface includes cavities in the interior of the molecule, even if they are not accessible to a solvent molecule coming from the outside.

The molecular surface calculated is that defined by F. M. Richards (1977, *Ann. Rev. Biophys. Bioeng.* ). According to Richards' definition the molecular surface consists of two parts: *contact surface* and *reentrant surface.* The contact surface is made up of ''those parts of the molecular van der Waals surface that can actually be in contact with the surface of the probe.'' The reentrant surface is defined by ''the interior-facing part of the probe when it is simultaneously in contact with more than one atom.''

*File* is an input file of coordinates. The input file must be in the Protein Data Bank format. The first letter or first two letters of the atom name is used to determine the element type. Implicit hydrogens are always included for carbon, nitrogen and oxygen atoms, thus aromatic carbons and nitrogens will have van der Waals radii that are somewhat too big. Note that only amino acid residues will be included unless **-a** is also specified.

The flags may be in any order. The meanings of the flags are described below:

**-a** Include all atoms, not just those in amino acid residues.

**-d** Change the density of points on the surface. *Density* is a factor affecting the density of points on the surface: the default of 1.0 produces about 5 points per square Angstrom. Only values between 0.1 and 1.0 are permitted. For large proteins, a density of 0.5 is recommended.

**-g** Write all the informative messages to *file,* instead of the standard error output. Genuine errors still go to the standard error output. This file is not rewound at any time, so messages from several runs may be accumulated.

**-i** Calculate the molecular surface only for those residues and atoms specified in *file,* but keeping the rest of the molecule for collision checks. This is equivalent to calculating the molecular surface for the entire molecule and then selecting out the surface belonging to the specified residues and atoms. The file consists of a series of lines such as the following:

```
ASP  205 CA
TYR   13 *
GLY  116 FRM
HIS  178 TO
```

The asterisk means all atoms of the residue and the ''FRM'' and ''TO'' mean all residues from 116 to 178 inclusive. The sequence number may contain letters and if the PDB input file contains chain identifiers then those should be appended on the right of the sequence number. The surface generated using the **-i** flag is not always the same as the surface generated by running the entire molecule and afterwards selecting out the desired atoms. The first surface will not include reentrant surface lying between an atom in the **-i** file and atoms not in the file.

**-s** Use the supplied file argument to specify the atomic radii. The format of the file is an atomic symbol followed by its radius, one per line. */usr/local/lib/midas/connect.tpl* uses this format.

**-n** Include the unit normals to the surface with each surface point record.

**-o** The output is written to *file.* This flag is not optional.

**-w** Change the water probe radius from the default radius of 1.4 Angstroms. This parameter must be between 1.0 and 201.0.

```
S      1.85  1     1     0
H      1.0   1     1     1
P      1.9   1     0.5   0
F      1.35  0     1     0
CL     1.8   0     1     0
BR     1.95  0     1     0
I      2.15  0     1     0
B      1.8   0.5   0     0
FE     0.64  0.5   0     0
CU     1.28  0.5   0     0
ZN     1.38  0.5   0     0
```

**BUGS**

Light intensity does not attenuate with distance.

**SEE ALSO**

ipaste(1), midas(1), ilabel(1)

**FILES**

/usr/local/lib/conic.atinfo – default atom information file

**AUTHORS**

Eric F. Pettersen, Conrad Huang, Gregory S. Couch
UCSF Computer Graphics Laboratory

Store the computed image in *file* . The file is generated using the Silicon Graphics Image Library routines, and may be displayed using the *ipaste*(1) program. By default no image file is used and the computed image is displayed on the IRIS directly.

**point** *x y z r g b*
Define a point light source. The arguments are the same as those for the **light** option, except that (*x y z*) defines the light position rather than direction.

**rcone** *x y z r g b dx dy dz angle*
**Rcone** is to **cone** as **rpoint** is to **point.**

**rpoint** *x y z r g b*
Define a point light source relative to the scene, similar to **point.** The (*x y z*) coordinate is relative to the center of the scene, with lengths normalized such that the distance from the eye to the center of the scene is 1. Thus, the option

**rpoint 0 0 1 1 1**

would define a point light source that coincided with the eye.

**rspot** *x y z r g b dx dy dz power*
**Rspot** is to **spot** as **rpoint** is to **point.**

**size** *x y* Sets the image size. The default image size is 1280x1024.

**spot** *x y z r g b dx dy dz power*
Define a spot light. The absolute Cartesian coordinate of the light source is given by (*x y z*). The color of the light is given by (*r g b*). The Cartesian direction of the spot light is given by (*dx dy dz*). The intensity of the spot light drops off as the angle between the spot light direction and the pixel direction; the rate of decrease is the cosine of the angle raised to the *power*th power. *Power* must be an even integer; odd integers will be incremented silently.

## COLORING THE MOLECULE

*Conic* uses two sources of atom radius and coloring information. If neither source of information yields radius and color for an atom, then the atom is ignored.

The first source is embedded in the input to *conic,* which is an extended Protein Data Bank format. The format is identical to standard PDB format except that **ATOM** and **HETATM** records may be followed by **USER** records, whose text field contains a keyword and some values. (The **pdbrun** command of *midas*(1) generates output of this format.) The keywords that *conic* uses are **COLOR**, **RADIUS**, and **MATPROP**. **COLOR** is followed by an integer color index and three floating point RGB intensities. **RADIUS** is followed by a floating point number representing the atom radius in angstroms. If the radius is absent, then the color information is considered invalid. **MATPROP** is followed by the three parameters to the **matprop** option in the configuration file. An example of the extended format follows.

```
ATOM      1  C   HIS     1      49.168  26.701  10.916  1.00 16.00
USER  COLOR 1 0.000 1.000 0.000
USER  RADIUS 1.800
USER  MATPROP 0.5 0.25 16
```

If the input fails to specify the color and radius of an atom, *conic* uses an **atom information** file to supply simple default values. The file contain comment lines, which begin with '**#**', and information lines, which have five fields: atom type, radius, and RGB value. The atom type is either one or two characters and is used to match the atom type in the PDB input. The atom type '*' is a special case and matches any atom which does not match any other information lines. Using an **atom information** file, simple color-by-type images may be generated from raw PDB files.

The default **atom information** file contains the following lines:

```
C     1.8   0.5   0.5   0.5
N     1.8   0     0     1
O     1.5   1     0     0
```

small molecules, which have low startup times, going from mode **none** to **2x2** will increase the computation time four-fold. The relative increase is less for large molecules since the startup time for large molecules is a significant fraction of total computation time. The default antialias mode is **none .**

**atinfo** *file*
Use the given file as the **atom information** file, which contains default information on how each type of atom should be colored. Coloring the molecule is described in greater detail below. This option has no effect if **conic** is invoked from within *midas*(1), as *midas* fully specifies atom colors and radii.

**background** *r g b* [*r g b*]
Set the background color for the image. If only one RGB value is given, then the entire background is set in that color. If two RGB values are given, then the background is interpolated between the two colors from bottom to top. The default background color is (0 0 0).

**cone** *x y z r g b dx dy dz angle*
Define a cone light. The absolute Cartesian coordinate of the light source is given by (*x y z*). The color of the light is given by (*r g b*). The Cartesian direction of the cone light is given by (*dx dy dz*). And the half-angle of the cone is *angle* degrees.

**eye** *r b g*
*Conic* places an additional point light source which coincides with the eye position. The purpose of this light source is to weakly illuminate shadowed areas so that they have discernible features rather than a uniform color. The **eye** option sets the color of the point light source. The default value is (0.3 0.3 0.3).

**fov** *angle*
Sets the field-of-view half-angle, in degrees. The default value is 15 degrees.

**input** *file*
Use *file* as the Protein Data Bank file.

**light** *x y z r g b*
Add an infinite light source to the scene being computed. The direction of the light source is specified by (*x y z*). The color of the light source is specified by (*r g b*). By default, *conic* defines a light source with direction (1 1 1) and color (1 1 1). The default light source is removed if other sources are specified via the **light** option.

**ls_flags** *flags*
Change the default flags of subsequently specified light sources. By default, a light source only shines on a point if there are no intervening spheres. If the **noshadow** flag is specified, however, all points are considered to be lit. The **noshadow** flag is generally used if the scene is very complex, and having shadows makes the resulting image difficult to interpret. This problem may also be mitigated by using multiple light sources.

**matprop** *kd ks power*
Define default material properties. *Kd* is the diffuse reflection coefficient. *Ks* is the specular reflection coefficient. *Power* controls how sharply defined a specular light is, and must be a positive even integer. The higher the value of *power* , the smaller the specular reflection area. The default values are 0.5, 0.25, and 8, respectively.

**noshadow** [**type|seq**] *residue*
Most atoms should cast shadows on other atoms in the scene. However, one may not want some fake atoms to cast shadows. For example, electron density ‘‘residues’’ as produced by **render**(1) can greatly complicate a scene with their shadows. Shadows from these residues may be eliminated by giving the **noshadow** option and specifying either the residue type or sequence number. (The problem of shadows may also be solved by using multiple light sources.)

**output** *file*

**NAME**

conic − generate CPK-style molecular models with shadows

**SYNOPSIS**

**conic** [ **−p** ] [ **−f** ] [ **−s** ] [ **−a** *mode* ] [ **−o** *output-file* ] [ **−x** *pixels-wide* ] [ **−y** *pixels-high* ] [ **−c** *config-file* ] [ **−e** *shell-command* ] [ **−v** ] [ **−W** ] [ *PDB-file* ]

**DESCRIPTION**

*Conic* reads a Protein Data Bank file and generates a Corey-Pauling-Koltun style image of the molecule. If no PDB file is specified, standard input is used. There can be an arbitrary number of light sources. Specular highlights, diffuse reflections, and shadows are all computed properly.

**COMMAND LINE FLAGS**

The command line flags interpreted by *conic* are:

**−p** Use preview mode. Set the image size to 645x484 and antialias mode to **none** (see below).

**−f** Set the image size to be the full screen.

**−s** Invoke *ipaste*(1) on the computed image file. This flag is only meaningful when used in conjunction with the **−o** flag or the **output** option.

**−a** *mode*

Set the antialias mode. *Mode* is the same as the argument to the **antialias** option in the configuration file (see below).

**−o** *file* Store the computed image in *file* in IRIS image library format. The image is not displayed unless the **−s** flag is also specified. This file may also be used with the *ilabel (1)* program to add titles and labels.

**−x** *size* Set the horizontal image size to *size* pixels.

**−y** *size* Set the vertical image size to *size* pixels.

**−e** *shell-command*

Execute the shell command when the image has finished drawing and exit when the command is done.

**−c** *file* Use *file* as the *conic* configuration file.

**−v** Print progress messages.

**−W** Force *midas*(1) to wait until conic has exited before continuing.

**NeXT DIFFERENCES**

The **-s** option is not supported because all output is in EPSF format (Encapsulated PostScript File). You should place the output in a file whose name ends with **.eps**, so the Workspace may open it correctly. *Midas*(1) simulates the effects of the **-s** option for compatibility with other systems.

**CONFIGURATION FILE**

The scene computed by *conic* is described by a list of options in a configuration file. If the configuration file is absent, or the option is omitted, then a default value will be used. Lines beginning with '**#**' are comments and are ignored. All other lines are options, which begin with a keyword and are followed by space-separated values. The available options are listed below.

**ambient** *r g b*

Set the ambient light to the given RGB value, which is three floating point intensities ranging from 0 to 1. The default ambient lighting is (0.2 0.2 0.2).

**antialias** *mode*

Set the antialiasing algorithm. *Mode* may be **none ,** for no antialiasing; **3/2 ,** for mapping 3x3 calculation pixels onto 2x2 image pixels; or **2x2 ,** for mapping 2x2 calculation pixels onto single image pixels. Antialiasing improves the picture quality at the expense of computation time. The time increase is proportional to the number of pixels computed modulo the startup time. Thus, for

and 5 respectively. Same as the −**u** and −**v** command line flags.

**printer** *printer_name*
Send PostScript output to printer *printer_name*. Same as the −**P** command line flag.

**scale** *scale_factor*
Scale the picture. The degree of scaling is proportional to the scale factor.

**sheet_color** *r g b*
Specify the ribbon color of residues which are part of β-sheets. If this option is not specified, the residue color will be the same as the α-carbon in the residue.

**show_atoms**
Display atoms and bonds as balls and sticks. Same as the −**a** command line flag.

**show_rectangles**
Show rectangles in PostScript output. Same as the −**R** command line flag.

**size** *width height*
Specify the display window width and height. When used in conjunction with the **location** option, the window and image will appear without user intervention (*i.e.*, having to sweep out a window).

**turn_color** *r g b*
Specify the ribbon color of residues which are part of turns. If this option is not specified, the residue color will be the same as the α-carbon in the residue.

## SEE ALSO

Carson, M and Bugg, C E, **Algorithm for ribbon models of proteins**, *Journal of Molecular Graphics* Vol 4 (1986) pp 121-122.
conic(1), lpr(1), midas(1).

## FILES

/usr/local/lib/cartoon/atinfo − default atom information file
/usr/local/lib/cartoon/xsection − default cross-section file
/usr/mol/models/*.ins − default residue drawing templates

## BUGS

This program has such a stupid name because all the good ones were taken.

## AUTHORS

Conrad Huang
UCSF Computer Graphics Laboratory

**–R** Display rectangular patches along ribbon for PostScript output. Mostly used for debugging although this rendition produces a better silhouette.

**–W** Force *midas*(1) to wait until cartoon has exited before continuing.

**–X** *file* Use *file* as the cross-section file rather than the default version.

**CONFIGURATION FILE**

The image computed by *cartoon* is described by a list of options in a configuration file. If the configuration file is absent, or the option is omitted, then a default value will be used. Lines beginning with '**#**' are comments and are ignored. All other lines are options, which begin with a keyword and are followed by space-separated values. The available options are listed below.

**alpha_only**
Use only the α-carbons for generating the ribbon. The image generated this way is generally inferior to using both α-carbons and carboxy oxygens.

**arrow_size** *length width*
Each β-sheet is terminate with an arrow. The length of the arrow is defined as a fraction of the inter-residue distance, and the width is defined as a fraction of the sheet width. The default length and width are 0.5 and 3 respectively.

**atinfo** *file*
Use the given file as the default **atom information** file, which contains information on how each type of atom should be colored. Coloring the molecule is described in the *conic*(1) manual page under section ''Coloring the Molecule.'' This option has no effect if **cartoon** is invoked from within *midas*(1), as *midas* fully specifies atom colors and radii.

**background** *r g b* [*r g b*]
Set the background color for the image. If only one RGB value is given, then the entire background is set in that color. If two RGB values are given, then the background is interpolated between the two colors from bottom to top. The default background color is (0 0 0).

**bs_size** *sphere_size cylinder_size*
Atoms and bonds may be displayed as balls and sticks in the computed image (see the **show_atoms** option below). The radius of the balls (spheres) and the diameter of the sticks (cylinders) are specified as fractions of the atomic radii. The default values are 0.3 for both sizes.

**hardcopy**
Generate PostScript output instead of displaying image on screen (same as the **–h** command line flag).

**helix_color** *r g b*
Specify the ribbon color of residues which are part of α-helices. If this option is not specified, the residue color will be the same as the α-carbon in the residue.

**location** *x y*
Specifies the location of the lower left corner of the display window. Due to a limitation of the IRIS graphics library, this option is only effective when the window size is specified as well (see the **size** option below).

**matprop** *ambient diffuse specular*
Specifies the material property of ribbons, balls, and sticks. The three values are the ambient, diffuse, and specular reflectance of the material and should all range between 0 and 1. The default values are 0.2, 0.4 and 0.2 respectively.

**output** *file*
Send PostScript output to *file*. Same as the **–o** command line flag.

**precision** *u v*
Specify the number of divisions per bicubic patch. The first parameter controls the number of divisions along the ribbon and the second controls the number across. The default values are 10

**NAME**

cartoon − generate ribbon representation of proteins

**SYNOPSIS**

**cartoon** [ **−a** ] [ **−c** *config-file* ] [ **−f** ] [ **−h** ] [ **−o** *output-file* ] [ **−p** ] [ **−s** *residue-file* ] [ **−u** *count* ] [ **−v** *count* ] [ **−e** *shell-command* ] [ **−A** *file* ] [ **−N** ] [ **−R** ] [ **−P** *printer* ] [ **−X** *cross-section-file* ] [ **−W** ] [ *PDB-file* ]

**DESCRIPTION**

*Cartoon* reads a Protein Data Bank file and generates ribbon image of the molecule. The PDB file may carry extra atom information such as color and radius in the same fashion described in the *conic*(1) manual page (under section ‘‘Coloring the Molecule’’). The color of the ribbon is the same as the color of the α-carbons. If no PDB file is specified, standard input is used.

Atoms and bonds may also be optionally displayed as balls and sticks. When the ball-and-stick option is selected, most mainchain atoms, including N, C, O, and OXT, are not displayed; the α-carbon, CA, is displayed if it is connected to a displayed atom; all other atoms are displayed. The bonds are derived either from CONECT records if they exist in the PDB file, or from drawing templates found in *midas*(1) template directories.

**COMMAND LINE FLAGS**

The command line flags interpreted by *cartoon* are:

**−a** Display all atoms using balls and sticks. The only atoms that will **not** appear in the image are N, C, O, and OXT of amino acids that form the ribbon.

**−c** *file* Use *file* as the *cartoon* configuration file.

**−f** Use full screen mode. Set the image size to use the entire screen.

**−h** Generate a PostScript file instead of displaying the image on the screen. The PostScript image is different from the screen image in that the ribbon for the former case is strictly two dimensional, while the ribbon for the latter case has a non-zero cross-section. The PostScript output will be sent to the default printer queue via the *lpr*(1), unless either the **−o** or **−P** flag is specified.

**−o** *file* When used with the **−h** flag, the PostScript output is sent to *file* instead of the default printer.

**−p** Use preview mode. Set the image size to 645x484.

**−s** *file* The content of *file* is a list of residues which should not be used in the construction of ribbons. The atoms in these residues are still displayed with the **−a** flag. The residues are specified one per line in *file*, and may be specified either by sequence or by type.

**−u** *count*
The ribbon is formed using a series of bicubic patches between residues. Each patch is subdivided into quadrilaterals, which are rendered on the screen. The **−u** flag specifies the number of divisions to use length-wise along ribbon. The default value is 10.

**−v** *count*
Specify the number of divisions to use width-wise across the ribbon. The default value is 5.

**−e** *shell-command*
Execute the shell command when the image has finished drawing and exit when the command is done.

**−A** *file* Default atom radius and color information are read from *file*. The format of the file is the same as that used by *conic*(1).

**−N** Display normal vectors along the ribbon. The resulting image has been compared to porcupines and cacti.

**−P***printer*
PostScript output is sent to *printer* instead of the default printer. If both **−o** and **−P** are specified, the output will be sent to the file rather than the printer.

## Appendix 6: MIDAS Utilities

Several MIDAS utilities are available for generating MIDAS databases, preparing surface files, building templates and preparing models for display. These utilities are typically run directly from the UNIX shell and *not* from the graphics system keyboard during a MIDAS session. The manual pages for MidasPlus and all associated utility programs are included here and the table below summarizes the function of each program.

**MIDAS Utility Programs**

| Program Name | Function |
|---|---|
| cartoon | generate ribbon representation of proteins on IRIS workstations |
| conic | generate CPK-style molecular models with shadows |
| esp | calculate electrostatic potential |
| fixatname | correct AMBER pseudo-PDB files so they are in standard PDB format |
| gentpl | generate a MIDAS template from a Protein Data Bank coordinate file |
| ilabel | label an IRIS image with arbitrary text |
| itops | convert IRIS image to color PostScript |
| midas | MidasPlus molecular interactive display program |
| midas.tty | terminal based version of MidasPlus display program |
| dms | calculate a solvent accessible molecular surface |
| neon | generate a molecular model with solid stick bonds and shadows |
| unmtrix | expand MTRIX records in Protein Data Bank coordinate file |

Each utility description contains a synopsis line indicating the correct usage of the command. The usage includes the command name in **boldface** type followed by command line parameters. These command line parameters appear in:

**boldface** print — indicating a flag. The flag is usually a single character and is preceded by a ‘‘–’’ character and is typed as is.

Roman print — indicating a parameter for which the user substitutes the appropriate name, digit, *etc*. In the text of the manual page, these parameters appear in *italic* print.

```
	fputs("> ", record_fp);
		vfprintf(record_fp, fmt, args);
	}
	va_end(args);
	(void) fflush(stdout);		/* Make sure buffered data get sent */

	/*
	 * Keep reading until we see a line containing only SYNC,
	 * which denotes end of MidasPlus replies
	 */
	while (fgets(buf, sizeof buf, stdin) != NULL) {
		if (record_fp != NULL)
			fprintf(record_fp, "< %s", buf);
		if (strcmp(buf, "SYNC\n") == 0)
			break;
	}

	return;
}
```

```
FILE    *record_fp;

/*
 * Sample MidasPlus delegate
 */
main(int ac, char **av)
{
        register int    c;
        int             verbose = FALSE;
        char            buf[BUFSIZ];
        extern int      optind;
        extern char     *optarg;
        static int      send_command(char *, ...);

        /*
         * Process command line arguments
         */
        while ((c = getopt(ac, av, "vr:")) != EOF)
                switch (c) {
                  case 'v':
                        verbose = TRUE;
                        break;
                  case 'r':
                        record_fp = fopen(optarg, "w");
                        if (record_fp != NULL)
                                setbuf(record_fp, (char *) NULL);
                        break;
                }

        /*
         * First we sync with MidasPlus, which is expecting us to notify
         * it of proper start up.
         */
        (void) printf("SYNC\n");
        (void) fflush(stdout);

        /*
         * We simply echo back any commands to MidasPlus.  If we are
         * in verbose mode, we notify the user before and after
         * each command
         */
        while (fgets(buf, sizeof buf, stdin) != NULL) {
                if (verbose)
                        send_command("echo Delegate executing %s", buf);
                send_command(buf);
                if (verbose)
                        send_command("echo Delegate done\n");
                (void) printf("SYNC\n");
                (void) fflush(stdout);
        }

        exit(0);
}

/*
 * send_command:
 *      Send a command to MidasPlus and wait until the
 *      synchronizing string comes back
 */
static
int
send_command(char *fmt, ...)
{
        va_list args;
        char    buf[BUFSIZ];

        va_start(args, fmt);
        (void) vfprintf(stdout, fmt, args);
        if (record_fp != NULL) {
```

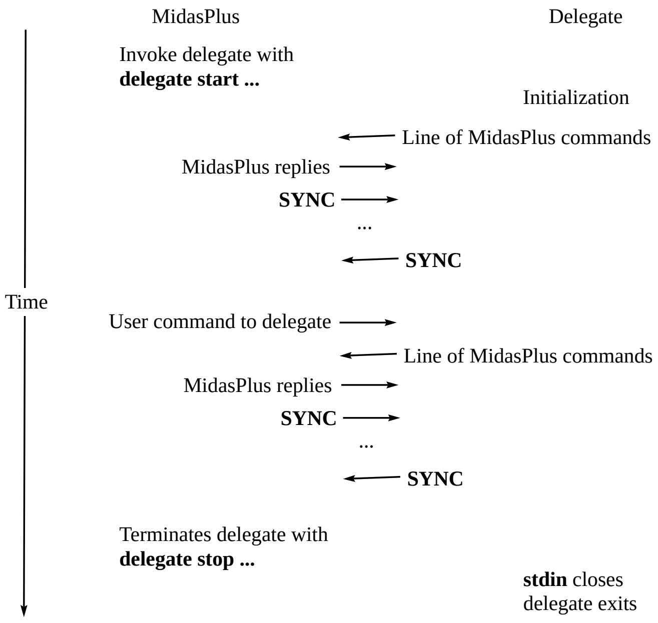



Figure 1 – Event diagram of delegate communications protocol

When the delegate receives an user command, it, once again, gets to send lines of commands to MidasPlus, using exactly the same synchronization as on start up. Between the time it forwards an user command to the delegate and the time it receives the terminating **SYNC** message from the delegate, MidasPlus will not accept any input from the user. Thus, a buggy delegate can cause MidasPlus to appear to hang until the delegate exits. When the delegate receives an end-of-file indication on **stdin**, it should terminate gracefully without trying to communicate with MidasPlus, as **stdout** may already been closed.

While waiting for an user command, a delegate may spontaneously generate MidasPlus commands. This is useful for programs that need to run for a substantial period of time before yielding results and can let the user manipulate the model while the computation occurs. These delegates can send the **SYNC** message before entering background computation mode, and then spontaneously generate MidasPlus commands once the calculation completes. The only drawback to using background computation is that the user may try to send more commands to the delegate, resulting in a race condition, where the user command may be interpreted as a reply to a MidasPlus command. Implementors of this type of delegates should clearly document which user commands use background computation modes, and possibly warn the user at run-time that further input is not advisable.

An example of a delegate that simply echoes user input follows.

```
#include <stdio.h>
#include <stdarg.h>

#ifndef TRUE
#define TRUE    1
#define FALSE   0
#endif
```

## Appendix 5: The MidasPlus Delegate Mechanism

### What are delegates?

MidasPlus has a rich command language, and users can specify nearly all operations by typing them in on the keyboard. Occasionally, however, it is useful to have other computer programs compose the commands. This functionality is partially provided by the **pdbrun** command, which sends the current transformed coordinates of molecules to an user-specified program, and treats the output of that program as MidasPlus commands. **pdbrun** is most useful for ''one-shot'' type computations, such as volume rendering or coloring atoms according to packing density. For computations that require information at several different times during a single MidasPlus session, however, **pdbrun** is too inefficient.

The solution is a mechanism that allows designated programs, called **delegates**, to communicate with MidasPlus while executing in parallel. For example, there is a rotation delegate that supports two commands: **snapshot** and **interpolate**. Users can use the **snapshot** command to save molecule positions at selected points during a session, and the **interpolate** command to smoothly interpolate between two saved positions. While it was possible to add the **snapshot** and **interpolate** commands directly to MidasPlus, this approach requires one to have both an understanding of the internal program structure, and permission to change source files. Writing the rotation delegate required no modifications to MidasPlus, and, once the matrix arithmetic was solved, took less that a day to implement. Less than 300 lines of new code (including comments) were written.

The delegate facility provides an alternative to modifying MidasPlus every time additional functionality is desired. Users who are willing to program can easily implement their own flavors of delegates and need not wait for MidasPlus developers to implement desired new features. In addition, delegates can use information sources other than MidasPlus. Thus, they can, potentially, inject some much needed chemistry information into MidasPlus.

### User Perspective

Delegates are controlled from MidasPlus using the *delegate* command, which supports three operations: **start**, **stop**, and **list**. New delegates are invoked with the command

> **delegate start** *delegate_name command arguments...*

where *delegate_name* is the name that MidasPlus will use to refer to the started delegate process, and *command* and *arguments* are the Unix command to execute the delegate program. Once a delegate is running, the user can send commands to it by prefixing the command with the name of the delegate, *i.e.*,

> *delegate_name delegate_command arguments...*

To terminate an active delegate, the user can issue the command

> **delegate stop** *delegate_name*

Finally, the command

> **delegate list**

lists the names of all active delegates.

### Implementor Perspective

When a delegate is executed, its standard input (C standard I/O library **stdin** or Unix file descriptor 0) and standard output (**stdout** or descriptor 1) are connected to MidasPlus. Data sent to **stdout** will be interpreted by MidasPlus. Data received on **stdin** are either commands from the user (via the *delegate_name* mechanism), or replies from MidasPlus commands (which are normally displayed to the user).

The communications protocol between the delegate and MidasPlus is very simple. An event diagram of the protocol is shown in Figure 1. On start up, the delegate gets to send lines of commands to MidasPlus for execution. For each line of command, MidasPlus sends back to the delegate all the reply lines, followed by a line containing only the word **SYNC**. When the delegate is finished with its initialization, it informs MidasPlus by sending a line containing only the word **SYNC**. At this point, the delegate should wait for user commands, which will arrive on **stdin** via MidasPlus.

## Appendix 4: Default Options, Aliases and Device Assignments

The following is a list of the default options, aliases and device assignments made by MidasPlus at the start of each MidasPlus session. These default assignments are stored in */usr/local/lib/midas/midas.rc* on the IRIS or */LocalLibrary/Midas/midas.rc* on the *NeXT*. The user may replace these defaults with an alternate file defined by the UNIX environment variable MIDASRC. If this variable is set to a legal source file name, it is executed *instead of* the MidasPlus default file. This is especially useful for making video tapes, as the user may not want extraneous text appearing on the screen at the beginning of the session.

The default assignments are:

| | |
|---|---|
| assign 0 scaling | *assign useful functions to the first few sliders* |
| assign 1 section | |
| assign 2 thickness | |
| | |
| alias model # | *a few useful aliases* |
| alias molecule # | |
| alias residue : | |
| alias atom @ | |
| alias sidechain @ cb - * | |
| alias mainchain @ n,ca,c,o | |
| alias close ˜open | |
| alias conic pdbrun /usr/local/bin/conic | ***conic*** *and* ***ribbon*** |
| alias ribbon pdbrun /usr/local/bin/cartoon | *are implemented using* ***pdbrun*** |
| set record | *start remembering commands for later* ***record****ing* |
| set text | *show command line and reply area* |
| set labels | *show distance, angle, and rotation monitors* |
| set control | *show control panel* |
| set verbose autocolor | |
| set vpsep 42 | *the optimal value for* **vpsep** *on your workstation can be determined by following the procedure outlined in the MidasPlus Installation Guide.* |

| Symbol | Function | Usage |
|---|---|---|
| **&** | intersection | Find the set of atoms that appear in both atom specifiers on left and right. *e.g.* **#1 & #2:1 zr<10** gives all residues in model one that are within 10 angstroms of residue one in model two. |
| **+** | atom picking | enables use of the mouse to select atoms whose names are substituted for the leftmost appearance of ‘‘**+**’’ symbol in the MIDAS command line. |
| **;** | command separator | separates multiple commands on a single line. |
| **RETURN** | return | accept the line. |
| **LINEFEED** | linefeed | accept the line. |
| **RUBOUT** | backspace | erase the character before the cursor. |
| **CTRL**-H | backspace | erase the character before the cursor. |
| **CTRL**-U | line kill | erase the whole line. |
| **CTRL**-W | word kill | erase the word before the cursor. |
| **CTRL**-D | delete | erase the character under the cursor. |
| **CTRL**-K | | erase to end of line. |
| **CTRL**-P | history | retrieve previous command. |
| **CTRL**-N | history | retrieve following command. |
| **CTRL**-A | | go to beginning of line. |
| **CTRL**-E | | go to the end of line. |
| **CTRL**-B | | move back a single character. |
| **CTRL**-F | | move forward a single character. |
| **CTRL**-L | | move cursor one word left. |
| **CTRL**-R | | move cursor one word right. |
| **CTRL**-G | | insert next character without interpretation. |
| **ESC** | break | break after the completion of the current command.<br>(see **source** command.) |

Note: Control characters are typed by holding down the **CTRL** key on the keyboard and typing the corresponding alphabetic character. For example, to type **CTRL**-H hold down the key marked ‘‘**CTRL**’’ while at the same time striking the ‘‘H’’ key.

## Appendix 3: Special Characters and Symbols Used in MIDAS

The following table describes symbols which have special meaning to MIDAS. In addition to these symbols, several special characters are available for use in command line editing (user's of the EMACS text editor will readily recognize most of these special editing characters).

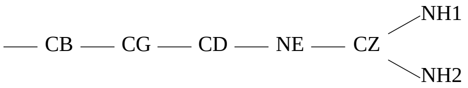
| Symbol | Function | Usage |
|---|---|---|
| **#** | model number | **#** *model_number*<br>where *model_number* is an integer. |
| **:** | residue | **:** *residue*<br>where *residue* is a residue name, residue sequence number, or range of residues. |
| **@** | atom name | **@** *atom_name*<br>where *atom_name* is an atom name or range of atoms. |
| – | range | specifies a range of atoms such as @CB–* (beta carbon to the last atom in residue branch), a range of residues such as :35-66 (residues 35 through 66) or a range of colors such as red-blue (shades of red, magenta, and blue). |
| **,** | name separator | separates names or ranges in an atom specifier *e.g.* #1@CA,CB,CG *or* :21-30,45 |
| ***** | whole wildcard match | matches whole atom or residue names. For example, #0:*****@CA selects the alpha carbon atoms of all residues. |
| **=** | partial wildcard match | matches partial atom or residue names. *e.g.* #0:*@C= matches all atoms whose names begin with C. |
| **?** | single character wildcard | used for atom and residue *names* only. For example :G**??** selects all three letter residue names beginning with ''G''. |
| **%** | every *nth* residue or atom | For example, :***%**5 selects every fifth residue in the sequence. |
| **z**> | zone specifier | **z**>*zone* and **zr**>*zone* select all residues within *zone* angstroms of the indicated atoms. **za**>*zone* selects all atoms (not residues) within *zone* angstroms. Using < instead of > results in the complementary set of atoms. |
| **b**> | temperature factor | **b**> *temp_factor* selects all atoms with temperature factors greater than *temp_factor*.<br>**b**< *temp_factor* selects all atoms with temperature factors less than *temp_factor*.<br>For example, **b**>20 **b**<25 selects all atoms with temperature factors greater than 20 and less than 25. |
| **e**> | electrostatic potential | **e**> *potential* selects all atoms with electrostatic potentials greater than *potential*.<br>**e**< *potential* selects all atoms with electrostatic potentials less than *potential*.<br>For example, **e**>10 **e**<20 selects all atoms with electrostatic potentials between 10 and 20 kcal/mole. |

## Appendix 2: PDB Atom Naming Conventions for Amino Acids

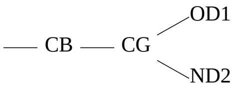
Alanine

— CB

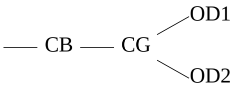
Arginine




Asparagine



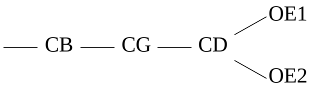

Aspartic acid



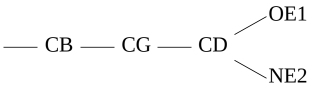

Cysteine

— CB — SG

Glutamic acid



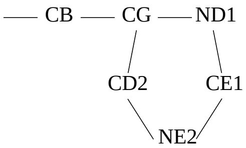

Glutamine



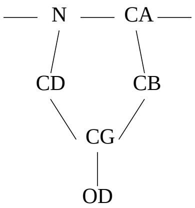

Glycine

— X

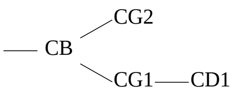
Histidine



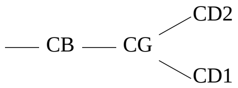

Hydroxyproline




Isoleucine




Leucine



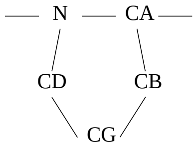

Lysine

— CB — CG — CD — CE — NZ

Methionine

— CB — CG — SD — CE

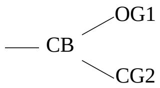
Proline



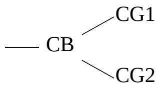

Serine

— CB — OG

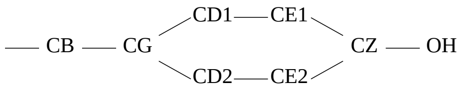
Threonine



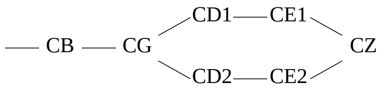

Valine



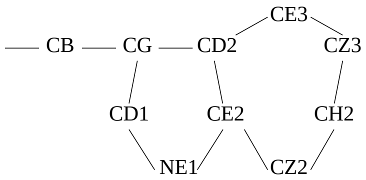

Tyrosine




Phenylalanine




Tryptophan



| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 3CLA | 1.75 | TYPE III CHLORAMPHENICOL ACETYLTRANSFERASE ($CAT_{III}$) ... | (ESCHERICHIA COLI), ... | A.G.W.LESLIE |
| 4CLA | 2.0 | TYPE III CHLORAMPHENICOL ACETYLTRANSFERASE ($CAT_{III}$) ... | (ESCHERICHIA COLI), ... | A.G.W.LESLIE |
| 2TS1 | 2.3 | TYROSYL-TRANSFER RNA SYNTHETASE (E.C.6.1.1.1) | (BACILLUS ...) | P.BRICK,T.N.BHAT,D.M.BLOW |
| 3TS1 | 2.7 | TYROSYL-TRANSFER RNA SYNTHETASE (E.C.6.1.1.1) COMPLEXED WITH ... | (BACILLUS ...) | C.MONTEILHET,P.BRICK *et al.* |
| 1UBQ | 1.8 | UBIQUITIN | HUMAN (HOMO SAPIENS) ... | S.VIJAY-KUMAR *et al.* |
| 2UTG | 1.64 | UTEROGLOBIN | UTERINE SECRETIONS ... | R.BALLY,J.DELETTRE |
| 1UTG | 1.34 | UTEROGLOBIN (OXIDIZED) | RABBIT (ORYCTOLAGUS ...) | I.MORIZE,E.SURCOUF *et al.* |
| 2SNM | 2.0 | VAL-66 TO LYS MUTANT OF STAPHYLOCOCCAL NUCLEASE (E.C.3.1.4.4) | (STAPHYLOCOCCUS ...) | W.E.STITES *et al.* |
| 1VSG | 2.9 | VARIANT SURFACE GLYCOPROTEIN (N-TERMINAL DOMAIN) | (TRYPANOSOMA BRUCEI) | D.FREYMANN,J.DOWN *et al.* |
| 7WGA | 2.0 | WHEAT GERM AGGLUTININ (ISOLECTIN 1) | WHEAT (TRITICUM ...) | C.S.WRIGHT |
| 1WGC | 2.2 | WHEAT GERM AGGLUTININ (ISOLECTIN 1) COMPLEX WITH ... | WHEAT (TRITICUM ...) | C.S.WRIGHT |
| 9WGA | 1.8 | WHEAT GERM AGGLUTININ (ISOLECTIN 2) | WHEAT (TRITICUM ...) | C.S.WRIGHT |
| 2WGC | 2.2 | WHEAT GERM AGGLUTININ (ISOLECTIN 2) COMPLEX WITH ... | WHEAT (TRITICUM ...) | C.S.WRIGHT |
| 1CCP | 2.2 | YEAST CYTOCHROME C PEROXIDASE (E.C.1.11.1.5) | YEAST (SACCHAROMYCES ...) | J.WANG,J.M.MAURO *et al.* |
| 2CCP | 2.2 | YEAST CYTOCHROME C PEROXIDASE (E.C.1.11.1.5) MUTANT WITH ASP ... | YEAST (SACCHAROMYCES ...) | J.WANG,J.M.MAURO *et al.* |
| 3CCP | 2.2 | YEAST CYTOCHROME C PEROXIDASE (E.C.1.11.1.5) MUTANT WITH TRP ... | YEAST (SACCHAROMYCES ...) | J.WANG,J.M.MAURO *et al.* |
| 4CCP | 2.2 | YEAST CYTOCHROME C PEROXIDASE (E.C.1.11.1.5) MUTANT WITH TRP ... | YEAST (SACCHAROMYCES ...) | J.WANG,J.M.MAURO *et al.* |
| 2YHX | 2.1 | YEAST HEXOKINASE B (E.C.2.7.1.1) COMPLEX WITH ... | BAKER'S YEAST ... | T.A.STEITZ *et al.* |
| 3ZNF | N/A | ZINC FINGER (NMR) | HUMAN (HOMO SAPIENS) ... | A.M.GRONENBORN *et al.* |
| 4ZNF | N/A | ZINC FINGER (NMR) | HUMAN (HOMO SAPIENS) ... | A.M.GRONENBORN *et al.* |
| 2ZNF | N/A | ZINC FINGERLIKE DOMAIN OF THE GAG PROTEIN P55 OF HIV (ZN(P55F1)) | SYNTHETIC ... | M.F.SUMMERS *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 3TMS | 2.1 | THYMIDYLATE SYNTHASE (E.C.2.1.1.45) | (ESCHERICHIA COLI) | K.M.PERRY,R.M.STROUD |
| 4TMS | 2.35 | THYMIDYLATE SYNTHASE (E.C.2.1.1.45) | (LACTOBACILLUS CASEI) | J.FINER-MOORE,R.STROUD |
| 2TSC | 1.97 | THYMIDYLATE SYNTHASE (E.C.2.1.1.45) COMPLEX WITH DUMP AND AN ... | (ESCHERICHIA COLI) | W.R.MONTFORT,R.M.STROUD |
| 2TBV | 2.90 | TOMATO BUSHY STUNT VIRUS | TOMATO BUSHY STUNT VIRUS | S.C.HARRISON |
| 1TON | 1.8 | TONIN (E.C. NUMBER NOT ASSIGNED) | RAT (RATTUS RATTUS) ... | M.FUJINAGA,M.N.G.JAMES |
| 1EST | 2.5 | TOSYL-ELASTASE (E.C.3.4.21.11) | PORCINE (SUS SCROFA) ... | L.SAWYER,D.M.SHOTTON *et al.* |
| 1TRA | 3.0 | TRANSFER RIBO-NUCLEIC ACID (YEAST, PHE), TRNA | YEAST (SACCHAROMYCES ...) | M.SUNDARALINGAM ET AL. |
| 2TRA | 3.0 | TRANSFER RIBO-NUCLEIC ACID (YEAST,ASP) TRNA (A FORM) | YEAST (SACCHAROMYCES ...) | E.WESTHOF,P.DUMAS,D.MORAS |
| 3TRA | 3.0 | TRANSFER RIBO-NUCLEIC ACID (YEAST,ASP) TRNA (B FORM) | YEAST (SACCHAROMYCES ...) | E.WESTHOF,P.DUMAS,D.MORAS |
| 4TNA | 2.5 | TRANSFER RIBO-NUCLEIC ACID (YEAST,PHE) TRNA | YEAST (SACCHAROMYCES ...) | A.JACK,J.E.LADNER,A.KLUG |
| 4TRA | 2.7 | TRANSFER RIBO-NUCLEIC ACID (YEAST,PHE),TRNA | YEAST (SACCHAROMYCES ...) | E.WESTHOF,P.DUMAS,D.MORAS |
| 6TNA | 2.7 | TRANSFER RIBO-NUCLEIC ACID (YEAST,PHE),TRNA | YEAST (SACCHAROMYCES ...) | J.L.SUSSMAN *et al.* |
| 1TGL | 1.9 | TRIACYLGLYCEROL ACYLHYDROLASE (E.C.3.1.1.3) | (RHIZOMUCOR MIEHEI) | L.BRADY *et al.* |
| 1TIM | 2.5 | TRIOSE PHOSPHATE ISOMERASE (E.C.5.3.1.1) | CHICKEN (GALLUS ...) | D.W.BANNER *et al.* |
| 1YPI | 1.9 | TRIOSE PHOSPHATE ISOMERASE (TIM) (E.C.5.3.1.1) | YEAST (SACCHAROMYCES ...) | T.ALBER,E.LOLIS *et al.* |
| 2YPI | 2.5 | TRIOSE PHOSPHATE ISOMERASE (TIM) (E.C.5.3.1.1) COMPLEX WITH ... | YEAST (SACCHAROMYCES ...) | E.LOLIS,G.A.PETSKO |
| 3TIM | 2.8 | TRIOSEPHOSPHATE ISOMERASE (E.C.5.3.1.1) | (TRYPANOSOMA BRUCEI ...) | R.K.WIERENGA |
| 6TIM | 2.2 | TRIOSEPHOSPHATE ISOMERASE (E.C.5.3.1.1) COMPLEX WITH ... | (TRYPANOSOMA BRUCEI ...) | M.E.M.NOBLE *et al.* |
| 2TIM | 1.83 | TRIOSEPHOSPHATE ISOMERASE (E.C.5.3.1.1) COMPLEX WITH SULPHATE | (TRYPANOSOMA BRUCEI ...) | R.K.WIERENGA |
| 5TIM | 1.83 | TRIOSEPHOSPHATE ISOMERASE (E.C.5.3.1.1) COMPLEX WITH SULPHATE | (TRYPANOSOMA BRUCEI ...) | R.K.WIERENGA,W.G.J.HOL |
| 4TIM | 2.4 | TRIOSEPHOSPHATE ISOMERASE (E.C.5.3.1.1) COMPLEXED WITH ... | (TRYPANOSOMA BRUCEI ...) | M.E.M.NOBEL *et al.* |
| 2TMA | 15.0 | TROPOMYOSIN | RABBIT (ORYCTOLAGUS ...) | G.N.PHILLIPS JUNIOR *et al.* |
| 1TNC | N/A | TROPONIN - CALCIUM-BINDING COMPONENT | RABBIT (ORYCTOLAGUS ...) | R.H.KRETSINGER,C.D.BARRY |
| 4TNC | 2.0 | TROPONIN C | CHICKEN (GALLUS ...) | M.SUNDARALINGAM |
| 5TNC | 2.0 | TROPONIN-C | TURKEY (MELEAGRIS ...) | O.HERZBERG,M.N.G.JAMES |
| 3WRP | 1.8 | TRP APOREPRESSOR | (ESCHERICHIA COLI) | R.-G.ZHANG,P.B.SIGLER |
| 2WRP | 1.65 | TRP REPRESSOR (ORTHORHOMBIC FORM) | (ESCHERICHIA COLI) | C.L.LAWSON,P.B.SIGLER |
| 1WRP | 2.2 | TRP REPRESSOR (TRIGONAL FORM) | (ESCHERICHIA COLI) | R.W.SCHEWITZ *et al.* |
| 1TAB | 2.3 | TRYPSIN (E.C.3.4.21.4) COMPLEX WITH BOWMAN-BIRK INHIBITOR (AB-I) | BOVINE (BOS TAURUS) ... | Y.TSUNOGAE,I.TANAKA *et al.* |
| 2PTN | 1.55 | TRYPSIN (ORTHORHOMBIC, 2.4 M AMMONIUM SULFATE) (E.C.3.4.21.4) | BOVINE (BOS TAURUS) ... | J.WALTER *et al.* |
| 1SGT | 1.7 | TRYPSIN (SGT) (E.C.3.4.21.4) | (STREPTOMYCES ...) | R.J.READ,M.N.G.JAMES |
| 3PTN | 1.7 | TRYPSIN (TRIGONAL, 2.4 M AMMONIUM SULFATE) (E.C.3.4.21.4) | BOVINE (BOS TAURUS) ... | J.WALTER *et al.* |
| 4PTI | 1.5 | TRYPSIN INHIBITOR | BOVINE (BOS TAURUS) ... | R.HUBER,D.KUKLA *et al.* |
| 2BTI | 2.2 | TRYPSIN INHIBITOR (BPTI) MUTANT (PHE 22 REPLACED BY ALA) (F22A) | BOVINE (BOS TAURUS) ... | D.HOUSSET,F.TAO *et al.* |
| 5PTI | 1.0 | TRYPSIN INHIBITOR (CRYSTAL FORM II) | BOVINE (BOS TAURUS) ... | A.WLODAWER,R.HUBER |
| 2CTI | N/A | TRYPSIN INHIBITOR (NMR, 5 SIMULATED ANNEALING STRUCTURES) | SQUASH (CUCURBITA ...) | T.A.HOLAK,D.GONDOL *et al.* |
| 3CTI | N/A | TRYPSIN INHIBITOR (NMR, 6 SIMULATED ANNEALING STRUCTURES) ... | SQUASH (CUCURBITA ...) | M.NILGES,J.HABAZETTL *et al.* |
| 1CTI | N/A | TRYPSIN INHIBITOR (NMR, MINIMIZED MEAN STRUCTURE) | SQUASH (CUCURBITA ...) | T.A.HOLAK,D.GONDOL *et al.* |
| 2ETI | N/A | TRYPSIN INHIBITOR II (EETI II) | (ECBALLIUM ELATERIUM) | A.HEITZ,L.CHICHE *et al.* |
| 1EFM | 2.7 | TRYPSIN-MODIFIED ELONGATION FACTOR TU (EF-TU-GDP) | (ESCHERICHIA COLI) | F.JURNAK |
| 1TGN | 1.65 | TRYPSINOGEN | BOVINE (BOS TAURUS) ... | A.A.KOSSIAKOFF,R.M.STROUD |
| 1TGC | 1.8 | TRYPSINOGEN (0.50 METHANOL, 0.50 WATER) | BOVINE (BOS TAURUS) ... | J.WALTER *et al.* |
| 2TGT | 1.7 | TRYPSINOGEN (103 DEGREES K, 0.70 METHANOL, 0.30 WATER) | BOVINE (BOS TAURUS) ... | J.WALTER *et al.* |
| 1TGT | 1.7 | TRYPSINOGEN (173 DEGREES K, 0.70 METHANOL, 0.30 WATER) | BOVINE (BOS TAURUS) ... | J.WALTER *et al.* |
| 2TGA | 1.8 | TRYPSINOGEN (2.4 M MAGNESIUM SULFATE) | BOVINE (BOS TAURUS) ... | J.WALTER *et al.* |
| 2TPI | 2.1 | TRYPSINOGEN - PANCREATIC TRYPSIN INHIBITOR - ILE-VAL COMPLEX ... | BOVINE (BOS TAURUS) ... | J.WALTER *et al.* |
| 2TGP | 1.9 | TRYPSINOGEN COMPLEX WITH PANCREATIC TRYPSIN INHIBITOR | BOVINE (BOS TAURUS) ... | R.HUBER,W.BODE *et al.* |
| 3TPI | 1.9 | TRYPSINOGEN COMPLEX WITH PANCREATIC TRYPSIN INHIBITOR AND ILE-VAL | BOVINE (BOS TAURUS) ... | R.HUBER,W.BODE *et al.* |
| 1TGS | 1.8 | TRYPSINOGEN COMPLEX WITH PORCINE PANCREATIC SECRETORY ... | BOVINE (BOS TAURUS) ... | M.BOLOGNESI,G.GATTI *et al.* |
| 4TPI | 2.2 | TRYPSINOGEN COMPLEX WITH THE $ARG^{15}$-ANALOGUE OF PANCREATIC ... | BOVINE (BOS TAURUS) ... | W.BODE,J.WALTER |
| 2TGD | 2.1 | TRYPSINOGEN, DIISOPROPYLPHOSPHORYL INHIBITED | BOVINE (BOS TAURUS) ... | M.O.JONES,R.M.STROUD |
| 1TGB | 1.8 | TRYPSINOGEN-CA FROM PEG | BOVINE (BOS TAURUS) ... | W.BODE,H.FEHLHAMMER *et al.* |
| 1WSY | 2.5 | TRYPTOPHAN SYNTHASE (E.C.4.2.1.20) | (SALMONELLA ...) | C.HYDE,S.AHMED *et al.* |
| 1TNF | 2.6 | TUMOR NECROSIS FACTOR-ALPHA (CACHECTIN) | HUMAN (HOMO SAPIENS) ... | M.J.ECK,S.R.SPRANG |
| 1CLA | 2.34 | TYPE III CHLORAMPHENICOL ACETYLTRANSFERASE ($CAT_{III}$) ... | (ESCHERICHIA COLI), ... | M.R.GIBBS,A.G.W.LESLIE |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 2ST1 | 1.8 | SUBTILISIN BPN’ (BAS) (E.C.3.4.21.14) | RECOMBINANT ... | R.BOTT |
| 1ST2 | 2.0 | SUBTILISIN BPN’ (BASOX) - PEROXIDE INACTIVATED (E.C.3.4.21.14) | RECOMBINANT ... | R.BOTT |
| 1SIC | 2.0 | SUBTILISIN BPN(PRIME) (E.C.3.4.21.14) COMPLEX WITH ... | PROBABLY (BACILLUS ...) | Y.MITSUI,S.HIRONO *et al.* |
| 1S01 | 1.7 | SUBTILISIN BPN(PRIME) 8350 (E.C.3.4.21.14) (MUTANT WITH MET ...) | (BACILLUS ...) | M.WHITLOW,A.J.HOWARD *et al.* |
| 1CSE | 1.2 | SUBTILISIN CARLSBERG (E.C.3.4.21.14) (COMMERCIAL PRODUCT ...) | (BACILLUS SUBTILIS) ... | W.BODE |
| 2SEC | 1.8 | SUBTILISIN CARLSBERG (E.C.3.4.21.14) COMPLEX WITH ... | (BACILLUS SUBTILIS) ... | C.A.MCPHALEN,M.N.G.JAMES |
| 1SBC | 2.5 | SUBTILISIN CARLSBERG (SUBTILOPEPTIDASE A) (E.C.3.4.21.14) | (BACILLUS SUBTILIS) | D.J.NEIDHART,G.A.PETSKO |
| 1SBN | 2.1 | SUBTILISIN NOVO (BPN’)(E.C.3.4.21.14) COMPLEXED WITH L45R ... | SUBTILISIN FROM ... | M.G.GRUETTER *et al.* |
| 2SBT | 2.8 | SUBTILISIN NOVO (E.C.3.4.21.14) | PROBABLY BACILLUS ... | J.DRENTH,W.G.J.HOL *et al.* |
| 2SNI | 2.1 | SUBTILISIN NOVO (E.C.3.4.21.14) COMPLEX WITH CHYMOTRYPSIN ... | (BACILLUS ...) | C.A.MCPHALEN,M.N.G.JAMES |
| 3SIC | 1.8 | SUBTILISINBPN’(PRIME)(E.C.3.4.21.14) COMPLEXED WITH A ... | SUBTILISIN FROM ... | Y.MITSUI,Y.TAKEUCHI *et al.* |
| 1S02 | 1.9 | SUBTILISN BPN’ (E.C.3.4.21.14) (MUTANT WITH GLN 19 REPLACED ...) | (BACILLUS ...) | C.R.ERWIN *et al.* |
| 1COB | 2.0 | SUPEROXIDE DISMUTASE (CO SUBSTITUTED) | BOVINE (BOS TAURUS) ... | K.DJINOVIC,A.CODA *et al.* |
| 1L03 | 1.7 | $S^{GAMMA157}$-BETA-MERCAPTOETHANOL-LYSOZYME (E.C.3.2.1.17) ... | BACTERIOPHAGE T4 ... | S.DAO-PIN,K.WILSON *et al.* |
| 1L26 | 1.7 | $S^{GAMMA86}$-BETA-MERCAPTOETHANOL-LYSOZYME (E.C.3.2.1.17) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L11 | 1.7 | $S^{GAMMA97}$-BETA-MERCAPTOETHANOL-LYSOZYME (E.C.3.2.1.17) ... | BACTERIOPHAGE T4 ... | S.DAO-PIN,K.WILSON *et al.* |
| 1L83 | 1.7 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L84 | 1.9 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L85 | 2.00 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L86 | 1.80 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L87 | 1.80 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L88 | 1.85 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L89 | 1.90 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L90 | 1.75 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L91 | 1.80 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L92 | 1.70 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L94 | 1.80 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1L95 | 2.00 | T4 LYSOZYME MUTANT WHERE CYSTEINE 54 IS REPLACED BY ... | BACTERIOPHAGE T4 ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 1LYD | 2.0 | T4-LYSOZYME | SYNTHETIC CODING DNA ... | D.R.ROSE |
| 2TAA | 3.0 | TAKA-AMYLASE A (E.C.3.2.1.1) | (ASPERGILLUS ORYZAE) | M.KUSUNOKI *et al.* |
| 2AIT | N/A | TENDAMISTAT | (STREPTOMYCES TENDAE) | A.D.KLINE,W.BRAUN *et al.* |
| 3AIT | N/A | TENDAMISTAT (ENERGY MINIMIZED MODEL USING "AMBER" 3.0) (NMR) | (STREPTOMYCES TENDAE) | M.BILLETER *et al.* |
| 4AIT | N/A | TENDAMISTAT (ENERGY MINIMIZED MODEL USING "FANTOM") (NMR) | (STREPTOMYCES TENDAE) | M.BILLETER *et al.* |
| 1THI | 3.2 | THAUMATIN I | KETEMFE ... | S.-H.KIM |
| 1TEC | 2.2 | THERMITASE (E.C.3.4.21.14) COMPLEX WITH EGLIN-C | (THERMOACTINOMYCES ...) | P.GROS,B.W.DIJKSTRA *et al.* |
| 3TEC | 2.0 | THERMITASE (E.C.3.4.21.14) COMPLEX WITH EGLIN-C (100 ...) | (THERMOACTINOMYCES ...) | P.GROS,K.H.KALK,W.G.J.HOL |
| 2TEC | 1.98 | THERMITASE (E.C.3.4.21.14) COMPLEX WITH EGLIN-C (5 ...) | (THERMOACTINOMYCES ...) | P.GROS,C.BETZEL *et al.* |
| 3TLN | 1.6 | THERMOLYSIN (E.C.3.4.24.4) | (BACILLUS ...) | B.W.MATTHEWS,M.A.HOLMES |
| 1TMN | 1.9 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH ... | (BACILLUS ...) | A.F.MONZINGO,B.W.MATTHEWS |
| 2TMN | 1.6 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH ... | (BACILLUS ...) | D.E.TRONRUD *et al.* |
| 5TLN | 2.3 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH ... | (BACILLUS ...) | B.W.MATTHEWS,M.A.HOLMES |
| 6TMN | 1.6 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH ... | (BACILLUS ...) | D.E.TRONRUD *et al.* |
| 5TMN | 1.6 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH CBZ-$GLY^{P}$-LEU-LEU ... | (BACILLUS ...) | H.M.HOLDEN *et al.* |
| 4TMN | 1.7 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH CBZ-$PHE^{P}$-LEU-ALA ... | (BACILLUS ...) | H.M.HOLDEN *et al.* |
| 7TLN | 2.3 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH CH2CO(N-OH)LEU-OCH3 | (BACILLUS ...) | B.W.MATTHEWS *et al.* |
| 7TMN | N/A | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH GLY-TPH-LEU-LEU ... | (BACILLUS ...) | H.M.HOLDEN *et al.* |
| 4TLN | 2.3 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH L-LEUCYL-HYDROXYLAMINE | (BACILLUS ...) | B.W.MATTHEWS,M.A.HOLMES |
| 1TLP | 2.3 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH PHOSPHORAMIDON | (BACILLUS ...) | D.E.TRONRUD *et al.* |
| 3TMN | 1.7 | THERMOLYSIN (E.C.3.4.24.4) COMPLEX WITH VAL-TRP (VW) | (BACILLUS ...) | H.M.HOLDEN,B.W.MATTHEWS |
| 2TRX | 1.68 | THIOREDOXIN (E.C.1.6.4.5) | (ESCHERICHIA COLI) | S.K.KATTI *et al.* |
| 1SRX | 2.8 | THIOREDOXIN (E.C.1.6.4.5) (OXIDIZED FORM) | (ESCHERICHIA COLI B) | B.-O.SODERBERG |
| 1TRX | N/A | THIOREDOXIN (E.C.1.6.4.5) (REDUCED FORM) | (ESCHERICHIA COLI) | H.J.DYSON *et al.* |
| 3TRX | N/A | THIOREDOXIN (E.C.1.6.4.5) (REDUCED FORM) | HUMAN (HOMO SAPIENS) ... | J.D.FORMAN-KAY *et al.* |
| 4TRX | N/A | THIOREDOXIN (E.C.1.6.4.5) (REDUCED FORM) | HUMAN (HOMO SAPIENS) ... | J.D.FORMAN-KAY *et al.* |
| 1TPT | 2.8 | THYMIDINE PHOSPHORYLASE (E.C.2.4.2.4) | (ESCHERICHIA COLI) ... | M.R.WALTER,W.J.COOK *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 2RM2 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN II(SR) | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 2RS3 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN III(S) | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 2R04 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN IV | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 1R09 | 2.9 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN R61837 | HUMAN (HOMO SAPIENS) ... | M.S.CHAPMAN,I.MINOR *et al.* |
| 2RS5 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN V(S) | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 2R06 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN VI | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 2R07 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN VII | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 1R08 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN VIII | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 1R1A | 3.2 | RHINOVIRUS SEROTYPE 1 (HRV1) COAT PROTEIN | HUMAN (HOMO SAPIENS) ... | S.KIM,M.G.ROSSMANN |
| 1RHD | 2.5 | RHODANESE (E.C.2.8.1.1) | BOVINE (BOS TAURUS) LIVER | W.G.J.HOL *et al.* |
| 3RN3 | 1.45 | RIBONUCLEASE A (E.C.3.1.27.5) | BOVINE (BOS TAURUS) ... | B.HOWLIN,D.S.MOSS *et al.* |
| 5RSA | 2.0 | RIBONUCLEASE A (E.C.3.1.27.5) (JOINT NEUTRON AND X-RAY) | BOVINE (BOS TAURUS) ... | A.WLODAWER |
| 6RSA | 2.0 | RIBONUCLEASE A (E.C.3.1.27.5) COMPLEX WITH URIDINE VANADATE ... | BOVINE (BOS TAURUS) ... | A.WLODAWER |
| 7RSA | 1.26 | RIBONUCLEASE A (PHOSPHATE-FREE) (E.C.3.1.27.5) | BOVINE (BOS TAURUS) ... | A.WLODAWER,G.L.GILLILAND |
| 8RSA | 1.8 | RIBONUCLEASE A (PHOSPHATE-FREE) (E.C.3.1.27.5) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | J.NACHMAN,A.WLODAWER |
| 9RSA | 1.8 | RIBONUCLEASE A (PHOSPHATE-FREE) (E.C.3.1.27.5) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | J.NACHMAN,A.WLODAWER |
| 1RBB | 2.5 | RIBONUCLEASE B(E.C.3.1.4.22) | BOVINE (BOS TAURUS) ... | R.L.WILLIAMS *et al.* |
| 1HRH | 2.4 | RIBONUCLEASE H DOMAIN OF HIV-1 REVERSE TRANSCRIPTASE | HUMAN ... | J.F.DAVIES II *et al.* |
| 1SAR | 1.8 | RIBONUCLEASE SA (E.C.3.1.4.8) | (STREPTOMYCES ...) | J.SEVCIK,E.J.DODSON *et al.* |
| 2SAR | 1.8 | RIBONUCLEASE SA (E.C.3.1.4.8) COMPLEX WITH 3'-GUANYLIC ACID | (STREPTOMYCES ...) | J.SEVCIK,E.J.DODSON *et al.* |
| 1RNT | 1.9 | RIBONUCLEASE $T_1$(E.C.3.1.27.3) ISOZYME-2(PRIME)-GUANYLIC ... | (ASPERGILLUS ORYZAE) | W.SAENGER,R.ARNI *et al.* |
| 4RNT | 2.2 | RIBONUCLEASE T1 (E.C.3.1.27.3) (H92A) (MUTANT WITH HIS 92 ...) | (ASPERGILLUS ORYZAE) ... | W.SAENGER,G.KOELLNER |
| 1RNS | 2.0 | RIBONUCLEASE-S (E.C.3.1.4.22) | BOVINE (BOS TAURUS) ... | F.M.RICHARDS,H.W.WYCKOFF |
| 6RNT | 1.8 | RIBONUCLEASE-$T_1$ (E.C.3.1.27.3) COMPLEX WITH 2'-ADENYLIC ACID | (ESCHERICHIA COLI) | G.KOELLNER *et al.* |
| 8RNT | 1.8 | RIBONUCLEASE-$T_1$ (E.C.3.1.27.3) COMPLEX WITH ZN($^{2+}$) | (ESCHERICHIA COLI) | J.DING,H.-W.CHOE *et al.* |
| 7RNT | 1.9 | RIBONUCLEASE-$T_1$ (E.C.3.1.27.3) MUTANT WITH TYR45 REPLACED ... | (ESCHERICHIA COLI) | G.KOELLNER *et al.* |
| 5RNT | 3.2 | RIBONUCLEASE-T1 (E.C.3.1.27.3) COMPLEX WITH ... | (ASPERGILLUS ORYZAE) | W.SAENGER *et al.* |
| 1RNA | 2.25 | RNA DUPLEX (U(U-A)$_6$A)2 | SYNTHETIC RNA | A.C.DOCK-BREGEON *et al.* |
| 1ROP | 1.7 | ROP: COLE1 REPRESSOR OF PRIMER | (ESCERICHIA COLI) K14 | M.KOKKINIDIS *et al.* |
| 2RSP | 2.0 | ROUS SARCOMA VIRUS PROTEASE (RSV PR) | ROUS SARCOMA VIRUS ... | A.WLODAWER,M.MILLER *et al.* |
| 1RUS | 2.9 | RUBISCO (RIBULOSE-1,5-BISPHOSPHATE ...) | (RHODOSPIRILLUM ...) | T.LUNDQVIST,G.SCHNEIDER |
| 2RUS | 2.3 | RUBISCO (RIBULOSE-1,5-BISPHOSPHATE ...) | (RHODOSPIRILLUM ...) | T.LUNDQVIST,G.SCHNEIDER |
| 5RUB | 1.7 | RUBISCO (RIBULOSE-1,5-BISPHOSPHATE ...) | (RHODOSPIRILLUM ...) | G.SCHNEIDER *et al.* |
| 1RDG | 1.4 | RUBREDOXIN | (DESULFOVIBRIO GIGAS) | M.FREY,L.C.SIEKER,F.PAYAN |
| 6RXN | 1.5 | RUBREDOXIN | (DESULFOVIBRIO ...) | R.E.STENKAMP *et al.* |
| 7RXN | 1.5 | RUBREDOXIN | (DESULFOVIBRIO VULGARIS) | E.T.ADMAN,L.C.SIEKER *et al.* |
| 8RXN | 1.0 | RUBREDOXIN | (DESULFORIBRIS VULGARIS) | Z.DAUTER,L.SIEKER *et al.* |
| 5RXN | 1.20 | RUBREDOXIN (OXIDIZED, FE(III)) (CONSTRAINED MODEL) | (CLOSTRIDIUM ...) | K.D.WATENPAUGH |
| 4RXN | 1.20 | RUBREDOXIN (OXIDIZED, FE(III)) (UNCONSTRAINED MODEL) | (CLOSTRIDIUM ...) | K.D.WATENPAUGH *et al.* |
| 2SCP | 2.0 | SARCOPLASMIC CALCIUM BINDING PROTEIN | SANDWORM (NEREIS ...) | W.J.COOK,S.VIJAY-KUMAR |
| 1SCP | 3.0 | SARCOPLASMIC CALCIUM-BINDING PROTEIN | SANDWORM (NEREIS ...) | W.J.COOK,S.E.EALICK *et al.* |
| 2STV | 2.50 | SATELLITE TOBACCO NECROSIS VIRUS | COAT PROTEIN OF ... | T.A.JONES,L.LILJAS |
| 1SN3 | 1.8 | SCORPION NEUROTOXIN (VARIANT 3) | SCORPION ... | R.J.ALMASSY *et al.* |
| 1RNH | 2.0 | SELENOMETHIONYL RIBONUCLEASE H (E.C.3.1.26.4) | (ESCHERICHIA COLI) ... | W.YANG *et al.* |
| 1SRN | 1.8 | SEMISYNTHETIC RIBONUCLEASE A (RNASE 1-118(COLON)111-124) ... | BOVINE (BOS TAURUS) ... | P.D.MARTIN *et al.* |
| 2SC2 | 2.2 | SERINE CARBOXYPEPTIDASE II (E.C.3.4.6.1) (CPDW-II) | WHEAT (TRITICUM ...) | D.-I.LIAO,S.J.REMINGTON |
| 4SGB | 2.1 | SERINE PROTEINASE B COMPLEX WITH THE POTATO INHIBITOR PCI-1 | (STREPTOMYCES ...) | M.JAMES,H.GREENBLATT |
| 1SNV | 3.0 | SINDBIS VIRUS CAPSID PROTEIN | SINDBIS VIRUS | L.TONG,M.ROSSMANN |
| 1SDG | N/A | SORBITOL DEHYDROGENASE (E.C.1.1.1.14) (MODEL) | SHEEP (OVIS ARIES) LIVER | H.EKLUND,E.HORJALES *et al.* |
| 4SBV | 2.8 | SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN | SOUTHERN BEAN MOSAIC ... | M.G.ROSSMANN |
| 1SNC | 1.65 | STAPHYLOCOCCAL NUCLEASE (E.C.3.1.31.1) COMPLEX WITH A ... | (STAPHYLOCOCCUS ...) | P.J.LOLL,E.E.LATTMAN |
| 1SNM | 1.74 | STAPHYLOCOCCAL NUCLEASE (E.C.3.1.31.1) MUTANT (GLU 43 ...) | (STAPHYLOCOCCUS ...) | P.J.LOLL,E.E.LATTMAN |
| 2SNS | 1.5 | STAPHYLOCOCCAL NUCLEASE (E.C.3.1.4.7) COMPLEX WITH ... | (STAPHYLOCOCCUS ...) | M.J.LEGG,F.A.COTTON *et al.* |
| 2SSI | 2.6 | STREPTOMYCES SUBTILISIN INHIBITOR | (STREPTOMYCES ...) | Y.MITSUI,Y.SATOW *et al.* |
| 1SBT | 2.5 | SUBTILISIN BPN (E.C.3.4.21.14) | PROBABLY BACILLUS ... | R.A.ALDEN *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 3PGM | 2.8 | PHOSPHOGLYCERATE MUTASE (E.C.2.7.5.3) DE-PHOSPHO ENZYME | DRIED BAKER,S YEAST ... | J.W.CAMPBELL *et al.* |
| 3BP2 | 2.1 | PHOSPHOLIPASE $A_2$ (E.C.3.1.1.4) (PHOSPHATIDE ...) | BOVINE (BOS TAURUS ...) | B.W.DIJKSTRA,J.DRENTH |
| 1BP2 | 1.7 | PHOSPHOLIPASE $A_2$ (E.C.3.1.1.4) (PHOSPHATIDE ACYL-HYDROLASE) | BOVINE (BOS TAURUS ...) | B.W.DIJKSTRA *et al.* |
| 1P2P | 2.6 | PHOSPHOLIPASE $A_2$ (E.C.3.1.1.4) (PHOSPHATIDE ACYL-HYDROLASE) | PORCINE (SUS SCROFA) ... | B.W.DIJKSTRA *et al.* |
| 4P2P | 2.4 | PHOSPHOLIPASE $A_2$ (PHOSPHATIDE-2-ACYL HYDROLASE) (E.C.3.1.1.4) | PORCINE (SUS SCROFA) ... | *et al.* |
| 3P2P | 2.1 | PHOSPHOLIPASE $A_2$ (PHOSPHATIDE-2-ACYL-HYDROLASE) MUTANT ... | PORCINE (SUS SCROFA) ... | B.W.DIJKSTRA *et al.* |
| 5P2P | 2.4 | PHOSPHOLIPASE $A_2$ (PHOSPHATIDE-2-ACYL-HYDROLASE) MUTANT ... | PORCINE (SUS SCROFA) ... | B.W.DIJKSTRA *et al.* |
| 4ICD | 2.5 | PHOSPHORYLATED ISOCITRATE DEHYDROGENASE (E.C.1.1.1.42) | (ESCHERICHIA COLI) | J.H.HURLEY,A.M.DEAN *et al.* |
| 1PHY | 2.4 | PHOTOACTIVE YELLOW PROTEIN | (ECTOTHIORHODOSPIRA ...) | D.E.MCREE,J.A.TAINER *et al.* |
| 5GCH | 2.7 | PHOTOLYSIS PRODUCT OF P-DIETHYLAMINO-O-HYDROXY-ALPHA-METHYL ... | BOVINE (BOS TAURUS) ... | B.L.STODDARD,D.RINGE *et al.* |
| 1PRC | 2.3 | PHOTOSYNTHETIC REACTION CENTER | (RHODOPSEUDOMONAS ...) | J.DEISENHOFER,O.EPP *et al.* |
| 7PCY | 1.8 | PLASTOCYANIN | GREEN ALGA ... | C.A.COLLYER,J.M.GUSS *et al.* |
| 4PCY | 2.15 | PLASTOCYANIN (CROSS-LINKED WITH GLUTERALDEHYDE, CU1+, PH 7.8) | POPLAR (POPULUS ...) | J.M.GUSS,H.C.FREEMAN |
| 6PCY | 1.90 | PLASTOCYANIN (CU1+,PH 3.8) | POPLAR (POPULUS ...) | J.M.GUSS,H.C.FREEMAN |
| 5PCY | 1.80 | PLASTOCYANIN (CU1+,PH 7.0) | POPLAR (POPULUS ...) | J.M.GUSS,H.C.FREEMAN |
| 1PCY | 1.6 | PLASTOCYANIN (CU2+, PH 6.0) | POPLAR (POPULUS ...) | J.M.GUSS,H.C.FREEMAN |
| 3PCY | 1.9 | PLASTOCYANIN ($HG^{2+}$ SUBSTITUTED) | POPLAR (POPULUS ...) | W.B.CHURCH,J.M.GUSS *et al.* |
| 2PLV | 2.88 | POLIOVIRUS (TYPE 1, MAHONEY STRAIN) | HUMAN (HOMO SAPIENS) ... | D.J.FILMAN,J.M.HOGLE |
| 4EST | 1.78 | PORCINE PANCREATIC ELASTASE (E.C.3.4.21.11) COMPLEX WITH ... | PORCINE (SUS SCROFA) ... | L.H.TAKAHASHI *et al.* |
| 5EST | 2.09 | PORCINE PANCREATIC ELASTASE (E.C.3.4.21.11) COMPLEX WITH ... | PORCINE (SUS SCROFA) ... | L.H.TAKAHASHI *et al.* |
| 2PAB | 1.8 | PREALBUMIN (HUMAN PLASMA) | HUMAN (HOMO SAPIENS) | S.J.OATLEY,C.C.F.BLAKE |
| 2BP2 | 3.0 | PROPHOSPHOLIPASE $A_2$ | BOVINE (BOS TAURUS ...) | B.W.DIJKSTRA *et al.* |
| 4BP2 | 1.6 | PROPHOSPHOLIPASE $A_2$ (PHOSPHATIDE-2-ACYL HYDROLASE) ... | BOVINE (BOS TAURUS) ... | *et al.* |
| 1AAP | 1.5 | PROTEASE INHIBITOR DOMAIN OF ALZHEIMER'S AMYLOID ... | HUMAN (HOMO SAPIENS) ... | T.R.HYNES,M.RANDAL *et al.* |
| 1GB1 | N/A | PROTEIN G (B1 DOMAIN) (60 MODELS) | GROUP G ... | A.M.GRONENBORN,G.M.CLORE |
| 2GB1 | N/A | PROTEIN G (B1 DOMAIN) (RESTRAINED MINIMIZED AVERAGED STRUCTURE) | GROUP G ... | A.M.GRONENBORN,G.M.CLORE |
| 2SGA | 1.5 | PROTEINASE A (COMPONENT OF THE EXTRACELLULAR FILTRATE ...) | (STREPTOMYCES ...) | M.N.G.JAMES,A.R.SIELECKI |
| 3SGA | 1.8 | PROTEINASE A (COMPONENT OF THE EXTRACELLULAR FILTRATE ...) | (STREPTOMYCES ...) | A.R.SIELECKI,M.N.G.JAMES |
| 4SGA | 1.8 | PROTEINASE A (COMPONENT OF THE EXTRACELLULAR FILTRATE ...) | (STREPTOMYCES ...) | A.R.SIELECKI,M.N.G.JAMES |
| 5SGA | 1.8 | PROTEINASE A (COMPONENT OF THE EXTRACELLULAR FILTRATE ...) | (STREPTOMYCES ...) | A.R.SIELECKI,M.N.G.JAMES |
| 1SGC | 1.8 | PROTEINASE A COMPLEX WITH CHYMOSTATIN | (STREPTOMYCES ...) | L.T.J.DELBAERE,G.D.BRAYER |
| 3SGB | 1.8 | PROTEINASE B FROM STREPTOMYCES GRISEUS (SGPB) (E.C. NUMBER ...) | (STREPTOMYCES ...) | R.J.READ,M.FUJINAGA *et al.* |
| 1BUS | N/A | PROTEINASE INHIBITOR IIA (BUSI IIA) (NMR, 5 DISTANCE ...) | BOVINE (BOS TAURUS) ... | P.GUNTERT *et al.* |
| 2BUS | N/A | PROTEINASE INHIBITOR IIA (BUSI IIA) (NMR, ENERGY MIMIMIZED ...) | BULL (BOS TAURUS) ... | P.GUNTERT *et al.* |
| 2PRK | 1.5 | PROTEINASE K (E.C.3.4.21.14) | FUNGUS (TRITIRACHIUM ...) | C.BETZEL,G.P.PAL *et al.* |
| 1PCD | 2.8 | PROTOCATECHUATE 3,4-DIOXYGENASE (E.C.1.13.11.3) | (PSEUDOMONAS ...) | *et al.* |
| 2PAZ | 2.0 | PSEUDOAZURIN (CUPREDOXIN) | (ALCALIGENES ...) | E.T.ADMAN,K.PETRATOS |
| 1PAZ | 1.55 | PSEUDOAZURIN (OXIDIZED CU ++ AT PH 6.8) | (ALCALIGENES ...) | K.PETRATOS,Z.DAUTER *et al.* |
| 2PNP | 3.2 | PURINE NUCLEOSIDE PHOSPHORYLASE (E.C.2.4.2.1) | HUMAN (HOMO SAPIENS) ... | S.E.EALICK,S.A.RULE *et al.* |
| 1PYK | 2.6 | PYRUVATE KINASE (E.C.2.7.1.40) | CAT MUSCLE (FELIS ...) | H.MUIRHEAD,M.LEVINE *et al.* |
| 1F19 | 2.8 | R19.9 (IGG2$B_K$, $CRI^-_A$) FAB FRAGMENT | MOUSE (MUS MUSCULUS) ... | M.B.LASCOMBE *et al.* |
| 3RP2 | 1.9 | RAT MAST CELL PROTEASE II (RMCPII) | RAT (RATTUS RATTUS) ... | R.REYNOLDS *et al.* |
| 2REB | 2.3 | RECA PROTEIN | (ESCHERICHIA COLI) | R.M.STORY,T.A.STEITZ |
| 1REA | 2.7 | RECA PROTEIN-ADENOSINE DIPHOSPHATE COMPLEX (RECA-ADP) | (ESCHERICHIA COLI) | R.M.STORY,T.A.STEITZ |
| 1RLX | N/A | RELAXIN | PIG (SUS SCROFA) OVARY | N.W.ISAACS,G.DODSON *et al.* |
| 2RLX | N/A | RELAXIN | PIG (SUS SCROFA) OVARY | N.W.ISAACS,G.DODSON *et al.* |
| 3RLX | N/A | RELAXIN | PIG (SUS SCROFA) OVARY | N.W.ISAACS,G.DODSON *et al.* |
| 4RLX | N/A | RELAXIN | PIG (SUS SCROFA) OVARY | N.W.ISAACS,G.DODSON *et al.* |
| 1RBP | 2.0 | RETINOL BINDING PROTEIN | HUMAN (HOMO SAPIENS) ... | T.A.JONES *et al.* |
| 4RHV | 3.0 | RHINOVIRUS 14 (HRV14) | HUMAN (HOMO SAPIENS) ... | E.ARNOLD,M.G.ROSSMANN |
| 1RMU | 3.0 | RHINOVIRUS 14 (HRV14) (MUTANT WITH CYS 1 199 REPLACED BY ...) | HUMAN (HOMO SAPIENS) ... | J.BADGER *et al.* |
| 2RMU | 3.0 | RHINOVIRUS 14 (HRV14) (MUTANT WITH VAL 1 188 REPLACED BY ...) | HUMAN (HOMO SAPIENS) ... | J.BADGER *et al.* |
| 2RR1 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN I(R) | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |
| 2RS1 | 3.0 | RHINOVIRUS 14 (HRV14) COMPLEX WITH ANTIVIRAL AGENT WIN I(S) | HUMAN (HOMO SAPIENS) ... | J.BADGER,T.J.SMITH *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 3MBA | 2.0 | MYOGLOBIN (FLUORIDE COMPLEX) (PH 7.0) | SEA HARE (APLYSIA ...) | M.BOLOGNESI,S.ONESTI *et al.* |
| 4MBA | 2.0 | MYOGLOBIN (IMIDAZOLE COMPLEX) (PH 7.0) | SEA HARE (APLYSIA ...) | M.BOLOGNESI,S.ONESTI *et al.* |
| 2MM1 | 2.8 | MYOGLOBIN (K45R,C110A MUTANT) | HUMAN (HOMO SAPIENS) ... | S.R.HUBBARD *et al.* |
| 1MBS | 2.5 | MYOGLOBIN (MET) | COMMON SEAL (PHOCA ...) | H.SCOULOUDI |
| 4MBN | 2.0 | MYOGLOBIN (MET) | SPERM WHALE ... | T.TAKANO |
| 1MBW | 1.9 | MYOGLOBIN (MET) (MUTANT WITH INITIATOR MET AND WITH ASP 122 ...) | SYNTHETIC GENE FOR ... | G.N.PHILLIPS JUNIOR |
| 1MBA | 1.6 | MYOGLOBIN (MET) (PH 7.0) | SEA HARE (APLYSIA ...) | M.BOLOGNESI,S.ONESTI *et al.* |
| 5MBA | 1.9 | MYOGLOBIN (MET) AZIDE COMPLEX | SEA HARE (APLYSIA ...) | M.BOLOGNESI,S.ONESTI *et al.* |
| 1MBO | 1.6 | MYOGLOBIN (OXY, PH 8.4) | SPERM WHALE ... | S.E.V.PHILLIPS |
| 2MHR | 1.71.3 | MYOHEMERYTHRIN | SIPUNCULAN WORM ... | S.SHERIFF,W.A.HENDRICKSON |
| 2TPR | 2.4 | NAD(P)H:OXIDIZED-TRYPANOTHIONE OXIDOREDUCTASE (E.C.1.6.4.-) ... | (CRITHIDIA FASCICULATA) | J.KURIYAN,X.-P.KONG *et al.* |
| 3EST | 1.65 | NATIVE ELASTASE (E.C.3.4.21.11) | PORCINE (SUS SCROFA) ... | E.F.MEYER,G.COLE *et al.* |
| 1NSB | 2.2 | NEURAMINIDASE SIALIDASE (E.C.3.2.1.18) | INFLUENZA VIRUS - ... | W.P.BURMEISTER *et al.* |
| 1NXB | 1.38 | NEUROTOXIN B (PROBABLY IDENTICAL TO ERABUTOXIN B) | SEA SNAKE (LATICAUDA ...) | D.TSERNOGLOU,G.A.PETSKO |
| 2SH1 | N/A | NEUROTOXIN I (SH I) | SEA ANEMONE ... | R.H.FOGH,R.S.NORTON |
| 1SH1 | N/A | NEUROTOXIN I (SH I) (ENERGY MINIMIZED AVERAGE STRUCTURE) | SEA ANEMONE ... | R.H.FOGH,R.S.NORTON |
| 1NRD | 2.3 | NITRITE REDUCTASE (E.C.1.7.99.3) | (ACHROMOBACTER ...) | J.W.GODDEN,E.T.ADMAN *et al.* |
| 2CLN | N/A | $N^{Z115}$ TRIMETHYLCALMODULIN COMPLEX WITH TRIFLUOPERAZINE (MODEL) | BOVINE (BOS TAURUS) BRAIN | N.C.J.STRYNADKA *et al.* |
| 1OMD | 1.85 | ONCOMODULIN | RAT (RATTUS ...) | F.R.AHMED *et al.* |
| 1OVA | 1.95 | OVALBUMIN (EGG ALBUMIN) | HEN (GALLUS DOMESTICUS) | P.E.STEIN,A.G.W.LESLIE |
| 1OVO | 1.9 | OVOMUCOID THIRD DOMAIN | JAPANESE QUAIL ... | E.WEBER,E.PAPAMOKOS *et al.* |
| 2OVO | 1.5 | OVOMUCOID THIRD DOMAIN | SILVER PHEASANT ... | W.BODE,O.EPP |
| 1EGO | N/A | OXIDIZED GLUTAREDOXIN | (ESCHERICHIA COLI) ... | T.-H.XIA *et al.* |
| 1HIP | 2.0 | OXIDIZED HIGH POTENTIAL IRON PROTEIN (HIPIP). | (CHROMATIUM ...) | C.W.CARTER JUNIOR *et al.* |
| 2PHH | 2.7 | P-HYDROXYBENZOATE HYDROXYLASE (PHBH) (E.C.1.14.13.2) - ... | (PSEUDOMONAS FLUORESCENS) | J.M.VAN DER LAAN *et al.* |
| 1PHH | 2.3 | P-HYDROXYBENZOATE HYDROXYLASE (PHBH) (E.C.1.14.13.2) - FAD - ... | (PSEUDOMONAS FLUORESCENS) | H.A.SCHREUDER,J.DRENTH |
| 1PAD | 2.8 | PAPAIN (E.C.3.4.22.2) -ACETYL-ALANYL-ALANYL- ... | PAPAYA (CARICA ...) | J.DRENTH,K.H.KALK *et al.* |
| 6PAD | 2.8 | PAPAIN (E.C.3.4.22.2) -BENZYLOXYCARBONYL- ... | PAPAYA (CARICA ...) | J.DRENTH,K.H.KALK *et al.* |
| 5PAD | 2.8 | PAPAIN (E.C.3.4.22.2) -BENZYLOXYCARBONYL-GLYCYL- ... | PAPAYA (CARICA ...) | J.DRENTH,K.H.KALK *et al.* |
| 2PAD | 2.8 | PAPAIN (E.C.3.4.22.2) -CYSTEINYL DERIVATIVE OF CYSTEINE-25 ... | PAPAYA (CARICA ...) | J.DRENTH,K.H.KALK *et al.* |
| 4PAD | 2.8 | PAPAIN (E.C.3.4.22.2) -TOSYL-METHYLENYLLYSYL DERIVATIVE OF ... | PAPAYA (CARICA ...) | J.DRENTH |
| 9PAP | 1.65 | PAPAIN (E.C.3.4.22.2) CYS-25 OXIDIZED | PAPAYA (CARICA ...) | I.G.KAMPHUIS,J.DRENTH |
| 3DPA | 2.5 | PAPD | (ESCHERICHIA COLI) ... | A.HOLMGREN,C.-I.BRANDEN |
| 5PAL | 1.54 | PARVALBUMIN (ALPHA LINEAGE) | LEOPARD SHARK ... | F.ROQUET *et al.* |
| 3PAL | 2.4 | PARVALBUMIN (PI 4.10) COMPLEX WITH CA, CA, AND MG | PIKE (ESOX LUCIUS) MUSCLE | J.P.DECLERCQ *et al.* |
| 1PAL | 1.65 | PARVALBUMIN (PI 4.10) COMPLEX WITH CA, CA, AND NH4 | PIKE (ESOX LUCIUS) MUSCLE | J.P.DECLERCQ *et al.* |
| 4PAL | 1.8 | PARVALBUMIN (PI 4.10) COMPLEX WITH CA, MG, AND MG | PIKE (ESOX LUCIUS) MUSCLE | J.P.DECLERCQ *et al.* |
| 2PAL | 1.8 | PARVALBUMIN (PI 4.10) COMPLEX WITH MN, MN, AND MN | PIKE (ESOX LUCIUS) MUSCLE | J.P.DECLERCQ *et al.* |
| 1TN2 | 3.0 | PB(II)-TRANSFER RIBO-NUCLEIC ACID (YEAST,PHE) TRNA (PH 5.0) | YEAST (SACCHAROMYCES ...) | J.C.DEWAN,R.S.BROWN *et al.* |
| 1TN1 | 3.0 | PB(II)-TRANSFER RIBO-NUCLEIC ACID (YEAST,PHE) TRNA (PH 7.4) | YEAST (SACCHAROMYCES ...) | J.C.DEWAN,R.S.BROWN *et al.* |
| 2LTN | 1.7 | PEA LECTIN | GARDEN PEA (PISUM ...) | F.L.SUDDATH *et al.* |
| 3PEP | 2.3 | PEPSIN (E.C.3.4.23.1) | PIG (SUS SCROFA) | C.ABAD-ZAPATERO *et al.* |
| 4PEP | 1.8 | PEPSIN (E.C.3.4.23.1) | PIG (SUS SCROFA) | N.ANDREEVA *et al.* |
| 5PEP | 2.34 | PEPSIN (E.C.3.4.23.1) | PORCINE (SUS SCROFA) | J.B.COOPER,G.KHAN *et al.* |
| 1PSG | 1.65 | PEPSINOGEN | PORCINE (SUS SCROFA) | J.A.HARTSUCK *et al.* |
| 1PFC | 3.125 | PFC(PRIME) FRAGMENT OF AN IGG1 | GUINEA PIG (CAVIA ...) | S.H.BRYANT,L.M.AMZEL *et al.* |
| 1PHS | 3.0 | PHASEOLIN | FRENCH BEAN ... | M.C.LAWRENCE *et al.* |
| 1F3G | 2.1 | PHOSPHOCARRIER $III^{GLC}_{FAST}$ | (ESCHERICHIA COLI) | D.WORTHYLAKE *et al.* |
| 2PFK | 2.4 | PHOSPHOFRUCTOKINASE (E.C.2.7.1.11) | (ESCHERICHIA COLI) | W.R.RYPNIEWSKI,P.R.EVANS |
| 3PFK | 2.4 | PHOSPHOFRUCTOKINASE (E.C.2.7.1.11) | (BACILLUS ...) | P.R.EVANS,P.J.HUDSON |
| 5PFK | 7.0 | PHOSPHOFRUCTOKINASE (E.C.2.7.1.11) (INHIBITED T-STATE ...) | (BACILLUS ...) | P.R.EVANS *et al.* |
| 1PFK | 2.4 | PHOSPHOFRUCTOKINASE (E.C.2.7.1.11) (R-STATE) COMPLEX WITH ... | (ESCHERICHIA COLI) | Y.SHIRAKIHARA,P.R.EVANS |
| 4PFK | 2.4 | PHOSPHOFRUCTOKINASE (E.C.2.7.1.11) COMPLEX WITH ... | (BACILLUS ...) | P.R.EVANS,P.J.HUDSON |
| 3PGK | 2.5 | PHOSPHOGLYCERATE KINASE (E.C.2.7.2.3) COMPLEX WITH ATP, ... | BAKER'S YEAST ... | P.J.SHAW,N.P.WALKER *et al.* |
| 2PGK | 3.0 | PHOSPHOGLYCERATE KINASE (HORSE,MUSCLE) (E.C.2.7.2.3) | HORSE (EQUUS ...) | R.D.BANKS *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 1L68 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH SER 44 REPLACED BY ALA, ...) | BACTERIOPHAGE T4 ... | D.HEINZ,B.W.MATTHEWS |
| 1L37 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 115 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L52 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 152 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L02 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L04 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L05 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L06 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,K.WILSON *et al.* |
| 1L07 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,R.FABER *et al.* |
| 1L08 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L09 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,J.BELL *et al.* |
| 1L10 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,K.WILSON *et al.* |
| 1L12 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L13 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L14 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L15 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH THR 157 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |
| 1L33 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH VAL 131 REPLACED BY ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L70 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH VAL 131 REPLACED BY ...) | BACTERIOPHAGE T4 ... | X.ZHANG,B.W.MATTHEWS |
| 1L53 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH VAL 149 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 8LYZ | 2.5 | LYSOZYME (E.C.3.2.1.17) IODINE-INACTIVATED | HEN (GALLUS GALLUS) ... | C.R.BEDDELL *et al.* |
| 7LYZ | 2.5 | LYSOZYME (E.C.3.2.1.17) TRICLINIC CRYSTAL FORM | HEN (GALLUS GALLUS) ... | J.MOULT,A.YONATH *et al.* |
| 1LZT | 1.97 | LYSOZYME (E.C.3.2.1.17), TRICLINIC CRYSTAL FORM | HEN (GALLUS GALLUS) ... | J.M.HODSDON *et al.* |
| 2LZT | 1.97 | LYSOZYME (E.C.3.2.1.17), TRICLINIC CRYSTAL FORM | HEN (GALLUS GALLUS) ... | M.RAMANADHAM *et al.* |
| 1LZH | 6.0 | LYSOZYME (MONOCLINIC) (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | P.J.ARTYMIUK *et al.* |
| 4LYM | 2.1 | LYSOZYME (MUCOPEPTIDE N-ACETYLMURAMYL HYDROLASE) (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | R.KODANDAPANI *et al.* |
| 9LYZ | 2.5 | LYSOZYME (NAM-NAG-NAM SUBSTRATE ONLY) (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | J.A.KELLY,M.N.G.JAMES |
| 2LZH | 6.0 | LYSOZYME (ORTHORHOMBIC) (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | P.J.ARTYMIUK *et al.* |
| 6LDH | 2.0 | $M_4$ APO-LACTATE DEHYDROGENASE (E.C.1.1.1.27) | DOGFISH (SQUALUS ...) | C.ABAD-ZAPATERO *et al.* |
| 8LDH | 2.8 | $M_4$ APO-LACTATE DEHYDROGENASE (E.C.1.1.1.27) COMPLEX WITH ... | DOGFISH (SQUALUS ...) | C.ABAD-ZAPATERO *et al.* |
| 1LDM | 2.1 | $M_4$ LACTATE DEHYDROGENASE (E.C.1.1.1.27) TERNARY COMPLEX ... | DOGFISH (SQUALUS ...) | J.P.GRIFFITH,M.G.ROSSMANN |
| 1MSB | 2.3 | MANNOSE BINDING PROTEIN A (LECTIN DOMAIN) COMPLEX WITH HOLMIUM | RAT (RATTUS RATTUS) ... | W.I.WEIS,K.DRICKAMER *et al.* |
| 2MLT | 2.0 | MELITTIN | HONEY BEE (APIS ...) | D.EISENBERG *et al.* |
| 2MEV | 3.0 | MENGO ENCEPHALOMYOCARDITIS VIRUS COAT PROTEIN | MONKEY BRAIN,MIDDLE ... | M.G.ROSSMANN |
| 1MEE | 2.0 | MESENTERICOPEPTIDASE WITH EGLIN-C PEPTIDYL PEPTIDE HYDROLASE ... | (BACILLUS ...) | Z.DAUTER,C.BETZEL *et al.* |
| 1MAD | 2.25 | METHYLAMINE DEHYDROGENASE (MADH) (E.C.1.4.99.3) | GRAM NEGATIVE ... | F.M.D.VELLIEUX,W.G.J.HOL |
| 1IPT | 0.0 | MODEL OF THE CORE STRUCTURE OF THE INTRON IN THE LARGE ... | (TETRAHYMENA THERMOPHILA) | F.MICHEL,E.WESTHOF |
| 7API | 3.0 | MODIFIED $ALPHA_1$-ANTITRYPSIN (MODIFIED $ALPHA_1$-PROTEINASE ...) | HUMAN (HOMO SAPIENS) | H.LOEBERMANN *et al.* |
| 8API | 3.1 | MODIFIED $ALPHA_1$-ANTITRYPSIN (MODIFIED $ALPHA_1$-PROTEINASE ...) | HUMAN (HOMO SAPIENS) | H.LOEBERMANN *et al.* |
| 9API | 3.0 | MODIFIED $ALPHA_1$-ANTITRYPSIN (MODIFIED $ALPHA_1$-PROTEINASE ...) | HUMAN (HOMO SAPIENS) | H.LOEBERMANN *et al.* |
| 1NTP | 1.8 | MODIFIED BETA TRYPSIN (MONOISOPROPYLPHOSPHORYL INHIBITED) ... | BOVINE (BOS TAURUS) ... | A.A.KOSSIAKOFF |
| 1MON | 2.75 | MONELLIN | SERENDIPITY ... | S.-H.KIM |
| 1MCA | N/A | MONOCYTE CHEMO-ATTRACTANT AND ACTIVATING PROTEIN ... | HUMAN (HOMO SAPIENS) | A.M.GRONENBORN,G.M.CLORE |
| 1MLE | 2.5 | MUCONATE LACTONIZING ENZYME (CIS,CIS MUCONATE ...) | (PSEUDOMONAS PUTIDA, ...) | A.GOLDMAN,D.L.OLLIS *et al.* |
| 1MLI | 3.3 | MUCONOLACTONE ISOMERASE (E.C.5.3.3.4) | (PSEUDOMONAS PUTIDA) | S.K.KATTI,B.A.KATZ *et al.* |
| 1MLP | N/A | MUREIN LIPOPROTEIN | (ESCHERICHIA COLI) | A.D.MCLACHLAN |
| 1L36 | 1.7 | MUTANT LYSOZYME WITH THREE ALANINE SUBSTITUTIONS ... | BACTERIOPHAGE T4 ... | X.-J.ZHANG,W.A.BAASE *et al.* |
| 1MVP | 2.2 | MYELOBLASTOSIS ASSOCIATED VIRAL PROTEASE (E.C.3.4.23) | MYELOBLASTOSIS ... | *et al.* |
| 2MVP | N/A | MYELOBLASTOSIS ASSOCIATED VIRAL PROTEASE (E.C.3.4.23) ... | MYELOBLASTOSIS ... | *et al.* |
| 1PMB | 2.5 | MYOGLOBIN (AQUOMET, PH 7.1) | PORCINE (SUS SCROFA) ... | S.J.SMERDON *et al.* |
| 2MBA | 2.0 | MYOGLOBIN (AZIDE COMPLEX) (PH 7.0) | SEA HARE (APLYSIA ...) | M.BOLOGNESI,S.ONESTI *et al.* |
| 2MB5 | 1.8 | MYOGLOBIN (CARBONMONOXYMYOGLOBIN) (NEUTRON STUDY) | SPERM WHALE ... | B.P.SCHOENBORN,X.CHENG |
| 5MBN | 2.0 | MYOGLOBIN (DEOXY) | SPERM WHALE ... | T.TAKANO |
| 1MBD | 1.4 | MYOGLOBIN (DEOXY, PH 8.4) | SPERM WHALE ... | S.E.V.PHILLIPS |
| 1MBC | 1.5 | MYOGLOBIN (FE II, CARBONMONOXY, 260 DEGREES K) | SPERM WHALE ... | J.KURIYAN,G.A.PETSKO |
| 1MBN | 2.0 | MYOGLOBIN (FERRIC IRON - METMYOGLOBIN) | SPERM WHALE ... | H.C.WATSON,J.C.KENDREW |
| 1MBI | 2.0 | MYOGLOBIN (FERRIC) COMPLEX WITH IMIDAZOLE | SPERM WHALE ... | C.LIONETTI *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 3LHM | 1.8 | LYSOZYME (E.C.3.2.1.17) (HOLO) (MUTANT WITH GLN 86 REPLACED ...) | HUMAN (HOMO SAPIENS) | K.INAKA,M.MATSUSHIMA |
| 1L24 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ALA 82 REPLACED BY PRO) ... | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L48 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ALA 98 REPLACED BY VAL) ... | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L49 | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ALA 98 REPLACED BY VAL, ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L50 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ALA 98 REPLACED BY VAL, ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L51 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ALA 98 REPLACED BY VAL, ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L44 | 1.70 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ARG 119 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L47 | 1.70 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ARG 154 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L34 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ARG 96 REPLACED BY HIS) ... | BACTERIOPHAGE T4 ... | L.H.WEAVER,B.W.MATTHEWS |
| 1L57 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASN 116 REPLACED BY ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L20 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASN 144 REPLACED BY ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L64 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASN 40 REPLACED BY ALA, ...) | BACTERIOPHAGE T4 ... | D.HEINZ,B.W.MATTHEWS |
| 1L21 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASN 55 REPLACED BY GLY) ... | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L72 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASP 127 REPLACED BY ...) | BACTERIOPHAGE T4 ... | X.ZHANG,B.W.MATTHEWS |
| 1L73 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASP 127 REPLACED BY ...) | BACTERIOPHAGE T4 ... | X.ZHANG,B.W.MATTHEWS |
| 1L75 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASP 127 REPLACED BY ...) | BACTERIOPHAGE T4 ... | X.ZHANG,B.W.MATTHEWS |
| 1L65 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ASP 47 REPLACED BY ALA, ...) | BACTERIOPHAGE T4 ... | D.HEINZ,B.W.MATTHEWS |
| 1L39 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L40 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L41 | 1.75 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L54 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L55 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L59 | 1.75 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L62 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L63 | 1.75 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L76 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 54 REPLACED BY THR, ...) | BACTERIOPHAGE T4 ... | U.SAUER,B.W.MATTHEWS |
| 1LHM | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH CYS 77 REPLACED BY ALA ...) | HUMAN (HOMO SAPIENS) | K.INAKA,M.MATSUSHIMA |
| 1L38 | 1.80 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH GLN 123 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L71 | 1.85 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH GLU 128 REPLACED BY ...) | BACTERIOPHAGE T4 ... | X.ZHANG,B.W.MATTHEWS |
| 1L74 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH GLU 128 REPLACED BY ...) | BACTERIOPHAGE T4 ... | X.ZHANG,B.W.MATTHEWS |
| 1L60 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH GLY 113 REPLACED BY ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L16 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH GLY 156 REPLACED BY ...) | BACTERIOPHAGE T4 ... | T.M.GRAY,B.W.MATTHEWS |
| 1L23 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH GLY 77 REPLACED BY ALA) ... | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L18 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ILE 3 REPLACED BY TYR) (I3Y) | BACTERIOPHAGE T4 ... | M.MATSUMURA *et al.* |
| 1L35 | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ILE 3 REPLACED BY TYR, ...) | BACTERIOPHAGE T4 ... | P.E.PJURA *et al.* |
| 1L17 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH ILE 3 REPLACED BY VAL) (I3V) | BACTERIOPHAGE T4 ... | M.MATSUMURA *et al.* |
| 1L69 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LEU 133 REPLACED BY ...) | BACTERIOPHAGE T4 ... | X.ZHANG,B.W.MATTHEWS |
| 1L67 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LEU 46 REPLACED BY ALA, ...) | BACTERIOPHAGE T4 ... | D.HEINZ,B.W.MATTHEWS |
| 1L22 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LYS 124 REPLACED BY ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L45 | 1.70 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LYS 135 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L46 | 1.70 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LYS 147 REPLACED BY ...) | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L42 | 1.80 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LYS 16 REPLACED BY GLU) ... | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L43 | 1.80 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LYS 16 REPLACED BY GLU) ... | BACTERIOPHAGE T4 ... | S.DAOPIN,B.W.MATTHEWS |
| 1L66 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LYS 43 REPLACED BY ALA, ...) | BACTERIOPHAGE T4 ... | D.HEINZ,B.W.MATTHEWS |
| 1L56 | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH LYS 60 REPLACED BY PRO) ... | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L58 | 1.65 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 143 REPLACED BY ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L25 | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 86 REPLACED BY ALA) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L31 | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 86 REPLACED BY ARG) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L27 | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 86 REPLACED BY ASP) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L28 | 1.9 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 86 REPLACED BY GLY) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L29 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 86 REPLACED BY HIS) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L30 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 86 REPLACED BY LEU) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L32 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH PRO 86 REPLACED BY SER) ... | BACTERIOPHAGE T4 ... | J.A.BELL,S.DAO-PIN *et al.* |
| 1L61 | 1.8 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH SER 38 REPLACED BY ASN, ...) | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |
| 1L19 | 1.7 | LYSOZYME (E.C.3.2.1.17) (MUTANT WITH SER 38 REPLACED BY ASP) ... | BACTERIOPHAGE T4 ... | H.NICHOLSON,B.W.MATTHEWS |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 2KAI | 2.5 | KALLIKREIN A (E.C.3.4.21.8) COMPLEX WITH BOVINE PANCREATIC ... | PORCINE (SUS SCROFA) ... | W.BODE,Z.CHEN |
| 1KES | 3.0 | KERATAN SULFATE (SULFATED POLY(GALACTOSYL-N-ACETYL GLUCOSAMINE)) | BOVINE (BOS TAURUS) ... | S.ARNOTT |
| 1TPK | 2.4 | KRINGLE-2: THE SECOND KRINGLE DOMAIN OF TISSUE PLASMINOGEN ... | HUMAN (HOMO SAPIENS) | A.M.DE VOS *et al.* |
| 1ABP | 2.4 | L-ARABINOSE-BINDING PROTEIN | (ESCHERICHIA COLI) | F.A.QUIOCHO,G.L.GILLILAND |
| 6ABP | 1.67 | L-ARABINOSE-BINDING PROTEIN (MUTANT WITH MET 108 REPLACED BY ...) | (ESCHERICHIA COLI) | P.S.VERMERSCH *et al.* |
| 7ABP | 1.67 | L-ARABINOSE-BINDING PROTEIN (MUTANT WITH MET 108 REPLACED BY ...) | (ESCHERICHIA COLI) | P.S.VERMERSCH *et al.* |
| 8ABP | 1.49 | L-ARABINOSE-BINDING PROTEIN (MUTANT WITH MET 108 REPLACED BY ...) | (ESCHERICHIA COLI) | P.S.VERMERSCH *et al.* |
| 1APB | 1.76 | L-ARABINOSE-BINDING PROTEIN (MUTANT WITH PRO 254 REPLACED BY ...) | (ESCHERICHIA COLI) | P.S.VERMERSCH *et al.* |
| 1BAP | 1.75 | L-ARABINOSE-BINDING PROTEIN (MUTANT WITH PRO 254 REPLACED BY ...) | (ESCHERICHIA COLI) | P.S.VERMERSCH *et al.* |
| 9ABP | 1.97 | L-ARABINOSE-BINDING PROTEIN (MUTANT WITH PRO 254 REPLACED BY ...) | (ESCHERICHIA COLI) | P.S.VERMERSCH *et al.* |
| 1LLC | 3.0 | L-LACTATE DEHYDROGENASE (E.C.1.1.1.27) COMPLEX WITH ... | (LACTOBACILLUS CASEI) | M.BUEHNER,H.J.HECHT *et al.* |
| 2LDB | 3.0 | L-LACTATE DEHYDROGENASE (E.C.1.1.1.27) COMPLEX WITH NAD AND ... | (BACILLUS ...) | K.PIONTEK,M.G.ROSSMANN |
| 1CTF | 1.7 | L7(SLASH)L12 50 S RIBOSOMAL PROTEIN (C-TERMINAL DOMAIN) | (ESCHERICHIA COLI, ...) | M.LEIJONMARCK,A.LILJAS |
| 3LDH | 3.0 | LACTATE DEHYDROGENASE (E.C.1.1.1.27) M4 ENZYME, TERNARY ... | DOGFISH (SQUALUS ...) | J.L.WHITE *et al.* |
| 5LDH | 2.7 | LACTATE DEHYDROGENASE $H_4$ AND S-LAC-$NAD^+$ COMPLEX ... | PIG (SUS SCROFA) HEART | U.M.GRAU,M.G.ROSSMANN |
| 3FAB | 2.0 | LAMBDA IMMUNOGLOBULIN FAB(PRIME) | HUMAN (HOMO SAPIENS) ... | R.J.POLJAK,L.M.AMZEL *et al.* |
| 1LRP | 3.20 | LAMBDA REPRESSOR (N-TERMINAL DOMAIN) | (LAMBDA) | C.PABO,M.LEWIS |
| 1LMB | 1.8 | LAMBDA REPRESSOR-OPERATOR COMPLEX | (BACTERIOPHAGE LAMBDA) | L.J.BEAMER,C.O.PABO |
| 1LRD | 2.5 | LAMBDA REPRESSOR-OPERATOR COMPLEX | BACTERIOPHAGE (LAMBDA) | S.JORDAN,C.PABO |
| 1LH1 | 2.0 | LEGHEMOGLOBIN (ACETATE,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 2LH1 | 2.0 | LEGHEMOGLOBIN (ACETATE,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 1LH2 | 2.0 | LEGHEMOGLOBIN (AQUO,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 2LH2 | 2.0 | LEGHEMOGLOBIN (AQUO,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 1LH3 | 2.0 | LEGHEMOGLOBIN (CYANO,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 2LH3 | 2.0 | LEGHEMOGLOBIN (CYANO,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 1LH4 | 2.0 | LEGHEMOGLOBIN (DEOXY) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 2LH4 | 2.0 | LEGHEMOGLOBIN (DEOXY) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 1LH5 | 2.0 | LEGHEMOGLOBIN (FLUORO,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 2LH5 | 2.0 | LEGHEMOGLOBIN (FLUORO,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 1LH6 | 2.0 | LEGHEMOGLOBIN (NICOTINATE,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 2LH6 | 2.0 | LEGHEMOGLOBIN (NICOTINATE,MET) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 1LH7 | 2.0 | LEGHEMOGLOBIN (NITROSOBENZENE) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 2LH7 | 2.0 | LEGHEMOGLOBIN (NITROSOBENZENE) | YELLOW LUPIN ... | B.K.VAINSHTEIN *et al.* |
| 1LAP | 2.7 | LEUCINE AMINOPEPTIDASE (E.C.3.4.11.1) | BOVINE (BOS TAURUS) LENS | S.K.BURLEY,P.R.DAVID *et al.* |
| 2LIV | 2.4 | LEUCINE(SLASH)ISOLEUCINE(SLASH)VALINE-BINDING PROTEIN (LIVBP) | (ESCHERICHIA COLI) | J.S.SACK,M.A.SAPER *et al.* |
| 2LBP | 2.4 | LEUCINE-BINDING PROTEIN (LBP) | (ESCHERICHIA COLI) ... | J.S.SACK *et al.* |
| 2RNT | 1.8 | LYS 25-RIBONUCLEASE $T_1$ (LYS 25-RNASE $T_1$) (E.C.3.1.27.3 ...) | (ASPERGILLUS ORYZAE) | W.SAENGER,J.KOEPKE *et al.* |
| 3RNT | 1.8 | LYS 25-RIBONUCLEASE $T_1$ (LYS 25-RNASE $T_1$) (E.C.3.1.27.3 ...) | (ASPERGILLUS ORYZAE) | D.KOSTREWA,H.-W.CHOE *et al.* |
| 1RSM | 2.0 | LYS-7-(DINITROPHENYLENE)-LYS-41 CROSS-LINKED RIBONUCLEASE A ... | BOVINE (BOS TAURUS) ... | P.C.WEBER,S.SHERIFF *et al.* |
| 1LZ2 | 2.8 | LYSOZYME | TURKEY (MELEAGRIS ...) | R.BOTT,R.SARMA |
| 1LYM | 2.5 | LYSOZYME (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | J.HOGLE,S.T.RAO *et al.* |
| 1LYZ | 2.0 | LYSOZYME (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | R.DIAMOND *et al.* |
| 1LZ1 | 1.5 | LYSOZYME (E.C.3.2.1.17) | HUMAN (HOMO SAPIENS) | P.J.ARTYMIUK,C.C.F.BLAKE |
| 2LYZ | 2.0 | LYSOZYME (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | R.DIAMOND *et al.* |
| 2LZ2 | 2.2 | LYSOZYME (E.C.3.2.1.17) | TURKEY (MELEAGRIS ...) | M.R.PARSONS *et al.* |
| 2LZM | 1.7 | LYSOZYME (E.C.3.2.1.17) | (ESCHERICHIA COLI ...) | L.H.WEAVER,B.W.MATTHEWS |
| 3LYZ | 2.0 | LYSOZYME (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | R.DIAMOND *et al.* |
| 3LZM | 1.7 | LYSOZYME (E.C.3.2.1.17) | (ESCHERICHIA COLI ...) | K.WILSON,R.FABER *et al.* |
| 4LYZ | 2.0 | LYSOZYME (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | R.DIAMOND *et al.* |
| 5LYZ | 2.0 | LYSOZYME (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | R.DIAMOND *et al.* |
| 6LYZ | 2.0 | LYSOZYME (E.C.3.2.1.17) | HEN (GALLUS GALLUS) ... | R.DIAMOND *et al.* |
| 2LYM | 2.0 | LYSOZYME (E.C.3.2.1.17) (1 ATMOSPHERE, 1.4 M NACL) | HEN (GALLUS GALLUS) ... | C.E.KUNDROT,F.M.RICHARDS |
| 3LYM | 2.0 | LYSOZYME (E.C.3.2.1.17) (1000 ATMOSPHERES, 1.4 M NACL) | HEN (GALLUS GALLUS) ... | C.E.KUNDROT,F.M.RICHARDS |
| 2LHM | 1.8 | LYSOZYME (E.C.3.2.1.17) (APO) (MUTANT WITH GLN 86 REPLACED B ...) | HUMAN (HOMO SAPIENS) | K.INAKA,M.MATSUSHIMA |
| 1L01 | 1.7 | LYSOZYME (E.C.3.2.1.17) (DOUBLE MUTANT WITH THR 155 REPLACED ...) | BACTERIOPHAGE T4 ... | S.DAO-PIN,T.ALBER *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 2HYA | 3.0 | HYALURONIC ACID (POLY D-GLUCURONIC ...) | HUMAN (HOMO SAPIENS) ... | S.ARNOTT |
| 3HYA | 3.0 | HYALURONIC ACID (POLY D-GLUCURONIC ...) | HUMAN (HOMO SAPIENS) ... | S.ARNOTT |
| 4HYA | 3.0 | HYALURONIC ACID (POLY D-GLUCURONIC ...) | HUMAN (HOMO SAPIENS) ... | S.ARNOTT |
| 2FBJ | 1.95 | IGA FAB FRAGMENT (J539) (GALACTAN-BINDING) | MOUSE (MUS MUSCULUS) | T.N.BHAT,E.A.PADLAN *et al.* |
| 1FVB | N/A | IGA FV FRAGMENT (19.1.2, ANTI-ALPHA(1(RIGHT ARROW)6) ...) | MOUSE (MUS MUSCULUS) | E.A.PADLAN,E.A.KABAT |
| 2FVB | N/A | IGA FV FRAGMENT (19.1.2, ANTI-ALPHA(1(RIGHT ARROW)6) ...) | MOUSE (MUS MUSCULUS) | E.A.PADLAN,E.A.KABAT |
| 1FVW | N/A | IGA FV FRAGMENT (W3129, ANTI-ALPHA(1(RIGHT ARROW)6) DEXTRAN) ... | MOUSE (MUS MUSCULUS) | E.A.PADLAN,E.A.KABAT |
| 2FVW | N/A | IGA FV FRAGMENT (W3129, ANTI-ALPHA(1(RIGHT ARROW)6) DEXTRAN) ... | MOUSE (MUS MUSCULUS) | E.A.PADLAN,E.A.KABAT |
| 1FDL | 2.5 | IGG1 FAB FRAGMENT (ANTI-LYSOZYME ANTIBODY D1.3, KAPPA) - ... | MOUSE (MUS MUSCULUS) ... | T.O.FISCHMANN,R.J.POLJAK |
| 3HFM | 3.0 | IGG1 FAB FRAGMENT (HYHEL-10) AND LYSOZYME (E.C.3.2.1.17) COMPLEX | MOUSE (MUS MUSCULUS) ... | E.A.PADLAN,D.R.DAVIES |
| 2HFL | 2.54 | IGG1 FAB FRAGMENT (HYHEL-5) AND LYSOZYME (E.C.3.2.1.17) COMPLEX | BALB(SLASH)C MOUSE ... | S.SHERIFF,D.R.DAVIES |
| 1IGF | 2.8 | IGG1 FAB' FRAGMENT (B13I2) | MOUSE (MUS MUSCULUS) ... | R.L.STANFIELD,I.A.WILSON |
| 2IGF | 2.8 | IGG1 FAB' FRAGMENT (B13I2) COMPLEX WITH PEPTIDE (RESIDUES ...) | MOUSE (MUS MUSCULUS) ... | R.L.STANFIELD,I.A.WILSON |
| 1HFM | N/A | IGG1 FV FRAGMENT (HYHEL-10) (MODEL) | MOUSE (MUS MUSCULUS) | S.J.SMITH-GILL *et al.* |
| 2HFM | N/A | IGG1 FV FRAGMENT (HYHEL-10) AND LYSOZYME (E.C.3.2.1.17) ... | MOUSE (MUS MUSCULUS) ... | S.J.SMITH-GILL *et al.* |
| 2FB4 | 1.9 | IMMUNOGLOBULIN FAB | HUMAN (HOMO SAPIENS) ... | M.MARQUART,R.HUBER |
| 1MCP | 2.7 | IMMUNOGLOBULIN FAB FRAGMENT (MCPC603) | MOUSE (MUS MUSCULUS) | Y.SATOW,G.H.COHEN *et al.* |
| 1FC2 | 2.8 | IMMUNOGLOBULIN FC AND FRAGMENT B OF PROTEIN A COMPLEX | HUMAN (HOMO SAPIENS) ... | J.DEISENHOFER |
| 2IG2 | 3.0 | IMMUNOGLOBULIN G1 | HUMAN (HOMO SAPIENS) ... | M.MARQUART,R.HUBER |
| 1MCW | 3.5 | IMMUNOGLOBULIN HETEROLOGOUS LIGHT CHAIN DIMER (MCG-WEIR HYBRID) | HUMAN (HOMO SAPIENS) | K.R.ELY,J.N.HERRON *et al.* |
| 3MCG | 2.0 | IMMUNOGLOBULIN LAMBDA LIGHT CHAIN DIMER (MCG) (ORTHORHOMBIC FORM) | HUMAN (HOMO SAPIENS) | K.R.ELY,J.N.HERRON *et al.* |
| 2MCG | 2.0 | IMMUNOGLOBULIN LAMBDA LIGHT CHAIN DIMER (MCG) (TRIGONAL FORM) | HUMAN (HOMO SAPIENS) | K.R.ELY,J.N.HERRON *et al.* |
| 2MCP | 3.1 | IMMUNOGLOBULIN MCPC603 FAB-PHOSPHOCHOLINE COMPLEX | MOUSE (MUS MUSCULUS) | E.A.PADLAN,G.H.COHEN *et al.* |
| 1PYP | 3.0 | INORGANIC PYROPHOSPHATASE (E.C.3.6.1.1) | BAKER'S YEAST ... | E.H.HARUTYUNYAN *et al.* |
| 4INS | 1.5 | INSULIN | PIG (SUS SCROFA) | G.G.DODSON *et al.* |
| 9INS | 1.7 | INSULIN | PIG (SUS SCROFA) | J.BADGER,G.G.DODSON |
| 1GF1 | N/A | INSULIN-LIKE GROWTH FACTOR I (IGF I) (SOMATOMEDIN) | HUMAN (HOMO SAPIENS) | T.L.BLUNDELL *et al.* |
| 1GF2 | N/A | INSULIN-LIKE GROWTH FACTOR II (IGF II) (SOMATOMEDIN) | HUMAN (HOMO SAPIENS) | T.L.BLUNDELL *et al.* |
| 2TMV | 2.9 | INTACT TOBACCO MOSAIC VIRUS (FIBER DIFFRACTION STUDY) | TOBACCO MOSAIC VIRUS ... | G.STUBBS *et al.* |
| 1HIG | 3.5 | INTERFERON-GAMMA | HUMAN (HOMO SAPIENS) ... | S.E.EALICK,W.J.COOK *et al.* |
| 1RIG | 2.7 | INTERFERON-GAMMA | RABBIT (ORYCTOLAGUS ...) | C.T.SAMUDZI *et al.* |
| 5I1B | 2.1 | INTERLEUKIN 1-BETA | HUMAN (HOMO SAPIENS) ... | *et al.* |
| 8I1B | 2.4 | INTERLEUKIN 1-BETA | MURINE, RECOMBINANT | *et al.* |
| 1IL8 | N/A | INTERLEUKIN 8 (IL-8) (NEUTROPHIL ACTIVATION PROTEIN) NAP ... | HUMAN (HOMO SAPIENS) ... | G.M.CLORE,A.M.GRONENBORN |
| 2IL8 | N/A | INTERLEUKIN 8 (IL-8) (NEUTROPHIL ACTIVATION PROTEIN) NAP ... | HUMAN (HOMO SAPIENS) ... | G.M.CLORE |
| 1I1B | 2.0 | INTERLEUKIN-1BETA (IL-1BETA) | HUMAN (HOMO SAPIENS) ... | B.C.FINZEL *et al.* |
| 1MIB | 2.8 | INTERLEUKIN-1BETA (IL-1BETA) | MOUSE (MUS MUSCULUS) | J.P.PRIESTLE *et al.* |
| 2I1B | 2.0 | INTERLEUKIN-1BETA (IL-1BETA) | HUMAN (HOMO SAPIENS) ... | J.P.PRIESTLE *et al.* |
| 4I1B | 2.0 | INTERLEUKIN-1BETA (IL-1BETA) | HUMAN (HOMO SAPIENS) ... | B.VEERAPANDIAN *et al.* |
| 21BI | 2.0 | INTERLEUKIN-1BETA (IL-1BETA) (MUTANT WITH CYS 71 REPLACED BY ...) | HUMAN (HOMO SAPIENS) ... | B.VEERAPANDIAN *et al.* |
| 31BI | 2.0 | INTERLEUKIN-1BETA (IL-1BETA) (MUTANT WITH CYS 71 REPLACED BY ...) | HUMAN (HOMO SAPIENS) ... | B.VEERAPANDIAN *et al.* |
| 41BI | 2.9 | INTERLEUKIN-1BETA (IL-1BETA) (MUTANT WITH CYS 8 REPLACED BY ...) | HUMAN (HOMO SAPIENS) ... | B.VEERAPANDIAN *et al.* |
| 1IFB | 1.96 | INTESTINAL FATTY ACID BINDING PROTEIN (APO FORM 1) (I-FABP) | RAT (RATTUS RATTUS) ... | J.C.SACCHETTINI *et al.* |
| 2IFB | 2.0 | INTESTINAL FATTY ACID BINDING PROTEIN (HOLO FORM) (I-FABP) | RAT (RATTUS RATTUS) ... | J.C.SACCHETTINI *et al.* |
| 1CAR | 3.0 | IOTA CARRAGEENAN (AN ALTERNATING COPOLYMER OF ...) | RED SEAWEED ... | S.ARNOTT |
| 1YEA | 1.9 | ISO-2-CYTOCHROME C (REDUCED STATE) | BAKER'S YEAST ... | M.E.P.MURPHY,G.D.BRAYER |
| 3ICD | 2.5 | ISOCITRATE DEHYDROGENASE (E.C.1.1.1.42) | (ESCHERICHIA COLI) | J.H.HURLEY *et al.* |
| 6ICD | 2.8 | ISOCITRATE DEHYDROGENASE (E.C.1.1.1.42) (MUTANT WITH SER 113 ...) | (ESCHERICHIA COLI) | J.H.HURLEY,A.M.DEAN *et al.* |
| 7ICD | 2.4 | ISOCITRATE DEHYDROGENASE (E.C.1.1.1.42) (MUTANT WITH SER 113 ...) | (ESCHERICHIA COLI) | J.H.HURLEY,A.M.DEAN *et al.* |
| 8ICD | 2.5 | ISOCITRATE DEHYDROGENASE (E.C.1.1.1.42) (MUTANT WITH SER 113 ...) | (ESCHERICHIA COLI) | J.H.HURLEY,A.M.DEAN *et al.* |
| 5ICD | 2.5 | ISOCITRATE DEHYDROGENASE (E.C.1.1.1.42) COMPLEX WITH MG2+ ... | (ESCHERICHIA COLI) | J.H.HURLEY,A.M.DEAN *et al.* |
| 9ICD | 2.5 | ISOCITRATE DEHYDROGENASE (E.C.1.1.1.42) COMPLEX WITH NADP+ | (ESCHERICHIA COLI) | J.H.HURLEY,A.M.DEAN *et al.* |
| 1GST | 2.2 | ISOENZYME 3-3 OF GLUTATHIONE S-TRANSFERASE (2.5.1.18) ... | RAT (RATTUS RATTUS) LIVER | X.JI,P.ZHANG *et al.* |
| 7ADH | 3.2 | ISONICOTINIMIDYLATED LIVER ALCOHOL DEHYDROGENASE (E.C.1.1.1.1) | HORSE (EQUUS ...) | B.PLAPP,H.EKLUND |
| 2PKA | 2.05 | KALLIKREIN A (E.C.3.4.21.8) | PORCINE (SUS SCROFA) ... | W.BODE,Z.CHEN |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 3HMG | 2.9 | HEMAGGLUTININ (L226(A)Q) (BROMELAIN DIGESTED) (MUTANT WITH ...) | INFLUENZA VIRUS ... | W.I.WEIS *et al.* |
| 4HMG | 3.0 | HEMAGGLUTININ (L226(A)Q) (BROMELAIN DIGESTED) (MUTANT WITH ...) | INFLUENZA VIRUS ... | W.I.WEIS *et al.* |
| 2HMZ | 1.66 | HEMERYTHRIN (ADIZOMET) | SIPUNCULID WORM ... | M.A.HOLMES,R.E.STENKAMP |
| 1HR3 | 5.5 | HEMERYTHRIN (AZIDO,MET) | (SIPHONOSOMA SPECIES ...) | J.L.SMITH *et al.* |
| 1HMD | 2.0 | HEMERYTHRIN (DEOXY) | SIPUNCULID WORM ... | M.A.HOLMES *et al.* |
| 2HMQ | 1.66 | HEMERYTHRIN (MET) | SIPUNCULID WORM ... | M.A.HOLMES,R.E.STENKAMP |
| 1HMO | 2.0 | HEMERYTHRIN (OXY) | SIPUNCULID WORM ... | M.A.HOLMES *et al.* |
| 1HRB | 5.5 | HEMERYTHRIN B | MARINE WORM ... | W.A.HENDRICKSON,K.B.WARD |
| 1PBX | 2.5 | HEMOGLOBIN (CARBOMONOXY) | ANTARTIC FISH ... | G.FERMI |
| 1HCO | 2.7 | HEMOGLOBIN (CARBONMONOXY) | HUMAN (HOMO SAPIENS) | J.M.BALDWIN |
| 1SDH | 2.4 | HEMOGLOBIN (CARBONMONOXY) | ARCID (BLOOD) CLAM ... | W.E.ROYER JUNIOR *et al.* |
| 2HCO | 2.7 | HEMOGLOBIN (CARBONMONOXY) | HUMAN (HOMO SAPIENS) | J.M.BALDWIN |
| 2HHB | 1.74 | HEMOGLOBIN (DEOXY) | HUMAN (HOMO SAPIENS) | G.FERMI,M.F.PERUTZ |
| 2SDH | 2.4 | HEMOGLOBIN (DEOXY) | ARCID (BLOOD) CLAM ... | W.E.ROYER JUNIOR *et al.* |
| 3HHB | 1.74 | HEMOGLOBIN (DEOXY) | HUMAN (HOMO SAPIENS) | G.FERMI,M.F.PERUTZ |
| 4HHB | 1.74 | HEMOGLOBIN (DEOXY) | HUMAN (HOMO SAPIENS) | G.FERMI,M.F.PERUTZ |
| 1FDH | 2.5 | HEMOGLOBIN (DEOXY, HUMAN FETAL $F_{II}$) | HUMAN FETUS (HOMO ...) | J.A.FRIER JUNIOR |
| 1ECA | 1.4 | HEMOGLOBIN (ERYTHROCRUORIN, AQUO MET) | (CHIRONOMOUS THUMMI ...) | W.STEIGEMANN,E.WEBER |
| 1ECO | 1.4 | HEMOGLOBIN (ERYTHROCRUORIN, CARBONMONOXY) | (CHIRONOMOUS THUMMI ...) | W.STEIGEMANN,E.WEBER |
| 1ECN | 1.4 | HEMOGLOBIN (ERYTHROCRUORIN, CYANO MET) | (CHIRONOMOUS THUMMI ...) | W.STEIGEMANN,E.WEBER |
| 1ECD | 1.4 | HEMOGLOBIN (ERYTHROCRUORIN, DEOXY) | (CHIRONOMOUS THUMMI ...) | W.STEIGEMANN,E.WEBER |
| 2MHB | 2.0 | HEMOGLOBIN (HORSE, AQUO MET) | HORSE (EQUUS CABALLUS) | R.C.LADNER *et al.* |
| 2DHB | 2.8 | HEMOGLOBIN (HORSE,DEOXY) | HORSE (EQUUS CABALLUS) | M.F.PERUTZ ET AL. |
| 1HDS | 1.98 | HEMOGLOBIN (SICKLE CELL) | VIRGINIA ... | E.L.AMMA,R.L.GIRLING |
| 1THB | 1.5 | HEMOGLOBIN (T STATE, PARTIALLY OXYGENATED) | HUMAN (HOMO SAPIENS) | D.A.WALLER,R.C.LIDDINGTON |
| 1HHO | 2.1 | HEMOGLOBIN A (OXY) | HUMAN (HOMO SAPIENS) | B.SHAANAN |
| 1HBS | 3.0 | HEMOGLOBIN S (DEOXY) | HUMAN (HOMO SAPIENS) | E.A.PADLAN,W.E.LOVE |
| 2LHB | 2.0 | HEMOGLOBIN V (CYANO,MET) | SEA LAMPREY ... | R.B.HONZATKO *et al.* |
| 1HKG | 3.5 | HEXOKINASE A AND GLUCOSE COMPLEX (E.C.2.7.1.1) | YEAST (SACCHAROMYCES ...) | W.S.BENNETT JUNIOR *et al.* |
| 2HIP | 2.5 | HIGH POTENTIAL IRON SULFUR PROTEIN (HIPIP) | (ECTOTHIORHODOSPIRA ...) | D.R.BREITER *et al.* |
| 6HIR | N/A | HIRUDIN (MUTANT WITH LYS 47 REPLACED BY GLU) (K47E) (NMR, ...) | LEECH (HIRUDO ...) | G.M.CLORE,A.M.GRONENBORN |
| 4HIR | N/A | HIRUDIN (MUTANT WITH LYS 47 REPLACED BY GLU) (K47E) (NMR,32 ...) | LEECH (HIRUDO ...) | G.M.CLORE,A.M.GRONENBORN |
| 5HIR | N/A | HIRUDIN (WILD-TYPE) | LEECH (HIRUDO ...) | G.M.CLORE,A.M.GRONENBORN |
| 2HIR | N/A | HIRUDIN (WILD-TYPE) (NMR,32 SIMULATED ANNEALING STRUCTURES) | LEECH (HIRUDO ...) | G.M.CLORE,A.M.GRONENBORN |
| 1HTC | 2.3 | HIRUDIN VARIANT 2-LYSINE$^{47}$ COMPLEX WITH HUMAN ... | HIRUDIN (HIRUDO ...) | A.TULINSKY,T.J.RYDEL *et al.* |
| 2HVP | 3.0 | HIV-1 PROTEASE | ESCHERICHIA COLI (IN ...) | M.A.NAVIA *et al.* |
| 4HVP | 2.3 | HIV-1 PROTEASE (HIV-1 PR) COMPLEX WITH INHIBITOR ... | SYNTHETIC ENZYME ... | M.MILLER,J.SCHNEIDER *et al.* |
| 3PHV | 2.7 | HIV-1 PROTEASE (ISOLATE HXB2) | HIV-1 RETROVIRUS ... | R.LAPATTO *et al.* |
| 9HVP | 2.8 | HIV-1 PROTEASE COMPLEX WITH A-74704 | BH102 HIV-1 ... | D.J.NEIDHART,J.ERICKSON |
| 5HVP | 2.0 | HIV-1 PROTEASE COMPLEX WITH ACETYL-PEPSTATIN (NY5 STRAIN) | NY5 STRAIN OF HUMAN ... | P.M.D.FITZGERALD *et al.* |
| 1HVP | N/A | HIV-1 PROTEASE COMPLEX WITH SUBSTRATE (MODEL) | HIV-1 RETROVIRUS ... | I.T.WEBER |
| 1PHV | N/A | HIV-2 PROTEASE (HIV-2 PR) MODEL COMPLEX WITH INHIBITOR ... | HIV-2 ROD ISOLATE | A.GUSTCHINA,I.T.WEBER |
| 2PHV | N/A | HIV-2 PROTEASE (HIV-2 PR) MODEL COMPLEX WITH RENIN INHIBITOR ... | HIV-2 ROD ISOLATE | A.GUSTCHINA,I.T.WEBER |
| 1GD1 | 1.8 | HOLO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (E.C.1.2.1.12) | (BACILLUS ...) | T.SKARZYNSKI *et al.* |
| 6ADH | 2.9 | HOLO-LIVER ALCOHOL DEHYDROGENASE (E.C.1.1.1.1) COMPLEX WITH ... | HORSE (EQUUS ...) | H.EKLUND |
| 1HOM | N/A | HOMEODOMAIN OF THE ANTENNAPEDIA PROTEIN | (DROSOPHILA MELANOGASTER) | Y.-Q.QIAN,M.BILLETER *et al.* |
| 2HOA | N/A | HOMEODOMAIN OF THE ANTENNAPEDIA PROTEIN MUTANT(C39S) | (DROSOPHILA MELANOGASTER) | P.GUNTERT,Y.Q.QIAN *et al.* |
| 1HLA | 3.5 | HUMAN CLASS I HISTOCOMPATIBILITY ANTIGEN A2 (HLA-A2, HUMAN ...) | HUMAN (HOMO SAPIENS) ... | P.J.BJORKMAN *et al.* |
| 3HLA | 2.6 | HUMAN CLASS I HISTOCOMPATIBILITY ANTIGEN A2.1 (HLA-A2.1 ...) | HUMAN (HOMO SAPIENS) ... | M.A.SAPER *et al.* |
| 2HLA | 2.6 | HUMAN CLASS I HISTOCOMPATIBILITY ANTIGEN AW 68.1 (HLA-AW ...) | HUMAN (HOMO SAPIENS) ... | T.P.J.GARRETT *et al.* |
| 4PHV | 2.10 | HUMAN IMMUNODEFICIENCY VIRUS TYPE-1 PROTEASE + ... | HIV TYPE-1 PROTEASE ... | R.BONE |
| 1HNE | 1.84 | HUMAN NEUTROPHIL ELASTASE (HNE) (E.C.3.4.21.37) (ALSO ...) | HUMAN (HOMO SAPIENS) ... | M.A.NAVIA *et al.* |
| 1PK4 | 1.9 | HUMAN PLASMINOGEN KRINGLE 4 | HUMAN (HOMO SAPIENS) | A.TULINSKY,A.M.MULICHAK |
| 2PK4 | 2.25 | HUMAN PLASMINOGEN KRINGLE 4 - EPSILON-AMINOCAPROIC ACID COMPLEX | HUMAN (HOMO SAPIENS) | A.TULINSKY,T.-P.WU |
| 1HYA | 3.0 | HYALURONIC ACID (POLY D-GLUCURONIC ...) | SYNTHESIZED BY ... | S.ARNOTT |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 1FNR | 2.2 | FERREDOXIN:NADP$^+$ OXIDOREDUCTASE (FERREDOXIN REDUCTASE) ... | SPINACH (SPINACIA ...) | P.A.KARPLUS *et al.* |
| 2FNR | 3.0 | FERREDOXIN:NADP$^+$ OXIDOREDUCTASE (FERREDOXIN REDUCTASE) ... | SPINACH (SPINACIA ...) | P.A.KARPLUS *et al.* |
| 1CYC | 2.3 | FERROCYTOCHROME C | BONITO (KATSUWONUS ...) | N.TANAKA,T.YAMANE *et al.* |
| 3FIS | 2.3 | FIS PROTEIN (FACTOR FOR INVERSION STIMULATION) | (ESCHERICHIA COLI) | H.S.YUAN,S.E.FINKEL *et al.* |
| 4FIS | 2.3 | FIS PROTEIN (FACTOR FOR INVERSION STIMULATION) MUTANT WITH ... | (ESCHERICHIA COLI) | H.S.YUAN,S.E.FINKEL *et al.* |
| 1FKF | 1.7 | FK506 BINDING PROTEIN (FKBP) COMPLEX WITH IMMUNOSUPPRESSANT FK506 | RECOMBINANT HUMAN ... | G.D.VAN DUYNE *et al.* |
| 1FCB | 2.4 | FLAVOCYTOCHROME $B_2$ (E.C.1.1.2.3) | YEAST (SACCHAROMYCES ...) | F.S.MATHEWS,Z.-X.XIA |
| 1FX1 | 2.0 | FLAVODOXIN | (DESULFOVIBRIO VULGARIS) | K.D.WATENPAUGH *et al.* |
| 2FCR | 1.8 | FLAVODOXIN | (CHONDRUS CRISPUS) | K.FUKUYAMA |
| 2FX2 | 1.9 | FLAVODOXIN | (DESULFOVIBRIO VULGARIS) | W.WATT,K.D.WATENPAUGH |
| 3FXN | 1.9 | FLAVODOXIN (OXIDIZED FORM) | (CLOSTRIDIUM MP) | M.L.LUDWIG |
| 4FXN | 1.8 | FLAVODOXIN (SEMIQUINONE FORM) | (CLOSTRIDIUM MP) | M.L.LUDWIG |
| 5FX2 | 1.9 | FLAVODOXIN LOW TEMPERATURE (-150C) FULLY REDUCED (HYDROQUINON) | (DESULFOVIBRIO ...) | W.WATT,K.D.WATENPAUGH |
| 3FX2 | 1.9 | FLAVODOXIN LOW TEMPERATURE (-150C) OXIDIZED FORM | (DESULFOVIBRIO ...) | W.WATT,K.D.WATENPAUGH |
| 4FX2 | 1.9 | FLAVODOXIN LOW TEMPERATURE (-150C) REDUCED FORM | (DESULFOVIBRIO ...) | W.WATT,K.D.WATENPAUGH |
| 1FBP | 2.5 | FRUCTOSE-1,6-BISPHOSPHATASE (D-FRUCTOSE-1,6-BISPHOSPHATE ...) | PIG (SUS SCROFA) ... | H.KE,Y.ZHANG,W.N.LIPSCOMB |
| 2FBP | 2.8 | FRUCTOSE-1,6-BISPHOSPHATASE (D-FRUCTOSE-1,6-BISPHOSPHATE ...) | PIG (SUS SCROFA) ... | H.KE,C.M.THORPE *et al.* |
| 3FBP | 2.8 | FRUCTOSE-1,6-BISPHOSPHATASE (D-FRUCTOSE-1,6-BISPHOSPHATE ...) | PIG (SUS SCROFA) ... | H.KE,C.M.THORPE *et al.* |
| 3GBP | 2.4 | GALACTOSE-BINDING PROTEIN COMPLEX WITH GLUCOSE | (SALMONELLA ...) | S.L.MOWBRAY |
| 3GCH | 1.9 | GAMMA CHYMOTRYPSIN (E.C.3.4.21.1) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | B.L.STODDARD,D.RINGE *et al.* |
| 4GCH | 1.9 | GAMMA CHYMOTRYPSIN (E.C.3.4.21.1) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | B.L.STODDARD,D.RINGE *et al.* |
| 8GCH | 1.6 | GAMMA CHYMOTRYPSIN (E.C.3.4.21.1) COMPLEX WITH GLY-ALA-TRP | BOVINE (BOS TAURUS) ... | M.HAREL.J.L.SUSSMAN *et al.* |
| 6GCH | 2.1 | GAMMA CHYMOTRYPSIN (E.C.3.4.21.1) WITH ... | BOVINE (BOS TAURUS) ... | K.BRADY,A.WEI *et al.* |
| 7GCH | 1.8 | GAMMA CHYMOTRYPSIN (E.C.3.4.21.1) WITH ... | BOVINE (BOS TAURUS) ... | K.BRADY,D.RINGE *et al.* |
| 2GCH | 1.9 | GAMMA CHYMOTRYPSIN A (E.C.3.4.21.1) | BOVINE (BOS TAURUS) ... | G.H.COHEN,D.R.DAVIES *et al.* |
| 1RSL | 2.3 | GAMMA DELTA RESOLVASE (LARGE FRAGMENT, CATALYTIC DOMAIN) | (ESCHERICHIA COLI) | M.R.SANDERSON *et al.* |
| 2GCR | 2.3 | GAMMA IVA-CRYSTALLIN | BOVINE LENS (BOS TAURUS) | H.E.WHITE *et al.* |
| 3GCT | 1.6 | GAMMA-CHYMOTRYPSIN A (E.C.3.4.21.1) (PH 10.5) | BOVINE (BOS TAURUS) ... | M.M.DIXON,B.W.MATTHEWS |
| 2GCT | 1.8 | GAMMA-CHYMOTRYPSIN A (E.C.3.4.21.1) (PH 2.0) | BOVINE (BOS TAURUS) ... | M.M.DIXON,B.W.MATTHEWS |
| 1GCT | 1.6 | GAMMA-CHYMOTRYPSIN A (E.C.3.4.21.1) (PH 7.0) | BOVINE (BOS TAURUS) ... | M.M.DIXON,B.W.MATTHEWS |
| 1GCR | 1.6 | GAMMA-II CRYSTALLIN | CALF (BOS TAURUS) ... | C.SLINGSBY,P.LINDLEY *et al.* |
| 2ZTA | 1.8 | GCN4 LEUCINE ZIPPER | YEAST (SACCHAROMYCES ...) | E.K.O'SHEA,J.D.KLEMM *et al.* |
| 2GN5 | 2.3 | GENE 5 DNA BINDING PROTEIN | FILAMENTOUS ... | G.D.BRAYER,A.MCPHERSON |
| 1GCN | 3.0 | GLUCAGON (PH 6 - PH 7 FORM) | PORCINE (SUS SCROFA) ... | T.L.BLUNDELL *et al.* |
| 1GLY | 2.2 | GLUCOAMYLASE (GLUCAN 1,4-ALPHA-GLUCOSIDASE) (E.C.3.2.1.3) | (ASPERGILLUS ...) | A.ALESHIN,A.GOLUBEV *et al.* |
| 2GLS | 3.5 | GLUTAMINE SYNTHETASE (E.C.6.3.1.2) | (SALMONELLA TYPHIMURIUM) | D.EISENBERG *et al.* |
| 1GSG | 2.8 | GLUTAMINYL-TRNA SYNTHETASE (GLNRS) COMPLEX WITH $TRNA^{GLN}$ AND ATP | (ESCHERICHIA COLI) | M.A.ROULD,J.J.PERONA *et al.* |
| 1EGR | N/A | GLUTAREDOXIN (REDUCED) | (ESCHERICHIA COLI) ... | P.SODANO,T.-H.XIA *et al.* |
| 1GP1 | 2.0 | GLUTATHIONE PEROXIDASE (E.C.1.11.1.9) | BOVINE (BOS TAURUS) ... | O.EPP,R.LADENSTEIN |
| 3GRS | 1.54 | GLUTATHIONE REDUCTASE (E.C.1.6.4.2), OXIDIZED FORM (E) | HUMAN (HOMO SAPIENS) ... | G.E.SCHULZ,P.A.KARPLUS |
| 4GR1 | 2.4 | GLUTATHIONE REDUCTASE (EC 1.6.4.2), OXIDIZED FORM IN COMPLEX ... | HUMAN (HOMO SAPIENS) ... | G.E.SCHULZ,W.JANES |
| 1GOX | 2.0 | GLYCOLATE OXIDASE (E.C.1.1.3.1) | SPINACH (SPINACIA ...) | Y.LINDQVIST |
| 1GMA | 0.86 | GRAMICIDIN A | (BACILLUS BREVIS) | D.A.LANGS |
| 1GMF | 2.4 | GRANULOCYTE-MACROPHAGE COLONY-STIMULATING FACTOR | HUMAN (HOMO SAPIENS) ... | P.A.KARPLUS,K.DIEDERICHS |
| 1GKY | 2.0 | GUANYLATE KINASE (E.C.2.7.4.8) ATP:GMP-PHOSPHOTRANSFERASE | BAKER'S YEAST ... | T.STEHLE,G.E.SCHULZ |
| 1HF1 | N/A | HANNUKA FACTOR (MODEL) | HUMAN (HOMO SAPIENS) | M.MURPHY,M.N.G.JAMES |
| 1HGG | 2.9 | HEMAGGLUTININ (BROMELAIN DIGESTED) COMPLEX WITH ... | INFLUENZA VIRUS, ... | D.C.WILEY |
| 1HGH | 2.7 | HEMAGGLUTININ (BROMELAIN DIGESTED) COMPLEX WITH ... | INFLUENZA VIRUS, ... | D.C.WILEY |
| 1HGI | 2.7 | HEMAGGLUTININ (BROMELAIN DIGESTED) COMPLEX WITH ... | INFLUENZA VIRUS, ... | D.C.WILEY |
| 1HGJ | 2.7 | HEMAGGLUTININ (BROMELAIN DIGESTED) COMPLEX WITH ... | INFLUENZA VIRUS, ... | D.C.WILEY |
| 1HGD | 2.7 | HEMAGGLUTININ (BROMELAIN DIGESTED) CONTAINING GLY 135 TO ARG ... | INFLUENZA VIRUS, ... | D.C.WILEY |
| 1HGE | 2.6 | HEMAGGLUTININ (BROMELAIN DIGESTED) CONTAINING GLY 135 TO ARG ... | INFLUENZA VIRUS, ... | D.C.WILEY |
| 1HGF | 3.0 | HEMAGGLUTININ (BROMELAIN DIGESTED) UNCOMPLEXED | INFLUENZA VIRUS, ... | D.C.WILEY |
| 5HMG | 3.2 | HEMAGGLUTININ (D112(B)G) (BROMELAIN DIGESTED) (MUTANT WITH ...) | INFLUENZA VIRUS ... | W.I.WEIS *et al.* |
| 2HMG | 3.0 | HEMAGGLUTININ (G146(A)D) (BROMELAIN DIGESTED) (MUTANT WITH ...) | INFLUENZA VIRUS ... | W.I.WEIS *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 2ZNA | N/A | DNA (Z-I, 5-D(PCPGPCPGPCPGPCPGPCPGPCPG)-3) | SYNTHETIC DNA | A.H.-J.WANG *et al.* |
| 3ZNA | N/A | DNA (Z-II, 5-D(PCPGPCPGPCPGPCPGPCPGPCPG)-3) | SYNTHETIC DNA | A.H.-J.WANG *et al.* |
| 1NDN | 3.0 | DNA NICKED DODECAMER DOUBLE HELIX ... | SYNTHETIC | J.AYMANI,M.COLL *et al.* |
| 1DPI | 2.8 | DNA POLYMERASE I (KLENOW FRAGMENT) (E.C.2.7.7.7) - DCMP COMPLEX | (ESCHERICHIA COLI) | L.BEESE,D.OLLIS,T.STEITZ |
| 2DND | 2.2 | DNA-5(PRIME)- D(CPGPCPAPAPAPTPTPTPGPCPG)-3(PRIME)) COMPLEX ...) | SYNTHETIC DNA | M.COLL,C.A.FREDERICK *et al.* |
| 1DNH | 2.25 | DNA-5(PRIME)- D(CPGPCPGPAPAPTPTPCPGPCPG)-3(PRIME)) COMPLEX ...) | SYNTHETIC DNA | M.-K.TENG,N.USMAN *et al.* |
| 4DNB | 2.0 | DNA-5(PRIME)- D(CPGPCPGPAPM$^{6}$APTPTPCPGPCPG)-3(PRIME) | SYNTHETIC DNA | C.A.FREDERICK *et al.* |
| 1DNE | 2.4 | DNA-5(PRIME)- D(CPGPCPGPAPTPAPTPCPGPCPG)-3(PRIME)) COMPLEX ...) | SYNTHETIC DNA | M.COLL,J.AYMAMI *et al.* |
| 1D16 | 2.1 | DNA-5(PRIME)- D(CPGPCPGPCPGPTPTPTPTPCPGPCPGPCPG)-3(PRIME) | SYNTHETIC DNA | R.CHATTOPADHYAYA *et al.* |
| 1DN7 | N/A | DNA-5(PRIME)-D( GPGPGPGGPGPGPGGPGPGPGGPGPGPG) ... | SYNTHETIC | M.J.MCCALL,T.BROWN *et al.* |
| 1DN4 | 1.4 | DNA-5(PRIME)-D(5BRCPGP5BRCPGP5BRCPGP)-3(PRIME)) (18 DEGREES C) | SYNTHETIC DNA | B.CHEVRIER,A.C.DOCK *et al.* |
| 1DN5 | 1.4 | DNA-5(PRIME)-D(5BRCPGP5BRCPGP5BRCPGP)-3(PRIME)) (37 DEGREES C) | SYNTHETIC DNA | B.CHEVRIER,A.C.DOCK *et al.* |
| 3DNB | 1.3 | DNA-5(PRIME)-D(CPCPAPAPGPAPTPTPGPG)-3(PRIME) | SYNTHETIC DNA | G.G.PRIVE,R.E.DICKERSON |
| 1DCG | 1.0 | DNA-5(PRIME)-D(CPGPCPGPCPG)-3(PRIME) COMPLEX WITH MAGNESIUM | SYNTHETIC DNA | R.V.GESSNER *et al.* |
| 2DCG | 0.9 | DNA-5(PRIME)-D(CPGPCPGPCPG)-3(PRIME) COMPLEX WITH MAGNESIUM ... | SYNTHETIC DNA | A.H.-J.WANG *et al.* |
| 1DN6 | 3.0 | DNA-5(PRIME)-D(GPGPAPTPGPGPGPAPG)-3(PRIME) | SYNTHETIC DNA | M.J.MCCALL,T.BROWN *et al.* |
| 3ANA | 2.5 | DNA-5(PRIME)-D(GPGPGPAPTPCPCPC)-3(PRIME) (A CONFORMATION) | SYNTHETIC DNA | U.HEINEMANN,H.LAUBLE |
| 1DN8 | 1.5 | DNA-5(PRIME)-D(PCPGPTPAPCPGPTPAPCPG) - COBALT HEXAMMINE COMPLEX | SYNTHETIC DNA | M.SUNDARALINGAM |
| 1R1E | 2.7 | ECO RI ENDONUCLEASE (E.C.3.1.21.4) COMPLEX WITH ... | (ESCHERICHIA COLI) | Y.KIM,J.C.GRABLE *et al.* |
| 2RVE | 3.0 | ECO RV ENDONUCLEASE COMPLEX WITH DNA | (ESCHERICHIA COLI) ... | F.K.WINKLER |
| 2EST | 2.5 | ELASTASE (E.C.3.4.21.11) COMPLEX WITH TRIFLUOROACETYL ... | PORCINE (SUS SCROFA) ... | L.C.SIEKER,D.L.HUGHES |
| 7EST | 1.8 | ELASTASE (E.C.3.4.21.11) COMPLEX WITH TRIFLUOROACETYL ... | PORCINE (SUS SCROFA) ... | I.LI DE LA SIERRA *et al.* |
| 6EST | 1.8 | ELASTASE (E.C.3.4.21.11) CRYSTALLIZED IN 10% DMF | PORCINE (SUS SCROFA) ... | T.PRANGE *et al.* |
| 1ETU | 2.9 | ELONGATION FACTOR TU (DOMAIN I) - GUANOSINE DIPHOSPHATE COMPLEX | (ESCHERICHIA COLI B) | B.F.C.CLARK *et al.* |
| 1ER8 | 2.0 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | A.M.HEMMINGS *et al.* |
| 2ER0 | 3.0 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | J.B.COOPER *et al.* |
| 2ER6 | 2.0 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | J.B.COOPER *et al.* |
| 2ER7 | 1.6 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | B.VEERAPANDIAN *et al.* |
| 2ER9 | 2.2 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | J.B.COOPER *et al.* |
| 3ER3 | 2.0 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | S.AL-KARADAGHI *et al.* |
| 3ER5 | 1.8 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | D.BAILY *et al.* |
| 4ER1 | 2.0 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | J.W.QUAIL,J.B.COOPER *et al.* |
| 4ER2 | 2.0 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | D.BAILEY *et al.* |
| 4ER4 | 2.1 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | S.I.FOUNDLING *et al.* |
| 5ER1 | 2.0 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | J.B.COOPER *et al.* |
| 5ER2 | 1.8 | ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) (E.C.3.4.23.6) ... | CHESTNUT BLIGHT ... | A.SALI *et al.* |
| 1HDD | 2.8 | ENGRAILED HOMEODOMAIN COMPLEX WITH DNA | FRUIT FLY ... | C.R.KISSINGER,B.LIU *et al.* |
| 3ENL | 2.25 | ENOLASE (E.C.4.2.1.11) (2-PHOSPHO-D-GLYCERATE HYDROLASE) (APO) | BAKER'S YEAST ... | L.LEBIODA,B.STEC |
| 4ENL | 1.9 | ENOLASE (E.C.4.2.1.11) (2-PHOSPHO-D-GLYCERATE HYDROLASE) (HOLO) | BAKER'S YEAST ... | L.LEBIODA,B.STEC |
| 5ENL | 2.2 | ENOLASE (E.C.4.2.1.11) (2-PHOSPHO-D-GLYCERATE HYDROLASE) ... | BAKER'S YEAST ... | L.LEBIODA,B.STEC |
| 6ENL | 2.2 | ENOLASE (E.C.4.2.1.11) (2-PHOSPHO-D-GLYCERATE HYDROLASE) ... | BAKER'S YEAST ... | L.LEBIODA,B.STEC |
| 7ENL | 2.2 | ENOLASE (E.C.4.2.1.11) (2-PHOSPHO-D-GLYCERATE HYDROLASE) ... | BAKER'S YEAST ... | L.LEBIODA,B.STEC |
| 5EBX | 2.0 | ERABUTOXIN A | SEA SNAKE (LATICAUDA ...) | P.W.R.CORFIELD *et al.* |
| 3EBX | 1.4 | ERABUTOXIN B | SEA SNAKE (LATICAUDA ...) | J.L.SMITH *et al.* |
| 1IGE | N/A | FC FRAGMENT (IGE(PRIME)CL) (MODEL) | HUMAN (HOMO SAPIENS) | E.A.PADLAN,D.R.DAVIES |
| 1FC1 | 2.9 | FC FRAGMENT (IGG1 CLASS) | HUMAN (HOMO SAPIENS) ... | J.DEISENHOFER |
| 1FLX | N/A | FELIX (DE NOVO DESIGNED PROTEIN) (MODEL 1) | RECOMBINANT USING A ... | T.P.QUINN *et al.* |
| 3FLX | N/A | FELIX (DE NOVO DESIGNED PROTEIN) (MODEL 2) | RECOMBINANT USING A ... | T.P.QUINN *et al.* |
| 1FDX | 2.0 | FERREDOXIN | (PEPTOCOCCUS AEROGENES) | E.T.ADMAN,L.C.SIEKER *et al.* |
| 2FXB | 2.3 | FERREDOXIN | (BACILLUS ...) | K.FUKUYAMA *et al.* |
| 3FXC | 2.5 | FERREDOXIN | (SPIRULINA PLATENSIS) | M.KAKUDO,T.TSUKIHARA *et al.* |
| 4FD1 | 1.9 | FERREDOXIN | (AZOTOBACTER ...) | C.D.STOUT |
| 1FD2 | 1.9 | FERREDOXIN (MUTANT WITH CYS 20 REPLACED BY ALA) (C20A) | (AZOTOBACTER ...) | C.D.STOUT |
| 2FD2 | 1.9 | FERREDOXIN (MUTANT WITH CYS 24 REPLACED BY ALA) (C24A) | (AZOTOBACTER ...) | C.D.STOUT |
| 1FXI | 2.2 | FERREDOXIN I | BLUE-GREEN ALGA ... | T.TSUKIHARA |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 2D47 | 2.00 | DNA (5’-D(CPCPCPCPCPGPCPGPGPGPG)-3’), COMPLEX WITH SPERMINE | SYNTHETIC DNA | N.VERDAGUER,J.AYMAMI *et al.* |
| 1D23 | 1.5 | DNA (5’-D(CPGPAPTPCPCPAPTPCPGP)-3’) | SYNTHETIC DNA | K.GRZESKOWIAK *et al.* |
| 1D15 | 1.5 | DNA (5’-D(CPGPAPTPCPGP)-3’) COMPLEX WITH 4’-EPIADRIAMYCIN ... | SYNTHETIC DNA | L.D.WILLIAMS *et al.* |
| 1D49 | 1.50 | DNA (5’-D(CPGPAPTPTPAPAPTPCPG)-3’) | SYNTHETIC DNA | J.R.QUINTANA *et al.* |
| 1D24 | 1.9 | DNA (5’-D(CPGPCP(O$^{6}$ME)GPCPG)-3’) | SYNTHETIC DNA | S.L.GINELL,S.KUZMICH *et al.* |
| 1BDN | 2.6 | DNA (5’-D(CPGPCPAPAPAPAPAPTPGPCPGP)-3’) AND ITS ... | SYNTHETIC | A.D.DIGABRIELE *et al.* |
| 1DNM | 2.5 | DNA (5’-D(CPGPCPAPAPGPCPTPGPGPCPGP)-3’) | SYNTHETIC DNA | G.D.WEBSTER *et al.* |
| 1D32 | 1.7 | DNA (5’-D(CPGPCPG)-3’) COMPLEX WITH DITERCALINIUM | SYNTHETIC DNA | Q.GAO,L.D.WILLIAMS *et al.* |
| 9BNA | 1.9 | DNA (5’-D(CPGPCPGPAPAPTPTPCPGPCPG)-3’) (B-DNA DODECAMER) | SYNTHETIC DNA | E.WESTHOF |
| 1D30 | 2.4 | DNA (5’-D(CPGPCPGPAPAPTPTPCPGPCPG)-3’) COMPLEX WITH ... | SYNTHETIC DNA | T.A.LARSEN *et al.* |
| 1D43 | 2.00 | DNA (5’-D(CPGPCPGPAPAPTPTPCPGPCPG)-3’) COMPLEX WITH HOECHST ... | SYNTHETIC DNA | J.R.QUINTANA *et al.* |
| 1D44 | 2.00 | DNA (5’-D(CPGPCPGPAPAPTPTPCPGPCPG)-3’) COMPLEX WITH HOECHST ... | SYNTHETIC DNA | J.R.QUINTANA *et al.* |
| 1D45 | 1.90 | DNA (5’-D(CPGPCPGPAPAPTPTPCPGPCPG)-3’) COMPLEX WITH HOECHST ... | SYNTHETIC DNA | J.R.QUINTANA *et al.* |
| 1D46 | 2.00 | DNA (5’-D(CPGPCPGPAPAPTPTPCPGPCPG)-3’) COMPLEX WITH HOECHST ... | SYNTHETIC DNA | J.R.QUINTANA *et al.* |
| 2DBE | 2.5 | DNA (5’-D(CPGPCPGPAPAPTPTPCPGPCPGP)-3’) COMPLEXED WITH ... | SYNTHETIC DNA | D.G.BROWN *et al.* |
| 1D33 | 1.5 | DNA (5’-D(CPGPCPGPCPG)-3’) COMPLEX WITH DAUNORUBICIN (DAUNOMYCIN) | SYNTHETIC DNA | A.H.-J.WANG,Y.-G.GAO *et al.* |
| 1D48 | 1.00 | DNA (5’-D(CPGPCPGPCPG)-3’) COMPLEX WITH SPERMINE | SYNTHETIC DNA | M.EGLI,L.D.WILLIAMS *et al.* |
| 1D27 | 2.0 | DNA (5’-D(CPGPCPM$^{6}$GPAPAPTPTPTPGPCPG)-3’) | SYNTHETIC DNA | G.A.LEONARD *et al.* |
| 2D34 | 1.4 | DNA (5’-D(CPGPTP+APCPG)-3’) COMPLEX WITH DAUNORUBICIN ... | SYNTHETIC DNA | A.H.-J.WANG,Y.-G.GAO *et al.* |
| 1D28 | 2.7 | DNA (5’-D(CPGPTPGPAPAPTPTPCPAPCPG)-3’) | SYNTHETIC DNA | N.NARAYANA *et al.* |
| 1D29 | 2.5 | DNA (5’-D(CPGPTPGPAPAPTPTPCPAPCPG)-3’) | SYNTHETIC DNA | T.A.LARSEN,M.L.KOPKA *et al.* |
| 1D26 | 2.12 | DNA (5’-D(GPCPCPCP+GPGPGPC)-3’) (+G 5 CARRIES A CHARGED, ...) | SYNTHETIC DNA | U.HEINEMANN |
| 28DN | 2.4 | DNA (5’-D(GPTPAPCPGPTPAPC)-3’) | SYNTHETIC DNA | C.COURSEILLE *et al.* |
| 1D19 | N/A | DNA (5’-D(GPTPAPCPGPTPAPCP)-3’) | SYNTHETIC DNA | J.D.BALEJA,B.D.SYKES |
| 1D21 | 1.7 | DNA (5’-D(M$^{5}$CPGPT(PS)APM$^{5}$CPGP)-3’) COMPLEX WITH NOGALAMYCIN | SYNTHETIC DNA | A.H.-J.WANG *et al.* |
| 1D22 | 1.8 | DNA (5’-D(M$^{5}$CPGPT(PS)APM$^{5}$CPGP)-3’) COMPLEX WITH U-58872 ... | SYNTHETIC DNA | A.H.-J.WANG *et al.* |
| 1D17 | 2.0 | DNA (5’-D(M$^{5}$CPGPTSPAPM$^{5}$CPGP) COMPLEX WITH NOGALAMYCIN | SYNTHETIC DNA | M.EGLI,L.D.WILLIAMS *et al.* |
| 1D20 | N/A | DNA (5’-D(TPCPTPAPTPCPAPCPCPGP)-3’) | SYNTHETIC DNA | J.D.BALEJA,B.D.SYKES |
| 1DNN | N/A | DNA (5(PRIME)-D((APTPCPGPGPCPTPAPAPG))- 3(PRIME)) MODEL | NOT APPLICABLE ... | J.L.SUSSMAN,E.N.TRIFONOV |
| 1D13 | 2.0 | DNA (5(PRIME)-D(APCPCPGPGPCPCPGPGPT)-3(PRIME)) | SYNTHETIC DNA | C.A.FREDERICK *et al.* |
| 1D12 | 1.7 | DNA (5(PRIME)-D(CPGPAPTPCPG)-3(PRIME)) COMPLEX WITH ADRIAMYCIN | SYNTHETIC DNA | C.A.FREDERICK *et al.* |
| 1D10 | 1.5 | DNA (5(PRIME)-D(CPGPAPTPCPG)-3(PRIME)) COMPLEX WITH DAUNOMYCIN | SYNTHETIC DNA | C.A.FREDERICK *et al.* |
| 1DN9 | 2.2 | DNA (5(PRIME)-D(CPGPCPAPTPAPTPAPTPGPCPGP)-3(PRIME)) | SYNTHETIC | C.YOON,R.E.DICKERSON |
| 1DNF | 1.5 | DNA (5(PRIME)-D(CPGPCPGPUFPGP)-3(PRIME)) | SYNTHETIC | M.COLL,D.SAAL *et al.* |
| 1D14 | 1.5 | DNA (5(PRIME)-D(CPGPTPAPCPG)-3(PRIME)) (A 4 IS ...) | SYNTHETIC DNA | L.D.WILLIAMS,M.EGLI *et al.* |
| 1D11 | 1.2 | DNA (5(PRIME)-D(CPGPTPAPCPG)-3(PRIME)) COMPLEX WITH DAUNOMYCIN | SYNTHETIC DNA | A.H.-J.WANG *et al.* |
| 5ANA | 2.25 | DNA (5(PRIME)-D(GPTPAPCPGPTPAPCP)-3(PRIME)) | SYNTHETIC | F.TAKUSAGAWA |
| 1DNS | 2.0 | DNA (5(PRIME)-D(GPTPGPTPAPCPAPCP)) COMPLEX WITH SPERMINE | SYNTHETIC | M.SUNDARALINGAM |
| 1D31 | 2.6 | DNA (5-D(CPGPCPAPGPAPAPTPTPCPGPCPG)-3’) | SYNTHETIC DNA | L.JOSHUA-TOR,J.L.SUSSMAN |
| 1ANA | 2.1 | DNA (A, 5(PRIME)-D($^{I}$CPCPGPG)-3(PRIME)) | SYNTHETIC DNA | B.N.CONNER,R.E.DICKERSON |
| 2ANA | 2.5 | DNA (A,5(PRIME)-D(GPGPGPGPCPCPCPC)-3(PRIME)) | SYNTHETIC DNA | M.MCCALL,T.BROWN *et al.* |
| 2D25 | 1.75 | DNA (B, 5’-D(CPCPAPGPGPCPM$^{5}$CPTPGPG)-3’) | SYNTHETIC DNA | U.HEINEMANN,M.HAHN |
| 6BNA | 2.21 | DNA (B, 5(PRIME)- D(CPGPCPGPAPAPTPTP=$_{BR}$=CPGPCPG)-3(PRIME)) ... | SYNTHETIC DNA | M.L.KOPKA,C.YOON *et al.* |
| 3BNA | 3.0 | DNA (B, 5(PRIME)- D(CPGPCPGPAPAPTPTPBRCPGPCPG)-3(PRIME)) (60 ...) | SYNTHETIC DNA | M.L.KOPKA *et al.* |
| 4BNA | 2.3 | DNA (B, 5(PRIME)- D(CPGPCPGPAPAPTPTPBRCPGPCPG)-3(PRIME)) (60 ...) | SYNTHETIC DNA | M.L.KOPKA *et al.* |
| 8BNA | 2.2 | DNA (B, 5(PRIME)- D(CPGPCPGPAPAPTPTPCPGPCPG)-3(PRIME)) ... | SYNTHETIC DNA | P.PJURA *et al.* |
| 2BNA | 2.7 | DNA (B, 5(PRIME)-D(CPGPCPGPAPAPTPTPCPGPCPG)-3(PRIME)) (16 ...) | SYNTHETIC DNA | H.R.DREW,R.E.DICKERSON |
| 1BNA | 1.9 | DNA (B, 5(PRIME)-D(CPGPCPGPAPAPTPTPCPGPCPG)-3(PRIME)) (290 ...) | SYNTHETIC DNA | H.R.DREW,R.E.DICKERSON |
| 7BNA | 1.9 | DNA (B, 5(PRIME)-D(CPGPCPGPAPAPTPTPCPGPCPG)-3(PRIME)) (290 ...) | SYNTHETIC DNA | S.R.HOLBROOK *et al.* |
| 5BNA | 2.6 | DNA (B, 5-D(CPGPCPGPAPAPTPTPCPGPCPG)-3) COMPLEX WITH CISPLATIN | SYNTHETIC DNA | R.WING,P.PJURA *et al.* |
| 1D39 | 1.2 | DNA (Z, 5’-D(CPGPCPGPCPG)-3’) COPPER(II) CHLORIDE SOAKED | SYNTHETIC DNA | T.F.KAGAWA *et al.* |
| 1D41 | 1.3 | DNA (Z, 5’-D(M$^{5}$CPGPUPAPM$^{5}$CPGP)-3’) | SYNTHETIC DNA | G.ZHOU,P.S.HO |
| 1D40 | 1.3 | DNA (Z, 5’-D(M$^{5}$CPGPUPAPM$^{5}$CPGP)-3’) COPPER(II) CHLORIDE SOAKED | SYNTHETIC DNA | B.H.GEIERSTANGER *et al.* |
| 1ZNA | 1.6 | DNA (Z, 5-D(CPGPCPG)-3, HIGH SALT) | SYNTHETIC DNA | H.R.DREW,R.E.DICKERSON |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 351C | 1.6 | CYTOCHROME $C_{551}$ (OXIDIZED) | (PSEUDOMONAS AERUGINOSA) | Y.MATSUURA,T.TAKANO *et al.* |
| 451C | 1.6 | CYTOCHROME $C_{551}$ (REDUCED) | (PSEUDOMONAS AERUGINOSA) | Y.MATSUURA,T.TAKANO *et al.* |
| 155C | 2.5 | CYTOCHROME C550 | (PARACOCCUS ...) | R.TIMKOVICH |
| 3CPP | 1.9 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) - ... | (PSEUDOMONAS PUTIDA) | R.RAAG,T.L.POULOS |
| 4CPP | 2.11 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) - ... | (PSEUDOMONAS PUTIDA) | R.RAAG,T.L.POULOS |
| 5CPP | 2.08 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) - ... | (PSEUDOMONAS PUTIDA) | R.RAAG,T.L.POULOS |
| 6CPP | 1.9 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) - ... | (PSEUDOMONAS PUTIDA) | R.RAAG,T.L.POULOS |
| 7CPP | 2.0 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) - ... | (PSEUDOMONAS PUTIDA) | R.RAAG,T.L.POULOS |
| 8CPP | 2.1 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) - ... | (PSEUDOMONAS PUTIDA) | R.RAAG,T.L.POULOS |
| 1CP4 | 1.9 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) ... | (PSEUDOMONAS PUTIDA) | R.RAAG,T.L.POULOS |
| 2CPP | 1.63 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) ... | (PSEUDOMONAS PUTIDA) | T.L.POULOS |
| 3CP4 | 2.3 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) ... | (PSEUDOMONAS PUTIDA) ... | R.RAAG,T.L.POULOS |
| 4CP4 | 2.1 | CYTOCHROME P450CAM (CAMPHOR MONOOXYGENASE) (E.C.1.14.15.1) ... | (PSEUDOMONAS PUTIDA) ... | R.RAAG,T.L.POULOS |
| 4MDH | 2.5 | CYTOPLASMIC MALATE DEHYDROGENASE (E.C.1.1.1.37) | PORCINE (SUS SCROFA) ... | J.J.BIRKTOFT,L.J.BANASZAK |
| 1AAT | 2.8 | CYTOSOLIC ASPARTATE AMINOTRANSFERASE (E.C.2.6.1.1) COMPLEX ... | CHICKEN (GALLUS ...) | E.G.HARUTYUNYAN *et al.* |
| 2CP1 | N/A | CYTOTOXIC T-LYMPHOCYTE PROTEINASE I (CCP1) (MODEL) | MOUSE (MUS MUSCULUS) | M.MURPHY,M.N.G.JAMES |
| 256B | 1.4 | CYTROCHROME B562 (OXIDIZED) | (ESCHERICHIA COLI) | K.HAMADA,P.H.BETHGE *et al.* |
| 1PTE | 2.8 | D-ALANYL-D-ALANINE CARBOXYPEPTIDASE(SLASH)TRANSPEPTIDASE | (STREPTOMYCES R61) | J.A.KELLY,J.R.KNOX *et al.* |
| 2GBP | 1.9 | D-GALACTOSED-GLUCOSE BINDING PROTEIN (GGBP) | (ESCHERICHIA COLI ...) | N.K.VYAS,M.N.VYAS *et al.* |
| 1PGI | 3.5 | D-GLUCOSE 6-PHOSPHATE ISOMERASE (E.C.5.3.1.9) | PORCINE (SUS SCROFA) ... | H.MUIRHEAD |
| 3GPD | 3.5 | D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (E.C.1.2.1.12) | HUMAN (HOMO SAPIENS) ... | H.C.WATSON,J.C.CAMPBELL |
| 1GPD | 2.9 | D-GYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (E.C.1.2.1.12) | LOBSTER (HOMARUS ...) | D.MORAS,K.W.OLSEN *et al.* |
| 1XIA | 2.3 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) | (ARTHROBACTER, ...) | D.M.BLOW |
| 3XIA | 3.0 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) | (STREPTOMYCES ...) | G.FARBER,G.PETSKO |
| 7XIA | 1.9 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) | (STREPTOMYCES ...) | H.L.CARRELL,J.P.GLUSKER |
| 6XIA | 1.65 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) (GLUCOSE ISOMERASE) | (STREPTOMYCES ALBUS) | Z.DAUTER,H.TERRY *et al.* |
| 8XIA | 1.9 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) COMPLEX WITH D-XYLOSE | (STREPTOMYCES ...) | H.L.CARRELL,J.P.GLUSKER |
| 9XIA | 1.9 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) COMPLEX WITH INACTIVATOR | (STREPTOMYCES ...) | H.L.CARRELL,J.P.GLUSKER |
| 1XIM | 2.2 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) COMPLEXED WITH XYLITOL-CO | (ACTINOPLANES ...) | N.T.MRABET *et al.* |
| 2XIM | 2.3 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) MUTANT WITH LYS 253 ... | (ACTINOPLANES ...) | N.T.MRABET *et al.* |
| 3XIM | 2.3 | D-XYLOSE ISOMERASE (E.C.5.3.1.5) MUTANT WITH LYS 309 ... | (ACTINOPLANES ...) | N.T.MRABET *et al.* |
| 4XIA | 2.3 | D-XYLOSE ISOMERASE (E.C.5.3.1.5), D-SORBITOL COMPLEX | (ARTHROBACTER, ...) | K.HENRICK *et al.* |
| 5XIA | 2.5 | D-XYLOSE ISOMERASE (E.C.5.3.1.5), XYLITOL COMPLEX | (ARTHROBACTER, ...) | K.HENRICK *et al.* |
| 1DFN | 1.9 | DEFENSIN HNP-3 | HUMAN (HOMO SAPIENS) ... | C.P.HILL,J.YEE *et al.* |
| 1DHL | N/A | DELTA HEMOLYSIN (MODEL) | (STAPHYLOCOCCUS AUREUS) | G.RAGHUNATHAN,H.R.GUY |
| 2DHL | N/A | DELTA HEMOLYSIN (MODEL) | (STAPHYLOCOCCUS AUREUS) | G.RAGHUNATHAN,H.R.GUY |
| 3DHL | N/A | DELTA HEMOLYSIN (MODEL) | (STAPHYLOCOCCUS AUREUS) | G.RAGHUNATHAN,H.R.GUY |
| 4TS1 | 2.5 | DES-(ILE 318-ARG 417)-TYROSYL-TRANSFER RNA SYNTHETASE ... | (BACILLUS ...) | P.BRICK,D.M.BLOW |
| 1C5A | N/A | DES-$ARG^{74}$-COMPLEMENT C5A | PIG (SUS SCROFA ...) | M.P.WILLIAMSON *et al.* |
| 2INS | 2.5 | DES-PHE B1 INSULIN | BOVINE (BOS TAURUS) | G.D.SMITH,W.L.DUAX *et al.* |
| 4TGF | N/A | DES-$VAL^{1}$,$VAL^{2}$-TRANSFORMING GROWTH FACTOR ALPHA (TGFA) | HUMAN (HOMO SAPIENS) | T.P.KLINE,F.K.BROWN *et al.* |
| 8DFR | 1.7 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) | CHICKEN (GALLUS ...) | D.A.MATTHEWS *et al.* |
| 2DHF | 2.3 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) (DHFR) COMPLEX WITH ... | HUMAN (HOMO SAPIENS) ... | J.F.DAVIES II,J.KRAUT |
| 7DFR | 2.5 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) (DHFR) COMPLEX WITH ... | (ESCHERICHIA COLI) ... | C.BYSTROFF *et al.* |
| 1DHF | 2.3 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) (DHFR) COMPLEX WITH FOLATE | HUMAN (HOMO SAPIENS) ... | J.F.DAVIES II,J.KRAUT |
| 6DFR | 2.4 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) (DHFR) COMPLEX WITH $NADP^{+}$ | (ESCHERICHIA COLI) ... | C.BYSTROFF *et al.* |
| 1DRF | 2.0 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) COMPLEX WITH FOLATE | HUMAN (HOMO SAPIENS) ... | C.OEFNER,A.D'ARCY *et al.* |
| 4DFR | 1.7 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) COMPLEX WITH METHOTREXATE | (ESCHERICHIA COLI ...) | D.J.FILMAN *et al.* |
| 3DFR | 1.7 | DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) COMPLEX WITH NADPH AND ... | (LACTOBACILLUS ...) | D.J.FILMAN *et al.* |
| 1D37 | 1.8 | DNA (5'-(CPGPAPTPCPGP)-3') COMPLEX WITH ... | SYNTHETIC DNA | Y.-G.GAO,A.H.-J.WANG |
| 1D38 | 1.7 | DNA (5'-(CPGPAPTPCPGP)-3') COMPLEX WITH IDARUBICIN ... | SYNTHETIC DNA | Y.-G.GAO,A.H.-J.WANG |
| 1D36 | 1.5 | DNA (5'-(CPGPTPAPCPGP)-3') COMPLEX WITH MAR70 | SYNTHETIC DNA | Y.-G.GAO,Y.-C.LIAW *et al.* |
| 1D35 | 1.3 | DNA (5'-(CPGPTP$^{NH2}$APCPGP)-3') COMPLEX WITH MAR70 | SYNTHETIC DNA | Y.-G.GAO,Y.-C.LIAW *et al.* |
| 1D18 | N/A | DNA (5'-D(CPAPTPGPCPAPTPGP)-3') | SYNTHETIC DNA | J.D.BALEJA,B.D.SYKES |
| 5DNB | 1.4 | DNA (5'-D(CPCPAPAPCPGPTPTPGPGP)-3') | SYNTHETIC DNA | G.G.PRIVE,K.YANAGI *et al.* |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 7CAT | 2.5 | CATALASE (E.C.1.11.1.6) | BEEF (BOS TAURUS) LIVER | M.R.N.MURTHY *et al.* |
| 8CAT | 2.5 | CATALASE (E.C.1.11.1.6) | BEEF (BOS TAURUS) LIVER | M.R.N.MURTHY *et al.* |
| 1MHU | N/A | CD-7 METALLOTHIONEIN-2 (ALPHA DOMAIN) (NMR) | HUMAN (HOMO SAPIENS) ... | W.BRAUN,B.A.MESSERLE *et al.* |
| 1MRT | N/A | CD-7 METALLOTHIONEIN-2 (ALPHA DOMAIN) (NMR) | RAT (RATTUS RATTUS) LIVER | W.BRAUN,P.SCHULTZE *et al.* |
| 2MHU | N/A | CD-7 METALLOTHIONEIN-2 (BETA DOMAIN) (NMR) | HUMAN (HOMO SAPIENS) ... | W.BRAUN,B.A.MESSERLE *et al.* |
| 2MRT | N/A | CD-7 METALLOTHIONEIN-2 (BETA DOMAIN) (NMR) | RAT (RATTUS RATTUS) LIVER | W.BRAUN,P.SCHULTZE *et al.* |
| 1MRB | N/A | CD-7 METALLOTHIONEIN-2A (ALPHA DOMAIN) (NMR) | RABBIT (ORYCTOLAGUS ...) | W.BRAUN,A.ARSENIEV *et al.* |
| 2MRB | N/A | CD-7 METALLOTHIONEIN-2A (BETA DOMAIN) (NMR) | RABBIT (ORYCTOLAGUS ...) | W.BRAUN,A.ARSENIEV *et al.* |
| 1CD4 | 2.3 | CD4 (1 - 183 PLUS ASP - THR) (D1D2) (N-TERMINAL FRAGMENT OF ...) | RECOMBINANT HUMAN ... | S.-E.RYU,P.D.KWONG *et al.* |
| 2CD4 | 2.4 | CD4(1-182) (N-TERMINAL FRAGMENT OF CD4 CONSISTING OF ...) | HUMAN (HOMO SAPIENS) ... | J.WANG,Y.YAN *et al.* |
| 3CBH | 2.0 | CELLOBIOHYDROLASE II CORE PROTEIN (E.C.3.2.1.91) (CBHII) | (TRICHODERMA REESEI) | T.A.JONES,J.ROUVINEN |
| 2CHY | 2.7 | CHEY (MUTANT WITH SER 56 REPLACED BY CYS) (S56C) | (SALMONELLA ...) | J.M.MOTTONEN *et al.* |
| 2CLA | 2.35 | CHLORAMPHENICOL ACETYLTRANSFERASE (E.C.2.3.1.28) ($CAT_{III}$) ... | (ESCHERICHIA COLI), ... | M.R.GIBBS *et al.* |
| 1COX | 1.8 | CHOLESTEROL OXIDASE (E.C.1.1.3.6) | (BREVIBACTERIUM ...) | A.VRIELINK,L.F.LLOYD *et al.* |
| 1C4S | 3.0 | CHONDROITIN-4-SULFATE (AN ALTERNATING COPOLYMER OF ...) | BOVINE (BOS TAURUS) ... | S.ARNOTT |
| 2C4S | 3.0 | CHONDROITIN-4-SULFATE (AN ALTERNATING COPOLYMER OF ...) | SWARM RAT ... | S.ARNOTT |
| 1CMS | 2.3 | CHYMOSIN B (FORMERLY KNOWN AS RENNIN) (E.C.3.4.23.4) | BOVINE (BOS TAURUS) ... | G.L.GILLILAND *et al.* |
| 4CMS | 2.2 | CHYMOSIN B (FORMERLY KNOWN AS RENNIN) (E.C.3.4.23.4) | BOVINE (BOS TAURUS) ... | M.NEWMAN,C.FRAZAO *et al.* |
| 2CI2 | 2.0 | CHYMOTRYPSIN INHIBITOR 2 (CI-2) | BARLEY (HORDEUM ...) | C.A.MCPHALEN,M.N.G.JAMES |
| 1CHG | 2.5 | CHYMOTRYPSINOGEN A | COW (BOS TAURUS) | S.T.FREER,J.KRAUT *et al.* |
| 2CGA | 1.8 | CHYMOTRYPSINOGEN A | BOVINE (BOS TAURUS) ... | D.WANG,W.BODE,R.HUBER |
| 5CSC | 2.8 | CITRATE SYNTHASE (E.C.4.1.3.7) | CHICKEN (GALLUS ...) | D.-I.LIAO,M.KARPUSAS *et al.* |
| 2CTS | 2.0 | CITRATE SYNTHASE (E.C.4.1.3.7) - (COA, CITRATE) COMPLEX | PIG (SUS SCROFA) HEART | S.REMINGTON *et al.* |
| 3CTS | 1.7 | CITRATE SYNTHASE (E.C.4.1.3.7) - (COA, CITRATE) COMPLEX | CHICKEN (GALLUS ...) | S.REMINGTON *et al.* |
| 1CTS | 2.7 | CITRATE SYNTHASE (E.C.4.1.3.7) - CITRATE COMPLEX | PIG (SUS SCROFA) HEART | S.REMINGTON *et al.* |
| 6CTS | 2.5 | CITRATE SYNTHASE (E.C.4.1.3.7) - CITRYLTHIOETHER - COENZYME ... | CHICKEN (GALLUS ...) | M.KARPUSAS *et al.* |
| 4CTS | 2.9 | CITRATE SYNTHASE (E.C.4.1.3.7) - OXALOACETATE COMPLEX | PIG (SUS SCROFA) HEART | S.REMINGTON *et al.* |
| 4CSC | 1.9 | CITRATE SYNTHASE (E.C.4.1.3.7)- D-MALATE - ACETYL COENZYME A ... | CHICKEN (GALLUS ...) | M.KARPUSAS,D.HOLLAND *et al.* |
| 2CSC | 1.7 | CITRATE SYNTHASE (E.C.4.1.3.7)- D-MALATE - CARBOXYMETHYL ... | CHICKEN (GALLUS ...) | M.KARPUSAS,D.HOLLAND *et al.* |
| 3CSC | 1.9 | CITRATE SYNTHASE (E.C.4.1.3.7)- L-MALATE - ACETYL COENZYME A ... | CHICKEN (GALLUS ...) | M.KARPUSAS,D.HOLLAND *et al.* |
| 1CSC | 1.7 | CITRATE SYNTHASE (E.C.4.1.3.7)- L-MALATE - CARBOXYMETHYL ... | CHICKEN (GALLUS ...) | M.KARPUSAS,D.HOLLAND *et al.* |
| 5CTS | 1.9 | CITRATE SYNTHASE (E.C.4.1.3.7)- OXALOACETATE - CARBOXYMETHYL ... | CHICKEN (GALLUS ...) | M.KARPUSAS *et al.* |
| 1CCD | 3.0 | CLARA CELL 17 KDA PROTEIN | RAT (RATTUS RATTUS) ... | T.C.UMLAND *et al.* |
| 2CNA | 2.0 | CONCANAVALIN A | JACK BEAN (CANAVALIA ...) | G.N.REEKE JUNIOR *et al.* |
| 3CNA | 2.4 | CONCANAVALIN A | JACK BEAN (CANAVALIA ...) | K.D.HARDMAN,C.F.AINSWORTH |
| 1CN1 | 3.2 | CONCANAVALIN A (DEMETALLIZED) | JACK BEAN (CANAVALIA ...) | M.SHOHAM,A.YONATH *et al.* |
| 1CRN | 1.5 | CRAMBIN | ABYSSINIAN CABBAGE ... | W.A.HENDRICKSON *et al.* |
| 1CRO | 2.2 | CRO REPRESSOR | BACTERIOPHAGE (LAMBDA) | D.H.OHLENDORF *et al.* |
| 4CRO | 3.9 | CRO REPRESSOR | BACTERIOPHAGE (LAMBDA) | R.G.BRENNAN *et al.* |
| 2SOD | 2.0 | CU,ZN SUPEROXIDE DISMUTASE (E.C.1.15.1.1) | BOVINE (BOS TAURUS) ... | J.A.TAINER *et al.* |
| 1CBP | 2.5 | CUCUMBER BASIC PROTEIN | CUCUMBER (CUCUMIS ...) | J.M.GUSS |
| 3B5C | 1.5 | CYTOCHROME B5 (OXIDIZED) | BOVINE (BOS TAURUS) ... | F.S.MATHEWS,R.C.E.DURLEY |
| 1CCR | 1.5 | CYTOCHROME C | RICE EMBRYOS (ORYZA ...) | H.OCHI,Y.HATA *et al.* |
| 1YCC | 1.23 | CYTOCHROME C (ISOZYME 1) (REDUCED) | BAKER'S YEAST ... | G.V.LOUIE,G.D.BRAYER |
| 3CYT | 1.8 | CYTOCHROME C (OXIDIZED) | ALBACORE TUNA ... | T.TAKANO |
| 5CYT | 1.5 | CYTOCHROME C (REDUCED) | ALBACORE TUNA ... | T.TAKANO |
| 2CYP | 1.7 | CYTOCHROME C PEROXIDASE (E.C.1.11.1.5) (FERROCYTOCHROME C ...) | BAKER'S YEAST ... | B.C.FINZEL *et al.* |
| 2CCY | 1.67 | CYTOCHROME C(PRIME) | (RHODOSPIRILLUM ...) | B.C.FINZEL,P.C.WEBER *et al.* |
| 1C53 | 1.8 | CYTOCHROME C-553 | (DESULFOVIBRIO ...) | A.NAKAGAWA,Y.HIGUCHI *et al.* |
| 1C2R | 2.5 | CYTOCHROME $C_2$ | (RHODOBACTER CAPSULATUS) | M.M.BENNING *et al.* |
| 2C2C | 2.0 | CYTOCHROME $C_2$ (OXIDIZED) | (RHODOSPIRILLUM RUBRUM) | G.BHATIA,B.C.FINZEL *et al.* |
| 3C2C | 1.68 | CYTOCHROME $C_2$ (REDUCED) | (RHODOSPIRILLUM RUBRUM) | G.BHATIA,B.C.FINZEL *et al.* |
| 1CY3 | 2.5 | CYTOCHROME $C_3$ | (DESULFOVIBRIO ...) | R.HASER,M.FREY,F.PAYAN |
| 2CDV | 1.8 | CYTOCHROME $C_3$ | (DESULFOVIBRIO ...) | Y.HIGUCHI,M.KUSUNOKI *et al.* |
| 1CC5 | 2.5 | CYTOCHROME $C_5$ (OXIDIZED) | (AZOTOBACTER VINELANDII) | C.D.STOUT,D.C.CARTER |

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 1REI | 2.0 | BENCE-JONES IMMUNOGLOBULIN REI VARIABLE PORTION | HUMAN (HOMO SAPIENS) | O.EPP,E.E.LATTMAN *et al.* |
| 2RHE | 1.6 | BENCE-JONES PROTEIN (LAMBDA, VARIABLE DOMAIN) | HUMAN (HOMO SAPIENS) ... | W.FUREY JUNIOR *et al.* |
| 1BJL | 3.0 | BENCE-JONES PROTEIN LOC (CRYSTALLIZED FROM AMMONIUM SULFATE) | HUMAN (HOMO SAPIENS) | M.SCHIFFER,Z.-B.XU *et al.* |
| 2BJL | 2.8 | BENCE-JONES PROTEIN LOC (CRYSTALLIZED FROM DISTILLED WATER) | HUMAN (HOMO SAPIENS) | M.SCHIFFER,Z.-B.XU *et al.* |
| 4PTP | 1.34 | BETA TRYPSIN, DIISOPROPYLPHOSPHORYL INHIBITED (E.C.3.4.21.4) | BOVINE (BOS TAURUS) ... | J.L.CHAMBERS *et al.* |
| 3BLM | 2.0 | BETA-LACTAMASE (E.C.3.5.2.6) | (STAPHYLOCOCCUS ...) | O.HERZBERG,J.MOULT |
| 2BLM | 2.0 | BETA-LACTAMASE (PENICILLINASE) (E.C.3.5.2.6) | (BACILLUS ...) | P.C.MOEWS,J.R.KNOX *et al.* |
| 3PTB | 1.7 | BETA-TRYPSIN (BENZAMIDINE INHIBITED) AT PH7 (E.C.3.4.21.4) | BOVINE (BOS TAURUS) ... | W.BODE,P.SCHWAGER *et al.* |
| 1TPP | 1.4 | BETA-TRYPSIN (E.C.3.4.21.4) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | J.WALTER,W.BODE,R.HUBER |
| 2PTC | 1.9 | BETA-TRYPSIN (E.C.3.4.21.4) COMPLEX WITH PANCREATIC TRYPSIN ... | BOVINE (BOS TAURUS) ... | R.HUBER,J.DEISENHOFER |
| 1TLD | 1.5 | BETA-TRYPSIN (ORTHORHOMBIC) AT PH 5.3 (E.C.3.4.21.4) | BOVINE (BOS TAURUS) ... | H.D.BARTUNIK *et al.* |
| 1TPO | 1.7 | BETA-TRYPSIN (ORTHORHOMBIC) AT PH5.0 (E.C.3.4.21.4) | BOVINE (BOS TAURUS) ... | W.BODE,J.WALTER,R.HUBER |
| 1BBP | 2.0 | BILIN BINDING PROTEIN (BBP) | CABBAGE BUTTERFLY ... | R.HUBER,M.SCHNEIDER *et al.* |
| 4ICB | 1.6 | BOVINE CALBINDIN D9K (MINOR A FORM) FORMERLY CALLED ... | BOVINE (BOS TAURUS) ... | L.A.SVENSSON |
| 1BN2 | 2.8 | BOVINE NEUROPHYSIN II COMPLEX WITH P-IODO-PHE-TYR AMIDE | BOVINE (BOS TAURUS) ... | J.P.ROSE,B.-C.WANG |
| 7PTI | 1.6 | BOVINE PANCREATIC TRYPSIN INHIBITOR (BPTI) MUTANT (CYS 30 ...) | BOVINE (BOS TAURUS) ... | C.EIGENBROT,M.RANDAL *et al.* |
| 8PTI | 1.8 | BOVINE PANCREATIC TRYPSIN INHIBITOR (BPTI) MUTANT (TYR 35 ...) | BOVINE (BOS TAURUS) ... | D.HOUSSET,K.-S.KIM *et al.* |
| 6PTI | 1.7 | BOVINE PANCREATIC TRYPSIN INHIBITOR (BPTI,CRYSTAL FORM III) | BOVINE (BOS TAURUS) ... | A.WLODAWER |
| 1PI2 | 2.5 | BOWMAN-BIRK PROTEINASE INHIBITOR PI-II | TRACY SOYBEAN ... | P.CHEN,J.ROSE,B.C.WANG |
| 1CPK | 2.7 | C-AMP-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) ... | RECOMBINANT MOUSE ... | D.R.KNIGHTON,J.ZHENG *et al.* |
| 5P21 | 1.35 | C-H-RAS P21 PROTEIN (AMINO ACIDS 1 - 166) COMPLEX WITH ... | HUMAN (HOMO SAPIENS) ... | E.F.PAI *et al.* |
| 2P21 | 2.2 | C-H-RAS P21 PROTEIN CATALYTIC DOMAIN | TRANSFORMED ... | S.-H.KIM |
| 3P21 | 2.2 | C-H-RAS P21 PROTEIN CATALYTIC DOMAIN (MUTANT WITH GLY 12 ...) | TRANSFORMED ... | S.-H.KIM |
| 1POM | 0.0 | C-MYB PROTO-ONCOGENE DNA-BINDING DOMAIN REPEAT 3 (MODEL) | CHICKEN (GALLUS ...) | T.J.GIBSON |
| 1CBH | N/A | C-TERMINAL DOMAIN OF CELLOBIOHYDROLASE I (CT-CBH I) ... | CHEMICALLY ... | G.M.CLORE,A.M.GRONENBORN |
| 2CBH | N/A | C-TERMINAL DOMAIN OF CELLOBIOHYDROLASE I (CT-CBH I) ... | SYNTHETIC ... | G.M.CLORE,A.M.GRONENBORN |
| 1CDP | 1.6 | CADMIUM-SUBSTITUTED CALCIUM-BINDING PARVALBUMIN B | CARP (CYPRINUS CARPIO) | A.L.SWAIN *et al.* |
| 4CPV | 1.5 | CALCIUM-BINDING PARVALBUMIN (PI=4.25) | CARP (CYPRINUS CARPIO) | V.D.KUMAR,L.LEE *et al.* |
| 5CPV | 1.6 | CALCIUM-BINDING PARVALBUMIN B | CARP (CYPRINUS CARPIO) | A.L.SWAIN *et al.* |
| 3ICB | 2.3 | CALCIUM-BINDING PROTEIN (VITAMIN D-DEPENDENT, MINOR A FORM) ... | BOVINE (BOS TAURUS) ... | D.M.E.SZEBENYI,K.MOFFAT |
| 1PP2 | 2.5 | CALCIUM-FREE PHOSPHOLIPASE $A_2$ (E.C.3.1.1.4) | WESTERN DIAMONDBACK ... | S.BRUNIE,P.B.SIGLER |
| 3CLN | 2.2 | CALMODULIN | RAT (RATTUS RATTUS) ... | Y.S.BABU,C.E.BUGG *et al.* |
| 4CLN | 2.2 | CALMODULIN | (DROSOPHILA ...) | D.A.TAYLOR,J.S.SACK *et al.* |
| 1TRC | 3.6 | CALMODULIN ($TR_2C$ FRAGMENT COMPRISING RESIDUES 78 - 148 OF ...) | BULL (BOS TAURUS) TESTES | L.SJOLIN *et al.* |
| 1APK | N/A | CAMP DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) TYPE I, DOMAIN ... | BOVINE (BOS ...) | I.T.WEBER |
| 1BPK | N/A | CAMP DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) TYPE I, DOMAIN ... | BOVINE (BOS ...) | I.T.WEBER |
| 2APK | N/A | CAMP DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) TYPE II, DOMAIN ... | BOVINE (BOS ...) | I.T.WEBER |
| 2BPK | N/A | CAMP DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) TYPE II, DOMAIN ... | BOVINE (BOS ...) | I.T.WEBER |
| 1CAP | 3.0 | CAPSULAR POLYSACCHARIDE | (ESCHERICHIA COLI) ... | S.ARNOTT |
| 2CAB | 2.0 | CARBONIC ANHYDRASE FORM B (CARBONATE DEHYDRATASE) (E.C.4.2.1.1) | HUMAN (HOMO SAPIENS) ... | K.K.KANNAN *et al.* |
| 4CAC | 2.2 | CARBONIC ANHYDRASE FORM C (CARBONATE DEHYDRATASE II) ... | HUMAN (HOMO SAPIENS) ... | M.LINDHAL,D.HABASH *et al.* |
| 5CAC | 2.2 | CARBONIC ANHYDRASE FORM C (CARBONATE DEHYDRATASE II) ... | HUMAN (HOMO SAPIENS) ... | M.LINDHAL,D.HABASH *et al.* |
| 1CA2 | 2.0 | CARBONIC ANHYDRASE II (CARBONATE DEHYDRATASE) (HCA II) ... | HUMAN (HOMO SAPIENS) ... | A.E.ERIKSSON *et al.* |
| 2CA2 | 1.9 | CARBONIC ANHYDRASE II (CARBONATE DEHYDRATASE) (HCA II) ... | HUMAN (HOMO SAPIENS) ... | A.E.ERIKSSON *et al.* |
| 3CA2 | 2.0 | CARBONIC ANHYDRASE II (CARBONATE DEHYDRATASE) (HCA II) ... | HUMAN (HOMO SAPIENS) ... | A.E.ERIKSSON *et al.* |
| 6CPA | 2.0 | CARBOXYPEPTIDASE A (E.C.3.4.17.1) COMPLEX WITH THE ... | BOVINE (BOS TAURUS) ... | H.KIM,W.N.LIPSCOMB |
| 5CPA | 1.54 | CARBOXYPEPTIDASE $A_{ALPHA}$ (COX) (E.C.3.4.17.1) | BOVINE (BOS TAURUS) ... | W.N.LIPSCOMB |
| 1CBX | 2.0 | CARBOXYPEPTIDASE $A_{ALPHA}$ (COX) (E.C.3.4.17.1) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | S.MANGANI,P.CARLONI *et al.* |
| 3CPA | 2.0 | CARBOXYPEPTIDASE $A_{ALPHA}$ (COX) (E.C.3.4.17.1) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | W.N.LIPSCOMB |
| 4CPA | 2.5 | CARBOXYPEPTIDASE $A_{ALPHA}$ (COX) (E.C.3.4.17.1) COMPLEX WITH ... | BOVINE (BOS TAURUS) ... | W.N.LIPSCOMB,D.C.REES |
| 1CPB | 2.8 | CARBOXYPEPTIDASE B (E.C.3.4.12.3) FRACTION II | BOVINE (BOS TAURUS) ... | M.F.SCHMID,J.R.HERRIOTT |
| 1CDT | 2.5 | CARDIOTOXIN $V_4^{II}$ (TOXIN III) | (NAJA MOSSAMBICA ...) | B.REES,A.BILWES *et al.* |
| 3GAP | 2.5 | CATABOLITE GENE ACTIVATOR PROTEIN - CYCLIC AMP COMPLEX (CAP) | (ESCHERICHIA COLI) | I.T.WEBER,T.A.STEITZ |
| 2GAP | N/A | CATABOLITE GENE ACTIVATOR PROTEIN - DNA COMPLEX (MODEL) | (ESCHERICHIA COLI) | I.T.WEBER,T.A.STEITZ |
| 4CAT | 3.0 | CATALASE (E.C.1.11.1.6) | (PENICILLIUM VITALE) | B.K.VAINSHTEIN *et al.* |

| Id | Å | Molecule | Source | Depositors |
| --- | --- | --- | --- | --- |
| 1CGJ | 2.3 | ALPHA-CHYMOTRYPSINOGEN COMPLEX WITH HUMAN PANCREATIC ... | BOVINE (BOS TAURUS) ... | H.J.HECHT *et al.* |
| 1DTX | 2.2 | ALPHA-DENDROTOXIN | GREEN MAMBA ... | T.SKARZYNSKI |
| 1COH | 2.9 | ALPHA-FERROUS-CARBONMONOXY, BETA-COBALTOUS-DEOXY HEMOGLOBIN ... | HUMAN (HOMO SAPIENS) | B.LUISI |
| 1ALC | 1.7 | ALPHA-LACTALBUMIN | BABOON (PAPIO ...) | K.R.ACHARYA *et al.* |
| 2ALP | 1.7 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) | (LYSOBACTER ENZYMOGENES) | M.FUJINAGA *et al.* |
| 1P07 | 2.25 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) (MUTANT WITH MET 192 ...) | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P08 | 2.25 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) (MUTANT WITH MET 192 ...) | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P09 | 2.20 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) (MUTANT WITH MET 213 ...) | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P10 | 2.25 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) (MUTANT WITH MET 213 ...) | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P01 | 2.0 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) COMPLEX WITH ... | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P02 | 2.0 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) COMPLEX WITH ... | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P03 | 2.15 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) COMPLEX WITH ... | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P04 | 2.55 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) COMPLEX WITH ... | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P05 | 2.10 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) COMPLEX WITH ... | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1P06 | 2.34 | ALPHA-LYTIC PROTEASE (E.C.3.4.21.12) COMPLEX WITH ... | (LYSOBACTER ...) | R.BONE,D.A.AGARD |
| 1TPA | 1.9 | ANHYDRO-TRYPSIN (E.C.3.4.21.4) COMPLEX WITH PANCREATIC ... | BOVINE (BOS TAURUS) ... | R.HUBER,W.BODE *et al.* |
| 1ATF | N/A | ANTIFREEZE POLYPEPTIDE (AFP) | WINTER FLOUNDER ... | K.-C.CHOU |
| 2GD1 | 2.5 | APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (E.C.1.2.1.12) | (BACILLUS ...) | T.SKARZYNSKI,A.J.WONACOTT |
| 4GPD | 2.8 | APO-D-GYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE (E.C.1.2.1.12) | LOBSTER (HOMARUS ...) | J.P.GRIFFITH,S.SONG *et al.* |
| 5DFR | 2.3 | APO-DIHYDROFOLATE REDUCTASE (E.C.1.5.1.3) (DHFR) | (ESCHERICHIA COLI) ... | C.BYSTROFF,J.KRAUT |
| 1LDB | 2.8 | APO-L-LACTATE DEHYDROGENASE (E.C.1.1.1.27) | (BACILLUS ...) | K.PIONTEK,M.G.ROSSMANN |
| 2LDX | 2.96 | APO-LACTATE DEHYDROGENASE (E.C.1.1.1.27), ISOENZYME $C_4$ | MOUSE (MUS MUSCULUS) ... | J.P.GRIFFITH,M.G.ROSSMANN |
| 5ADH | 2.9 | APO-LIVER ALCOHOL DEHYDROGENASE (E.C.1.1.1.1) COMPLEX WITH ... | HORSE (EQUUS ...) | H.EKLUND,T.A.JONES |
| 8ADH | 2.4 | APO-LIVER ALCOHOL DEHYDROGENASE (E.C.1.1.99.8) | HORSE (EQUUS ...) | T.A.JONES,H.EKLUND |
| 2PCY | 1.8 | APO-PLASTOCYANIN (PH 6.0) | POPLAR (POPULUS ...) | T.P.J.GARRETT *et al.* |
| 1APD | N/A | APOLIPOPROTEIN D (MODEL) | HUMAN (HOMO SAPIENS) | M.C.PEITSCH,M.S.BOGUSKI |
| 1TRM | 2.3 | $ASN^{102}$TRYPSIN (E.C.3.4.21.4) (MUTANT WITH ASP 102 REPLACED ...) | RAT (RATTUS RATTUS) | S.SPRANG,T.STANDING *et al.* |
| 2TRM | 2.8 | $ASN^{102}$TRYPSIN (E.C.3.4.21.4) (MUTANT WITH ASP 102 REPLACED ...) | RAT (RATTUS RATTUS) | R.M.STROUD,J.FINER-MOORE |
| 3AAT | 2.8 | ASPARTATE AMINOTRANSFERASE (E.C.2.6.1.1) (MUTANT WITH ARG ...) | (ESCHERICHIA COLI) | A.T.DANISHEFSKY *et al.* |
| 2AAT | 2.8 | ASPARTATE AMINOTRANSFERASE (E.C.2.6.1.1) MUTANT K258A ... | (ESCHERICHIA COLI) | D.SMITH,S.ALMO *et al.* |
| 1AT1 | 2.8 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | J.E.GOUAUX,W.N.LIPSCOMB |
| 2AT1 | 2.8 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | J.E.GOUAUX,W.N.LIPSCOMB |
| 2ATC | 3.0 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | R.B.HONZATKO *et al.* |
| 3AT1 | 2.8 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | J.E.GOUAUX,W.N.LIPSCOMB |
| 4AT1 | 2.6 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | R.C.STEVENS *et al.* |
| 5AT1 | 2.6 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | R.C.STEVENS *et al.* |
| 6AT1 | 2.6 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | R.C.STEVENS *et al.* |
| 7AT1 | 2.8 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | J.E.GOUAUX *et al.* |
| 8AT1 | 2.8 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | J.E.GOUAUX *et al.* |
| 8ATC | 2.5 | ASPARTATE CARBAMOYLTRANSFERASE (ASPARTATE TRANSCARBAMYLASE) ... | (ESCHERICHIA COLI) | H.KE,W.N.LIPSCOMB *et al.* |
| 1ATX | N/A | ATX IA (NMR, 8 STRUCTURES) | SEA ANEMONE ... | M.BILLETER,H.WIDMER *et al.* |
| 1PPT | 1.37 | AVIAN PANCREATIC POLYPEPTIDE | TURKEY (MELEAGRIS ...) | T.L.BLUNDELL *et al.* |
| 1AZU | 2.7 | AZURIN | (PSEUDOMONAS AERUGINOSA) | E.T.ADMAN,L.C.SIEKER *et al.* |
| 2AZA | 1.8 | AZURIN (OXIDIZED) | (ALCALIGENES ...) | E.N.BAKER,G.E.NORRIS |
| 1YEB | 1.95 | B-2036 COMPOSITE CYTOCHROME C (REDUCED STATE) | BAKER'S YEAST ... | M.E.P.MURPHY,G.D.BRAYER |
| 1BD1 | 1.6 | B-DNA-5(PRIME)-D(CPCPAPGPGPCPCPTPGPG)-3(PRIME) | SYNTHETIC DNA | U.HEINEMANN |
| 3BCL | 1.9 | BACTERIOCHLOROPHYLL-A PROTEIN | (PROSTHECOCHLORIS ...) | D.TRONRUD,M.F.SCHMID *et al.* |
| 1BRD | 3.5 | BACTERIORHODOPSIN | (HALOBACTERIUM HALOBIUM) | R.HENDERSON *et al.* |
| 1RNB | 1.9 | BARNASE (G SPECIFIC ENDONUCLEASE) COMPLEXED WITH ... | RECOMBINANT FORM ... | J.JANIN,S.BAUDET |
| 2FGF | 1.77 | BASIC FIBROBLAST GROWTH FACTOR | HUMAN (HOMO SAPIENS) ... | J.ZHANG,S.R.SPRANG |
| 3FGF | 1.6 | BASIC FIBROBLAST GROWTH FACTOR (HBFGF) | HUMAN (HOMO SAPIENS) ... | A.E.ERIKSSON,B.W.MATTHEWS |
| 9PTI | 1.22 | BASIC PANCREATIC TRYPSIN INHIBITOR (MET 52 OXIDIZED) | BOVINE (BOS TAURUS) ... | C.EIGENBROT,M.RANDAL *et al.* |
| 2BDS | N/A | BDS-I (NMR, 42 SIMULATED ANNEALING STRUCTURES) | SEA ANEMONE ... | G.M.CLORE *et al.* |
| 1BDS | N/A | BDS-I (NMR, MINIMIZED MEAN STRUCTURE) | SEA ANEMONE ... | G.M.CLORE *et al.* |
| 1BMV | 3.0 | BEAN POD MOTTLE VIRUS (MIDDLE COMPONENT) | BOUNTIFUL BEAN | J.E.JOHNSON |

# Appendix 1: Available Protein Data Bank Models

| Id | Å | Molecule | Source | Depositors |
|---|---|---|---|---|
| 3HVP | 2.8 | (ABA$^{67,95}$)-HIV-1 PROTEASE (SF2 ISOLATE) | SYNTHETIC ENZYME ... | A.WLODAWER *et al.* |
| 1XY2 | 1.20 | 1 BETA-MERCAPTOPROPIONATE-OXYTOCIN (DRY FORM) | SYNTHETIC | S.COOPER *et al.* |
| 1XY1 | 1.04 | 1 BETA-MERCAPTOPROPIONATE-OXYTOCIN (WET FORM) | SYNTHETIC | J.HUSAIN *et al.* |
| 1HCC | N/A | 16TH COMPLEMENT CONTROL PROTEIN (CCP) OF FACTOR H | HUMAN (HOMO SAPIENS) ... | D.G.NORMAN *et al.* |
| 1PPD | 2.0 | 2-HYDROXYETHYLTHIOPAPAIN (E.C.3.4.22.2)- CRYSTAL FORM D | PAPAYA (CARICA ...) | J.N.JANSONIUS |
| 1KGA | 3.5 | 2-KETO-3-DEOXY-6-PHOSPHOGLUCONATE (KDPG) ALDOLASE (E.C.4.1.2.14) | (PSEUDOMONAS PUTIDA) | A.TULINSKY |
| 3INS | 1.5 | 2ZN-INSULIN (JOINT X-RAY AND NEUTRON REFINEMENT) | PIG (SUS SCROFA) | A.WLODAWER,H.SAVAGE |
| 1ZNF | N/A | 31ST ZINC FINGER FROM XFIN (XFIN-31) (37 MODELS) | CHEMICALLY ... | M.S.LEE,G.P.GIPPERT *et al.* |
| 1HSD | 2.6 | 3ALPHA,20BETA-HYDROXYSTEROID DEHYDROGENASE (HOLO FORM) | (STREPTOMYCES ...) | D.GHOSH,W.L.DUAX |
| 4FAB | 2.7 | 4-4-20 (IGG2A$_{KAPPA}$) FAB FRAGMENT - FLUORESCEIN (DIANION) ... | MOUSE (MUS MUSCULUS) | J.N.HERRON,X.HE *et al.* |
| 2CRO | 2.35 | 434 CRO PROTEIN | PHAGE 434 | A.MONDRAGON *et al.* |
| 3CRO | 2.5 | 434 CRO PROTEIN COMPLEX WITH 20 BASE PAIR PIECE OF DNA ... | PHAGE 434 | A.MONDRAGON,S.C.HARRISON |
| 1R69 | 2.0 | 434 REPRESSOR (AMINO-TERMINAL DOMAIN) (R1-69) | PHAGE 434 | A.MONDRAGON *et al.* |
| 2OR1 | 2.5 | 434 REPRESSOR (AMINO-TERMINAL DOMAIN) (R1-69) COMPLEX WITH ... | PHAGE 434 | A.K.AGGARWAL *et al.* |
| 1HSC | 2.2 | 44K ATPASE FRAGMENT (N-TERMINAL) OF 7OK HEAT-SHOCK COGNATE ... | BOVINE (BOS TAURUS) BRAIN | K.M.FLAHERTY *et al.* |
| 1RRN | 0.0 | 5S RIBOSOMAL RNA MODEL | (XENOPUS LAEVIS) OOCYTES | E.WESTHOF,P.ROMBY *et al.* |
| 1PGD | 2.5 | 6-PHOSPHOGLUCONATE DEHYDROGENASE (6-PGDH) | (OVIS ORIENTALIS ...) | M.J.ADAMS,S.GOVER *et al.* |
| 9DNA | 1.8 | A-DNA-5(PRIME)-D(GPCPCPCGPGPGPC)-3(PRIME) | SYNTHETIC DNA | U.HEINEMANN |
| 1ACE | 2.8 | ACETYLCHOLINESTERASE (E.C.3.1.1.7) | ELECTRIC RAY ... | J.L.SUSSMAN,M.HAREL *et al.* |
| 4APE | 2.1 | ACID PROTEINASE (E.C.3.4.23.10), ENDOTHIAPEPSIN | CHESTNUT BLIGHT ... | L.H.PEARL,B.T.SEWELL *et al.* |
| 3APP | 1.8 | ACID PROTEINASE (PENICILLOPEPSIN) (E.C.3.4.23.7) | FUNGUS (PENICILLIUM ...) | A.R.SIELECKI,M.N.G.JAMES |
| 2APR | 1.8 | ACID PROTEINASE (RHIZOPUSPEPSIN) (E.C.3.4.23.6) | BREAD MOLD (RHIZOPUS ...) | K.SUGUNA,D.R.DAVIES |
| 3APR | 1.8 | ACID PROTEINASE (RHIZOPUSPEPSIN) (E.C.3.4.23.6) COMPLEX WITH ... | BREAD MOLD (RHIZOPUS ...) | K.SUGUNA,D.R.DAVIES |
| 4APR | 2.5 | ACID PROTEINASE (RHIZOPUSPEPSIN) (E.C.3.4.23.6) COMPLEX WITH ... | BREAD MOLD (RHIZOPUS ...) | K.SUGUNA,D.R.DAVIES |
| 5APR | 2.1 | ACID PROTEINASE (RHIZOPUSPEPSIN) (E.C.3.4.23.6) COMPLEX WITH ... | BREAD MOLD (RHIZOPUS ...) | K.SUGUNA,D.R.DAVIES |
| 6APR | 2.5 | ACID PROTEINASE (RHIZOPUSPEPSIN) (E.C.3.4.23.6) COMPLEX WITH ... | BREAD MOLD (RHIZOPUS ...) | K.SUGUNA,D.R.DAVIES |
| 6ACN | 2.5 | ACONITASE (E.C.4.2.1.3) (ACTIVATED (4FE-4S) CLUSTER FORM) | PIG (SUS SCROFA) HEART | A.H.ROBBINS,C.D.STOUT |
| 5ACN | 2.1 | ACONITASE (E.C.4.2.1.3) (INACTIVE (3FE-4S) CLUSTER FORM) | PIG (SUS SCROFA) HEART | A.H.ROBBINS,C.D.STOUT |
| 2ACT | 1.7 | ACTINIDIN (SULFHYDRYL PROTEINASE) (E.C. NUMBER NOT ASSIGNED) | CHINESE GOOSEBERRY ... | E.N.BAKER |
| 1ACX | 2.0 | ACTINOXANTHIN | (ACTINOMYCES ...) | V.Z.PLETNEV,A.P.KUZIN |
| 1APS | N/A | ACYLPHOSPHATASE (E.C.3.6.1.7) | HORSE (EQUUS ...) | V.SAUDEK,A.PASTORE *et al.* |
| 1ADA | 2.4 | ADENOSINE DEAMINASE (E.C.3.5.4.4) COMPLEX WITH ... | MOUSE (MUS MUSCULUS) ... | D.K.WILSON,F.A.QUIOCHO |
| 3ADK | 2.1 | ADENYLATE KINASE (E.C.2.7.4.3) | PORCINE (SUS SCROFA) ... | G.E.SCHULZ |
| 1AKE | 1.9 | ADENYLATE KINASE (E.C.2.7.4.3), ... | (ESCHERICHIA COLI) | C.W.MUELLER,G.E.SCHULZ |
| 1AK3 | 1.9 | ADENYLATE KINASE ISOENZYME-3, GTP:AMP PHOSPHOTRANSFERASE ... | BOVINE (BOS TAURUS) ... | K.DIEDERICHS,G.E.SCHULZ |
| 1AGA | 3.0 | AGAROSE (AN ALTERNATING COPOLYMER OF 3-LINKED ...) | RED SEAWEED ... | S.ARNOTT |
| 1AMT | 1.5 | ALAMETHICIN | (TRICHODERMA VIRIDE) | R.O.FOX,F.M.RICHARDS |
| 1ALD | 2.0 | ALDOLASE A (E.C.4.1.2.13) | HUMAN (HOMO SAPIENS) ... | H.C.WATSON |
| 1AL1 | 2.7 | ALPHA - 1 (AMPHIPHILIC ALPHA HELIX) | SYNTHETIC | C.P.HILL *et al.* |
| 5CHA | 1.67 | ALPHA CHYMOTRYPSIN A (E.C.3.4.21.1) | COW (BOS TAURUS) | R.A.BLEVINS,A.TULINSKY |
| 6CHA | 1.8 | ALPHA CHYMOTRYPSIN A (E.C.3.4.21.1) COMPLEX WITH ... | COW (BOS TAURUS) | A.TULINSKY,R.A.BLEVINS |
| 2CHA | 2.0 | ALPHA CHYMOTRYPSIN A (TOSYLATED) (E.C.3.4.21.1) | COW (BOS TAURUS) | J.J.BIRKTOFT,D.M.BLOW |
| 1CTX | 2.8 | ALPHA COBRATOXIN | COBRA (NAJA NAJA ...) | W.SAENGER,M.D.WALKINSHAW |
| 2CTX | 2.4 | ALPHA COBRATOXIN | COBRA (NAJA NAJA ...) | C.BETZEL,G.LANGE *et al.* |
| 1HOE | 2.0 | ALPHA-AMYLASE INHIBITOR HOE-467A | (STREPTOMYCES TENDAE ...) | J.W.PFLUGRATH *et al.* |
| 2ABX | 2.5 | ALPHA-BUNGAROTOXIN | BRAIDED KRAIT ... | R.LOVE,R.STROUD |
| 4CHA | 1.68 | ALPHA-CHYMOTRYPSIN (E.C.3.4.21.1) | COW (BOS TAURUS) | H.TSUKADA,D.M.BLOW |
| 1ACB | 2.0 | ALPHA-CHYMOTRYPSIN (E.C.3.4.21.1) COMPLEX WITH EGLIN C | OX (BOS TAURUS) AND ... | M.BOLOGNESI *et al.* |
| 1CHO | 1.8 | ALPHA-CHYMOTRYPSIN (E.C.3.4.21.1) COMPLEX WITH TURKEY ... | BOVINE (BOS TAURUS) ... | M.FUJINAGA *et al.* |
| 1CGI | 2.3 | ALPHA-CHYMOTRYPSINOGEN COMPLEX WITH HUMAN PANCREATIC ... | BOVINE (BOS TAURUS) ... | H.J.HECHT *et al.* |

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See also: **fix**, **save**

### 11.82. Version

Usage: **version**

**Version** reports information about which version of MIDAS is currently being executed and is displayed in the reply area of the MIDAS window. It is useful to supply this information when reporting MIDAS bugs, so that it is possible to determine if the problem has already been solved in a more recent version of the program.

The **wait** may be interrupted by pressing the **ESC** key. This breaks out of **wait** but does not freeze the screen (*i.e.* any active motion continues until completion).

See also: **sleep**

### 11.79. Watch/Watchopt

Usage: **watch** *atom_specification*

Usage: **watchopt** [ distance *distance* ]

**Watch** monitors interatomic distances. By default, it checks for distances less than the sum of the van der Waals radii of two atoms. Atoms in the *atom_specification* are checked against all other atoms to whom their distance can potentially vary (i.e. to atoms on other models or atoms on the same model across from active bond rotations) Close contacts are displayed as yellow dotted lines, in the same manner as distance monitors. One can specify a fixed distance by using the **distance** option to the **watchopt** command, where *distance* is in angstroms. A *distance* of zero means to use the default vdw radii for comparison. Only distances that potentially vary are checked, *i.e.*, atoms that are fixed relative to each other are not checked.

**˜watch** will terminate **watch** monitoring.

See also: **distance**

### 11.80. Window

Usage: **window** [ *atom_specification* ]

With no arguments, **window** puts all displayed models on the screen by changing the scale and position of the view. The orientation of the models is not changed. If the image has drifted off the screen, this is an excellent way of making it visible again.

If given an *atom_specification* as an argument, **window** will recalculate the view to enclose just those atoms instead of all of the models.

See also: **align**, **center**, **push/pop**, **reset**, **savepos**

### 11.81. Write

Usage: **write** [ surface ] [ relative *n* ] *model_number* [ *filename* ] [ relative *n* ]

This command causes the specified *model* to be written out as a PDB file. Current bond rotations must be **fix**ed before the **write** if they are to be reflected in the written file.

The **relative** option specifies that the atomic coordinates written out are relative to the untransformed atomic coordinates of model *n*.

If a *filename* is not given, then the file that the model was opened from will be overwritten.

If the **surface** option is given, then the model's surface is written instead. The surface is written in MS format. Note that the **relative** option is not supported for surfaces.

The **vdw** command may be interrupted by the ESC key. Atoms whose vdw surfaces were already computed when the interrupt occurred will have their surfaces displayed. Since computing the vdw surface is much faster than displaying it, pressing the ESC key might not help.

Note that the default vdw radii used by MIDAS assume that no explicit hydrogens are present in the model(s). This behavior can be changed with the **vdwopt** command.

See also: **vdwopt**, **surface**

### 11.77. Vdwopt

Usage: **vdwopt** [radii *file*] [density *value*] [hydrogen | default] [extend *len*] [define *atom_type radius*]

**Vdwopt** sets user options for displaying van der Waals surfaces. The options are as follows:

**radii** *file* — Indicates a file containing alternate van der Waals radii. The alternate file must contain a complete set of radii for all atoms in the model. The file contains a series of records consisting of an atom name (character string) followed by a space and the atom radii in angstroms (floating point number). This is the same format as used by **ms** program (see Appendix 6). Optionally, a third field can specify the residue type. Use the **default** or **hydrogen** options to return to default values.

**density** *value* — The user may change the dot density of the displayed surface relative to the initial value of 1, which corresponds to 5 dots per square Angstrom. The density of dots varies linearly with the *value* provided. Thus, a density *value* of 2 gives 10 dots per square angstrom.

**hydrogen** — Indicates that hydrogen atoms are included in the model and van der Waals radii should not compensate for missing hydrogens. The result is smaller atom radii and distinct hydrogen atoms.

**default** — Indicates that van der Waals radii should compensate for missing hydrogen atoms. **Vdwopt default** essentially undoes the effects of **vdwopt hydrogen**.

**extend** *len* — Increases all van der Waals radii by the constant *len* angstroms.

**define** *atom_type radius* — Indicates that all atoms with an atomic symbol of *atom_type* should be assigned a van der Waals radius of *radius* angstroms.

See also: **vdw**

### 11.78. Wait

Usage: **wait**

**Wait** suspends command processing until all model movement has ceased. Thus, if a **roll** has been activated for a given number of frames, that motion is completed before the next command is executed.

See also: **run**, **pdbrun**, **midaspush**, **save**

### 11.73. Thickness

Usage: **thickness** *units* [*frames* [*wait_frames*] ]

The **thickness** command changes the distance between the hither and yon clipping planes by the specified number of angstrom *units*. A positive *unit* value increases the distance between the clipping planes, whereas a negative value decreases the it. This results in displaying an increased or decreased cross section of the current model(s).

*Frames* moves the clipping planes in the specified manner for the specified number of image update frames. *Wait_frames*, if specified, indicates the number of frames to wait before beginning the move. **˜thickness** will halt an ongoing thickness. *Frames* and *wait_frames* default to 1 and 0, respectively. These parameters are useful for controlling the rate of clipping and are helpful when constructing MIDAS command scripts and making videos.

See also: **section**, **clip**

### 11.74. Turn

Usage: **turn** [ *axis* [*angle* [*frames* [*wait_frames*] ] ] ]

**Turn** functions the same as **roll** except that the default values for the *angle* and number of *frames* are 3 degrees and 1 frame, respectively. Thus, the command **turn** *y* will generate an approximate left-eye stereo image, although **stereo lefteye** and **stereo righteye** are preferable since these commands generate a more technically accurate stereo image pair.

See also: **roll**, **stereo**

### 11.75. Update

Usage: **Update** transformed **|** original *filename*

**Update** changes the coordinates of a subset of atoms in a model. The user must supply either the **transformed** or **original** keywords and a PDB filename containing atom records with new atom coordinates. If PDB `MODEL` record(s) are present in the file, then the indicated models are updated, otherwise the lowest numbered model is updated. If the keyword is **transformed**, then the new coordinates are considered as having already been transformed by the current rotation and translation matrices. If the keyword is **original**, then the new coordinates are treated as untransformed coordinates and the current rotation and translation matrices are applied to the new coordinates before they are integrated with the rest of the model.

### 11.76. Vdw

Usage: **vdw** *atom_specification*

**Vdw** displays the van der Waals surface for the selected atoms. The syntax is the same as for the **display** command, except that it applies to surface points instead of bonds.

Examples:

| | |
|---|---|
| **surface** #0 | display the surface for model 0 |
| **surface** #1:5 | display the surface for model 1 residue 5 |
| ˜**surface** #1:5,32,64 | remove surface for model 1 residues 5, 32 and 64 |

See also: **vdw**

### 11.70. Swapaa

Usage: **swapaa** *new_residue_type* [,preserve] *residue*

**Swapaa** replaces *residue* with a *new_residue_type* residue. Both the old and new residues must be standard amino acids. The side chain of the new residue will be in standard conformation unless the **preserve** keyword is given, in which case as much existing conformation as possible is saved. Preserving conformation can cause rings to become non-planar (*e.g.* swapping in a PHE for a LYS while preserving conformation).

The temperature factor for the new residue is set to the highest currently found in the model.

### 11.71. Swapna

Usage: **swapna** *new_residue_type* [,preserve] *residue*

**Swapna** replaces *residue* with a *new_residue_type* residue. Both the old and new residues must be standard nucleotides: A, T, G, C, or U.

The temperature factor for the new residue is set to the highest currently found in the model.

The keyword **preserve** is recognized, although it currently does not affect **swapna** behavior in any way.

### 11.72. System

Usage: **system** *command*

**System** executes the UNIX *command* under the user's preferred shell. *Command* may not be an interactive program. The output from *command* will appear as a `REPLY` on the graphics display screen. If the expected reply is more than five lines, the user should instead give the command:

**!***command*

(note ''!'' mark) which directs output to the user's shell window.

As an alternative to the **system** command, the **midaspush** command may be used to access other screen windows or icons (*i.e.* go off and do something else for awhile and then return to MIDAS). If MIDAS was started in its own window, the standard IRIS window manipulation menu may also be use for this purpose. Lastly, one could also use the **save** command to retain orientations, rotation and slider assignments, *etc.* and then quit MIDAS entirely and return later for another modeling session.

### 11.66. Speed

Usage: **speed** *value*

**Speed** changes the speed of functions activated by sliders or ‘‘spaceball’’. Thus, the sensitivity of the devices are altered for scaling and rotation functions. *Value* is a positive or negative integer which reflects the *relative* change in speed. The absolute range is 2 to 14 with default value of 10.

### 11.67. Stereo

Usage: **stereo** off **|** sequential **|** walleye **|** crosseye **|** lefteye **|** righteye

**Stereo** specifies how images are displayed. **Off** indicates a monocular image. **Sequential** indicates a time sequential stereographic image of the type that is utilized by ‘‘Crystal Eyes’’ stereo systems. Note that this command requires special hardware to work properly and not all workstations may support this hardware (in particular the *NeXT* doesn’t support hardware stereo). **Walleye** indicates side-by-side stereo pairs having positive horizontal parallax. That is, the left eye image is shown on the left hand side of the display window and the right eye image is shown on the right hand side of the window. This is the classic method of generating stereo image pairs, but the size of the images are constrained not to overlap. The size of the walleye image can be changed with the *walleye_scale* variable (see the **set** command). **Crosseye** indicates side-by-side stereo pairs having negative horizontal parallax. That is, the left eye image is shown on the right hand side of the display window and the right eye image is shown on the left hand side of the window. The user must look ‘‘crosseyed’’ at the images to perceive the stereopsis effect. Image size may fill the entire window in this mode. **Lefteye** and **righteye** show the left and right view of a stereo image, respectively. This is useful for taking stereo slides since you can photograph each eye view individually.

The command **˜stereo** is equivalent to **stereo off**.

See also: **set**

### 11.68. Stop

Usage: **stop**

**Stop** terminates the current MIDAS session without saving any of the currently displayed models.

See also: **save**

### 11.69. Surface

Usage: **surface** *atom_specification*

**Surface** selectively displays solvent accessible surface points for models. The syntax is the same as for the **display** command, except that it applies to surface points rather than to bonds.

To prepare a solvent accessible surface for display see ‘‘Solvent Accessible Surfaces’’ in Part II of this manual. The **open** command is used to open prepared MIDAS solvent accessible surface files followed by the **surface** command to display the surface.

Alternatively, the **vdw** command may be used to display the model’s van der Waals surface. Display of this surface requires no advance calculation and is more convenient unless the solvent accessible surface is specifically desired.

### 11.62. Setcom

Usage: **setcom** *model x_coord y_coord z_coord* [*radius* [*natoms*] ]

When MIDAS is asked to rotate one or more models, it needs to know the center of mass of the model(s). **Setcom** is used to change the center of mass parameters in the rare case where the ones automatically computed by MIDAS are unacceptable.

*X_coord*, *y_coord*, and *z_coord* specify the new center of mass for *model*. If *radius* is given, it should be the shortest radius (in angstroms) from the new center of mass that encloses the model. This helps MIDAS do a better job of framing the models in the graphics window. Specifying *natoms* essentially tells MIDAS how much weight this model has when computing a combined center of mass for multiple models.

**˜setcom** will cause MIDAS to revert to the default center of mass that it normally computes.

### 11.63. Show

Usage: **show** *atom_specification*

**Show** displays the specified atoms and removes all others from the display. Note that this differs from the **display** command in that the **show** command displays *only* those atoms specified (and will undisplay all others). **˜Show** removes the specified atoms completely from the display.

See also: **chain**, **display**

### 11.64. Sleep

Usage: **sleep** *number_of_seconds*

**Sleep** causes MIDAS to pause for *number_of_seconds* seconds and then resume operation. This command is useful in command scripts where a break in the action is required.

See also: **wait**

### 11.65. Source

Usage: **source** *filename*

**Source** reads a command file of MIDAS commands. **Source** differs from **read** in that **source** will display the results of each command as it is executed while **read** only updates the display after all commands have completed.

The user may interrupt the execution of the *source* file by pressing the **ESC** key. MIDAS completes execution of the current command before processing the interrupt.

See also: **read**

| Set/Unset Value Options | |
|---|---|
| Keyword | Function |
| bg_color | Sets the MIDAS background color. *Value* can be either a color keyword or color index as described in detail under **color**. |
| bg_intensity | Controls the brightness of the background color. *Value* can vary from 0 (black) to 1 (full intensity). For purposes of backwards compatibility, *value* can be in the range 0-255, in which case it will be interpolated into the range 0-1 and handled appropriately. This latter functionality is obsolescent and should not be relied upon to exist in future MIDAS releases. |
| eyesep | The separation between the centers of the viewer's eyes, in inches. This information is necessary to compute the projections for stereo viewing. It is rarely necessary to change the default setting for most adults, but it might be necessary for children viewing stereo. |
| font | This allows atom labels to be in any font style. The *value* is a font name concatenated with a point size, *i.e.*, **Helvetica10** would set the font to be Helvetica, and the point size to 10. |
| linewidth | This controls the thickness with which bonds are drawn. The default is 1, and larger values produce thicker lines (and slower interaction). |
| nameplate | This controls the placement of the MidasPlus logo on the bottom of the screen. A *value* of 0.0 puts it to the extreme left; 1.0 puts it to the right. |
| viewdist | The distance from the viewer to the screen, in inches. This information is needed to correctly compute stereo projections. Its default setting is appropriate for most modeling work, but the value may have to be increased if a demonstration is being given where many people are further from the screen than normal. |
| vpsep | Amount of vertical separation between left and right eye images in stereo mode, in scan lines. This option should only have to be set once for each machine with stereo. It controls the vertical convergence of the left and right images when the stereo system is turned on. Once the correct *value* is determined (empirically), it should be put in */usr/local/lib/midas/midas.rc* on the IRIS, */LocalLibrary/Midas/midas.rc* on the *NeXT*. |
| walleye_scale | This scales the size of walleye-type stereo image pairs (see **stereo** command). The default size is correct when using opticomechanical stereo viewers, while a larger scale is useful for taking pictures for publications. |

| Set/Unset Toggle Options | |
|---|---|
| Keyword | Function |
| autocolor | Give each newly opened model a different color. |
| cofg | Puts a '+' at the center of rotation for the selected models. The '+' corresponds to the center of gravity if there is only one molecule or if the rotations are independent (center of mass of selected molecules). |
| control | Display the control panel. |
| filenames | Make MIDAS display the filenames of the open models in the top left corner of the window above any bond rotation monitors. |
| fullscreen | Make MIDAS resize itself to use the full screen. Useful if MIDAS is started without a desired *-f* option. If then unset, MIDAS will revert to its original size. |
| halfbond | Atoms are colored by halfbond connections to other atoms instead of each atom having one whole bond associated with it. Note that using halfbond mode may degrade response time. |
| independent | If set, models rotate about their own centers of mass, otherwise models rotate about the combined center of mass. |
| labels | Turns on distance, rotation, and angle monitoring labels. |
| ortho | Use orthographic instead of perspective projection. |
| record | Initiates remembering of subsequent typed user commands. Note that commands that implicitly generate additional commands (*e.g.* **read**, **source**, **run**, **pdbrun**) are remembered but not expanded. Issuing a new **set record** when record mode is already set resets remembering from scratch. **˜set record** clears the command memory and prevents subsequent commands from being remembered. This will save some time and disk space since the commmands are remembered in a temporary disk file. |
| showsphere | Controls whether a circle defining the transition between ***x,y*** versus ***z*** rotation is shown when MidasPlus is in ''virtual trackball'' manipulation mode. |
| text | Displays the `Command` and `Reply` text lines on the bottom of the display screen. This option can be turned off using **unset text** when taking photographs. |
| verbose | MIDAS prints confirmation messages after each successful command. If verbose is **unset** these messages will not appear. |

See also: **assign**

## 11.61. Set/Unset

Usage: **set** *keyword* [*value*]

Usage: **unset** *keyword*

There are two types of display options in MIDAS, those that act as off/on toggles and those that vary over a range of values. For the toggle type of option, **set** with the appropriate *keyword* enables the option and **~set** *keyword* or **unset** *keyword* disables the option. For value type options, **set** *keyword value* sets the value while **set** *keyword* displays the current value.

Although initially all toggle options are disabled, MIDAS sets certain options on at the beginning of each session by reading the initialization file */usr/local/lib/midas/midas.rc* on the IRIS, */LocalLibrary/Midas/midas.rc* on the *NeXT*. See Appendix 4 of this document for a list of the display options enabled during initialization.

See also: **devopt**

The available MIDAS display options are:

(see next page)

halt an ongoing scale. *Frames* and *wait_frames* default to 1 and 0, respectively. These parameters are useful for controlling the rate of scaling and are helpful when constructing MIDAS command scripts and making videos.

### 11.59. Section

Usage: **section** *units* [*frames* [*wait_frames*] ]

**Section** moves the hither and yon clipping planes the specified number of angstrom *units*. This has the effect of displaying a different cross section of the displayed model(s). A positive number of units moves the cross section toward the user, whereas a negative number moves the cross section away from the user.

*Frames* moves the clipping planes in the specified manner for the specified number of image update frames. *Wait_frames*, if specified, indicates the number of frames to wait before beginning the clip. **˜section** will halt an ongoing section. *Frames* and *wait_frames* default to 1 and 0, respectively. These parameters are useful for controlling the rate of clipping and are helpful when constructing MIDAS command scripts and making videos.

See also: **thickness**, **clip**

### 11.60. Select

Usage: **select** *atom_specification*

Usage: **select** *model_number ...* | *model_range*

Usage: **select** all

**Select** selects a model or models for subsequent **move**, **rock**, **roll** and **turn** commands as well as interactive mouse manipulations.

If the argument to **select** is an atom specification, then the model(s) containing those atoms will be selected.

If **select** is used with the keyword ‘‘all’’, then all models will be selected. **˜select all** will then revert to the previous selection state. This feature is convenient for switching back and forth between moving models relative to one another and global motion of all models.

Otherwise the argument(s) to **select** should be one or more model numbers or ranges (of the form *#-#*), separated by spaces. Note that the *model* number does not permit a **#** symbol to be included in the number.

The numbered boxes on the lower part of the ‘‘control panel’’ portion of the display (referred to as pseudo-switches) are used to toggle the selection status of the corresponding model number. Clicking on the box will select a model if currently unselected (turning the box green), or deselect if selected (turning the box red). The box labeled ‘‘All’’ works in an analogous manner to the typed **select all**. Clicking on ‘‘All’’ once will cause all open models to become selected and turn the ‘‘All’’ box green. Clicking on the box again will return to the previous selection status and turn the ‘‘All’’ box red.

Examples:

| | |
|---|---|
| **select** 1 | selects model 1 |
| **select** 1 5–8 | selects models 1 and 5 through 8 |

**Run** passes its arguments *cmd* and *cmd_args* to the shell for execution and takes the output from these as a series of MIDAS commands.

The user may interrupt the execution of the MIDAS commands by pressing the **ESC** key. Execution of the current command is completed before processing the interrupt.

See also: **pdbrun**, **system**

### 11.56. Save

Usage: **save** *session_name*

**Save** stores the model orientation, bond rotations, distance calculations, slider assignments and user options for the current session in a MIDAS session file. The model coordinates are saved in PDB format. Since the model orientations are stored in the session file and not the data files, PDB files produced with **save** do not have their coordinates transformed. To get transformed coordinates, use the **write** or **pdbrun** command.

To restart a saved session, use the command:

% **midas** *session_name*

Note that if bond rotations have been made and the user wishes to have the saved PDB files reflect the new conformation, the **fix** command must be invoked before the session is saved.

See also: **fix**, **stop**, **write**

### 11.57. Savepos

Usage: **savepos** [*view_name*]

**Savepos** saves the current model orientations and associates *view_name* with it. If *view_name* is missing, the name ‘‘default’’ is used. The view may be retrieved using the **reset** command.

A view may be ‘‘forgotten’’ using the command **~savepos** *view_name*. This saves space in session files.

For a list of all existing *view_name*s, give the command:

**savepos list**

See also: **align**, **reset**, **push/pop**, **window**

### 11.58. Scale

Usage: **scale** *factor* [*frames* [*wait_frames*] ]

**Scale** increases the size of the displayed view by the specified scaling *factor*. The scaling factor must be positive — a scaling factor less than one will decrease the size of the displayed view. Note that this command does not modify the model coordinates.

*Frames* scales the models in the specified manner for the specified number of image update frames. *Wait_frames*, if specified, indicates the number of frames to wait before beginning the scaling. **~scale** will

**Roll** will rotate the selected structures about the ***x***, ***y***, or ***z*** *axis* continuously. If *axis* is an integer, it refers to the corresponding bond rotation.

If *angle* is specified, the structure is rolled through that angle (given in degrees) for each frame. If *angle* has a negative value the direction of the rotation is reversed. *Frames*, if specified, indicates the number of image update frames over which the **roll** operation is carried out. If *frames* is not specified, the structure continues to roll until explicitly turned off with the command **˜roll** *axis*. Note that two or three **roll**s may be active at the same time; that is, the user can roll the structure around two or three axes at the same time. Each must be turned off explicitly.

*Wait_frames*, if specified, indicates the number of frames to wait before beginning the roll. This is useful for making videos. For example,

**roll** x 2 90 30

rolls the model 180 degrees over 90 image updates (*i.e.* 2 degrees on each frame update) after waiting 30 image update cycles before beginning.

The default values for *axis* and *angle*, if omitted, are *y* and *3*, respectively.

If **roll** does not work, it is likely you have failed to **select** the target models.

See also: **freeze**, **select**, **turn**

### 11.54. Rotation

Usage: **rotation** [*rotation_number*] *atom1,atom2* [*,atom3,atom4*]

**Rotation** activates a bond rotation. All rotations are assigned a *rotation_number* between 0 and 15 inclusive, either by the user or automatically by MIDAS. Once a bond rotation is activated, the rotation may be manipulated and controlled by assigning the rotation to a slider via the **assign** command.

The rotation number and current bond angle are reported on the top of the display screen. If only *atom1* and *atom2* are specified, the angle reported is relative to the beginning position, *i.e.* the position when the assignment was made. If four atoms are specified, then the torsional angle is reported. The **˜rotation** command removes the rotation and returns the bond to its original conformation (use the **fix** command to preserve the new conformation).

In assigning multiple bond rotations to a model, two rotations cannot affect a common set of atoms unless one affected set is a complete subset of the other. That is, rotations must be properly nested.

Examples:

| | |
|---|---|
| **rotation** 1 #1:1@c8,c9 | assign rotation 1 to the bond between c8 and c9 in the first residue of model 1 |
| **rotation** 3 #1:2@205:3@1 | assign rotation 3 to the bond between the terminal atom of residue 2 (atom 205) and the first atom of residue 3 |

See also: **brotation**, **reverse**, **assign**, **fix**

### 11.55. Run

Usage: **run** *cmd* [*cmd_args...*]

See also: **brotation**, **rotation**

### 11.50. Ribbon

Usage: **ribbon** *options*

The **ribbon** command produces an aesthetic representation of the secondary structure of the displayed molecule(s), in a manner reminiscent of a ‘‘Jane Richardson drawing.’’ The current model orientation and coloring is retained. Clicking the left mouse button returns to MidasPlus.

In order for the ribbon command to know what the secondary structure of the model(s) is, each model must have been opened from a PDB file, and that PDB file has to have correct `HELIX` and `SHEET` records.

There are many options, which are detailed fully in the **cartoon** manual page included in Appendix 6 of this document. (The **ribbon** command is actually an alias that executes the **pdbrun** command and sends data to the **cartoon** program.)

See also: **conic**, **pdbrun**

### 11.51. Rlabel

Usage: **rlabel** *atom_list*

**Rlabel** enables residue labeling of the first displayed atom of each residue in *atom_list*. This condition is true by default in MIDAS. **~rlabel** may be used to turn off display of residue labels.

See also: **label**

### 11.52. Rock

Usage: **rock** [*axis* [*angle* [*frames* [*wait_frames*] ] ] ]

Rock will rotate the selected structures back and forth about the ***x***, ***y*** or ***z*** *axis*. The *angle* indicates the number of degrees the structure rotates at the fastest point in the sinusoidal period. (An *angle* value of 9 corresponds approximately to a 90 degree arc.)

The cycle time for **rock** is approximately 2.4 seconds. This corresponds to 18 frames forward and 18 frames back [15 frames per second].

If arguments are omitted, defaults will be used. These defaults are: *wait_frames – 0*, *frames –* infinite, *angle – 3, axis – y*.

If **rock** does not work, it is likely you have failed to **select** the target models.

See also: **freeze**, **select**

### 11.53. Roll

Usage: **roll** [*axis* [*angle* [*frames* [*wait_frames*] ] ] ]

**Record** saves all the commands remembered by the **set record** command in the file *filename*. Saved commands can later be re-executed with a **read** or **source** command, although the command file should first be edited since the **record** command itself will be in the file. **Record** is very useful for creating demonstration scripts for later playback. Note that there is normally a **set record** in the system startup file distributed with MIDAS so that, by default, all typed user input is remembered. Thus all commands used since MIDAS startup can easily saved with **record**. This is useful for reproducing results or applying commands used on one set of models to a different set of models.

See also: **read**, **set**, **source**

### 11.47. Redraw

Usage: **Redraw** *atom_specification*

This command no longer does anything. It is provided for backwards compatibility with old MIDAS command scripts.

### 11.48. Reset

Usage: **reset** [*view_name*]

**Reset** returns models back to saved orientations. In each MIDAS session, the original orientation of the *first* model(s) opened is saved as *view_name* ''default''. This orientation may be retrieved by the command **reset** or the command **reset default**. Other orientations may be saved using the **savepos** command:

**savepos** *view_name*

and retrieved using the **reset** command:

**reset** *view_name*

For a list of existing *view_name*s, give the command:

**reset list**

See also: **align**, **push/pop**, **savepos**, **window**

### 11.49. Reverse

Usage: **reverse** *rotation_number*

**Reverse** reverses the direction of a bond rotation. If the direction is reversed, then the portion of the molecule which rotated previously remains fixed and vice versa in subsequent rotations.

Warning: In assigning multiple bond rotations to a model, two rotations cannot affect a common set of atoms unless one affected set is a complete subset of the other. That is, rotations must be properly nested. In executing **reverse**, reversing the bond rotation may cause such a conflict and be disallowed. Reversing bond rotations must be done in an appropriate order such that all intermediate combinations are legal. (See **rotation**.)

When MIDAS accepts a **pickatom** command from a delegate, it will reply with

Waiting for pick

If another delegate program is already waiting for an atom to be selected, MIDAS will reply with

Already picking for delegate "XXX"

After MIDAS accepts a **pickatom** command and the user selects an atom, the command that MIDAS sends to the delegate is of the form

pickatom #*model_number*:*residue_sequence@atom_name*

If, instead of selecting an atom, the user types **pickabort**, MIDAS will send the command

pickabort

to the requesting delegate.

The commands and replies described above are primarily for use by delegate application programmers. The only important point that a user needs to remember is that typing **pickabort** will terminate a delegate picking request without actually selecting an atom. The **pickatom** command is only valid when sent by a delegate and has no effect when typed at the keyboard.

See also: **delegate**, **picking**

### 11.44. Push/Pop

Usage: **push**

Usage: **pop**

**Push** saves the current orientation of all open models on an image stack.† **Pop** retrieves the last ‘‘pushed’’ orientation. Any number of model orientations may be saved on the stack, memory allowing, and retrieved on a last-in first-out basis.

See also: **align**, **reset**, **savepos**, **window**

### 11.45. Read

Usage: **read** *filename*

**Read** executes the contents of the file *filename* as a list of commands. **Read** differs from **source** in that **source** updates the display after each command while **read** only updates the display after all commands are done.

See also: **record**, **source**

### 11.46. Record

Usage: **record** *filename*

† For those unfamiliar with the concept of a ‘‘stack’’, think of a pile of pictures which is created by ‘‘pushing’’ pictures one at a time onto the *top* of the pile and in which pictures are retrieved one at a time by taking the *top* picture off the pile.

A typical set of records describing an atom looks like this:

```
ATOM      1  C   HIS     1      49.168  26.701  10.916  1.00 16.00
USER  COLOR gray 0.500 0.500 0.500
USER  RADIUS 1.800
```

which indicates the C atom of histidine residue 1 is colored gray (color name *gray*, half red, half green, half blue) and has an atomic radius of 1.8 angstroms.

User records that have the `GFX` keyword are parts of an object description. The remainder of the user record consists of another keyword and arguments. The currently used keywords, arguments, and their semantics are shown in the following table.

**`GFX` Keywords**

| Keyword | Arguments | Semantics |
|---|---|---|
| `COLOR` | MIDAS color range and red, green, and blue values in the range 0 to 1 | Same as regular `USER COLOR` records |
| `MOVE` | Cartesian coordinates | Set the current drawing location to given coordinates |
| `DRAW` | Cartesian coordinates | Draw a line from the current drawing location to the given coordinates and set the current drawing location to the new coordinates |
| `POINT` | Cartesian coordinates | Set the current drawing location to given coordinates and draw a point there |
| `MARKER` | Cartesian coordinates | Set the current drawing location to given coordinates and draw a marker there |
| `LABEL` | Cartesian coordinates followed by a quoted string | Set the current drawing location to the given coordinates and display the given string, using the coordinates as its lower left-hand corner |
| `FONT` | Font name, size | Set the font that will be used to display subsequent strings |

See also: **delegate**, **run**, **system**, **write**, **vdwopt**

### 11.43. Pickatom/Pickabort

Usage: **pickatom**

Usage: **pickabort**

These commands are used in conjunction with the MIDAS delegate facility (see appendix 5). A delegate program can request that the user select a particular atom on the display by first sending a **pickatom** command to MIDAS, verifying that the command has been accepted by MIDAS, then waiting for the user to select an atom and for MIDAS to send the indication of the selected atom back to the delegate program.

| Pdbrun Keywords | | |
|---|---|---|
| Keyword | Where Found | Information |
| `PDBRUN` | First line of file | Pdbrun version number |
| `EYEPOS` | Second line of file | Where the viewer is assumed to be positioned ($x$,$y$,$z$) for purposes of calculating what to display. |
| `ATPOS` | Third line of file | The location the viewer is assumed to be looking towards for determining line of sight. |
| `WINDOW` | Fourth line of file | View volume displayed, relative to the line of sight. The 6 numbers are, respectively, $x_{left}$, $x_{right}$, $y_{bottom}$, $y_{top}$, $z_{hither}$, $z_{yon}$. Since in MIDAS the view volume is symmetric about the line of sight, $x_{left}$ and $y_{bottom}$ are both negative and equal in magnitude respectively to $x_{right}$ and $y_{top}$, which are both positive. $z_{hither}$ and $z_{yon}$ are positive distances from the viewer to the *hither* and *yon* clipping planes, respectively. |
| `FOCUS` | Fifth line of file | Distance from viewer to focal plane, along line of sight. Used primarily when making stereo projections. |
| `VIEWPORT` | Sixth line of file | Extent of the MIDAS window, in screen coordinates. ($x_{min}$, $x_{max}$, $y_{min}$, $y_{max}$) |
| `FILE` | After each `MODEL` record | Name of file corresponding model was **open**ed from |
| `COLOR` | After each `ATOM` record | MIDAS color range and red, green, and blue values in the range 0 to 1 |
| `RADIUS` | After each `ATOM` record | van der Waals radius in angstroms |
| `OBJECT` | Before a list of object description `USER` records | Number of the corresponding model |
| `ENDOBJ` | After a list of object description `USER` records | Number of the corresponding model |
| `GFX` | Between `OBJECT` and `ENDOBJ` records | Part of an object description (see below) |
| `ANGLE` | Towards the end of **pdbrun** output | Number of angle monitor, serial number of atoms involved, and the value of that is being displayed for the monitor |
| `DISTANCE` | Towards the end of **pdbrun** output | Number of distance monitor, serial number of atoms involved, and the value of that is being displayed for the monitor |
| `CHAIN` | After a model's `CONECT` records | Two atom serial numbers that are connected by a chain pseudo-bond. |

*Filename* may be a pathname to a file or the name of a file in the current working directory. To change directories, use the **cd** command.

See also: **cd**, **match**, **write**, **surface**

### 11.42. Pdbrun

Usage: **pdbrun** [ **all** ] [ **conect** ] [ **nouser** ] *command* [*command_args...*]

**Pdbrun** causes *command* and *command_args* to be passed to the user's preferred UNIX shell for execution. A PDB file describing the current models is also passed as standard input. Normal shell metacharacters (notably output redirection) can be used. Errors are ignored and any shell output is interpreted as MIDAS commands and executed.

The **all** option specifies that all atoms, not just those displayed, labeled, vdw'ed, or surfaced should be sent to the given *command*.

The **conect** [*sic*] option specifies that PDB-standard CONECT records should be generated for all residues, even if they have standard connectivity.

The **nouser** option specifies that no USER records should appear in the output.

Control returns to MIDAS when the **pdbrun** command terminates. This command facilitates extensions to the normal MIDAS command set. In particular, both the **conic** and the **ribbon** commands are implemented using **pdbrun.**

`TER` records are inserted normally in the PDB file and `ENDMDL` records follow each model. Fields in PDB records that are not wide enough to hold their associated values are filled with asterisks instead. Unless disabled as noted above, USER records are also added to give additional information. These remarks are of the general form:

`USER` *keyword information*

The following table describes each *keyword* and its associated *information*.

See also: **conic**, **ribbon**, **pdbrun**

### 11.41. Open

Usage: **open** [model **|** surface **|** ms **|** object ] [*model_number*] *filename* [*surface_filename*]

**Open** causes the contents of the file *filename* to be read and shown as model *model_number* (if *model_number* is omitted, the lowest available model number is used). The model number is used to uniquely reference the model in subsequent commands and therefore should be remembered.

How MIDAS interprets *filename* is controlled by the optional keyword specifier. If no keyword is given, or the keyword **model** is specified, MIDAS will try to open the *filename* as a PDB file.

The **ms** keyword indicates the *filename* is the output of the **ms** utility, used to generate solvent accessible surfaces, and that the surface should be associated with the indicated *model_number* (*model_number* cannot be omitted in this case).

MIDAS can read **ms** and PDB files that have been compressed using the UNIX ‘‘compress’’ command. Compressed **ms** and PDB files use substantially less disk space than regular files. There is no need to first uncompress the files or to specify any special keyword on the **open** command line.

The **surface** keyword indicates that *filename* is a surface. Currently, the only surface type supported is **ms** surfaces, but there are plans to add more surface types. Optionally, a surface file, *surface_filename*, may be specified as a fourth argument. This surface is associated with the open model.

If **open** is used with the **object** keyword, the file is assumed to specify a non-molecule graphic object, and can be opened as a new model, or associated with an existing model. Each line in the object file is a command or text. If it is text, then it is displayed in the current color and font at the current position. All of the commands start with a period and are as follows:

| | |
|---|---|
| **.comment** *text* | comments |
| **.c** *text* | comments |
| **.font** *name size* | set font and size |
| **.color** *color_designation* | set color (see below) |
| **.cmov** *x y* [ *z* ] | set character position |
| **.dot** *x y* [ *z* ] | show dot at position |
| **.marker** *x y* [ *z* ] | show marker at position |
| **.m** *x y* [ *z* ] | move to location |
| **.move** *x y* [ *z* ] | move to location |
| **.d** *x y* [ *z* ] | draw line from last location |
| **.draw** *x y* [ *z* ] | draw line from last location |

The *color_designation* parameter to the **.color** directive can be simply a single MIDAS color, including user-defined colors (see *colordef*), or two colors and a mixture fraction, separated by commas. The mixture fraction is a number between zero and one that indicates the relative amounts of the two colors to use to get the actual color. Zero indicates use exclusively the first color, while one would indicate use only the second color.

If the **autocolor** option has been set (using the command **set autocolor**), then each newly opened model without color definitions will be given a unique color so that different models can be easily distinguished.

To close a model, use **˜open** followed by either the model number or name. If the name is used, it must match exactly the name used in the open command.

In MidasPlus, if a model is closed and another model opened with the same model number, then none of the transformations applied to the previous model are applied to the newly opened model. Note that this is in direct contrast to previous versions of MIDAS where all the transformations were applied, in order to facilitate docking. If docking is necessary, two models can be placed in approximately the same orientation with the **match** command.

**Matrixget** prints the current 4x4 transformation matrices to a file named *filename*.

**Matrixset** reads matrices from the file named *filename* and sets the current transformation matrices (using the same file format as **matrixget**).

See also: **cofr**, **getcrd**

### 11.38. Midaspush/Midaspop

Usage: **midaspush**

Usage: **midaspop**

**Midaspush** pushes the MIDAS display window behind all other screen windows and icons. These windows and icons can then be used normally. **Midaspop** brings MIDAS back to the top. Make sure that the mouse cursor is over the MIDAS window when **midaspop** is typed because MIDAS will not receive keystrokes typed with the mouse cursor positioned over other screen windows. If you accidentally type with the mouse incorrectly positioned, erase your input in the other window, then move the mouse over the MIDAS window and type **midaspop**.

Note that if MIDAS is not using the full screen, and therefore has a window frame around it, it is possible to use the standard mouse techniques for pushing and popping windows.

### 11.39. Move

Usage: **move** *axis units* [*frames* [*wait_frames*] ]

The **move** command translates the selected molecule(s) along the specified *axis*. *Axis* may be *x*, *y* or *z*. *Units* is a floating point number in angstroms. A positive value for *units* indicates translation to the right, up, or toward the user and corresponds to the x, y, and z axes, respectively.

*Frames* moves the models in the specified manner for the specified number of image update frames. *Wait_frames*, if specified, indicates the number of frames to wait before beginning the move. **~move** will halt an ongoing move. *Frames* and *wait_frames* default to 1 and 0, respectively. These parameters are useful for controlling the rate of motion and are helpful when constructing MIDAS command scripts and making videos.

If the **move** command does not work, it is likely you have failed to **select** the target models.

See also: **select**

### 11.40. Neon

Usage: **neon** *options*

The **neon** command produces a three dimensional ball and stick representation of the displayed molecule(s) with appropriate shadows. The current orientation and coloring is retained. This image is not interactive and takes anywhere from a minute to several minutes to produce. After the image is displayed on an IRIS, clicking the left button returns to MidasPlus.

There are many options, which are detailed fully in the *neon* manual page included in Appendix 6 of this document. (The **neon** command is actually an alias that executes the **pdbrun** command and sends data to the **neon** and **conic** programs.)

### 11.35. Link

Usage: **link** *residue*

This command is obsolete and is provided for backwards compatibility with old MIDAS command scripts. Use **bond** instead.

See also: **bond**

### 11.36. Match

Usage: **match** [ selected ] *atom_specification*

The **match** command uses the least squares fit method to superimposes two models. The *atom_specification* should contain an equal number of atoms from two different models.

The atoms are matched according to the order in which they are specified, *i.e.* the first atom of the first model is matched to the first atom of the second model, second atom to second atom, etc. The MIDAS command syntax allows much flexibility in specification, *i.e.* atom specifications can use all the shorthands available for related atoms. For example, the user might match models 1 and 2 thus:

**match** #1:3@C1@C2@P@O2 #2:3@C1@C2@P@O2

MIDAS will transform the second model so that its atoms overlay those of the first model. Specifying the **selected** option will make **match** transform not only the second model but all selected models as well, using the same transformation that was applied to the second model.

The user should be aware that the order in which atoms are specified in a list does not necessarily force the order in the match. For example,

**match** #1:3@C1,C2,P,O2 #2:3,C1,C2,P,O2

is not specific as to the order of the atoms C1, C2, P and O2. In this case, MIDAS will order the atoms as they occur in the residue connectivity for residue 3. If residue 3 of model 1 and residue 3 of model 2 are the same, this is not a concern. If they different, however, then the order is not specific and the models may not be superimposed in the way the user would expect. Ordering may be forced by using the @ designation:

**match** #1:3@C1@C2@P@O2 #2:3@C1@C2@P@O2

The RMS error value from the least squares fit is returned in the command reply area at the bottom of the MIDAS window.

### 11.37. Matrixcopy/Matrixget/Matrixset

Usage: **matrixcopy** *from_model to_model*

Usage: **matrixget** *filename*

Usage: **matrixset** *filename*

**Matrixcopy** makes the 4x4 transformation matrix of model *to_model* the same as model *from_model*.

## 11.31. Getcrd

Usage: **getcrd** *atom_specification*

The **getcrd** command returns the untransformed x, y and z coordinates for the atom specified. The *atom_specification* must select one atom only using the standard #:@ syntax. The coordinates are returned in the command reply area at the bottom of the MIDAS window.

## 11.32. Help

Usage: **help** [*topic*]

The **help** command displays information on the selected topic. If no *topic* is specified, MIDAS displays a list of all available topics.

On the *NeXT*, if the *topic* isn't found, then the Librarian is used to search for the topic.

See also: **devopt**

## 11.33. Intensity

Usage: **intensity** *hither_value* [*yon_value*]

**Intensity** changes the value of the intensity at the hither and yon clipping planes. The values range from 0 to 1. Default values are 1 for the hither (maximum intensity) to 0.2 for the yon (minimum intensity). Note that the location of the hither and yon clipping planes may be changed with the **clip** command or by assigning thickness and section to the control panel sliders (which is done by default). For backwards compatibility, it is legal to use intensity values in the range 0-255 (which are then mapped to 0-1) but this functionality is obsolescent and should not be relied upon to exist in future versions of MIDAS.

See also: **clip**

## 11.34. Label

Usage: **label** *atom_specification*

Atoms and residues are labeled appropriately. *Atom_specification* may be any displayed atoms, residues or models. The residue name appears after the first labeled atom in the residue.

Examples:

| | |
|---|---|
| **label** #3 | label everything in model 3 |
| **label** #2:HIS | label all histidine residues in model 2 |
| **˜label** #2:40 | unlabel the 40th residue in model 2 |

See also: **rlabel**

standard MIDAS syntax.

Examples:

| | |
|---|---|
| **distance** 1 #1:12@CA #0:47@CA | assign distance 1 |
| ˜**distance** 0,1 | remove distances 0 and 1 |

See also: **watch**

### 11.27. Echo

Usage: **echo** *text*

**echo** places all of the *text* argument into the MidasPlus reply buffer visible at the bottom of the graphics window. **echo** may be used by custom MidasPlus scripts to send messages back the user.

### 11.28. Fix

Usage: **fix** *rotation_number*

The **fix** command removes a previously activated torsional bond rotation and leaves the structure as currently displayed. It is necessary to **fix** a rotation before giving a **save** command if the current position of the rotation is to be reflected in the **save**d PDB file of the model with the active rotation.

### 11.29. Fixreverse

Usage: **fixreverse** *rotation_number*

**Fixreverse** fixes the named bond rotation and activates the reverse bond rotation using the same *rotation_number*. This command insures that the model will not move relative to other displayed models as is often the case when the **reverse** command is used.

Warning: In the case of multiple bond rotations, *if* the set of atoms rotated by a given bond rotation includes the pivotal atom of another bond rotation and *if* the set of atoms rotated by this second rotation includes the pivotal atom of the first, *then* MIDAS will not allow such rotations. In executing **fixreverse**, reversing the bond rotation may cause such a conflict and be disallowed. Reversing bond rotations must be done in an appropriate order such that intermediate combinations are legal. (See **rotation**.)

### 11.30. Freeze

Usage: **freeze**

**Freeze** stops all motion on the screen.

See also: **rock**, **roll**

See also: **addgrp**

### 11.24. Devopt

Usage: **devopt** [ *option* [ on | off ] ]

**Devopt** sets device-specific options.

Issuing a **devopt** command with no arguments will list the options available on your machine as well as each option's current setting.

The **help_search** option turns on and off always searching for the help topic even when it is a known topic. (*NeXT* only.)

The **smooth** option turns antialiasing on and off. (IRIS only.)

The **colormap** option turns on and off colormap mode. This mode is provided because on many models of the IRIS antialiased lines are *much* faster in colormap mode than in RGB mode. The disadvantage of colormap mode is that you are limited to 22 colors. (IRIS only.)

The **blend** option turns on and off color-blending. Color blending is off by default because neither the Personal IRIS nor the IRIS VGX support depthcued color blending. (IRIS only.)

The **antialias_points** option controls whether points used to depict molecular surfaces are antialiased when the **smooth** option is on. Having **antialias_points** off will improve graphics performance and may improve or degrade image quality, depending on the specific model of workstation that MidasPlus is running on. (IRIS only.)

Setting the **ucsf_stereo** option on prevents the **stereo sequential** command from automatically switching the monitor to 120 Hz interlaced refresh rate. The monitor must instead be switched manually. (IRIS only.)

See also: **set**

### 11.25. Display

Usage: **display** *atom_specification*

**Display** allows the user to selectively display the atoms of a model. The *atom_specification* may be any combination of molecules, residues and atoms for the currently open models. To display only selected portions of a model the user may use **˜display** to remove the unwanted atoms and labels. When used with the **label**, **vdw** and **surface** commands, the user is able to display any combination of bonds, labels and atom surfaces.

See also: **chain**, **show**, **label**, **surface**, **vdw**

### 11.26. Distance

Usage: **distance** [*distance_number*] *atom1 atom2*

**Distance** dynamically calculates and displays distances in angstroms between specified atoms. A dotted line is drawn between each pair of atoms for which a distance calculation is active. The user may assign a *distance_number* between 0 and 15, inclusive, to each active distance calculation. If *distance_number* is not given, one will be assigned for you. The distance calculation may be deactivated using **˜distance** *distance_number*. *Atom1* and *atom2* may be any two atoms on the displayed models in

See also: **ribbon**, **pdbrun**

### 11.21. Copy

Usage: **copy** [date] [box] [flat] [bg|background *color*] [intensity *0-1*] [printer *printer*] [file *file*] [title *title* ...]

The **copy** command sends a PostScript description of the current picture to a printer or disk file.

The optional keyword **date** puts today's date in the lower left hand corner of the copy. The optional keyword **box** draws a heavy border around the copy. The **flat** option forces all vectors (line segments) to be the same thickness, thereby disabling the pseudo-depthcueing effect created with variable width lines.

The **background** option sets the background copy color without changing what is shown on the screen. Similarly, the **intensity** option controls the color intensity of the copy background without affecting the screen background.

If the **printer** keyword is given, the copy is sent to *printer*. If the **file** keyword is given, the Postscript is saved in *file*. If neither is given, the copy is sent to the default system printer.

If the **title** keyword is given, the entire rest of the line is taken to be the title for the picture. Therefore, if **title** is specified, it must be the last thing in the **copy** command. If no title is given, you will be prompted for the title. If no title is desired, simply hit RETURN at the prompt. The title is centered at the bottom of the picture.

Users should note that in order to get halfbond coloring on color hardcopies, halfbond mode will have to be set before issuing the **copy** command. (Users of an IRIS 4DGT should probably unset halfbond immediately after the copy, since MIDAS on GT's looks worse with halfbond mode set).

### 11.22. Delegate

Usage: **delegate** list

Usage: **delegate** *name* start *command* [ *command_arguments* ]

Usage: **delegate** *name* stop

The **list** option lists all the active delegates.

The **start** and **stop** options start up and terminate a delegate of the given *name*, respectively.

The delegate mechanism allows other programs to extend the interactive capabilities of MidasPlus. The delegate mechanism is discussed in detail in appendix 5 of this manual. For a detailed description of an application developed using delegates, see ''Automated Site-Directed Drug Design Using Molecular Lattices'' in the *Journal of Molecular Graphics*, volume 10, number 2, June 1992 [R. A. Lewis, *et al.*].

See also: **pdbrun**, **pickatom**, **run**, **system**

### 11.23. Delete

Usage: **delete** *new_residue_type atom_specification*

**Delete** removes a branch of atoms from a residue. All atoms from *atom_specification* to the end of the side chain are deleted from the residue. Deleting from a main chain atom produces unpredictable results. Because the structure of the residue changes after deletion, a *new_residue_type* must be specified to differentiate between the original and new residue types.

By convention, *red*, *green*, *blue*, *cyan*, *yellow*, *magenta*, *white*, *gray*, *grey*, and *black* are predefined. And for backwards compatibility, the color names that correspond to the integers ranging from 0 to 65, inclusive, are predefined and may not be redefined.

**Numerical Color Mapping**

| Color name | Equivalent color number | colordef value | | |
|---|---|---|---|---|
| | | red | green | blue |
| green | 1 | 0.0 | 1.0 | 0.0 |
| cyan | 8 | 0.0 | 1.0 | 1.0 |
| blue | 16 | 0.0 | 0.0 | 1.0 |
| magenta | 24 | 1.0 | 0.0 | 1.0 |
| red | 32 | 1.0 | 0.0 | 0.0 |
| yellow | 48 | 1.0 | 1.0 | 0.0 |
| white | 0 | 1.0 | 1.0 | 1.0 |
| black | 64 | 0.0 | 0.0 | 0.0 |
| gray/grey | 65 | 0.5 | 0.5 | 0.5 |

Examples:

**colordef** activesite red    create a special color for the active site

On the *NeXT*, the **colorpanel** color is constantly redefined to be the current color in the color panel when the Color Panel is active, but otherwise acts just like any normal color name.

See also: **color**, **colorrename**

### 11.19. Colorrename

Usage: **colorrename** *color_name new_color_name*

**colorrename** replaces the given *color_name* with the *new_color_name*. The new color name is an arbitrary sequence of letters, digits, and underscores. This command is most useful on the *NeXT*, where one might color the active site with the **colorpanel** color, and then rename it to a different name to save it.

See also: **color**, **colordef**

### 11.20. Conic

Usage: **conic** *options*

The **conic** command produces a space-filling rendering of the displayed molecule(s). The current orientation and coloring is retained. Each atom is depicted as a sphere of the appropriate radius with realistic highlighting and shadowing effects. This image is not interactive and takes anywhere from 30 seconds to a few minutes to produce. Clicking the left button returns to MidasPlus.

There are many options, which are detailed fully in the *conic* manual page included in Appendix 6 of this document. (The **conic** command is actually an alias that executes the **pdbrun** command and sends data to the **conic** program.)

| | |
|---|---|
| **color** red #0:4@* | color all bonds in the fourth residue of model 0 red. |
| **color** 20,s #3 | color model 3 surface color 20 (midway between blue and magenta). |
| **color** green #2:HIS | color all histidine residues on model 2 green. |
| **color** blue,s #1 e<5 | color all atom surfaces on model 1 with electrostatic potential less than 5 the color blue. |

Ranges of colors may be mapped onto models based on either surface electrostatic potential or atom temperature factor. A range of color is specified by either keywords or numbers, such as *blue-red* or *16-32*. By default, color hues are interpolated counter-clockwise on a standard color wheel, the **c** designation changes the interpolation to be in the clockwise direction. To color models by electrostatic potential use the surface designation, **s**, with the color range. Colors are mapped onto the surface from lowest to highest potential based on a scale determined by the lowest and highest potential values *of all open models*. If boundary conditions are given, *i.e.* **e>**, **e<**, the colors are mapped within the boundaries. Similarly, for temperature factors, use the **l**, **b**, or **v** designation and specify boundary conditions using **b<** and **b>**. The default designation maps bond color by temperature factor and surface color by electrostatic potential.

For finer distribution of potentials and temperature factors, broader color ranges should be used. For example, *blue-red* maps only 120 degrees of the color wheel, whereas *cyan-yellow* maps 240 degrees. Alternatively, the interpolation direction may be changed by specifying the **c** designator.

Examples:

| | |
|---|---|
| **color** blue-red,s #0 | color lowest potential surface blue and highest red. Intermediate potentials are mapped to shades of magenta. |
| **color** red-blue,b #0 | color the bonds of the lowest temperature factor atoms red and highest blue. |
| **color** 8-32,s #0 e>-20 e<20 | color *ms* surfaces with potential -20 kcal/mole cyan (color 8) and with potential +20 kcal/mole orange (color 40). Intermediate potentials are mapped to shades of blue, magenta, and red. |
| **color** red /color=blue | color red every atom that is blue |

Note that lots of color changes, especially color ranges, have the potential of slowing down interactive response time significantly.

See also: **colordef**, **colorrename**

### 11.18. Colordef

Usage: **colordef** *color_name red green blue*

Usage: **colordef** *color_name existing_color_name*

**colordef** adds the given *color_name* to the list of color names that MIDAS recognizes. A color name is an arbitrary sequence of letters, digits, and underscores. A color name may be redefined at will. The *red*, *green*, and *blue* arguments must be floating point numbers between zero and one, inclusive.

### 11.16. Cofr

Usage: **cofr** [ *atom_specification* | view ]

When invoked without any arguments, the **cofr** command reports the current center of rotation.

If given an *atom_specification*, the **cofr** command sets the center of the bounding box of the given atom(s) as the center of subsequent rotations.

If the **view** keyword is given instead, the center of rotation is set to be the center of the current view.

**˜cofr** causes MIDAS to use its default center of rotation, instead of any previous user-specified one.

### 11.17. Color

Usage: **color** *color_designation*[,s][,l][,b][,v][,c] *atom_specification*

The **color** command allows the user to selectively color bonds, labels and surfaces by model, residue, and atom. *Color_designation* is a name that has been previously defined by the **colordef** command. A special *color_designation* is **byatom**, which is a simple attempt at determining color from atom name. Atom name prefixes and their corresponding colors are as follows:

| | |
|---|---|
| CL/BR | magenta |
| FE | gray |
| C | gray |
| O | red |
| N | light blue |
| H/D/digit | white |
| S | yellow |
| I/F | magenta |
| B | gray |
| others | blue |

These colors are coded into MidasPlus and cannot be easily changed.

Optionally, the user may specify one of the designations **s**, **l**, **b** or **v** to color surfaces, labels, bonds, and van der Waals surfaces, respectively. In the absence of these specifiers, MIDAS colors everything, *e.g.* bonds, surfaces, labels and van der Waals surfaces of all specified atoms.

Note that the solvent accessible surface and the van der Waals surface may be displayed simultaneously, and thus colored separately. See the **surface** and **vdw** commands in this document.

The *atom_specification* uses the standard MIDAS syntax. Note that the **˜color** command will not work, *i.e.* models may not be ‘‘uncolored’’.

On Silicon Graphics IRIS systems with the ‘‘GT’’ graphics option, bond colors will smoothly change from atom to atom due to the GT’s automatic color blending if ‘‘**devopt** blend’’ is *on*. On other systems, the entire bond will be given the color of the bond’s initial atom. To get half bond coloring on these systems, use **set halfbond**. This may result in decreased interactive response due to the increased number of vectors that have to be drawn.

If no *atom_specification* is given, all open models are colored.

Examples:

### 11.12. Cd

Usage: **cd** *path_name*

**Cd** changes the current working directory to *path_name*. If you are not familiar with the concept of directories and path names, see ‘‘UNIX for Beginners’’ (Kernighan) and the description of the ‘‘cd’’ command in section 1 of the UNIX User’s Manual. Note that all subsequent commands that have filename arguments are executed in the new working directory, for example, **pdbrun**, **record**, **save**, **source**, **write**, *etc*.

Example: **cd** ../crodna

### 11.13. Center

Usage: **center** *atom_specification*

**Center** places the center of the atoms in the *atom_specification* at the center of the screen.

See also: **window**

### 11.14. Chain

Usage: **chain** *atom_specification*

The **chain** command draws pseudobonds between the specified atoms, undisplaying all others. This is particularly useful for displaying the backbone atoms of a protein.

Example: **chain** @ca          chain all alpha carbons

See also: **display**, **show**

### 11.15. Clip

Usage: **clip** *plane units* [*frames* [*wait_frames*] ]

The clipping planes may be moved relative to their current position by a specified number of angstrom *units*. *Units* is a positive or negative number in angstroms. A positive number moves the plane towards the user. A negative number moves it away from the user. *Plane* may be either **hither**, or **yon.**

*Frames* moves the clipping plane in the specified manner for the specified number of image update frames. *Wait_frames,* if specified, indicates the number of frames to wait before beginning the move. **˜clip** will halt an ongoing clip. *Frames* and *wait_frames* default to 1 and 0, respectively. These parameters are useful for controlling the rate of clipping and are helpful when constructing MIDAS command scripts and making videos.

See also: **intensity**, **section**, **thickness**

The *direction*, if applicable, may be any of:

| **Slider Directions** | | |
|---|---|---|
| Direction | Designation | Applicability |
| x | the x axis | translation, rotation |
| y | the y axis | translation, rotation |
| z | the z axis | translation, rotation |
| h | hither plane | clipping, section, thickness |
| y | yon plane | clipping, section, thickness |
| 0–15 | rotation number | rotation |

Note that if *direction* is an integer, the corresponding intramolecular bond rotation is assigned to the slider. *Direction* is required for the functions **translation**, **rotation**, and **clipping**.

The default device assignments are located in */usr/local/lib/midas/midas.rc* on the IRIS, */LocalLibrary/Midas/midas.rc* on the *NeXT*, and listed in Appendix 4 of this document. The user may find it convenient to make additional automatic assignments by constructing a ‘‘.midasrc’’ file in his or her home directory and/or present working directory. Each time MIDAS is executed, any ‘‘.midasrc’’ files in the user’s home directory *and* the current working directory are executed before user commands are processed.

The **assign** command without any arguments reports all current assignments.

Example: **assign** 0 clipping h

See also: **select**, **(b)rotation**

### 11.10. Bond

Usage: **bond** *atom1 atom2*

The **bond** command tells MIDAS that *atom1* and *atom2* are bonded. *Atom1* and *atom2* must be in the same model.

**˜bond** breaks an existing bond between two atoms.

See also: **link**

### 11.11. Brotation

Usage: **brotation** [ *rotation_number* ] *atom1, atom2*[, *atom3, atom4*]

**Brotation** produces a ‘‘backwards’’ rotation, *i.e.* the portion of the molecule which remains fixed in a **rotation** command is rotated in the **brotation** command and vice versa. See **rotation** for an explanation of the syntax.

See also: **rotation**, **reverse**

The **alias** command without any arguments reports all current aliases. The **alias** command with *name* only reports the alias for that *name*. **˜alias** *name* deletes the alias for that *name*.

### 11.7. Align

Usage: **align** *atom1 atom2*

**Align** positions the selected model(s) such that the two specified atoms lie along the z-axis at the center of the screen. *Atom1* is positioned in the front and *atom2* is in the back.

See also: **reset**, **push/pop**, **savepos**, **window**

### 11.8. Angle

Usage: **angle** [*angle_number*] *atom1 atom2 atom3* [*atom4*]

**Angle** monitors the angle in degrees between the three specified atoms. If four atoms are specified, the dihedral angle is monitored. The atoms need not be connected and no diagnostic is given if the atoms are not connected. Up to 16 angles (0–15) may be monitored simultaneously. If the angle number is not specified, MIDAS will assign one for you.

**˜angle** *angle_number* will remove the indicated angle monitor.

### 11.9. Assign

Usage: **assign** [ *slider_number function* [*direction*] ]

**Assign** is used to activate control panel sliders. Each slider's number is displayed just to the left or right of the slider itself on the control panel. Usually only one slider may be assigned to any one function and reassignment of a function cancels the previous assignment. This default action of canceling a previous assignment can be disabled via the **unset reassign** command (see **set/unset**).

*Function* may be any of the following key words or the first two letters of the appropriate key word:

**Slider Functions**

| Keyword | Function |
|---|---|
| translation | model translation |
| rotation | model and bond rotation |
| clipping | clipping planes |
| scaling | changes size of selected models |
| section | moves hither and yon planes in the same direction at the same rate |
| thickness | moves hither and yon planes in the opposing directions at the same rate |
| nothing | for canceling slider assignment |

### 11.4. Addaa

Usage: **addaa** *residue_type*, *residue_sequence* [, *conformation*] *residue*

**Addaa** adds an amino acid of type *residue_type*, with sequence number *residue_sequence*, in the specified conformation after the specified *residue*. *Conformation* may be one of:

| | |
|---|---|
| EXT | extended (default) |
| ALPHA | alpha helix |
| PBETA | parallel beta sheet |
| ABETA | antiparallel beta sheet |

Currently, *residue* may only be the very last residue of a molecule. (This restriction may be removed in future versions of MIDAS.)

The temperature factor for the new residue is set to the highest currently found in the model.

Example:

| | |
|---|---|
| **addaa** tyr,30 #0:29 | Add **tyr** as residue **30** after residue **#0:29** |

### 11.5. Addgrp

Usage: **addgrp** *group*, *bond_length*, *bond_angle* [, *dihedral_angle* [, *new_residue_name*] ] *atom1 atom2 atom3*

**Addgrp** adds a new chemical group whose position is determined by the three specified atoms. The parameters required are the group name (which corresponds to a file in a directory, see below) the *bond_length* from *atom1* to the first atom of the added group, and the *bond_angle* formed by the group being added, *atom1* and *atom2*. The *dihedral_angle*, which defaults to 0, and the *new_residue_name*, which defaults to the old residue name, are optional. The *dihedral_angle* must be a positive value between 0 and 360, inclusive.

On the *NeXT*, group files are searched for in $*{HOME}/Library/Mol/groups/* and */LocalLibrary/Mol/groups/*, in that order. On the IRIS, group files are search for in $*{HOME}/groups/* and */usr/mol/groups,* in that order. Users may create groups in the former using files in the latter as formatting guides. A group name must contain only alphanumeric characters.

Note that adding a group creates a new residue which is colored white and has no labels. The temperature factor for the new residue is set to the highest currently found in the model.

See also: **delete**

### 11.6. Alias

Usage: **alias** [ *name* [ *wordlist...* ] ]

**Alias** assigns to *name* the specified *wordlist.* All subsequent appearances of the space delimited *name* will be substituted with the *wordlist.* The *wordlist* may contain multiple commands separated by semicolons in which case the *wordlist* must be embedded in double quotes, like this:

alias name "command1 ; command2"

The action of many MIDAS commands may be reversed by preceding the command with the tilde character ‘‘~’’. This is essentially an ‘‘undo’’ for the following commands:

| Reverse Command Functions | |
|---|---|
| Command | Function |
| ~alias | delete an alias |
| ~angle | remove an angle monitor |
| ~assign | deactivate pseudo-sliders |
| ~bond | remove a bond between two atoms |
| ~brotation | remove a ‘‘backwards’’ rotation |
| ~chain | break chaining for all atoms listed |
| ~clip | halt an ongoing clipping operation |
| ~cofr | use default center of rotation |
| ~display | remove atoms from the display |
| ~distance | remove a distance calculation |
| ~label | remove atom and residue labels |
| ~link | break residue chain into two parts |
| ~move | stop an ongoing move operation |
| ~open | close a model |
| ~pop | equivalent to **push** |
| ~push | equivalent to **pop** |
| ~rlabel | don’t display residue labels |
| ~rock | stop **rock** motion |
| ~roll | stop **roll** motion |
| ~rotation | remove a rotation |
| ~savepos | delete saved position |
| ~scale | stop ongoing scaling operation |
| ~section | stop an ongoing section operation |
| ~select | deselect a model |
| ~set | unset an option |
| ~setcom | use default center of mass |
| ~show | remove atoms from the display |
| ~stereo | equivalent to ‘‘**stereo** off’’ |
| ~surface | undisplay a solvent accessible surface |
| ~thickness | stop an ongoing thickness operation |
| ~turn | stop **turn** motion |
| ~vdw | remove a van der Waals surface display |
| ~watch | stop **watch** monitoring |

| **MidasPlus Commands**<br>(continued) | |
|---|---|
| Command | Function |
| pickabort | abort a **pickatom** request from a delegate |
| pdbrun | pipe PDB file describing current models to UNIX command |
| push/pop | push or pop images on the picture stack |
| read | read a command file |
| record | record all executed MidasPlus commands in a file |
| reset | reset all models to original orientations |
| reverse | reverse the direction of a bond rotation |
| rlabel | enable residue labeling |
| ribbon | display secondary structure ribbon image |
| rock | rock a structure about the x, y or z axis |
| roll | roll a structure or bond rotation about the x, y, or z axis |
| rotation | initiate a bond rotation |
| run | execute a shell command and send output to MIDAS |
| save | save a MIDAS session |
| savepos | save a model's current orientation |
| scale | apply a scaling factor to all models |
| section | change displayed image's cross section |
| select | select models for move, rock, roll, or turn commands |
| set/unset | set options |
| setcom | set molecule's effective center of mass |
| show | display specified atoms and no others |
| sleep | temporarily suspend all input processing |
| source | read and execute a command file |
| speed | set the control speed of pseudo-sliders and spaceball |
| stereo | specify whether to use stereo and in what manner |
| stop | terminate the current MIDAS session |
| surface | display a model's solvent accessible surface |
| swapaa | exchange one amino acid for another |
| swapna | exchange one nucleotide for another |
| system | execute a UNIX shell command |
| thickness | change thickness of the displayed image cross section |
| turn | rotate a structure about the x, y, or z axis |
| update | change coordinates of a model from a PDB file |
| vdw | display van der Waals surface |
| vdwopt | set van der Waals surface options |
| version | report MIDAS version number |
| wait | suspend input processing until model has stopped moving |
| watch | graphically monitor interatomic distances |
| watchopt | specify parameters used by **watch** command |
| window | display the entire molecule on the screen |
| write | output a model into a file |

**MidasPlus Commands**

| Command | Function |
|---|---|
| addaa | add an amino acid to the end of a molecule |
| addgrp | add a new group to a residue |
| alias | define or display command aliases |
| align | align two atoms along the z-axis |
| angle | monitor bond or dihedral angle |
| assign | assign functions to pseudo-sliders |
| bond | make a bond between two atoms |
| brotation | initiate a ‘‘backwards’’ bond rotation |
| cd | change current working directory |
| center | specify center of image |
| chain | chain specified atoms together |
| clip | move clipping planes |
| cofr | change center of rotation |
| color | color bonds, labels and surfaces |
| colordef | define color name |
| colorrename | rename color name |
| conic | display shadowed, space-filling image |
| copy | send display image to a printer or file |
| delegate | specify an action involving delegate program(s) |
| delete | delete a group from a residue |
| devopt | set device specific option |
| display | display specified molecules, residues, atoms |
| distance | monitor atom distances |
| echo | display text in reply area |
| fix | make bond rotations permanent |
| fixreverse | fix and reverse bond rotation |
| freeze | stop all motion |
| getcrd | return <x,y,z> coordinates for an atom |
| help | show information about MidasPlus commands |
| intensity | set depth cue intensity at hither and yon clipping planes |
| label | label atoms and residues |
| link | join two residue chains |
| match | superimpose two models |
| matrixcopy | copy transformation matrix from one model to another |
| matrixget | output a transformation matrix to a file |
| matrixset | set a transformation matrix from a file |
| midaspop | pop MIDAS window to front of other screen windows |
| midaspush | push MIDAS window behind other screen windows |
| move | translate selected models |
| neon | generate a molecular model with solid stick bonds and shadows |
| open | open a PDB file, solvent accessible surface, or object file for display |

(continued on next page)

### 11.3. Command Synopsis

MIDAS commands may be grouped together on one line using the ‘‘;’’ character as a delimiter. For example:

**label #1; color 32,s #1; color green,b #1**

If a large system is being displayed, it might be advantageous to use such a compound command since the graphics image is drawn only after the entire command has been executed.

Each description of the MIDAS commands in this document contains a line indicating the correct usage of the command. The usage includes the command name appearing in **boldface** print followed by command line parameters in *italic* or roman print. Parameters appearing in *italics* require substitution of the appropriate name, digit, etc. by the user. Parameters appearing in roman print are literals and should be typed in as they appear in the usage line. Parameters which appear inside square brackets, ‘‘[...]’’, are optional. All parameters not appearing inside square brackets are required for the command to execute. Keyword parameters are sometimes separated by vertical bars (‘‘|’’), which indicate that the keywords are mutually exclusive. Parameters named *atom_specification* always refer to a selection of atoms, residues and/or models as described in sections 10.1 and 10.2 of this document. Note that giving a null *atom_specification* is the same as specifying all atoms in all models.

MIDAS accepts abbreviated forms for all commands. Abbreviations are disambiguated by a ranking commands by frequency of use. For example, ‘‘rec’’ may be substituted for **record**. Typing ‘‘re’’ happens to mean **reset** instead of **read**.

The commands available in MIDAS are summarized in the following tables and described individually in detail on subsequent pages:

(see next page)

Then ‘‘pick’’ the atoms with the mouse. After the atom names are substituted for the ‘‘+ +’’, press the RETURN key to execute the command. When picking atoms, it may be necessary to rotate the molecule so that the desired atom is not obscured by other atoms, or so that neighbor atoms are not picked by mistake.

# 11. Commands

## 11.1. Command Overview

MIDAS commands allow the user a variety of modes of execution. The user may:

(1) Type in commands at the graphics system keyboard,

(2) Set up a command file named *.midasrc* which is automatically read each time MIDAS is executed,

(3) Set up a command file which can be executed via the **source** or **read** commands,

(4) Control movements via the mouse or auxiliary devices such as a joystick or ‘‘Spaceball’’.

Commands which are typed in at the graphics system keyboard are echoed on the graphics display screen. Replies generated by MIDAS appear next to this line. There may be several lines of reply messages. For example:

```
Reply:  Clipping plane is missing
Usage: assign [ slider_num function [ direction ] ]
Command: assign 0 clipping
```

appears on the screen when the user inadvertently forgets to supply the required clipping plane argument to the **assign** command.

## 11.2. MIDAS Start-Up

The MIDAS commands in the start-up file *.midasrc*, are executed each time MIDAS is executed. There is also a system start-up file executed each time (*/usr/local/lib/midas/midas.rc* on the IRIS, */LocalLibrary/Midas/midas.rc* on the *NeXT*). The order of execution of start-up files proceeds as follows:

(1) The system start-up file OR the file specified by the user’s environment variable ‘‘MIDASRC’’. (See Appendix 4 of this document.)

(2) The *.midasrc* in the user’s home directory.

(3) The *.midasrc* in the user’s present working directory. †

Start-up files are conveniently used for assigning pseudo-sliders as well as defining aliases and setting display options. (See the **assign**, **alias**, and **set** commands.) Any legal MIDAS command, however, may be included in a start-up file.

MidasPlus starts up in window mode with a default window size of 645 x 484 pixels on the IRIS (484 x 484 on the *NeXT*). To get a full-screen window with no border, use the **–f** command line option. If you always want full screen behavior when running MIDAS, you can put the following line in your *.cshrc* file:

```
alias midas midas -f
```

On the Silicon Graphics IRIS, MidasPlus now will refuse to start up if you’re not logged in on the console. You can force opening a window on the console by giving the **–F** command line option.

† On the *NeXT* machine, note that if MIDAS is started by *open*ing a file with a *.pdb* extension or by double-clicking on the **MidasPlus** application icon, then MIDAS will be running in the user’s home directory.

must *not* have that property. The visible property is true if an atom actually appears on the screen. The color property must be followed by an equals sign, **=**, and a color designation (see the **color** command for details). The following specifier selects all atoms named CA which appear on the screen, are not labeled, and are not green nor red:

@ca/visible,!label,!color=green,!color=red

### 10.4. Zone Specifiers

Zone specifiers are used to select atoms and residues that are within a given distance of the referenced atom(s). **z<** and **zr<** specify all *residues* within the given distance from the referenced atoms. **za<** specifies all *atoms* within the given distance. **z>**, **zr>**, and **za>** yield the complementary set to their ‘<’ counterpart. For example,

#1 za<10

selects all atoms within 10 angstroms of model 1.

### 10.5. Temperature Factors and Electrostatic Potentials

Atoms may be selected by temperature factor and surface points by electrostatic potential using the ‘‘<’’ and ‘‘>’’ symbols. Electrostatic potential selection requires the symbol ‘‘e>’’ or ‘‘e<’’ to select potentials above or below a specified value, respectively. Temperature factor selection requires the symbol ‘‘b>’’ or ‘‘b<’’ to select factors above or below a specified value, respectively. These symbols follow the *entire* atom specification and *must* have a preceding blank. For example,

| | |
|---|---|
| #1:HIS  b>25.0 | (all atoms in histidine residues in model 1 which have temperature factors exceeding 25.0) |
| #1  e>10  e<20.0 | (all surface points in model 1 with potentials between 10 and 20 kcal/mole) |

Note that electrostatic potentials only apply to surface points and are calculated and incorporated into surface files by the **esp** utility program; see Appendix 6 of this document for details.

### 10.6. Atom Intersections

Intersections of groups of atoms are handled with the **&** operator. For example, one may want all atoms in model 1 which are within 10 angstroms of model 0:

#1 & #0 z<10

### 10.7. Atom Picking

Atom picking allows a user to select atoms using the mouse instead of typing in the atom names on the keyboard. This is useful for identifying atoms whose names are not known and for ‘‘non-typists’’. To use this mode, type the MidasPlus command substituting the symbol ‘‘+’’ in place of each desired atom specification. When you type the ‘‘+’’, the cursor will change shape into a picking arrow. Use the mouse to move the picking arrow displayed on the screen to the desired atom and press the left mouse button. MidasPlus substitutes the name of the selected atom for the first occurrence of the symbol ‘‘+’’. Each subsequent ‘‘picked atom’’ is likewise substituted for a ‘‘+’’ symbol in the typed command. As an alternative to typing a ‘‘+’’ and then picking an atom with the mouse, an atom can be picked by clicking the left or middle mouse button on it while the keyboard Alternate (ALT on an IRIS) key is depressed. Its atom specifier will then be inserted in front of the command line cursor.

The command may be edited at any point using the editing commands detailed in Appendix 3. The command is executed when the user hits the RETURN key. For example, to label two atoms, type:

**label + +**

| | |
|---|---|
| #0:12@CA@N | (alpha carbon of residue 12 in model 0 and nitrogen of residue 12 in model 0) |
| #0:12@CA,N | (alpha carbon and nitrogen of residue 12 in model 0) |
| #1:LYS | (all lysine residues in model 1) |
| #3:45-83 | (range of residues 45 through 83 in model 3) |

Notice in the above example that the two atoms, 'CA' and 'N', may be delimited by either a comma or the symbol '@'. MIDAS interprets each atom name specified with the '@' symbol as a separate entity. Thus, the @N is interpreted to mean ''use the preceding (most recent) residue and molecule information to determine the atom.'' The comma delimiter indicates a group of atoms which are not single entities. Thus, '@CA,N' means ''use the preceding (most recent) residue and molecule information to determine *both* carbon and nitrogen.'' Thus, in specifications where the *order* of appearance of the atoms is significant (*e.g.* the **match** command), the separate entity notation should be used. For residues, the same hierarchical notation is followed. For example, for atoms on different residues but same model:

| | |
|---|---|
| #1:12,14@CA | (alpha carbon in residue 12 and residue 14) |
| #1:12:14@CA | (all atoms in residue 12 and alpha carbon in residue 14) |
| #1:12-20@CA:14@N | (alpha carbon in residues 12 through 20 and nitrogen in residue 14) |
| :LYS@CA | (alpha carbons in all lysine residues) |

In the example above, the first statement gives two residues which make up a single residue specification. Therefore, the carbon atoms in both residues are selected. In the second example, the entire residue 12 and only the carbon in residue 14 are selected.

The residue sequence number has to be followed by the residue insertion code and the chain identifier (in that order) if they are present in the PDB file.

### 10.2. Wildcard Symbols

The global wildcard symbol ''*'' matches all atoms in a residue or all residues in a model. It stands alone as a symbol, *i.e.* it cannot be used to match parts of names or sequences, such as G* or *A. To do that, use the ''='' wildcard character. For example, **color red @c=** means to color all atoms whose names begin with the letter ''c''. This works for residue names too (but not residue sequence numbers). The single character wildcard symbol ''?'' is used to select atom *names* and residue *names* whose names follow patterns. ''?'' cannot be used to match sequence numbers. For example:

| | |
|---|---|
| #1:12@* | (all atoms in residue 12 of model 1) |
| #0,1,2:50-*@CA | (all alpha carbon atoms in residues 50 to the end of models 0, 1 and 2) |
| #2:G?? | (all three character residue names which begin with the letter 'G' in model 2) |
| #0:*@H@H?@H?? | (all hydrogen atoms with one, two or three letter names in model 0) |

The percent symbol, ''**%**'', may be used to specify every *n*th item where *n* is an integer. For example, #1:*%5 selects every fifth residue in model 1; #1:HIS@*%4 selects the fourth atom of each HIS residue.

### 10.3. Atom Properties

Atom properties are specified with the **/** operator. The currently supported properties include **display**, **label**, **vdw**, **surface**, **visible**, and **color**. If a property name is preceded by a **!**, it means the atom

# PART III: Command Reference Guide

## 10. Referencing Models, Residues and Atoms

### 10.1. Models, Residues and Atoms

MIDAS uses a hierarchical command syntax developed in 1980 by the U.C.S.F. Computer Graphics Laboratory for referencing models, residues and atoms. In each MIDAS model, molecules are made up of residues. The residues are chained together in a specific sequence to form the molecule. Each residue is made up of atoms organized according to the coordinates and connectivity information. This scheme reflects nature's organization of biomolecules: amino acid chains make up protein molecules and nucleotide chains make up DNA molecules.

MIDAS allows the user to display multiple models (molecules) simultaneously. These molecules are assigned model numbers by the user with the **open** command or a default by MIDAS. Each molecule consists of one or more residues, each of which has a unique associated residue number according to its location in the residue sequence. The atoms which make up the residue each have associated atom names which are unique within any single residue. Thus, any displayed atom may be uniquely described by its model number, residue number and atom name.

The residue and atom names are determined at the time the input file is read in, and generally match the standard Brookhaven Protein Data Bank (PDB) residue and atom names. The symbols for these reference levels are defined as follows: †

**Atom Specification Symbols**

| Symbol | Reference Level | Definition |
|---|---|---|
| # | model number | a number assigned to the displayed model by the user via the **open** command |
| : | residue | a residue type (standard Protein Data Bank abbreviation) *or* residue sequence number *or* range of sequence numbers |
| @ | atom | an atom name (standard Protein Data Bank abbreviation) |

The following examples illustrate the use of these symbols for referencing models, residues and atoms. Note that the lack of either a residue specifier or an atom specifier or both is interpreted to mean ‘‘all’’ units of the associated reference level.

| | |
|---|---|
| #0 | (all atoms in all residues in model 0) |
| #1:50 | (all atoms of residue 50 in model 1) |
| #0:12@CA | (alpha carbon of residue 12 in model 0) |

Groups of atoms or residues may be specified. For example:

† Note: A summary of all special symbols described in this section appears in Appendix 3 of this document.

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DRAW NA
DRAW NB
DRAW NC
END NC

The start atom, *FE1* is correct but the connection to the following residue should be made via *FE2* instead of *NC*. The file can be edited to read:

RESIDUE FEA
START FE1
DRAW O
DRAW FE2
DRAW NA
DRAW NB
DRAW NC
END FE2

Sometimes **gentpl** is unable to generate a template from the PDB file because the atoms in the file are too far apart to determine the correct connectivity. An error message appears indicating ‘‘unreachable atoms’’. **gentpl** uses a standard list of atomic radii for determining connectivity. This list is located in */usr/local/lib/connect.tpl*. Atoms falling within the standard distances in the list are joined. Any atoms which are not joined to the main body of the residue, are reported as ‘‘unreachable atoms.’’

One approach to solving the ‘‘unreachable atoms’’ problem is changing the standard radii to larger values so that atoms which failed to bond before can be appropriately connected. To do this one can:

(1) Make a copy of the atomic radii file in your own private directory using the command:

    **cp /usr/local/lib/connect.tpl connect**

(2) Edit this connect file to increase the atom radii so that the appropriate connections can be made.

(3) Use the **gentpl** program to create the new template. For example, if the residue for which we want to build a template is VLX and this residue occurs in the PDB file *glx.pdb*, the command used is:

    **gentpl -r VLX -i glx.pdb -c connect**

    where *connect* is the name of the atomic radii file just edited. **Gentpl** searches through the PDB file for the specified residue and uses the atomic radii in the *connect* file to generate the connectivity of atoms and the corresponding MIDAS template.

If this method fails to produce an accurate template, the user must resort to creating the template instruction file with a text editor. Refer to the previous section for a description and example of the connectivity instruction file. Look at some of the *.ins* files in the template library (*/usr/mol/models* on the IRIS, */LocalLibrary/Mol/models* on the *NeXT*) to use as examples. Do not worry about the order in which the DRAW and MOVE commands appear in your instruction file as long as they correctly specify the connectivity and all atoms are connected to at least one other atom in the residue.

## 9. Making Videos

Many MIDAS commands are useful for producing video tapes and movies, and commands such as **move**, **rock**, **roll** and **turn** have optional parameters for the number of image update frames over which to carry out the command execution and the number of frames to wait before beginning execution. Currently, there are no stop motion ‘‘frame by frame’’ movie features (*i.e.* image generation synchronized with a camera).

MIDAS videos are produced from ‘‘scripts’’ or command files which can be created by the user with a text editor or recorded during a MIDAS session using the **record** command. By using command scripts the disk space required for files is minimized. To review a script give a **push** command, run the script, and do a **pop** to return to the original picture (this only works if the displayed atoms remain the same). To stop MIDAS in the middle of a script you may have to press the ESC key multiple times.

(1) The residue has a name, GLY, a starting atom, N, and an ending atom C. Thus, if GLY were found in a chain of amino acids, this residue would be connected to the previous residue in the chain via atom N and to the next residue in the chain via atom C.

(2) If you follow the DRAW and MOVE instructions on paper with a pencil (starting at N, draw a bond to CA, draw a bond from CA to C, draw a bond from C to O, lift up the pencil and move it back to C, draw a bond to OXT), you will find a pattern of connectivity for glycine such as can be found in any standard biochemistry text.

(3) Templates specify connectivity only, and do not give any information about bond angle or bond length. *In MIDAS, connectivity is determined by the MOVE and DRAW instructions in the template files, not by the distance between atoms.* If the user provides coordinates for glycine in which the distance from the C to the O is 10 angstroms, MIDAS is constrained to draw the long bond because of the connectivity specification in the glycine template. It is the user who defines the templates and ultimately controls which atoms are connected.

(4) The observant reader may have noticed that the carboxyl acid group contains two oxygen atoms, OXT and O. If this *gly* residue is the terminal amino acid in a peptide chain, then both oxygen atoms are appropriate to the model. If, however, the residue appears within a sequence of amino acids, then only one oxygen is appropriate and the bond to the atom named OXT is not drawn but instead a bond is drawn between the ‘‘END’’ atom (in this example a carbon) and the ‘‘START’’ atom of the next residue (typically a nitrogen in the case of amino acids). MIDAS decides which bonds not to draw in this case by ignoring atoms which appear in the template but for which the user provides no coordinates. Thus, only if the user provides a coordinate value for the atom OXT will MIDAS draw OXT. If OXT does not appear in the template, however, providing coordinates for OXT is *not* sufficient for adding the additional atom since the associated connectivity information must also be provided. In other words, an atom must be included in the template in order to appear in the MIDAS model.

(5) Note that none of the hydrogen atoms contained within a real glycine amino acid are included in the above template specification. Historically hydrogen atom coordinates are not included in protein and nucleic acid structures because of the limited resolution provided by x-ray crystallography techniques. For structures where hydrogen atom information is available, appropriately named atoms (*e.g.* HA, 1HG1...) can be added to the residue definitions and thus incorporated into the template file in the same manner as other atoms in the template.

Most commonly used templates have already been constructed and reside in a library accessible to MIDAS (*/usr/mol/models* on the IRIS, */LocalLibrary/Mol/models* on the *NeXT*). The naming conventions used in these templates are those specified by the Brookhaven Protein Data Bank and include amino acids, nucleic acids, and many prosthetic groups. Thus, for the most part all the residues needed to build a molecular model are already available. For the exception, however, the user must construct his or her own set of MIDAS templates and use these alone or in combination with the existing MIDAS library of templates. A program exists to automatically construct new template files when needed; see **gentpl** in Appendix 6 for details.

### 8.1. Building and Modifying MIDAS Templates

Occasionally it is necessary to modify existing templates. For example, **gentpl** sometimes generates templates with incorrect START and END atoms. This results in the use of the wrong atoms to connect the current residue to the previous and next residues in the chain. To correct this problem, the user may edit the template directly. To do so, invoke the standard system text editor on the *.ins* file in the user’s private ‘‘models’’ directory. On the *NeXT*, the default private models directory is *${HOME}/Library/Mol/models/*. On the IRIS, the default private models directory is *${HOME}/models/*. This can be overridden by setting the ‘‘MODELS’’ environment variable. If that directory doesn’t exist nor does the default models directory, then the template will be found in the current directory. Since *.ins* suffix files contain only simple character text, they can be edited directly. The name of the START atom and the END atom can be changed as needed; see previous section for additional information on the format of template files. For example, suppose **gentpl** generated the following template:

```
RESIDUE     FEA
START  FE1
DRAW   O
DRAW   FE2
```

```
ATOM      1  N   VAL     1       0.330  15.770  15.090  3.30  1.46
ATOM      2  CA  VAL     1       1.650  16.390  15.360  0.96  1.50
ATOM      3  C   VAL     1       2.670  15.670  16.230  3.18  1.43
ATOM      4  O   VAL     1       3.170  16.250  17.200 -0.72  1.48
ATOM      5  CB  VAL     1       1.760  17.680  16.180  1.77  1.47
ATOM      6  CG1 VAL     1       3.120  18.310  15.900  4.31  1.50
ATOM      7  CG2 VAL     1       0.630  18.680  15.930  2.42  1.51
ATOM      8  D   VAL     1      -0.250  15.310  14.410  4.96  1.46
ATOM      9  HA  VAL     1       2.200  16.520  14.420 -2.30  1.50
ATOM     10  HB  VAL     1       1.750  17.420  17.260 -2.08  1.62
ATOM     11 1HG1 VAL     1       3.210  18.510  14.820 -0.21  1.60
ATOM     12 2HG1 VAL     1       3.230  19.250  16.460 -0.92  1.57
ATOM     13 3HG1 VAL     1       3.910  17.600  16.200 -1.79  1.56
ATOM     14 1HG2 VAL     1      -0.270  18.120  15.640 -3.19  1.55
ATOM     15 2HG2 VAL     1       0.440  19.240  16.860 -0.54  1.56
ATOM     16 3HG2 VAL     1       0.940  19.370  15.130  2.66  1.57
```

Note in this example that:

- All hydrogens appear after the other atoms of the residue.
- Atom 9, ‘‘HA’’ is attached to atom 2, ‘‘CA’’. The remoteness indicator, ‘‘A’’ is the same for both these atoms.
- There are three hydrogen atoms connected to ‘‘CG1’’. These three all have the same remoteness indicator, but contain a distinguishing digit in column 13. Thus, each has a unique name.
- It is not necessary to use a digit as a prefix to the atom name when only one hydrogen is attached to a given atom.

## 8. More on Connectivity and Templates

**MidasPlus** has an algorithm for constructing atom connectivity based on interatomic distances. With reasonable coordinate data, this algorithm generally produces the correct connectivity. If, however, it consistently produces incorrect connectivity for a particular residue, the user may override the algorithm with a template.

MIDAS uses files called *templates* to form the connectivity of atoms. Each template consists of a map which describes how the atoms are connected and which atoms link the residue to other residues. This includes the following information:

(1) the residue name,

(2) the starting atom of the residue (important for connecting this residue to the previous one),

(3) the ending atom of the residue (important for connecting this residue to the next residue), and

(4) connections between atoms in the residue.

Template file names must be the same as the residue name. It is the template file name that is used to determine the connectivity and atom naming information when reading in PDB files. The following example is a template instruction file for glycine:

```
RESIDUE     GLY
START  N
DRAW   CA
DRAW   C
DRAW   O
MOVE   C
DRAW   OXT
END    C
```

Notice that:

**open 1 dfr dfr.dms**

To display the surface, use the **surface** command:

**surface #1**

## 6. Electrostatic Potential Molecular Surfaces

Users who wish to display electrostatic potential molecular surfaces should run the **dms** program as described above with an additional flag, *-n*. This flag generates surface normals in the **dms** output file. The **dms** output file may be used to generate the electrostatic potential of the surface using the program **esp**.

**Esp** requires a **dms** file and a PDB file as input. Assuming the **dms** file name is *dfr.dms* and the PDB file name is *dfr*, the command to calculate electrostatic potential is:

**esp -i dfr.dms -o dfr.esp -a dfr**

The program generates an annotated **dms** surface file, which in this example is named *dfr.esp*.

The atomic charges for the various residue types are held in the system file */usr/local/lib/charges.esp*. The user may substitute his or her own file of charges if desired. Use the system file as a format guide to generate the appropriate file. Include this file in the command line:

**esp -i dfr.dms -o dfr.esp -q chrgs -a dfr**

where *chrgs* is the name of the charges file. The *-q* flag and charges file must precede the name of the PDB file in the command line. Note that the electrostatic surface potential computed by **esp** depends crucially on the charge data in the charges file, so users should verify the data given in this file is correct for their particular application.

The **esp** program has several other options which are described in the **esp** manual page; see Appendix 6 of this document.

## 7. Modeling Hydrogen Atoms

### 7.1. Hydrogens in Protein Data Bank Files

Users who have coordinate values for hydrogen atoms may include those values in the PDB data file using the Brookhaven Protein Data Bank convention for hydrogen atoms. The conventions for hydrogen atoms in PDB files are as follows:

(1) Hydrogen atoms appear as ATOM records following the ATOM records of all other atoms of a particular residue.

(2) The name of each hydrogen atom is determined by the name of the atom to which it is connected:

The first space of the name (column 13) is an optional digit to be used if two or more hydrogens are attached to the same atom.

The second column, 14, is used for the chemical symbol, ‘‘H’’.

The next two columns contain the remoteness indicator (one or two characters) of the atom to which the hydrogen is attached.

For example,

```
ASN    15   FRM
LYS    21   TO
HIS   123   *
GLU   141   CB
GLU   141   CG
```

selects residues 15 through 21, inclusive, residue 123 (the ‘‘*’’ selects all the atoms of the residue), and atoms ‘CB’ and ‘CG’ of residue 141. The surface is calculated only for these specified atoms and residues.

Usually the selected portion of the model is an active site. The user may determine which atoms are of interest by one of two methods:

(2a) display the model and choose the atoms visually.

(2b) display the model and choose the atoms within a given radius of a ligand (use the zone specifiers in the atom specification syntax).

In either case you would have to generate the site selection file by hand using a text editor.

(3) Use the **dms** program to generate the surface. An example command for creating a surface is:

**dms** *dfr* **-a -d 0.5 -g** *logfile* **-i** *site* **-o** *dfr.dms*

where:

| | |
|---|---|
| *dfr* | is the name of the PDB file. |
| −a | indicates that all atoms are to be included in the calculation. If this flag is missing only amino acids are included in the calculation. |
| −d *0.5* | indicates that the density of points on the surface. |
| −g *logfile* | directs informative messages from the program to the file *logfile*. |
| −i *site* | directs **dms** to calculate the surface for the entire molecule but report the surface for only those atoms and residues selected in the file *site*. |
| −o *dfr.dms* | directs the output from the program (*i.e.* the surface) to the file *dfr.dms.* |

At U.C.S.F., the **dms** program should always be run in the background using the **submit** command. This prevents long running compute-bound jobs from adversely affecting interactive users. Thus, the command line for the above example becomes:

**submit dms** *dfr* **-a -d 0.5 -g** *logfile* **-i** *site* **-o** *dfr.dms*

(4) The progress of the **dms** program may be monitored in two ways:

(4a) Use the **ps** command to see if the program is running.

(4b) Read the logfile (*i.e.* the file name given with the *-g* flag) and the *submit.out* file created by **submit**. If the program is left to run overnight, it is a good idea to check these two files before leaving the laboratory to make sure the program didn’t run into immediate difficulty and stop.

The completed **dms** output file is quite large, so be sure adequate disk space is available.

(5) To display the surface, invoke the **midas** display program. Open the PDB file first using the **open** command as described in the ‘‘Command Reference Guide’’ section of this document. Then using the same model number, open the surface file. For example:

**open 1 dfr**
**open surface 1 dfr.dms**

opens PDB file *dfr* as model 1 and associates the surface *dfr.dms* with it. This may be shortened to:

Data Bank naming conventions (*e.g.* if the first letter encountered in atom name is C, then the atom is carbon, and so forth for N (nitrogen), O (oxygen), *etc.*). MIDAS creates a surface around each atom, clipping off areas of overlap to create a Corey-Pauling-Koltun (cpk) type model. The radii used can be changed with the **vdwopt** command in MIDAS.

(2) A *solvent accessible* surface may be calculated for any molecule. This surface is defined by rolling a theoretical water ‘‘probe’’ around the van der Waals surface of the molecule and using the contact and reentrant points to determine the surface. This type of surface provides a smooth surface, free of ‘‘seams’’ between atoms, since the surface is determined by a probe water molecule.

These two types of molecular surface representation differ significantly in their speed of generation and utility. Vdw surfaces are generated quickly and do not break or ‘‘tear’’ with bond rotations. Solvent accessible surfaces take approximately 100 times longer to compute, and the surface tears with bond rotations.

### 5.1. VDW Surfaces

The **vdw** command in MIDAS will display the van der Waals surface for all atoms of a MIDAS model or a subset of atoms as described in the ‘‘Command Reference Guide’’ section of this document. The user selects those atoms, residues, and models for which the surface is displayed.

Often the user does not want the surfaces of all atoms, both interior and exterior, displayed, but rather only the surfaces of those atoms which comprise the surface of the molecule or the surface of an active site. It can be a tedious process in MIDAS to select each of these surface atoms individually or even residue by residue. The zone specifiers in atom specifications (section 10.4) provide a convenient way to select specific sites of interest.

**Example**: Site selection

Suppose the user wants to display the surfaces of only those atoms within a certain distance of a particular set of atoms or coordinate positions, as in determining an active site of a molecule. If the receptor’s PDB file were opened as model zero and the ligand’s PDB file were opened as model one, the following command

**show #1 za<8**

will show only those atoms within 8 angstroms of any ligand atom (coordinate value). If the user wishes to change the test radius from 8 angstroms to 12 angstroms, for example, the command line is:

**show #1 za<12**

See Part III Section 10 of this document for additional details on how to specify atoms and zones around atoms.

### 5.2. Solvent Accessible Surfaces

In order to create a solvent accessible surface for display with MIDAS it is necessary to use the **dms** program to create a surface file that can be opened in MIDAS. Because of the time required to generate the surface, it is important to prepare files carefully to prevent time-consuming errors.

(1) Begin with a PDB file which has been displayed and is known to be correct.

(2) The surface may be calculated for the entire model or specific sections. To select specific sections, prepare a file containing the residues and/or atoms of interest. The format for this file is a series of lines containing the residue name, residue number and atom specification separated by spaces. Chain identifiers (if present in the PDB file) should be appended to the residue number. An atom specification can be an atom name, ’’*’’ (any atom in the named residue), or ’’FRM’’ followed on the next line by ’’TO’’ (used in pairs to denote residue ranges). Note that atom names should correspond exactly to the name given to the same atom by MIDAS. This generally means that the names of atoms in `HETATM` records should have a ’’*’’ appended to them.

As an example, a file appearing as:

## Part II: Advanced Concepts: Surfaces, Hydrogen Atoms, and Templates

This section describes some additional features of MIDAS and some ancillary programs which may be used in conjunction with MIDAS for specific modeling problems. Beginning users may skip this section on first reading. Included are descriptions of:

- Connectivity and templates
- Calculation and display of a molecular surface
- Calculation of electrostatic potential for a surface

Note: The descriptions include sample command lines. In these examples the model name used is *dfr*, an acronym for dihydrofolate reductase, a system which has been extensively modeled. The file names containing ‘‘dfr’’ should be substituted with the user’s own file names when running commands.

### 1.1. Connectivity and Templates

Many macromolecules in nature, such as proteins and DNA, are built from component molecules which are chained linearly into large structures using amino acids and nucleic acids as the building blocks. MIDAS uses the same approach in building molecular models. Small component molecules are chained together to build images of complex models. In MIDAS, these building blocks are called *residues*.

Each residue is made up of *atoms* which are connected in a specific pattern. Each atom in the residue has a unique name, usually combining a key letter, such as C for carbon, N for nitrogen, *etc.* and additional letters to uniquely identify it. For example, atoms may be named CA, C1, C2, N1, O2, *etc.* Thus, a residue contains a fixed number of atoms with specific names.

The pattern of bonding between the atoms is termed *connectivity*. The connectivity within a residue must form a connected graph of uniquely named atoms. Since the atoms are uniquely named, the bonding can be defined in an unambiguous manner. The definition of a MIDAS residue includes both connectivity and atom naming information.

When residues are used to build models, the connectivity of atoms is the same for each occurrence of any given residue in the model. For example, if we build a residue named ‘‘gly,’’ then each time a ‘‘gly’’ residue appears in the model protein, it will have the same basic pattern of connectivity of atoms and the same atom names.

MIDAS uses files called *templates* to name each residue’s atoms and the connectivity of those atoms. Each template consists of a map which describes how the atoms are connected and which atoms link the residue to other residues. If a template doesn’t exist for a particular residue, then MIDAS will use atomic radii and distances to connect atoms within the residue.

In most cases, you can safely forget about the existence of template files, partially because MidasPlus usually gets the connectivity right, and because you can fix the connectivity with MidasPlus commands once the model is displayed (see the **bond** command). Templates are discussed in more detail in part II section 9.

### 5. Molecular Surfaces

MIDAS represents molecules by drawing three dimensional ‘‘wire frame’’ stick figures on the screen. Users often want to characterize the surfaces of these molecules as well. This can be accomplished in several ways within MIDAS: the two basic types are space filling ‘‘solid’’ models and surfaces represented by a densely spaced dot surface. Surfaces represented by dots offer the most utility, since they can be manipulated in real time in the same way as wire frame models. Space filling models, on the other hand, offer shading and shadows and produce photographic quality images; these models are generated using the **conic** command (see Appendix 6 for full details).

There are two different types of dot surfaces available:

(1) A *vdw* or van der Waals surface uses the van der Waals radii of the atoms in the model. MIDAS assigns a van der Waals radius to each atom according to its atom type as determined by the Protein

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```
ATOM      1  C   HIS     1       49.169  26.701  10.917  1.00 16.00
ATOM      2  CA  HIS     1       50.197  25.578  10.784  1.00 16.00
ATOM      3  CB  HIS     1       51.312  26.048   9.843  1.00 16.00
ATOM      4  CD2 HIS     1       51.797  26.043   7.286  1.00 16.00
ATOM      5  CE1 HIS     1       49.691  26.152   6.454  1.00 17.00
ATOM      6  CG  HIS     1       50.958  26.068   8.340  1.00 16.00
ATOM      7  N   HIS     1       49.668  24.248  10.436  1.00 25.00
ATOM      8  ND1 HIS     1       49.636  26.144   7.860  1.00 16.00
ATOM      9  NE2 HIS     1       51.046  26.090   6.098  1.00 17.00
ATOM     10  O   HIS     1       48.241  26.524  11.749  1.00 16.00
ATOM     11  C   SER     5       47.713  29.006  10.110  1.00 15.00
ATOM     12  CA  SER     5       49.138  29.147  10.620  1.00 15.00
ATOM     13  CB  SER     5       49.875  29.930   9.569  1.00 16.00
ATOM     14  N   SER     5       49.788  27.850  10.784  1.00 16.00
ATOM     15  O   SER     5       46.740  29.251  10.864  1.00 15.00
ATOM     16  OG  SER     5       49.145  31.057   9.176  1.00 19.00
ATOM     17  C   GLN     3       45.406  27.172   8.963  1.00 14.00
ATOM     18  CA  GLN     3       46.287  28.193   8.308  1.00 14.00
```

Another common error often arises in the data entry process. Sometimes the letter ‘‘l’’ may be erroneously substituted for the number ‘‘1’’. This error has different repercussions depending upon in what data field the error occurs. If the letter ‘‘l’’ appears in the residue number, MIDAS does not complain, but then the letter ‘‘l’’ (rather than the number ‘‘1’’) must be used in all subsequent references to that residue. This can be very confusing, especially when all the other residues in the model are numbered. If the letter ‘‘l’’ appears in place of a ‘‘1’’ in the coordinate values, MIDAS accepts the input and sets those coordinate values equal to 0.000. Thus, if the user finds some atoms grossly misplaced in the MIDAS model, the corresponding error in the PDB file may be the use of ‘‘l’’ instead of ‘‘1’’. Such errors may be readily located if the text of the data file appears in upper case, since the editor may be invoked to search for all occurrences of the lower case letter ‘‘l’’.

can be summarized as:

(1) All atoms within a single residue must have unique names. For example, residue ‘‘VAL’’ may have only one atom named ‘‘CA’’. Other residues may also have a ‘‘CA’’ atom but not more than one ‘‘CA’’ may appear in ‘‘VAL’’.

(2) Residue names are a maximum of three characters long and uniquely identify the residue type. Thus, all residues of a given name in a file will be the same type residue and have the same structure. For example, residue ‘‘SER’’ has a certain connectivity specified in the template for ‘‘SER’’. Each occurrence of a serine residue in the Protein Data Bank file will conform to this pattern of connectivity. Atoms may be deleted in the PDB file, but may not be added if they do not appear in the corresponding template file. If a residue requires additional atoms or a different pattern of connectivity, such as in homoserine, a new template must be built and the PDB file must use a different residue name (*i.e.* other than ‘‘SER’’) in specifying the coordinates for the new residue.

### 4.3. Common Errors in PDB Format Files

If a data file fails to produce a model or produces an incorrect model in MIDAS, it is sometimes difficult to determine where in the hundreds of lines of data the mistake occurred. One common pitfall is failure to uniquely name all atoms within a given residue. Notice in the following example that two atoms in residue VAL are named CA.

```
ATOM      1  N   VAL A   1       6.280  17.225   4.929  1.00  0.00
ATOM      2  CA  VAL A   1       6.948  18.508   4.671  1.00  0.00
ATOM      3  C   VAL A   1       8.436  18.338   4.977  1.00  0.00
ATOM      4  O   VAL A   1       8.813  17.657   5.941  1.00  0.00
ATOM      5  CA  VAL A   1       6.317  19.598   5.527  1.00  0.00
ATOM      6  CG1 VAL A   1       6.959  20.999   5.376  1.00  0.00
ATOM      7  CG2 VAL A   1       4.819  19.636   5.383  1.00  0.00
ATOM      8  N   LEU A   2       9.259  18.958   4.152  1.00  0.00
ATOM      9  CA  LEU A   2      10.715  18.872   4.330  1.00  0.00
ATOM     10  C   LEU A   2      11.156  20.058   5.187  1.00  0.00
```

This error often does not become apparent until the residue is labeled and the resulting model is found to be missing a ‘‘CB’’ atom. If the MidasPlus program is used to (implicitly) construct the model, then it will draw a bond to the closest atom and silently ignore the other set of coordinates. This is one of the reasons it is advisable to always construct a template using **gentpl** since this program is more rigorous in checking for input errors; see section 9.1 for more details.

In the following example, notice that the second residue (SER) appearing in the file is erroneously numbered residue 5. MIDAS will accept this input without complaint. The resulting model have residue 5 connected to residue 1 and residue 3. This is all well and good, but only if it is what was originally intended. If, however, residue number 5 was to appear between residue 4 and residue 6, then it should have appeared in that order in the PDB file. Thus, if one finds that residues are connected in an incorrect order, the ordering and not the numbering in the data file should be changed.

```
ATOM   1058  N   ARG A 141      -6.576  12.834 -10.275  1.00  0.00
ATOM   1059  CA  ARG A 141      -8.044  12.831 -10.214  1.00  0.00
ATOM   1060  C   ARG A 141      -8.186  14.096  -9.365  1.00  0.00
ATOM   1061  O   ARG A 141      -7.591  15.139  -9.671  1.00  0.00
ATOM   1062  CB  ARG A 141      -8.579  11.531  -9.580  1.00  0.00
ATOM   1063  CG  ARG A 141      -8.386  11.441  -8.054  1.00  0.00
ATOM   1064  CD  ARG A 141      -8.727  10.045  -7.568  1.00  0.00
ATOM   1065  NE  ARG A 141      -9.095  10.056  -6.143  1.00  0.00
ATOM   1066  CZ  ARG A 141      -9.268   8.931  -5.414  1.00  0.00
ATOM   1067  NH1 ARG A 141      -8.602   8.795  -4.282  1.00  0.00
ATOM   1068  NH2 ARG A 141     -10.097   7.962  -5.830  1.00  0.00
ATOM   1069  OXT ARG A 141      -8.973  13.984  -8.310  1.00  0.00
TER    1070      ARG A 141
HETATM 1071 FE   HEM A   1       8.133   8.321 -15.014  1.00  0.00
HETATM 1072  CHA HEM A   1       8.863   8.752 -18.417  1.00  0.00
HETATM 1073  CHB HEM A   1      10.362  10.946 -14.389  1.00  0.00
HETATM 1074  CHC HEM A   1       8.482   7.374 -11.743  1.00  0.00
HETATM 1075  CHD HEM A   1       6.982   5.180 -15.773  1.00  0.00
HETATM 1076  N A HEM A   1       9.452   9.545 -16.178  1.00  0.00
```

The last residue in the alpha chain is an ‘‘ARG’’ (arginine). Again, the extra oxygen atom ‘‘OXT’’ appears in the terminal carboxyl. Notice that the ‘‘TER’’ record terminates the alpha chain, thus separating it from the heme group. This is important in preventing MIDAS from drawing a connection between the last atom in ARG and the first atom of the HEM residues. The atom number, residue type, chain indicator and residue number in the ‘‘TER’’ record are optional.

The heme group is a single residue made up of ‘‘HETATM’’ records. These record types are interchangeable with ‘‘ATOM’’ records in MIDAS. Note that the residue numbering begins again with ‘‘1’’ as the new chain begins.

At the end of the heme group associated with the alpha chain, the gamma chain begins:

```
HETATM 1109  CAD HEM A   1       7.582   6.731 -20.480  1.00  0.00
HETATM 1110  CBD HEM A   1       8.992   6.848 -20.968  1.00  0.00
HETATM 1111  CGD HEM A   1       8.998   6.529 -22.465  1.00  0.00
HETATM 1112  O1D HEM A   1       9.693   5.683 -22.895  1.00  0.00
HETATM 1113  O2D HEM A   1       8.276   7.153 -23.229  1.00  0.00
ATOM   1114  C   ACE G   0       7.896 -18.462  -1.908  1.00  0.00
ATOM   1115  O   ACE G   0       7.246 -18.839   -.922  1.00  0.00
ATOM   1116  CH3 ACE G   0       9.415 -18.301  -1.832  1.00  0.00
ATOM   1117  N   GLY G   1       7.354 -18.174  -3.077  1.00  0.00
ATOM   1118  CA  GLY G   1       5.904 -18.282  -3.283  1.00  0.00
ATOM   1119  C   GLY G   1       7.139 -19.112  -2.930  1.00  0.00
ATOM   1120  O   GLY G   1       7.026 -20.248  -2.448  1.00  0.00
ATOM   1121  N   HIS G   2       8.300 -18.533  -3.176  1.00  0.00
ATOM   1122  CA  HIS G   2       9.565 -19.224  -2.889  1.00  0.00
```

Here the ‘‘TER’’ card is implicit in the start of a new chain. The new chain identifier is ‘‘G’’. The file continues in the same pattern as before until the entire gamma chain and its associated heme group have been specified.

Remember that the spacing of the data fields is crucial. Refer to the table given previously to determine the precise columns in which data *must* appear. If a data field does not apply, it should be left blank. For example, a protein which consists of a single amino acid chain has no chain identifier and thus column 22 is blank.

From this example, it is apparent that Protein Data Bank format relies on the concept of *residues* much in the same way as templates. The same rules apply for PDB residues and template residues. These

The next three data fields contain the X, Y, and Z coordinate values, respectively. The next data field is the occupancy and is not used by **MIDAS**. The final data item is an optional atom temperature factor.

The glucagon data file continues in this manner until the final residue is reached:

```
ATOM    239  N   THR    29       3.391  19.940  12.762  1.00 21.00
ATOM    240  CA  THR    29       2.014  19.761  13.283  1.00 21.00
ATOM    241  C   THR    29        .826  19.943  12.332  1.00 23.00
ATOM    242  O   THR    29        .932  19.600  11.133  1.00 30.00
ATOM    243  CB  THR    29       1.845  20.667  14.505  1.00 21.00
ATOM    244  OG1 THR    29       1.214  21.893  14.153  1.00 21.00
ATOM    245  CG2 THR    29       3.180  20.968  15.185  1.00 21.00
ATOM    246  OXT THR    29       -.317  20.109  12.824  1.00 25.00
TER     247      THR    29
```

Note that this residue includes the extra oxygen atom, OXT, on the terminal carboxyl. The ‘‘TER’’ record terminates the amino acid chain.

A more complicated protein, fetal hemoglobin, consists of two amino acid chains (alpha and gamma) and two heme groups. The first ten lines of the PDB file for this molecule appear as:

```
ATOM      1  N   VAL A   1       6.280  17.225   4.929  1.00  0.00
ATOM      2  CA  VAL A   1       6.948  18.508   4.671  1.00  0.00
ATOM      3  C   VAL A   1       8.436  18.338   4.977  1.00  0.00
ATOM      4  O   VAL A   1       8.813  17.657   5.941  1.00  0.00
ATOM      5  CB  VAL A   1       6.317  19.598   5.527  1.00  0.00
ATOM      6  CG1 VAL A   1       6.959  20.999   5.376  1.00  0.00
ATOM      7  CG2 VAL A   1       4.819  19.636   5.383  1.00  0.00
ATOM      8  N   LEU A   2       9.259  18.958   4.152  1.00  0.00
ATOM      9  CA  LEU A   2      10.715  18.872   4.330  1.00  0.00
ATOM     10  C   LEU A   2      11.156  20.058   5.187  1.00  0.00
```

This data file appears initially much the same as the file for glucagon with the exception that the fifth data field now contains the single character chain indicator. In this case, the chain indicator is ‘‘A’’, indicating the alpha chain of the hemoglobin molecule. This field was simply blank in the glucagon example. At the end of chain A, the heme group records appear:

| | |
|---|---|
| **ATOM** and **HETATM** | Format ( A6,I5,1X,A4,A1,A3,1X,A1,I4,A1,3X,3F8.3,2F6.2 ) |
| **SSBOND** | Format ( A6,1X,I3,1X,A3,1X,A1,1X,I4,4X,A3,1X,A1,1X,I4 ) |
| **CONECT** | Format ( A6,11I5 ) |

### 4.2. Examples of PDB Format

Glucagon is a small protein of 29 amino acids in a single chain. The first residue is the amino terminal amino acid, histidine, which is followed a serine residue and then a glutamine. The beginning portion of the PDB file appears thus:

```
ATOM      1  N   HIS     1      49.668  24.248  10.436  1.00 25.00
ATOM      2  CA  HIS     1      50.197  25.578  10.784  1.00 16.00
ATOM      3  C   HIS     1      49.169  26.701  10.917  1.00 16.00
ATOM      4  O   HIS     1      48.241  26.524  11.749  1.00 16.00
ATOM      5  CB  HIS     1      51.312  26.048   9.843  1.00 16.00
ATOM      6  CG  HIS     1      50.958  26.068   8.340  1.00 16.00
ATOM      7  ND1 HIS     1      49.636  26.144   7.860  1.00 16.00
ATOM      8  CD2 HIS     1      51.797  26.043   7.286  1.00 16.00
ATOM      9  CE1 HIS     1      49.691  26.152   6.454  1.00 17.00
ATOM     10  NE2 HIS     1      51.046  26.090   6.098  1.00 17.00
ATOM     11  N   SER     2      49.788  27.850  10.784  1.00 16.00
ATOM     12  CA  SER     2      49.138  29.147  10.620  1.00 15.00
ATOM     13  C   SER     2      47.713  29.006  10.110  1.00 15.00
ATOM     14  O   SER     2      46.740  29.251  10.864  1.00 15.00
ATOM     15  CB  SER     2      49.875  29.930   9.569  1.00 16.00
ATOM     16  OG  SER     2      49.145  31.057   9.176  1.00 19.00
ATOM     17  N   GLN     3      47.620  28.367   8.973  1.00 15.00
ATOM     18  CA  GLN     3      46.287  28.193   8.308  1.00 14.00
ATOM     19  C   GLN     3      45.406  27.172   8.963  1.00 14.00
```

Notice that each line or *record* begins with the record type, ATOM. The atom serial number is the next item in each record. Although each atom in the file is given a unique serial number, this information is not required by MIDAS.

The atom name is the third item in the record. Notice that the first one or two characters of the atom name consists of the chemical symbol for the atom type. All the atom names beginning with ‘‘C’’ are carbon atoms; ‘‘N’’ indicates a nitrogen and ‘‘O’’ indicates oxygen. The next character is the remoteness indicator code which is transliterated according to:

| | |
|---|---|
| α | A |
| β | B |
| δ | D |
| ε | E |
| γ | G |
| η | H |
| ζ | Z |

The last character of the atom name is a branch indicator, if required.

The next data field is the residue type. Notice that *each* record contains the residue type. In this example, the first residue in the chain is HIS (histidine) and the second residue is a SER (serine).

The next data field contains the residue sequence number. Notice that as the residue changes from histidine to serine, the residue number changes from ‘‘1’’ to ‘‘2’’. Two like residues may be adjacent to one another, so the residue number is very important for distinguishing between them.

| Protein Data Bank Format | | | | |
|---|---|---|---|---|
| Record Type | Columns | Data | Justification | Data Type |
| ATOM | 1-4 | ‘‘ATOM’’ | left | character |
| | 7-11 | Atom serial number | right | integer |
| | 13-16 | Atom name | left* | character |
| | 17 | Alternate location indicator | | character |
| | 18-20 | Residue name | right | character |
| | 22 | Chain identifier | | character |
| | 23-26 | Residue sequence number | right | integer |
| | 27 | Code for insertions of residues | | character |
| | 31-38 | X orthogonal Å coordinate | right | floating |
| | 39-46 | Y orthogonal Å coordinate | right | floating |
| | 47-54 | Z orthogonal Å coordinate | right | floating |
| | 55-60 | Occupancy | right | floating |
| | 61-66 | Temperature factor | right | floating |
| TER | 1-3 | ‘‘TER’’ | | character |
| | 7-11 | Serial number(optional) | right | integer |
| | 18-20 | Residue name(optional) | right | character |
| | 22 | Chain identifier(optional) | | character |
| | 23-26 | Residue sequence number(optional) | right | integer |
| | 27 | Code for insertions of residues(optional) | | character |
| HETATM | 1-6 | ‘‘HETATM’’ | | |
| | 7-66 | same as ATOM records | | |
| SSBOND | 1-6 | ‘‘SSBOND’’ | | character |
| | 8-10 | Sequence number (optional) | right | integer |
| | 12-14 | Residue name (CYS) | right | character |
| | 16 | Chain identifier | | character |
| | 18-21 | Residue sequence number | right | integer |
| | 26-28 | Residue name (CYS) | right | character |
| | 30 | Chain identifier | | character |
| | 32-35 | Residue sequence number | right | integer |
| CONECT | 1-6 | ‘‘CONECT’’ | | |
| | 7-11 | Atom serial number | right | integer |
| | 12-16 | Atom serial number (covalent bond) | right | integer |
| | 17-21 | Atom serial number (covalent bond) | right | integer |
| | 22-26 | Atom serial number (covalent bond) | right | integer |
| | 27-31 | Atom serial number (covalent bond) | right | integer |
| | 32-36 | Atom serial number (hydrogen bond) | right | integer |
| | 37-41 | Atom serial number (hydrogen bond) | right | integer |
| | 42-46 | Atom serial number (salt bridge) | right | integer |
| | 47-51 | Atom serial number (hydrogen bond) | right | integer |
| | 52-56 | Atom serial number (hydrogen bond) | right | integer |
| | 57-61 | Atom serial number (salt bridge) | right | integer |

For those who are familiar with the FORTRAN programming language, the following format descriptions will be meaningful. For those users unfamiliar with FORTRAN, ignore this gibberish:

*Atoms whose chemical symbols (as distinct from remoteness indicator) are one letter long are left justified in columns 14-16. Those which are 2 characters long (*e.g.* zinc symbol ‘‘ZN’’) are left justified starting in column 13. Refer to the Brookhaven document ‘‘Protein Data Bank File Record Formats’’ for details.

| Protein Data Bank Record Types<br>Recognized by MIDAS | |
|---|---|
| Record Type | Data Provided by Record |
| **ATOM** | atomic coordinate record containing the x,y,z orthogonal angstrom coordinates for the given atom |
| **HETATM** | atomic coordinate record containing x,y,z coordinates for non-standard atoms. These record types are used by BNL to distinguish standard residues, such a amino acids and nucleic acids, from non-standard groups, such as inhibitors, substrates, and saccharides. The only functional difference with ATOM records is that HETATM residues are by default not connected to other residues. |
| **SSBOND** | defines disulfide bond linkages between amino acid residues. Notice that the templates as described thus far allow only for linkage to the next residue in the chain and to the previous residue in the chain. SSBOND records are special case links which are handled separately in MIDAS and bond rotations about these links are not allowed. |
| **TER** | indicate the end of a chain of residues. For example, a hemoglobin molecule consists of 4 subunit chains which are not connected. TER indicates the end of a chain and prevents a connection (line) to the next chain. This record type is also used to prevent connection of substrates to other displayed parts of the model. |
| **CONECT** | gives explicit connectivity of atoms. |

The following table describes the format for each record type. The *record type* appears in columns 1 to 6 of each line of a PDB file. This *record type* determines the kind and format of information on the remainder of that line. Note that the data appears in specific *columns*. This refers to the spaces on the line in which the data appears. For example, in an ATOM record, the first four spaces contain the record type, ‘‘ATOM’’. The next two spaces are blank. The 7th through 11th spaces contain the atom serial number. The serial number is right justified, so if the serial number is ‘‘1’’, for example, the digit 1 will appear in the 11th space and the other spaces will be blank. For the atom with serial number ‘‘100’’ the number will appear in spaces 9 through 11 leaving space 7 and 8 blank. It is necessary to reproduce this format *exactly* in order for MIDAS to interpret the data properly. Any deviation is likely to cause errors preventing the successful construction of a model.

## 3. On-line Help

MIDAS features an on-line help system. All commands documented in Part III of this manual are also available on-line. The command

**help** *command*

will produce a short synopsis of the specific command in question. The command

**help**

without any arguments produces a list of all available MIDAS commands. The help facility is very useful for both the novice and experienced MIDAS user and alleviates constantly referring the User's Manual for every command.

On the *NeXT*, the MidasPlus **help** command with no arguments puts you in the Digital Librarian where you can search for the information you desire. Use the *Titles* button in the Librarian to list all of the available topics. If you wish to access the MidasHelp files directly with the Librarian (without starting up *MidasPlus* first), add */LocalLibrary/Midas/MidasHelp* as a target in the Librarian's bookshelf and select it as you would any other target.

By default, when you give the **help** command with an argument, MidasPlus interprets the argument as a topic name and displays the help file for that topic. If the topic isn't found, the Digital Librarian is invoked with the topic as the search string. If you want to always search for the topic using the Librarian (and not be limited to one word), put

**devopt help_search on**

in your private *.midasrc* file in your home directory, or change the default behavior for all users by putting the above command in */LocalLibrary/Midas/midas.rc.*

## 4. Protein Data Bank Format

The UCSF Computer Graphics Laboratory has adopted the Protein Data Bank (PDB) format as a standard for all coordinate text files. The Protein Data Bank at Brookhaven National Laboratory (BNL) is a clearing house for macromolecular coordinate data, and distribution tapes are written in a standardized format specified by BNL. A complete and concise description of the format is given in the document ''Protein Data Bank Atomic Coordinate Entry Format Description,'' which is published and distributed by Brookhaven National Laboratory. A newsletter is also published on a periodic basis by BNL. In this section, a shortened description of PDB format is presented that is sufficient for use in creating MIDAS input.

The complete PDB file structure contains a wealth of information including source, journal citations, and identification of substructures such as disulfide bonds, helices, beta sheets, and active sites. Since the entire Protein Data Bank entry contains much more information on a macromolecule than is needed for model building, knowledge of a subset of the format is sufficient for MIDAS users. Users should bear in mind, however, that adhering strictly to the format specifications is key to successful model building. The modeling programs are unforgiving about incorrect input formats, and much time and frustration can be saved by diligence in data preparation.

### 4.1. Description

Protein Data Bank format is a character oriented format which consists of lines of information in a file. One file generally contains enough information to characterize a single molecule or model. Each line of information in the file is called a *record*. There are usually several different types of records present in the same file, such as **ATOM** records, which contain coordinate values for atoms, **SSBOND** records, which contain disulfide linkage information, and **TER** records which signal the end of a chain of residues. These records are arranged in a specific sequence to characterize the molecule.

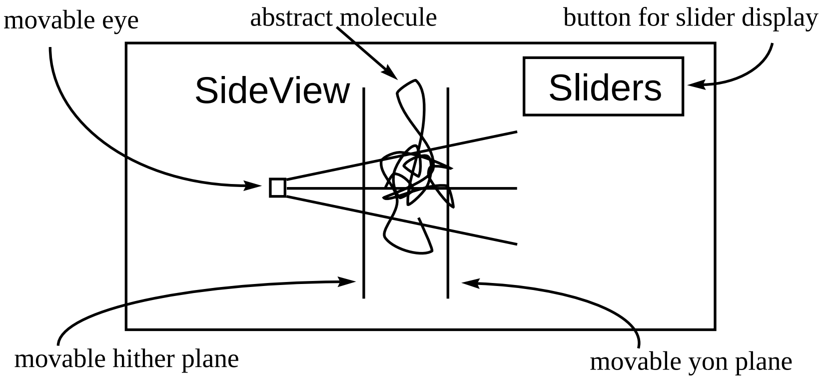


Figure 2. IRIS Side-view

The eyepoint and clipping planes can be moved by positioning the mouse over them, depressing the left button, and dragging the item. Moving the eyepoint changes the apparent size (scale) of the image. If the control panel isn't a separate window, then clicking on the box labelled *Sliders* replaces the sideview with the general purpose sliders. Each slider is numbered, and may be assigned a function, such as model rotation or translation, clipping plane manipulation or bond rotation adjustment. See the **assign** command in Part III for further details. To utilize a slider function, click and hold down the left mouse button over the slider labeled with the function of interest. For example, to translate a model along the z axis, click over the slider labeled ''z tran''. The left half of the slider moves the model further away, while the right half brings it closer. As one holds the button down, the rate of the translation, and even its direction, can be adjusted by moving the mouse within the slider region.

The lower part of the control panel contains two rows of numbered (except for one marked ''All'') small boxes, collectively known as *pseudo-switches* or simply *switches*. These control whether the corresponding model number is *selected*. Only models that are selected can be manipulated. When a model is first opened, it is automatically selected and the corresponding switch is highlighted. It may be necessary to deselect a model if one model is to be moved relative to another. Clicking over a switch toggles the selection mode of the corresponding model. Clicking over ''All'' selects all open models. Clicking on ''All'' again will return to the previous selection state. If there are more models open than there are switches, you will need to use the **select** command instead of the mouse to select and deselect them.

From this point on, there are many MIDAS commands available for manipulating the model. These are described in detail in Part III, ''Command Reference Guide'', of this document. The following categories of commands are provided to help you get started:

| For information on: | The pertinent commands are: |
|---|---|
| Adding groups or new residues | **addgrp addaa delete swapaa swapna** |
| Coloring models | **color intensity set** |
| Displaying molecular surfaces | **surface vdw vdwopt** |
| Interactive manipulation of models | **assign select** |
| Labeling model components | **label rlabel** |
| Making videos | **rock roll set sleep source wait** |
| Recovering coordinates | **fix getcrd save write** |
| Rotating bonds | **rotat brotat reverse assign angle** |
| Selective display of model components | **chain display show** |
| Viewing in stereo | **stereo** |

*''Menu Button'' has been enabled via the Preferences application.* Depressing and holding the left button controls model rotation. While the button is held down, a dashed blue circle is displayed on the screen. Moving the mouse outside the circle results in model rotation about the z axis. The area inside the circle is a ''virtual trackball''; when the mouse is within this area it ''grabs'' the trackball and rotates it. The model rotates as if it were inside the trackball. Once comfortable with this interaction method, display of the dashed circle can be suppressed, if desired, by typing **˜set showsphere**. The ''icon'' used for the mouse cursor changes when the left mouse button is depressed and also changes dependent on whether or not the mouse is inside or outside the trackball circle, regardless of whether or not the actual circle is displayed. Thus the mouse icon can be effectively used as a visual feedback clue to indicate the type of rotational motion currently in effect. Depressing and holding the middle mouse allows dragging the model(s) left/right and up/down. In other words, the middle button controls global translation of the selected model(s). Depressing and holding the left and middle mouse buttons simultaneously results in z translation of the selected model(s).

More mouse-based interactions can be done via the *control panel*, which is a separate window on a *NeXT*, or is in the lower right corner of the main window on an IRIS. In the control panel appear controls for manipulating the selection state of models, the viewing parameters, and some general purpose sliders.

The sideview shows a stylized representation of the molecule(s), as viewed from the side. Also represented are the viewer's eyepoint (the box at the junction of the convergent horizontal lines) and the hither and yon clipping planes (the left and right vertical lines, respectively). Typical side-view areas are shown in Figures 1 and 2.

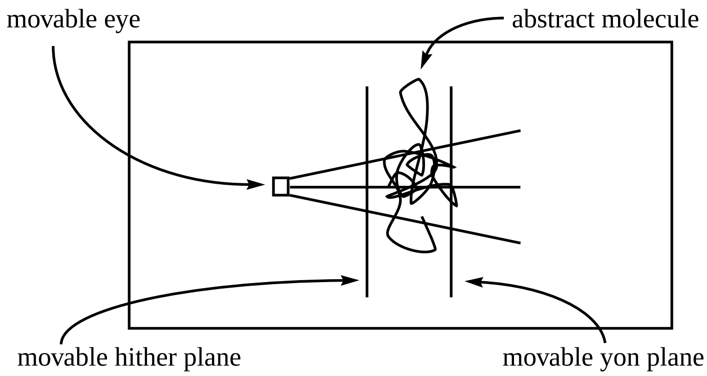


Figure 1. *NeXT* Side-view

# Part I: Molecular Modeling with MIDAS

## 1. Getting Started

MidasPlus is capable of displaying molecular structures and surfaces from information contained in Protein Data Bank* (PDB) format files, molecular surfaces from the solvent accessible surface computation program (DMS), or arbitrary collections of text, lines, and points. Using PDB format files directly provides for maximum convenience, since only a single human-readable file needs to be manipulated.

The only functional difference between the various file formats occurs with the ancillary programs, *e.g.*, the **ribbon** and **conic** commands, as these commands operate only on PDB format files — especially **ribbon** as it requires secondary structure information in the form of the PDB HELIX and SHEET records. The section ‘‘Protein Data Bank Format’’ discusses the details of PDB file format. If you have trouble displaying a file that is supposedly in PDB format, you should consult the aforementioned manual section to ensure that the file is indeed in adherence to the PDB standard.

If you already have a PDB format file that is known to be correct, or you want to try out MidasPlus with one of the test files included with the software distribution, the following section shows you how to quickly display a model and then manipulate it.

## 2. Displaying the Model

The MidasPlus display program is used to display the PDB file. To invoke the MidasPlus display program give the command:

**midas** (on SGI IRIS workstations)

*or*

**/LocalApps/Midas** (on *NeXT* workstations)

A default-sized window is initially presented, although the MIDAS window may be resized at any time by using the standard technique of ‘‘grabbing and pulling’’ a window corner with the mouse.

After a few seconds delay, **MidasPlus** should be ready for command line input at the ‘‘Command:’’ prompt. The *control panel* on the right side is described in detail below under **Manipulating the Model**.

Once the ‘‘Command:’’ prompt appears, characters typed on the keyboard are interpreted directly as commands to MIDAS.

The first step in displaying a model is to ‘‘open’’ the model. If the name of the PDB file were *1gcn*, the command used to open the model is:

**open 0 1gcn**

The model name may also be a pathname to a model in another directory. The 0 (zero) in the above example is the optional model number. If the model number is left out, then the smallest unused (non-negative) model number is used.

### 2.1. Manipulating the Model

After execution of the **open** command completes, the model should appear on the graphics display screen. On a three button mouse, the left and middle mouse buttons allow direct manipulation of the selected model(s) and the right button calls up a system menu. On a two button mouse (like the *NeXT*’s), the original system menu functionality of the right button is lost and the right button acts just like the middle button on a three button mouse. *On the NeXT, the right mouse button will not function unless the*

* Bernstein, F. C. The Protein Data Bank: a Computer Archive. J Mol. Biol. 112, 535-542 (1977). For information on obtaining copies of coordinates from the data bank write to Protein Data Bank, Chemistry Department – Building 555, Brookhaven National Laboratory, Upton, New York 11973 USA. Electronic mail can be sent to PDB@BNLCHM.BITNET or pdb@pb1.chm.bnl.gov.

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**Acknowledgements**

The original version of **MIDAS** was written by Prof. Thomas Ferrin and Dr. Conrad Huang. Dr. Huang is also the principal author of **MidasPlus**. Eric Pettersen, Greg Couch and Laurie Jarvis have all contributed to the significant effort required in programming, testing and documenting the many features the **MIDAS** system offers. All of these individuals are still affiliated with our laboratory. The Laboratory Director is Prof. Robert Langridge. Thanks are due to many of our existing MIDAS users for countless suggestions over the years that lead to improvements in the system. This work is supported by the National Institutes of Health, National Center for Research Resources (NCRR), RR-01081.

Because a substantial portion of the funding for our laboratory comes from a NCRR grant (RR-01081) from the National Institutes of Health, it is important that publications resulting from work using the **MIDAS** system or incorporating graphical images produced with **MidasPlus** acknowledge our laboratory. We ask that a statement similar to the following be used:

> Molecular graphics images were produced using the MidasPlus software system from the Computer Graphics Laboratory, University of California, San Francisco.

The article which describes the **MIDAS** system and should be included in your references is:

> T.E. Ferrin *et.al.*, ‘‘The MIDAS display system’’, *J. Mol. Graphics* **6**, 13-27 (1988).

We would also appreciate receiving two reprints of any publications resulting from your work with the **MIDAS** system.

- Full Protein Data Bank (PDB) support. Anything that used to be done with a **MIDAS** database can now be done directly from within **MidasPlus**. For example, **MidasPlus** can open PDB format files for input directly, without needing to use the antiquated *midas.in* program beforehand. ‘‘Compressed’’ PDB files are also supported. Because of direct PDB support, the *midas.in* program is no longer distributed.
- Graphical-based user interaction, including a ‘‘virtual trackball’’ technique for interactive rotations and direct manipulation of eye position and hither and yon clipping planes.
- Ability to generate space filling images with shadows cast from multiple light sources. These images can be simple CPK-style spheres (see the *conic* command) or ball and cylinder representations (see the *neon* command).
- Ability to generate ‘‘ribbon’’ drawings for depicting protein secondary structure.
- Ability to annotate space filling images with text (see the *ilabel* command).
- Ability to spawn and interactively communicate with other programs from within **MidasPlus**.
- Enhanced support for stereo viewing of images, including generating images with either positive or negative horizontal parallax.
- Support for Spatial Technology’s six degree-of-freedom ‘‘Spaceball’’ interactive input device.
- Enhanced control of van der Waals surfaces with immediate updating of the screen image. Non-standard atom radii can be defined directly on the **MidasPlus** command line.
- Interactive monitoring for interatomic contacts during bond and dihedral angles rotations.
- Direct support of MS surface files, including ‘‘compressed’’ MS files.
- Full integration with native windowing systems.

**Manual Organization**

The MidasPlus User’s Manual is divided into several sections. Part I discusses the important concepts in **MidasPlus** input file format and the user interface. Since the input data used by **MidasPlus** is critical to a productive modeling session, careful reading of this section is essential. Part II discusses many of the advanced concepts in **MIDAS** such as displaying molecular surfaces, computing electrostatic potential surfaces, adding hydrogen atoms, *etc*. Beginning users may skip Part II on first reading. Part III of the manual is intended as a reference guide and gives a concise description of each of the commands available in **MidasPlus**. Appendices near the end of this manual describe topics such as available models in the Protein Data Bank library, atom naming conventions, special characters and symbols used by **MidasPlus**, default options, aliases and device assignments, and differences between **MidasPlus** and previous versions of **MIDAS**. There is a descriptive index at the end of the manual which may be of use in locating particular topics of interest. Special attention should be given to Appendix 6, as this section describes the many **MIDAS** utility programs that are part of the overall system. Where there are differences between the way MIDAS acts on various workstations, they will be explicitly noted.

Recent changes to the MidasPlus User’s Manual are now indicated with a vertical bar in the right margin area of the manual, such as shown in this paragraph. Changes, additions and bug fixes are also detailed in the ‘‘Release Notes’’ document. Thus users already familiar with **MidasPlus** can quickly determine what all has changed when a new release is distributed.

**Future Development Plans**

The **MIDAS** system is used daily at UCSF as part of an active research program in pharmaceutical chemistry. As such, changes and enhancements are made from time to time, often in response to new ideas from our users. While we make no promises as to when new versions of **MIDAS** will be released, we do encourage your feedback. If you discover bugs or have ideas you think would be particularly useful to others, please send us electronic mail at **midas-ideas@cgl.ucsf.edu**. If the mail concerns a program bug, please include the version of **MidasPlus** you are using as determined from the output of the ‘‘version’’ command.

## Introduction

### Background

The Molecular Interactive Display and Simulation (**MIDAS**) System is a collection of programs developed by the Computer Graphics Laboratory at the University of California, San Francisco. The major component of the **MIDAS** system is an interactive graphics display program, **MidasPlus**™, designed for the display and manipulation of macromolecules such as proteins and nucleic acids. Several ancillary programs are also part of the system and allow for such features as computing the surface of a molecule, computation of electrostatic charge potentials, *etc.*

**MIDAS** is the most recent in a series of interactive molecular graphics systems whose direct lineage extends back to the first developments in molecular graphics at Project MAC, Massachusetts Institute of Technology, in 1964.[1,2] National Institutes of Health (NIH) support began with the formation of the Computer Graphics Laboratory at Princeton University in 1969 and resulted in a number of pioneering developments including CAAPS (Computer Aided Analysis of Protein Structure).[3] In 1976 this NIH research resource moved to U.C.S.F. A new graphics package[4] was designed to operate under the UNIX[5] operating system and a new molecular graphics system (MMS) designed, initially in collaboration with the group under Professor J. Kraut at U.C. San Diego. This evolved into a system, MIDS, which was good enough to accommodate the new developments in color graphics and which also made possible the display of interacting surfaces.[6] The MIDS system was used by numerous visitors to our laboratory in the late 1970's.

In 1980 we decided to redesign the system completely, making use of the lessons learned over the previous 15 years. The result, **MIDAS**,[7,8] emphasized highly interactive display and manipulation, with a data structure designed for very fast access to large and complex molecules such as proteins and nucleic acids.[9] Over 200 publications have resulted from work at the UCSF Computer Graphics Laboratory using **MIDAS**.

**MIDAS** was developed in a university research environment and has grown considerably in functionality and size in response to new ideas; often these ideas have come from **MIDAS** users themselves, now numbering over 190 from 33 states and 17 countries. **MIDAS** was originally developed on the UNIX operating system for use with an Evans and Sutherland Picture System 2 display, however between 1982 and 1989 **MIDAS** has run on a variety of graphics display engines (PS2, MPS, PS300 family, and Silicon Graphics IRIS family) and operating systems (BSD UNIX, System V UNIX and VMS).

### MidasPlus

Due to the substantial advances in graphics display technology and workstation functionality and performance in the mid-1980's, we decided in early 1989 that it was time to ''rewrite'' the display portion of the **MIDAS** system in order to take advantage of these advances. This work was done during the summer of 1989 and the resulting program was named **MidasPlus**. **MidasPlus** has significantly increased functionality and performance when compared to the previous version of the **MIDAS** display program; many commands execute 5x - 10x faster. This was accomplished while maintaining complete compatibility with the original **MIDAS** command language. New features in **MidasPlus** include:

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**MidasPlus** is a trademark of the UCSF Computer Graphics Laboratory.

[1] R. Langridge and A.W. MacEwan, in *Proceedings, IBM Scientific Computing Symposium on Computer Aided Experimentation* (1965).

[2] C. Levinthal, *Scientific American* **214** (6), 42-52 (1966).

[3] R. Langridge, *Federation Proceedings of the American Society of Experimental Biology* **33**, 2322-2328 (1974).

[4] T.E. Ferrin and R. Langridge, *Computer Graphics* **13**, 320-331 (1980).

[5] D.M. Ritchie and K. Thompson, *Communications of the ACM* **17**, 7 (1974). UNIX is a registered trademark of AT&T Bell Laboratories.

[6] R. Langridge, T.E. Ferrin, I.D. Kuntz, M.L. Connolly, *Science* **211**, 661-666 (1981).

[7] T.E. Ferrin *et.al.*, *J. Mol. Graphics* **2**, 55 (1984);

[8] T.E. Ferrin *et.al.*, *J. Mol. Graphics* **6**, 13-27 (1988).

[9] T.E. Ferrin *et.al.*, *J. Mol. Graphics* **6**, 2-12 (1988).

# MidasPlus User's Manual

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Additional copies of this manual are available for $10 each, including postage, by writing to MIDAS Software Distribution, Computer Graphics Laboratory, School of Pharmacy, University of California, San Francisco, CA 94143-0446. Please include a check or money order payable to The Regents of the University of California with your request. Sorry, but purchase orders cannot be accepted. Orders received without payment enclosed will be returned unprocessed.

# UCSF MidasPlus™

## Molecular Interactive Display And Simulation

# USER’S MANUAL

July 1992

Computer Graphics Laboratory
School of Pharmacy
University of California, San Francisco