MAIN 95 Dialog Mode Manual

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Contents

1.11.5

Chapter 1

DIALOG MODE ACCESSORIES MANUAL

Mouse usage

File: MOUSE.TXT Last Modified: 27-sept-94

When the cursor is in the IMAGE window, the mouse can be used beside for picking atoms as a substitute input from dials. (The dials substitution is disabled on the ESV computers.) The mouse has 3 buttons: left (L), middle (M) and right(R). When one or two of them are pressed and moved, they replace input from the current dials set. By default:

The left button (L) can control rotations around X, Y and Z axis. When the cursor is moved within a circle of the image window center, the horizontal movements correspond to rotation about Y axis and vertical about X axis. If cursor is moved outside the circle, its' movement results in rotation about Z axis.

The middle button (M) controls translations along X and Y direction.

The left and middle button (LM) pressed together and moved vertically; they translate image along the Z direction.

The right button (R) controls scaling of the image (zoom). When cursor is moved towards the center of the image window, the image is shrunk, and when it is moving away from it, the image is expanded.

The right and middle button (RM) pressed together control clipping. When the cursor is moved towards the center of the image window, the clipping planes are moved together, and when it is moving away from it, the separation between the clipping planes is increased.

Changing dial definitions will also change the mouse button functions. In general, pressed middle button (M) mimics dials 1 and 2, pressed left and middle button (LM) mimic dial 3, right button (R) mimic dial 4, left button (L) mimics dials 5, 6 and 7, and combination of right and middle button (RM) mimic dial 8.

Releasing a mouse button while still moving the cursor results in a continuation repetition of the last move before the release. So smooth rotations of image on the screen can be achieved.

Magic of a keyboard touch

File: keyboard.txt Last modified: 27-sept-94

Pressing keys is usually the quickest way for an experienced user to control the working of a program. programs work. In MAIN they serve to call certain actions that require no confirmation and are frequently applied. These keyboard functions will be greatly enhanced in the future.

Currently these functions are supported:

- 'a' accepts geometry of currently defined active objects,
- 'c' or 'C' sets the current rotation to the last picked atom,
- 'd' or 'D' drops the last picked atom from the history list,
- 'e' or 'E' exits the dialog mode,
- 'h' toggles menu documentation mode on and off,
- 'M' toggles the image menu on and off,
- 'm' minimizes the 'active' key selection of atoms,
- 'r' redraws entire image of molecular objects,
- 'R' redraws the maps around the current center,
- 's' or 'S' toggles stereo on and off,
- '-' rotates the image for the stereo angle in the - direction
- '+' rotates the image for the stereo angle in the + direction
- '1' to '0' includes or removes maps (1 to 10) from the image. (since 10 is no key 0 is used instead)

Strikes

```
File: strikes.txt
Last modified: 29-sept-94
```

Strikes window commands (MENUS) are spread over 10 PAGES. Only a single MENU PAGE is displayed at a time. EACH MENU PAGE can be composed of MENU BLOCKS following each other in a defined order. Some BLOCKS are defined inside the program, some can be loaded and organized while the program is running. A MENU BLOCK is a group of ITEMS. Each ITEM is the visible string you actually see and can press. When pressed, ITEMS actually send command(s) the the command senttence interpreter. See also the MENU commands in the Reference manual or try to retrieve information with the MENU HELP commands.

If the Strikes window is in the DOCUMENT mode, short description of the pressed BLOCK and ITEM is written to the standard outout window. The DOCUMENT mode can be turned on or off either by pressing 'h' on the keyboard or by typing the command MENU DOCUMENT ON/OFF.

When an item is pressed the cursor is changed from an arrow to a clock pointing that MAIN is executing the selected MENU commands. Arrow is retrieved when command input is returned to the interactive devices (mouse and dials).

Pages

```
$<< >>$ is used to switch between different MENU pages.
forward $$>>$ and backward $<<$.  The current page number id
is displayed in the middle of the page field.  The PAGE
switching is not disabled when the DOCUMENT mode is on.
```

BUILD

```
File: build.txt
Last modified: 28-sept-94
```

Enables the building of new residues into the model and replacement of existing ones. START, ATTACH and CHANGE are setup flags defining whether residue(s) will START a new chain at the current image center, ATTACH it to the last picked residue or CHANGE the last picked residue. No action is undertaken as long "RESID ??" is not pressed. "RESID ??" requires input from keyboard: a list of residue names. Each residue may be preceded by an integer number of its repetitions(e.g. '3 ALA CYS 2 MET ... ').

Newly built residues may start with s SEQUENCE root and obtain a new SEGMENT name when a new chain is STARTed. Inputs for SEQUENCE root and SEGMENT name are prompted from the keyboard.

Keyboard input is in the origin window (mono-screen).

DEFINE

Prepares atoms for energy calculation and enables interactive modification of energy term lists. Its purpose is to help creating new topology library residues.

DIALS

```
File: >doc/menu/dials.txt
Last modified: 14-nov-95
```

Enables you to perform the basic control of DIAL set definitions. (See also SET DIALS in reference manual.)

Current dial set definition is echoed in the Dials window in the lower left corner.

DIAL_INI

Set dials to their INITIAL (default) definition. (image center translation, scaling, rotation and clipping)

DIAL_SAV

```
> SET DIAL 1 WRITE
```

Saves the current DIAL set as the last one on the dial sets stack. (30 dial sets can be saved.)

DIAL_RST

```
> SET DIAL 1 READ
```

Restores a DIAL set definition and increases current dial set counter for one. Repeating hits allow you to sroll through entire set of saved dial set definitions.

DIAL_VIE

```
> SET DIAL 1 VIEW
```

Assigns DIALS to VIEW parameters as scaling of screen, stereo angle, distances from viewer position to the center, character scale (for PHIGS only).

DIAL_DRO

Drops all of saved DIAL sets from the memory and initialize dials.

DISPLAY_LONG

```
File: display_long.txt
Last modified: 27-sept-94
```

The DISPLAY_LONG menu BLOCK controls basics of the image re-processing and interaction with a user.

EXIT

EXIT is used to EXIT the DIALOG mode and return to MAIN>. It has no analog in command sentences. When CRYSTAL eyes STEREO screen is turned on, picking EXIT turns STEREO OFF and returns control to the mono screen.

Keyboard equivalent keys are 'e' and 'E'.

MENU

```
> IMAGE MENU ON
             OFF
```

MENU turns off MENU and expands the molecular image to the whole MAIN window size. The menu can be retrieved again by picking the item MENU once more.

Keyboard equivalent is key 'M'.

RE_DRAW

```
> IMAGE OVER FALSE
```

RE_DRAW redraws all 3-dimensional objects (except MAP(s)) stored in the program. Background IMAGE objects are not redrawn.

Keyboard equivalent is key 'r'.

RE_MAP

```
> IMAGE MAP OVER
```

RE_MAP redraws all MAP(s) centered at the current IMAGE CENTER.

Keyboard equivalent is key 'R'.

STEREO

```
> IMAGE STEREO ON
               OFF
```

STEREO toggles the STEREO ON or OFF.

Keyboard equivalent is key 's'.

PLOT

```
> inquire file_name "PLOT FILE NAME:"
> open unit 79 overwrite file file_name
> image unit 79 plot on initialize
> image over false map over
> image plot off
> close unit 79
```

Creates a plot file of the current IMAGE. The name of the plot file is INQUIRED by the prompt "PLOT FILE NAME" and should be typed in.

GRAPH objects can not be PLOTTED this way

CENTER

```
> IMAGE CENTER COORD 3*real
```

Centers the image to the current position of the last picked atom.

Keyboard equivalent is key 'c'.

DISPLAY_SHORT

```
File: display_short.txt
Last modified: 27-sept-94
```

DISPLAY_SHORT consist of 3 items from the DISPLAY_LONG: MENU, STEREO and CENTER.

ENERGY

Is used to turn separate ENERGY flags ON and OFF.

HISTORY

```
File: history.txt
Last modified: 27-sept-94
```

Picked atoms constitute the HISTORY list. An atom is PICKED, when the cursor is placed on its IMAGE location and a mouse button is pressed. The history information of the picked atom appears in white at the atom position.

HISTORY list is input for any other Strikes MENU function. In general atoms are first picked in desired order and then some other function is activated. This way mistakes by picking atoms can be corrected easily and the same picked atoms can be reused.

Through the HISTORY lists of interatomic distances, angles, dihedral angles or ramachandran plot position of a amino acid can be monitored while changing atom(s) positions.

HIS_ERAS

```
> IMAGE HISTORY INITIALIZE
```

HIS_ERAS empties the history array (set the counter of atoms present to zero and deletes all history images).

HIS_DROP

```
> IMAGE HISTORY DROP
```

Drops the last PICKED atom from the HISTORY list.

Keyboard equivalent key is 'd'.

HIS_NAME

```
> IMAGE HISTORY NAME ON
                     OFF
```

HIS_NAME removes the HISTORY atom information from the image without actually modifying the history list. Toggling the atomic history list is usefull when it gets large.

HIS_DIST

```
> IMAGE HISTORY DISTANCE
```

Displays DISTANCE between last two PICKED atoms and connects them with the white history line.

HIS_ANGL

```
> IMAGE HISTORY ANGLE
```

Displays the ANGLE among the last 3 PICKED atoms and connects them with the white history line.

HIS_DIHE

```
> IMAGE HISTORY DIHEDRAL
```

Displays the DIHEDRAL angle among the last 4 PICKED atoms and connects them with the white history line.

HIS_INTE

```
> IMAGE HISTORY INTERNAL
```

Displays DISTANCE, ANGLE and DIHEDRAL information of last 4 PICKED atoms.

HIS_NEIGH

```
> IMAGE HISTORY NEIGHBOUR his_neigh
```

Finds the NEIGHBOURS of the last PICKED atom. The neighbours are atoms closer than the specified distance, at least 3 covalent bonds away from the last picked atom and are included in the key 'image'. The distance criterion is stored in the variable named 'his_neigh'. The default value is 3.6Å and can be SET with a

```
MAIN> SET VARIABLE his_neigh  real
```

command sentence. Its value can be displayed with

```
MAIN> SHOW VARIABLES his_neigh
```

HIS_RAMA

```
> IMAGE HISTORY RAMACHANDRAN
```

HIS_RAMA draws a cross into Ramachandran plot when it is displayed as part of the GRAPH object number 1. It is enough to PICK any atom of the desired residue and then hit HIS_RAMA. The program finds required atoms atomatically (-C N CA C +N).

HISTORY_FLAGS

Turns ON and OFF flags for HISTORY record constituents (atom, residue names and numbers, ...).

MINIMIZE

```
File: minimize.txt
Last modified: 28-sept-1994
```

Atoms SELECTED in KEY 'active' are MINIMIZED against background of "passive" KEY atoms with the ENERGY terms turned ON. 'active' atoms are allowed to move and 'passive' atoms are there only to interact with 'active' atoms. The key 'passive' should include all 'active' atoms, otherwise 'active' atoms will not be treated properly.

When applying PAIR constraints take care that anchor do not become a part of the 'active' key. Anchors do not need to be included to the 'passive' key.

MINI_ANH minimizes anchors in an electron density map gradients. I recommand you to use this option a lot.

MODELER

```
File: >doc/menu/modeler.txt
Last modified: 14-nov-95
```

The modeling functions (ROT_TRAN, RT_CHAIN, MOV_ATOM, MOV_RESI, TRANSLATE, MOV_DIST, MOV_RT_6, RT_ANGLE) activate OBJECTS for interactive spatial modifications of molecular geometry and assign DIALS to them. (See also DIAL_SAV and DIAL_RST regarding DIAL set storage end retrivial.)

The INV_CHIR and CONNECT act instantaneously and do not need any DIAL action or aproval (OB_ACCEPT).

Remember first to pick atoms and afterwards pick an ITEM.

After activating an OBJECT the IMAGE must be redrawn by user intervention (pick RE_DRAW or press 'r') otherwise the image does not follow changes.

Most of modeling functions consist of more than one command sentence or even call some external command files. (So don't get confused when looking at the file INPUT.COP). The required data are transferred to command files via MAIN VARIABLES.

ROT_TRAN

Combines ROTATION and TRANSLATION of the molecule of the last PICKED atom. The center of rotation is defined at the position of the last PICKED atom.

Its DIAL set is saved automatically.

RT_CHAIN

RT_CHAIN activates rotation of all BONDS between the last 2 PICKED atoms. MAIN is only capable of checking each separate bond rotation. When there are more bonds to be rotated in the chain and one is a part of a ring, an error message will appear. In such case you should hit OB_REJECT and pick a different pair of atoms.

The menu item RT_CHAIN calls within a loop a variety of command files, one for each rotatable bond. After each 8th bond, the DIAL WRITE sentence is automatically done. The last DIAL set, however, should be saved by the user in order to keep it on the DIAL set stack.

MOV_ATOM

TRANSLATES the last PICKED atom disregarding its connectivities. (You don't have to break bonds as in the case of the TRANSLAT command.)

Does not save the DIAL set automatically.

MOV_RESI

ROTATES and TRANSLATES the residue of the last PICKED atom disregarding the connectivities of that particular residue. (You don't have to break bonds as in the case of the ROT_TRAN command.) The center of rotation is the last picked atom.

Automatically saves the DIAL set.

TRANSLATE

TRANSLATES the molecule of the last PICKED atom.

Does not save the DIAL set automatically.

RT_ANGLE

Takes the last 3 atoms from the HISTORY list (3,2, $1) and modifies angle between them. Atoms on the $2 atom side of the bond (3−2) are rotated about the axis perpendicular to the plane defined by the last three atoms and going through the atom $2.

Does not save the DIAL set automatically.

MOV_DIST

Moves (translates) the molecule of the last PICKED atom in the direction of the vector connecting the last two PICKED atoms. When the atoms are connected via a covalent bond, then on the atoms on the side $2 (first picked) atom is moved.

Does not save the DIAL set automatically.

MOV_RT_6

Activates 3 BOND and 2 ANGLE rotations and 1 DISTANCE movement. This is an INTERNAL (relative) coordinate way of ROTATION and TRANSLATION (ROT_TRAN) function that is applied in absolute (cartesian) coordinate space. The last 6 PICKED history atoms are required.

This is an internal coordinate alternative to ROT_TRAN function. It also includes 6 degrees of freedom.

Automatically saves the DIAL set.

INV_CHIR

```
> SET INVERSE atom-num1 atom-num2
```

Interchanges the positions of the two side chains attached to a single atom. In other words: inverts the chirality of the common neighbour of the last 2 PICKED atoms.

CONNECT

Moves the first picked molecule into a reasonable binding geometry against to the second picked molecule and forms a covalent bond between the last two picked atoms. You may wish to rotate about the newly formed bond to improve its' dihedral conformation (see RT_CHAIN).

Objects

```
OB_START
> OBJECT int SET INIT
```

OB_REJEC > OBJECT int SET TRUE

OB_ACCEP > OBJECT int SET FALSE

These commands affect all activated OBJECTS. The objects are either returned to their initial position (OB_START), rejected (OB_REJEC) or accepted (OB_ACCEP). Only OB_ACCEPT changes atom coordinates. After OB_REJEC and OB_ACCEP the complete image is redrawn.

SECONDARY

```
File: secondary.txt
Last modified: 28-sept-94
```

Hiting a secondary structure item sets conformation of 'active' protein atoms to standard helices, beta sheets or other regular patterns. Conformation conversion starts rotating 'active' atoms around predefined bonds from N-(FORWARD) or C-(BACKWARD) terminus, depending whether FORWARD or BACKWARD flag is set.

Hiting the DIHEDRAL item requires preceding atom picking and a dihedral value from the keyboard. DIHEDRAL is not limited to some standard atom types and dihedral angle value(s). You can define any dihedral angle among any four atoms you want.

Clicking standard (1-4 BETA, 1-3 GAMMA) turns items changes conforamtion of the second and third residue FORWARD or BACKWARD from the last picked residue by 1-4 turns while by 1-3 turn only the second residue conformation is changed.

All geometry changes are instantaneous, no confirmation is required. In the case you have messed up everything, you have to extract the last editing session commands from the 'input.cop' file and insert a return command before the command where the mess begun.

SELECT

```
File: select.txt
Last modified: 27-sept-94
```

Keys:

By using SELECT menu items a user is enabled to utilize flexibility of many menu item blocks. By picking the SELECT menu items four KEYs can be accessed ('active', 'pasive', 'image' and 'anchor') and modified by logical operations of the SELECT ... END command sentence. ITEMS including boxes are setup flags, that are at the moment, when a SELECT command item is picked, transformed into a SELECT ... END command sentence specifying a new key definition.

KEY 'active' is the selection used in most of menu driven actions. KEY 'passive' is used for ENERGY calculations serving as interaction to 'active'. Positions of atoms that are included in KEY 'passive' only and not in KEY 'active' as well, are not modified during an ENERGY MINIMIZATION run.

KEY 'image' defines pickable atoms from images.

KEY 'anchor' is the selection used for anchoring atoms by distance constraints, where atoms and their anchors can be moved and minimized separetely. For example picking MIN_ANCH minimizes the anchors in the specified electron density map.

Tags:

Tags are organized in three groups each consisting of three items: (SEL_LAST, SEL_RANG, SEL_HIST), (SELE_NAM, SELE_nn, SELE_SEQ) and (SEL_ATOM, SEL_RESI, SEL_MOLE). In each group only a single item flag can be set at a time. A tag is composed by putting together an item of each Tag group in a meaningful entity. The first group flag specifies how many atoms from the history list will enter a tag. The second group specifies wheter atoms will be selected according to names, numbers or sequence names. The third group specifies whether tag refers to atom, residue or a molecule (segment) level of molecular structure organization.

Setting flags does not affect any key as long an item in the Select group (SELE_ALL, SEL_COPY, SEL_ARO?, SEL.not., SEL .or., SEL_.and.) has been pressed.

KEY_ACTI

Sets current SELECTION to the 'active' key.

KEY_PASI

Sets current SELECTION to the 'passive' key.

KEY_IMAG

Sets current SELECTION to the 'image' key.

KEY_ANCH

Sets current SELECTION to the 'anchor' key.

SEL_CLEA

```
> key ... select .not. all end
```

Clears the currently ('...') chosen SELECTION. After this command the chosen selection includes NO atoms.

SELE_ALL

```
> key ... select all end
```

Includes ALL atoms into the currently ('...') chosen selection.

SEL_COPY

```
> key ... select active end
```

Copies the contents of 'active' to the currently ('...') chosen selection ('anchor' or 'image').

```
> key passive select active .or. by resid by bond active end
```

The 'passive' selection is thereby also enlarged for the residues, that form a covalent bond with an 'active' atom.

```
> key active select passive end
```

In the case when the currently chosen SELECTION is 'active' then the contents of KEY 'passive' is copied to key 'active'.

SEL_ARO?

```
> key ... select ... .or. -
>    by resid around key active dist real from image end
```

Modifies the currently chosen SELECTION. All residues that have at least one atom closer than the specified distance from the active KEY and are included in the KEY image are merged (.OR.) into the current selection. The distance should be typed in to the prompt appearing in the standard input window.

SEL.not.

```
> key ... select ... .and. .not. tag end
```

Modifies the currently ('...') chosen SELECTION so that the logical '.and. .not.' operation is performed.

SEL .or.

```
> key .. select ... .or. tag end
```

Modifies the currently ('...') chosen SELECTION so that the logical '.or.' operation is performed.

SEL.and.

```
> key ... select ... .and. tag end
```

Modifies the currently ('...') chosen SELECTION so that the logical '.and.' operation is performed.

SEL_LAST

The chosen tag refers to the last picked atom only.

SEL_RANG

The chosen tag refers to the last two picked atoms.

SEL_HIST

The chosen tag refers to all picked atoms available in the history list.

SELE_NAM

Selects atoms according to (ATOM, RESIDUE or SEGMENT) NAMES.

SELE_nn

Selects atoms according to (ATOM, RESIDUE or SEGMENT) NUMBERS. In the case when SEL_MOLE is chosen, there is a slight modification of the common rule (see SEL_MOLE).

SEL_SEQU

Selects atoms according to their SEQUENCE names.

SEL_ATOM

Selects atoms according to their ATOMic names or numbers.

SEL_RESI

Selects atoms according to their RESIDUE names or numbers.

SEL_MOLE

Selects atoms according to their SEGMENT names or numbers. In the case of SELE_NAM selection always relates to SEGMENT NAMES, while in the case of SELE_nn, the select sentence depends on the current range mode (SEL_LAST, SEL_RANG, SEL_HIST). When SEL_LAST mode is chosen, a molecule is selected. Molecule is defined as a group of atoms attached to the last picked atom through a network of covalent bonds. In both the other cases (SEL_RANG or SEL_HIST) tag refers to already existing SEGMENT numbers.

SHOW_KEY

```
> IMAGE MARK ON
             OFF
```

Controls displaying of the currently choosen key atom marks on the image screen.

ANCHOR

ANCHOR is an extremly flexible tool that in combination with the energy minimization enables you to model the desired geometry of a molecular model. Anchors are target positions for your atoms. They are pooling their origin atoms towards the desired position without destoring the geometry (bond length, angles, impropers) of a molecular model. Anchors positions can be easyly moved. Each atom can have its anchor.

When created anchors are displayed as green crosses connected with a line to their origin atoms so that you can always keep track of your atom - anchor pairs. Hiting ANCHOR creates an anchor for each atom included in the key 'anchor'. New anchors are created at positions of their origin atoms. Already existing anchors remain on their positions. Anchors that lose their partner atom (orig atom is not any more included in the key 'anchor') are deleted.

Anchor positions can be optimized regarding to their correlation within an electron density map (MIN_ANCH). This way a better (real space) fit of your model to an electron density can be derived.

IMAGE

Is not implemented yet.

XRAY_BUILD

```
File: xray_build.txt
Last modified: 14-nov-95
```

The functions herein support model building in electron density. It enables you to reconstruct image on the screen (RE_IMAGE), to create and display symmetry related molecules (SYMMETRY, SYMM_CA), set crystallographic weights to atoms (WEIG_ATO, WEIG_RES, WEIG_ACT), find symmetry equivalent segments of your current model (WHERE_IS), and change coordinates of your model segment by a symmetry equivalent one (COPY_COO). UN_DO returns your model coordinates one step back.

All cmds files are available in the cmds directory. Some files as ’re_image.cmds’, ’symmetry.cmds’ and ’symmetry_ca.cmds’ are there only as examples. You can use them as they are and copy them into your working directory or modify them to your needs (what I strongly recommend).

The SAVE command should save your current data to files. Write your own ’save_file.cmds’

This menu BLOCK is loaded with the command ’¡>cmds/load_xray_build’ as XRAY_BUILD to the PAGE 2.

RE_IMAGE

The available ’>cmds/re_image.cmds’ erases entire image and displays a bond presentation of all atoms excluding the ones generated by a symmetry command.

With the second part of the ’>cmds/re_image.cmds’ command file it is possible to draw a model presentation within a sphere around the current image center. This reduces amount of model vectors that should be redrawn and thus improves dial respond of an image especially when images of large molecular models are to be displayed.

Each particular case may require original approach, so you are encouraged to write your own ’re_image.cmds’ files.

A simple example (also available as >cmds/around.cmds) first ERASES the image objects, then assignes to the key ’aro’ only atoms that are closer than 15.AA to the current IMAGE CENTER, and afterwards displayes all with covalent bond connected atoms that are not part of the symmetry segments (segment names started with #). Solvent oxygen atoms of water molecules (assigned to key wat) are displayed as CROSSES. Finally the key image is updated, so that allows only the aro and CA atoms to be picked.

```
> image erase
> key aro select by residue around center current dist 15. -
    .and .not. segment name #* end
> ima select aro .and. .not. wat end set bond
> ima select aro .and. wat .and. atom name O* end set atom cros
> key image select aro .or. atom name CA end
> return
```

It is assumed that a main chain trace has been displayed as a background image object, thus preventing its deletion:

```
> make bond resi
> image color 1 sele atom name CA end bond
> image from
> image erase
> delete bond sele atom name CA end
```

SYMMETRY

First the already existing symmetrical parts of model are deleted. Then symmetry related atoms laying within a sphere of 20AA of segments named MOL* are generated, assigned to key SYMM_M and displayed in purple. Similarly solvent molecules are displayed as red crosses. So it is possible to differentiate symmetry images of different molecules of the same asymmetric unit by a different color and INCLUDE or REMOVE them from the image separately. It is assummed that this file resides in your working directory.

```
> delete atom select segment name #* end
> key old select all end

> symm select segment name MOL* end around center atom $1 dist 20. neigh 2
> key SYMM_M select .not old end
> image select SYMM_M end col 105 bond

> key old select all end
```

```
> symm select wat end around center atom $1 dist 20. neigh 2
> key SYMM_WAT select .not old end
> image select SYMM_WAT .and. atom name O* end col 125 atom cros
> return
```

SYMM_CA

SYMM_CA is essentially very similar to the above SYMMETRY item. Generates CA plot in a range of 50.0AA around the last picked atom. By changing the file it is possible to differentiate between different parts of molecular models by generating separate symm_ KEYs and display them in different colors. It is assummed that this file resides in your working directory.

```
> menu block XRAY_BUILD item SYMM_CA add text "<symmetry_ca.cmds"
```

A symmetry_ca.cmds (available as >cmds/symm_ca.cmds):

```
> delete atom sele symm_* end
> key old sele all end
> make bond from residue sele all end
> symmetry sele atom name CA end around center atom $1 -
>          distance 50. neigh 2
> key symm_ sele .not old end
> image sele symm_ end col 105 bond
> delete bond sele atom name CA end
> return
```

UN_DO

Restores aomic coordinates to the values before the last MINIMIZATION, SECONDARY structure change or SET GEOMETRY (CONNECT) click.

```
> menu block XRAY_BUILD item UN_DO add \
>      text "<>cmds/un_do.cmds"
```

WEIGH_0

Sets the variable 'set_weight' to 0 in order to define later dummy atoms by hiting items (WEIG_ATO, WEIG_RES, WEIG_ACT).

```
> menu block XRAY_BUILD item WEIGH_0 add \
> text "set vari set_weight 0.0"
```

WEIGH_1

Sets the variable 'set_weight' to 0 in order to define later crystallographic scatterers by hiting items (WEIG_ATO, WEIG_RES, WEIG_ACT).

```
> menu block XRAY_BUILD item WEIGH_1 add \
>      text "set vari set_weight 1.0"
```

WEIG_ATO

Sets the last picked atom WEIGHT to the variable 'set_weight' defined by the latest WEIGH_0 or WEIGH_1 command.

```
> set weight sele numb atom $1 end set_weight
```

WEIG_RES

Sets the WEIGHT of all non hydrogen atoms of the last picked residue to the variable 'set_weight' as set by the latest WEIGH_0 or WEIGH_1 command.

```
> set weight sele by resi numb atom $1 .and. \
>       .not. atom name H* end set_weight
```

WEIG_ACT

Sets the WEIGHT of 'active' atoms to the variable 'set_weight' as set by the latest WEIGH_0 or WEIGH_1 command.

```
> set weight sele active end set_weight
```

TEMP_ACT

Sets the TEMPERATURE factor of 'active' atoms to the value you should type in on the keybord.

WHERE_IS

Displays with white bonds all equivalent residues (with identical sequence names) of the segment you have just picked.

The procedure is in file "main/cmds/where_is_segment.cmds".

COPY_COOR

Copies coordinates of the segment you have just picked (a symmetry equivalent segment) to the original model. With this command you can move atoms around through symmetry equivalent positions you find on the screen. Useful especially when you realize that a segment should move to another asymetric unit (by model building or a molecular envelope construction).

Use this item only in combination with SYMMETRY generation.

The procedure is in the file "main/cmds/copy_coor.cmds".

INV_CHAIN

Inverts direction of a peptide chain (KEY "active") by keeping the initial secondary structure (phi, psi angles) as close as possible to the original values.

The procedure is in the files "main/cmds/invert_chain.cmds" and "main/cmds/invert_chain_rms.cmds".

SAVE

SAVE saves atom data, current connectivity table and the current view. SAVE is supposed to be a security measure. In a "read.com", the starting MAIN file, you should not use the same files as specified in your "save_file.cmds".

At least try to copy this files before starting MAIN, to the files MAIN will actually read at the beginning. Otherwise in a case of a crash restavration of the last editing session will not be possible any more. In the case of corrupted save files you may find yourself in a big trouble.

The save view command is only to make life easier. It does not effect any structural data so you can easily process it during your starting file (read.com).

Hint: Create SAVE_2 item so that you keep two file tracks.

```
> menu block XRAY_BUILD item SAVE add text "<save_file.cmds"
```

A 'save_file.cmds' (example present in main/cmds):

```
> write over file SAVE_FILE.PDB select segment name * end atom pdb
> write over file SAVE_FILE.CTAB select segment name * end ctab
> save over file SAVE_FILE.VIEW view
> return
```

MAP_ATOM

```
File: map_atom.txt
Last modified: 30-mar-95
```

MAP_ATOMS together with the MAP_IMAGE blocks enable you to interactively create and modify electron density maps with using molecular models (ATOMS) under visual control. (MAP_ACT? items of both blocks are identical - they both reffer to the same variable.)

Active map density can be modified in the radius (ATO_RAD?) around 'active' atoms. Density values can be either set to mask (ATO_MASK), empty (ATO_CLEA) or atom density values (ATO_DENS).

The ATO_DIFF creates a difference electron density map, where the generated density from the 'active' key atoms is subtracted from the active map.

The commands GET_PHASE, 2FO-FC_M, FO-FC_MA, REFINE, SKELTONIZE, MASK_FLAT, SOLV_FLAT govern structure factor and map calculations, crystallographics refinement and map skeletonization and two solvent flattening approaches.

MAP_PAS?

MAP_ACT?

ATO_RAD

```
> menu block MAPS_EDIT item ATO_RAD? add text "<>cmds/make_map_radius.cmds"
```

ATO_MASK

```
> menu block MAPS_EDIT item ATO_MASK add text -
>  "make map map_to atom mask map_rad select active end"
```

ATO_CLEA

```
> menu block MAPS_EDIT item ATO_CLEA add text -
>  "make map map_to atom clea map_rad select active end"
```

ATO_DENS

```
> menu block MAPS_EDIT item ATO_DENS add text -
>   "make map map_to atom dens select active end"
```

ATO_DIFF

```
> menu block MAPS_EDIT item ATO_DIFF add \
>       text "<>cmds/make_map_atom_diff.cmds"
```

RE_PHASE

Calucaulates structure factors (PHASES) and R-factor of your current model. You should always use your own files. The file "main/cmds/re_phase.cmds" is only an example that should be adjusted to almost each particular case.

2FO-FC_MAP

Calucaulates an 2Fobs-Fcalc map on the basis from the last calculated structure factors. You should always use your own files. The file "main/cmds/calc_2fofc_map.cmds" is only an example that should be adjusted to almost each particular case.

FO-FC_MAP

Calucaulates an Fobs-Fcalc map on the basis from the last calculated structure factors. You should always use your own files. The file "main/cmds/calc_fofc_map.cmds" is only an example that should be adjusted to almost each particular case.

REFINE

Refines your model against a Fobs-Fcalc map. Structure factor update step numb can be specifed.

The file "main/cmds/refine.cmds" is only an example that should be adjusted to almost each particular case.

SKELETONIZE

Skeletonizes a map. You should specify the density cutoff level and size of segments that should be drawn on the screen. The skeleton atoms are accessible through the key "skel".

The file "main/cmds/get_skel.cmds" is only an example that should be adjusted to almost each particular case.

MASK_FLAT

Calculates structure factors of a solvent flattened map. Envelope is created from an atom selection. You can use your model or skeleton atoms or whatever kind of atoms you may have.

The file "main/cmds/mask_flat.cmds" is only an example that should be adjusted to almost each particular case.

SOLV_FLAT

Calculates structure factors of a solvent flattened map. Envelope is created by the standard Wang sphere statistics procedure. Try to limit the procedure to a asymetric unit and later generate the whole unit cell from it. The procedure takes some time.

The file "main/cmds/solv_flat.cmds" is only an example that should be adjusted to almost each particular case.

MAPS_EDIT

```
File: maps_edit.txt
Last modified: 29-sept-94
```

MAPS_EDIT together with the MAPS_IMAGE blocks enable you to interactively create and modify electron density maps under visual control. (MAP_ACT? items of both blocks are identical

- they both reffer to the same variable.)

Essential oparations as map creations (MAP_NEW) to initial values (MAP_CLEA, MAP_MASK) can be performed.

Map values can be set directly (MAP_SET?), copied from another map (MAP_COPY) scaled (MAP_SC.?) or rescaled (MAP_RESC).

Two maps can be merged (MAP_MR.?) and added (MAP_ADD) together. Cavities within masks can be filled (MAP_FIL?) and a unit cell density can be generated (MAP_CELL).

Some previous knowledge of the MAKE MAP command syntax is recommended.

MAP_PAS?

MAP_ACT?

MAP_NEW

```
> make map map_to from map_from initial map_val number
```

MAP_AROU

```
> menu block MAPS_EDIT item MAP_AROU add \
>   text "<>cmds/make_map_around.cmds"
```

The '>cmds/make_map_around.cmds' file has the following syntax:

```
> inquire ato_grid "GRIDS AROUND ATOM BOX:"
> make map map_to from map_from init map_val number -
>    around ato_grid select active end
> return
```

MAP_CLEA

```
> menu block MAPS_EDIT item MAP_CLEA add text -
>  "set variable map_val = -9999"
```

MAP_MASK

```
> menu block MAPS_EDIT item MAP_MASK add text -
>  "set variable map_val = 9999"
```

MAP_SET?

```
> menu block MAPS_EDIT item MAP_SET? add text "<>cmds/make_map_set.cmds"
```

MAP_COPY

```
> menu block MAPS_EDIT item MAP_COPY add text -
>   "make map map_to from map_from copy"
```

MAP_SC.?

```
> menu block MAPS_EDIT item MAP_SC.? add text "<>cmds/make_map_scale.cmds"
```

MAP_RESC

```
> menu block MAPS_EDIT item MAP_RESC add text -
>  "make map map_to from  map_from rescale"
```

MAP_MR.?

```
> menu block MAPS_EDIT item MAP_MR.? add text "<>cmds/make_map_merge.cmds"
```

MAP_ADD

```
> menu block MAPS_EDIT item MAP_ADD  add text -
>  "make map map_to from map_from add"
```

MAP_FIL?

```
> menu block MAPS_EDIT item MAP_FIL? add text "<>cmds/make_map_fill.cmds"
```

MAP_CELL

```
> menu block MAPS_EDIT item MAP_CELL add text -
>  "make map map_to from map_from cell"
```

MAP_IMAGE

```
File: map_image.txt
Last Modified: 29-sept-94
```

This menu block enables you to gain complete map presentation control within the IMAGE DIALOG mode.

Maps can be drawn as vectors (MAP_VECT)or areas (MAP_AREA), along different axes (MAP_X-AX, MAP_Y-AX, MAP_Z-AX).

Maps can be turned on (MAP_ON) or off (MAP_OFF) in order to allow or prohibit their recontouring when RE_MAP or 'R' are hit. A map can also be erased (MAP_ERAS).

The current map setup can be retrieved (SHOW_MAP).

The menu is loaded with the command '¡>cmds/load_maps_image'. It includes some default variable setups as active map (1), box sizes (12 grid points), contouring level (1.0) and the currently active map. These values can be later modified with the MAP_ACT?, MAP_BOX and MAP_CONT.

The menu is loaded to the page 10.

RENAME

```
File: rename.txt
Last modified: 29-sept-94
```

RENAME menu is a set of commands that allow you to RENAME atom, resiude, sequence and segment names, DELETE atoms or whole reidues, MERGE The file is loaded with the command '¡>cmds/load_rename' and inserted to the menu page 1.

THE ACT_SEGM and ACT_2RES are two the most often rewuired combinations otherwise accessible through the SELECT menu.

REN_ATOM

RENAMES ATOM NAME of the last picked atom. You are prompted for a string

REN_RESI

RENAMES RESIDUE NAME of the last picked residue. You are prompted for a string

REN_SEQ

RENAMES SEUENCE NAME of the last picked residue. You are prompted for a string must be typed within double quotes, for example as "125" to force MAIN to interpret 125 as a string and not as an integer

REN_SEGM

RENAMES SEGMENT NAME of the last picked segment. You are prompted for a string

DELE_ATOM

Deletes the last picked atom. NO confirmation is required

DELE_RESIDUE

Deletes the last picked residue. NO confirmation is required

MERG_RES

Two consecutive residues (of the two last picked atoms) can be joined (MERG_RES). This is a useful tool when ATTACHING N and C terminals to a peptide chain. NTER and CTER are namely attached to a residue as a new residue that should be later on merged (joined) to the original one.

ACT_SEGM

ACT_SEGM selects in the KEY "active" the atoms attached to the last picked atom through a network of covalent bonds, the KEY "passive" includes all "active" atoms. ENERGY lists are initialized and rebuild.

ACT_2RES

ACT_2RES selects in the KEY "active" all atoms between the last two picked atoms. The KEY "passive" includes whole residues of all "active" atoms plus all covalently attached residues. ENERGY lists are initialized and rebuild.