MAIN 95 Command Reference Manual

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Contents

Chapter 1

COMMAND REFERENCE MANUAL

ANALYZE

```
File: main/doc/com/anal.txt
Last modified: 30-aug-95
```

Stores data for calculation of average, standard deviation (sigma) and maximal and minimal value for each SELECTED ATOM or RESIDUE record for the specified property. Five kinds of data are stored for each record: number of matches, summ of values, summ of squared values and minimal and maximal value. Average value can be later calculated by dividing summ of values with number of matches and standard deviation from square root of record variance divided by number of matches minus one. Record variance is calculated by formula sum of square values minus square of summ divided by number of matches. (In almost any book abouts statistics.) So it possible to pass each data set only once and to enlarge data set as long as the numerical accuracy allows it. These make possible to investigate large data basis, that can not be present in the program simultaneously.

Average and standard deviation for each record are calculated just before being written with a WRITE ANALYZES command sentence or displayed within GRAPH or use (SET) COLOR options follwoed by IMAGE SET commands to color each atom or residue according to the results of analysis.

Syntax

```
ANALYZE   INITIALIZE
          APPEND
          ATOMIC
          RESIDUAL
          SELECT ... END
          SET     inte
                  SELECT ... END
          COORDINATES
          CHARGES
          RADII
          TEMPERATURE
          INTERNAL       DISTANCE
                         ANGLE
                         DIHEDRAL
                         ALL
```

```
ENERGY        DISTANCE  real
              RESIDUES  int
              NEIGHBOR  int
POINTS        SURFACE
              POTENTIAL
              DENSITY
PAIR   inte
PARAMETER       BONDS
                ANGLES
                DIHEDRALS
                IMPROPER

MAP inte      STEP inte
```

INITIALIZE

`... INIT ...`

Initializes the analyzes arrays.

APPEND

`... APPEND ...`

Analized data will be added values already stored in the analysis arrays in contrary to INITAILIZE. APPEND is the default.

ATOMIC

`... ATOM ...`

Analysis records will be organized per ATOM basis. ATOM is default.

RESIDUAK

```
... RESIDUAL ...
```

Analysis records will be organized per RESIDUE basis. ATOM is default.

COORDINATES

```
... COORDINATES
```

Compares the atomic COORDINATES.

CHARGES

```
... CHARGES
```

Compares the partial atomic CHARGES.

RADII

```
... RADII
```

Compares the atomic RADII.

TEMPERATURE

```
... TEMPERATURE
```

Compares the TEMPERATURE factors.

SET

```
... SET  inte
         SELECT ... END
```

Defines number of records explicitly either directly by an integer number or indirectly through number of SELECTED atoms.

SELECT

```
... SELECT ... END ...
```

SELECTS atoms that are suposed to be analyzed. For syntax see SELECT.

INTERNAL

```
... INTERNAL DISTANCES
             ANGLES
             DIHEDRALS
```

Compares the INTERNAL coordinates: DISTANCE, ANGLES or DIHEDRALS.

ENERGY

```
...  ENERGY DISTANCE  real
            RESIDUES  int
            NEIGHBOR  int
            WHOLE
```

ANALYZE interaction energies on per atm basis are calculated and stored into analysis arrays for ATOMs or RESIDUEs.

Options enable you to choose part(s) of SELECTION that is within a certain neighborhood criteria: DISTANCE criteria (quality of packing), RESIDUES before and after the chosen atom, through network coalent bond steps (NEIGHBOR), or simply the WHOLE selection.

Interaction energies are calculated on per atom basis for all the ENERGY terms that are currently turned on.

POINTS

```
... POINT SURFACE
          POTENTIAL
          DENSITY
```

Analyzes SURFACE, POTENTIAL or density POINT values of SELECTED atoms per ATOM or RESIDUE record as specified above.

PAIR

```
... PAIR inte
```

Divides the whole PAIR list into the specified inte equal parts, and averages the values from the second to the last part in the first one. It works only with the SET flag. The compared distances must be set before by a

```
MAIN> DEFINE PAIR CALCULATE
```

statement.

PARAMETER

```
... PARAMETER GENERATE
              BOND
              ANGLE
              DIHEDRAL
              IMPROPER
```

Analyzes appearance and deviation for each particular force field parameter from average value and from its'ideal value present in the force. It measures force field reliability and accuracy. PARAMETERS are stored on order of appearance in force files parameter array. ATOM or RESIDUE organization of records has no effect.

GENERATE flag is an option that not only analyzes a kind of an ENERGY term but can also CREATE a new entry in the PARAMETER lists. A usefull option for a forcefield creation.

MAP

```
... MAP inte STEP inte
```

Analyzes the specified MAP by counting its points for a number of intervals specified by STEPS, where each step covers a density interval of the same size, between the map minimal and maximal value. (It creates a HISTROGRAM of a MAP). By writing this data with a WRITE ANALYZES command sentence, also the portions of eaxh partucal interval and their partial sum are being written.

Examples

Analysis of temperature factors of first ten segments. Each segment is supposed to have equal size of atoms.

```
MAIN> analyze atom init temperature
MAIN> analyze set sele numb seg 1 end  select segment numb 1 10 end
```

Analysis of PAIR list divided in 5 sets.

```
MAIN> analyze atom init
MAIN> analyze set pair 5 select all end select all end
```

Analysis of electron density along the chain. First density points are created at each selected atom center.

```
MAIN> analyze residue init
MAIN> analyze poin density sele segment name TRYP end
```

Analyzes of forcefield parameters (Force field parameters must be read and assigned to atoms.):

```
MAIN> analyze residue init
MAIN> analyze parameter bond sele all end
```

BREAK

```
BREAK.TEX        19-nov-91


Syntax
BREAK     BOND      atom-num  atom-num
          RESIDUE   atom-num  atom-num
          SEGMENT   atom-num  atom-num
```

BREAK BOND breaks a covalent bond between the two specified atoms. BREAK RESIDUE breaks a residue in 2 parts after the first specified atom BREAK SEGMENT breaks a segment in 2 parts between the two atoms. Different residues or segments can not be broken. 2 atom-numbers should be defined properly to avoid making non-sense.

BUILD

```
BUILD.TXT      23-FEB 1993
```

In the BUILD module molecules can be built from scratch, residues can be changed, chanes prolonged and new residies inserted. An EXIT command word must be applied to return from INTERNAL> to MAIN>.

SYNTAX

```
EXIT
START
APPEND   RESIDUE  string(s)
INSERT  atom-numb         RESIDUE  string(s)
SELE  ...  END
     [ALL]
CHANGE  RESIDUE string
FILL
DIHEDRAL
SEGMENT string
SEQUENCE string
CENTER   COORDINATES
         CALCULATED
         ATOM
```

APPEND

```
APPEND nn * (integer string)
```

APPENDs residues. Residues, when found in the topology library are appended to the end of atom list, however by INSERT they start apearing before the first SELECTED residue. As many as wanted residue names can be given. Each residue name can be preceded by an integer (number of repetitions). Default number of repetitions is 1.

INSERT

```
INSERT nn * (integer string)
```

INSERTs residues. Residues, when found in the topology library are inserted before the first SELECTED residue. The APPEND command adds them to the end of the list. As many as wanted residue names can be specified. Each residue name can be preceded by an integer (number of repetitions). Default number of repetitions is 1.

CHANGE

```
CHANGE string
```

CHANGEs the SELECTED residue by converting it into the new specified one. CHANGE acts only on one residue at a time (the first SELECTED residue).

Atoms of the old and new residue are compared by names. The matching atoms in both residues (except hydrogens) keep the old position (COORDINATES), TEMPERATURE factor and crystallographic WEIGHT. The rest of atoms are build from the INTERNAL coordinates data, when they are present in the topology library. Therefore sometimes atoms of the CHANGED residues appear in a weard conformations. To get around this either a RESIDUE should be CHANGED in two steps; in first step into a smaller residue (as ALA) and in second step the newly created residue (ALA) is CHANGED into the desired residue. The other solution is to energetically MINIMIZE such irregular parts.

When a larger range of residues should be changed, then it is recommanded to use combination of RENAME RESIDUE followed by a FILL command in the BUILD module.

FILL

```
FILL
```

FILLs residues by inserting missing atoms. It acts on the whole SELECTION in contrary to CHANGE. FILL calls CHANGE command within a loop, however it has no parameter (a new RESIDUE NAME). It keeps the current residue names. It can be used for hydrogen atom insertion or when a residue composition of a whole molecule is supposed to be replaced by a new one (in combination with RENAME).

DIHEDRAL

Corrects the bad DIHEDRAL angles resluted from a FILL command by adjusting DIHEDRAL angles of newly defined atoms present in INTERNAL coordinates to the DIHEDRAL angles in the TOPOLOGY library.

SEGMENT

```
SEGMENT string
```

Sets the name for a newly created SEGMENT. This segment name is used only when a new segment is created that is in combination with START.

SEQUENCE

```
SEQUENCE string
```

Sets a root for SEQUENCE names. Each newly created residue sequence name starts with the root string generating additional characters going from 1 to 9. For example root B generates series B1 ... B9 B10 ... B20 etc.

CENTER

```
CENTER   COORDINATES   3*real
         CALCULATED
         ATOM
```

Sets a CENTER that may be later used when STARTing a new chain.

START

```
START
```

Sets the START flag for the next INSERT or APPEND command. When START flag is set a new RESIDUE chain starts at the specified CENTER. The resulting chain of residues is not connected to already existing atoms.

CALCULATE

```
CALC.TXT          21-NOV-94
```

CALCULATES connectivity lists (BONDS, HBONDS, PAIRS by using geometric criteria), electrostatic POTENTIAL at selected points, a PLANE passing through an atom selection, converts INTERNAL (relative) into cartesian (absolute) atomic coordinates and vice versa. The first two command words (CALCULATE and for example BOND), must be specified in the correct order, the remaining words can follow in any order.

Syntax

```
CALCULATE BONDS    INITIALIZE
                   [APPEND]
                   SELECT ... END     [ALL]
                   NEIGHBOR
                   RESIDUE
                   DISULFIDE
                   DISTANCE           [1.71]

         HBONDS  INITIALIZE
                 [APPEND]
                 SELECT ... END  [SELECT ... END]
                 ANGLE real [100.0]
                 DISTANCE real  [3.5]
                 EXCLUDE  inte  [3]
                 HYDROGEN

         PAIRS   SELECT ... END   SELECT ... END
                 [APPEND] INITIALIZE
                 EXCLUDE  int [3]
                 RANG real  real [0.0  1.5]
                 CLOSEST
                 EACH_CLOSEST

         INTERNAL  SELECT ... END   [SELECT ALL END]

         COORDINATES     SELECT ... END    [SELECT ALL END]
                         [INITIALIZE]
```

```
                    APPEND
                    X-AX  [X-AX Y-AX]
                    Y-AX
                    Z-AX

POTENTIAL    SELECT ... END      SELECT ... END
            [ SELECT ALL END ]  [ SELECT ALL END ]
            FROM  SURFACE
                  VOLUME   ATOM
                           ACCESSIBLE
                  DENSITY
                  POTENTIAL
                  ATOM
            RANGE real real  (0. 15.)

PLANE    SELECT ... END
```

BONDS

```
CALCULATE BONDS    INITIALIZE
                   [APPEND]
                   SELECT ... END     [SELE ALL END]
                   NEIGHBOR
                   RESIDUE
                   DISULFIDE
                   DISTANCE           [1.75]
```

Calculates covalent BONDS from interatomic distances.

APPEND

```
... APPEND
```

The CALCULATED bonds will be appended to the list of already existing bonds. Otherwise (INITIALIZE) the bond list (connectivity table) of all atoms will be initialized. APPEND is the default.

INITIALIZE

```
... INITIALIZE
```

Before calculating the bond list, the bond list is INITIALIZED.

SELECT

```
... SELECT ... END
```

The calculation will be done on the SELECTED atom set. SELECT ALL END is the default.

DISULFIDE

```
... DISULFIDE
```

Only sulphur atoms from the selection will be considered by the DISULFIDE bonds calculation.

RESIDUE

```
... RESIDUE
```

Only interatomic distances of selected atoms for each separate RESIDUE will be calculated and then checked to form the BONDING list.

NEIGHBOR

```
... NEIGHBOR
```

Only interatomic distances for each two consecutive residues will be calculated and then checked to form the bonding list.

DISTANCE

```
... DISTANCE real
```

The maximal interatomic DISTANCE for a bond criterion can be changed to any real number. The default value is 1.75AA, exception are the S-S bonds where the default maximal DISTANCE is set to 2.3 A.

HBONDS

```
CALCULATE HBONDS  INITIALIZE
                  APPEND
                  SELECT ... END  (SELECT ALL END )
                  ANGLE real (90.0)
                  DISTANCE real  (3.5)
                  EXCLUDE inte
                  HYDROGEN
```

Calculates hydrogen bonds (HBONDS) for the SELECTED atoms. Hydrogen bond donors or acceptors may be only nitrogen and oxygen atoms. Hydrogen bonds with carbon aromatic rings (benzen) as donors or acceptors are not calculated.

APPEND

```
... APPEND
```

The calculated hydrogen bonds will be appended to existing ones. APPEND is the default.

INITIALIZE

```
... INITIALIZE
```

Before CALCULATING the hydrogen BOND list, the program deletes all present hydrogen bonds.

SELECT

```
... SELECT ... END
```

Hydrogens bonds are calculated between two SELECTIONS. When only one is defined then the second one is automatically made equal to the first one.

EXCLUDE

```
... EXCLUDE inte
```

The EXCLUDE inte parameter excludes the covalently attached atoms from the hydrogen bonds calculation. The inte is the number of covalent bonds steps from the hydrogen bond donor or acceptor to the compared atom. When inte is -1 then the whole network unit (molecule) is excluded, and only intermolecular hydrogen bonds are calculated. Default EXCLUDE parameter value is 3.

HYDROGEN

```
... HYDROGEN
```

Sets the HYDROGEN flag, which means, that the HYDROGEN atoms are present in the atom list and should be used in the calculation.

DISTANCE

```
... DISTANCE real  (3.5)
```

Sets the maximum DISTANCE criterion between HYDROGEN bond donor and acceptor atoms to form a hydrogen bond. The default value is 3.5 A. When the HYDROGEN flag is set, then the distance between acceptor and a hydrogen atom is checked. The default distance in this case is 2.5 A.

ANGLE

```
... ANGLE real
```

The ANGLE criterion is applied only when the HYDROGEN flag is set, since it calculates the ANGLE between the donor, hydrogen and acceptor atom. Hydrogen bond is created when the calculated ANGLE is larger than the specified value. 100.0 degrees is the default.

PAIRS

```
CALCULATE PAIRS   SELECT ... END
                  SELECT ... END
                  (APPEND) INITIALIZE
                  EXCLUDE  inte (3)
                  RANG real  real (0.0  1.5)
                  CLOSEST
                  EACH_CLOSEST
```

CALCULATES atom PAIRS between 2 defined SELECTIONS. A PAIR is formed when an interatomic distance is in the specified RANGE (default values are 0.0 to 1.5Å). EXCLUDES the neighbor atoms (default value 3). INITIALIZES or APPENDS the new pairs to the previous ones. When CLOSE is specified, only the PAIR of atoms with the shortest interatomic distance between the two selections will be added to the pair list. The EVERY_CLOSE forms a pair between each atom in the first selection and its closest atom from the second selection.

INTERNAL

```
... CALCULATE INTERNAL SELECT ... END
```

Calculates INTERNAL coordinates from cartesian coordinates and Z-mat-table (ZTABLE) for the selected atoms.

COORDINATES

```
... COORDINATES    SELECT ... END    INITIALIZE   X-AX  (X-AX Y-AX)
```

```
                        ( SELECT ALL END )  APPEND       Y-AX
                                                         Z-AX
```

```
Calculates cartesian COORDINATES from INTERNAL coordinates
and z-mat-table for selected atoms. INITIALIZE is the
default. That means that all selected atom coordinates are
calculated from internal coordinate values. When APPEND is
used, only coordinates of nondefined atom centers (having
9999.0 for x, y, and z absolute coordinate value) are
calculated.  X-AX, Y-AX and Z-AX command words specify the
rules for the first 3 atomic positions. The first atom
coordinates are always set to the coordinate system origin,
the second ones on the first specified axis, and the third
in the plane of the first two specified axes. X-AX Y-AX is
the default.
```

POTENTIAL

```
CALCULATE POTENTIAL    SELECT ... END      SELECT ... END
                     ( SELECT ALL END )  ( SELECT ALL END )
                     FROM  SURFACE
                           VOLUME   ATOM
                                    ACCESSIBLE
                           DENSITY
                           POTENTIAL
                           ATOM
                     RANGE real real  (0. 15.)
```

Calculates the electrostatic POTENTIAL at the generated or read points. The first selection defines points belonging to atoms (at least one atom should be confirmed), where the potential will be calculated. The second selection defines atoms to be included in the electrostatic potential calculation. Atom charges are used as the point charges in space. eps = 1.0 The points are selected FROM the specified kind of points. The default RANGE can be changed on order to calculated electrostatic potential only in specified interatomic distance range. Electrostatic potential can be calculated also in the ATOM positions. In this case the points are created at atom positions.

PLANE

```
CALCULATE PLANE SELECT ... END
```

Calculates the RMS fit plane of the SELECTED atomic set. Not implemented yet. See SET PLANE instead.

CHARGES

```
CHARGE.TEX    21-nov-91
```

```
Syntax
CHARGE SELECT ... END real
       INITIAL
       EXIT
```

To a given selection real value CHARGES can be set. See also DEFINE CHARGE.

CLASS

```
CLASS.TEX    21-nov-91


Syntax
CLASS  SELECT ... END string
       INITIAL
       EXIT
```

To a given selection class of atom can be set. See also DEFINE CLASS.

COLOR

```
File: main/doc/color.txt
Last modified: 24-aug-95
> COLOR
        [SELECT ... END]  RESIDUE int1 int2
                          SEGMENT int1 int2
                          COLOR int
                          ANALYSES  AVERAGE
                                    RMS
                                    MINIMUM
                                    MAXIMUM
                                    COLOR  int1 int2 int3
                                    RANGE  AUTOMATIC
                                           CURRENT
                                           DEFINE real real
                          DEFAULT
                          ATOMS int1
                          INITIAL
                          EXIT
```

The (SET) COLOR commands define color attribute of each individual SELECTED atom. By default all atoms are selected. The colors can be checked at the display by using IMAGE SET commands or with SHOW COLOR SELECT ... END.

RESIDUE

```
... RESIDUE int1 int2
```

The RESIDUE specifier colors a selection so that each next RESIDUE has the color value for int2 higher than the previous one. Atoms of the first RESIDUE obtain color int1. Similar rule is applied for the SEGMENT colors.

SEGMENT

```
... SEGMENT int1 int2
```

The SEGMENT specifier colors a selection so that each next SEGMENT has the color value for int2 higher than the previous one. Atoms of the first SEGMENT obtain color int1. Similar rule is applied for the RESIDUE colors.

COLOR

```
... COLOR int1
```

Sets a single COLOR to the whole atom SELCTION.

INITIAL

Makes atoms invisible (negative color value).

ANALYSES

```
... AVERAGE  COLOR int1 int2 int3
    RMS
    MINIMUM
    MAXIMUM
    RANGE  AUTOMATIC
           CURRENT
           DEFINE real real
```

Set colors acording to the analyses aray data. The procedure first finds minimum and maximum value of an ANALYSES array (AVERAGE, RMS, MINIMUM, MAXIMUM) and spans the vaules between the int1 and int2 COLORS. The int3 number is the COLOR step, so that only each int3 color number is taken. The COLOR command has an analogue in FORTRAN "do" loop sentence, which means that you can also inverse the coloring (128 64 -4).

RANGE Interval) of values spanned over the minimal and maximal color can be found by the program (AUTOMATIC), remain from a previous run (CURRENT) or DEFINED explicitly by a user.

ATOMS

```
... ATOMS int1 int2
```

Defines a new color for the atom number int1.

DEFAULT

```
... DEFAULT
```

Set the DEFAULT set color values to the selected atoms. (See also COLOR ATOMS.)

EXIT

EXIT returns command input back to the MAIN> interpreter.

COORDINATES

```
File: main/doc/coord.txt
Last modified: 17-oct-95
> SET COORDINATES  SELECT ... END
                   INITIALIZE
                   VALUES 3*real
                   DEORTHOGONALIZE
                   ORTHOGONALIZE
                   RESTORE
```

Sets COORDINATES to the SELECTED atoms. They can be set explicitly by X, Y and Z VALUES (3*real), INITIALIZED (set to 9999.0), DEORTHOGONALIZED (partial) or its reverse ORTHOGONALIZED.

RESTORE

With RESTORE it is possible to restore the atomic coordinate values to their values before the last MINIMIZE or SECONDARY command application. The command should be applied immediately after the catastrophic event, since the saved coordinate data set storage can be modified and therefore disabled with any IMAGE command.

```
MAIN> SET COORD SELECT ... END DEORTHOGONALIZE
```

COPY

```
COPY.TEX        18-nov-91
```

COPY command sentences copies an property from the first SELECTION to the second one. Two SELECTIONS and a property must always be specified.

Copying is made by pairing atoms (ATOM, CLASS, COORDINATES, CHARGE, COLOR, RADII) or residues (RESIDUE, SEQUENCE) according to their sequential position in the both selections from first to the second. For example atom property of the third atom found in the first selection is copied to the third selected atom found in the second selection. Copying is done from the first selection(A) to the second one(B). Relation is B := A.

Syntax

```
COPY  RESIDUE         SELECT ... END         SELECT ... END
      SEQUENCE
      COORDINATES
      ATOM_NAMES
      CLASS
      CHARGE
      COLOR
      RADII
      TEMPERATURE
      WEIGHT
      INTERNAL  DISTANCE
                ANGLES
                DIHEDRALS
                (ALL)
      POINTS    SURFACE
                POTENTIAL
```

Examples

```
MAIN> copy coordinate select atom number 1 29 end -
MAIN> select atom number 30 59 end
```

```
MAIN> copy sequence select segment number 1 end -
MAIN> select segment number 2 end
```

DEFINE

```
File: define.txt
Last modified: 14-mar-95
```

Define command sentences are used to define atom CLASS, CHARGE or BOND, ANGLE, DIHEDRAL AND IMPROPER ANGLE parameters from the TOPOLOGY library lists or by an AUTOMATIC procedure and assign them values for energy parameters necessary to carry out energy calculations. Without using the DEFINE command sentence, calculation of most potential ENERGY terms can not be performed.

Additionally distance (PAIRS) and dihedral (CONSTRAINTS) constraints can be defined to enforce desired interatomic distances and dihedral angles during an ENERGY MINIMIZATION procedure.

```
> DEFINE CLASS
         CHARGES
         BONDS
         ANGLES
         DIHEDRALS
         IMPROPERS CHECK
         CONSTRAINTS DIHEDRAL   4*atom-numb real real   COPY
                     INTERACTION  SELECT ... END  SELECT ... END
                     MAP inte SELECT ... END
                     NCS  SELECT ... END
                          FORCE real
                          NEXT_GROUP
                          AUTO_GUESS
                          RMS_GUESS
                          SET_GUESS inte 6*real
         PAIR         FORCE real
                      DISTANCE real
                      CALCULATE
         INITIALIZE
         BY  TOPOLOGY
             AUTOMATIC  RESIDUES
             ATOMS   x*atom-numb
         SELECT ... END
         NEIGHBOR  string
         SYMBOL  string
```

```
RESIDUE   string
```

SELECT

```
... SELECT ... END ...
```

SELECT ... END and ATOM are the two ways to select the atoms for which force field PARAMETERS are being DEFINED or chosen. With SELECT the whole SELECTION is used while the BY ATOMS option, only the particular energy term for the specified atoms is added to the list.

BY

```
... BY TOPOLOGY
       AUTOMATIC
       ATOMS
```

The search for ENERGY terms (BOND, ANGLES, DIHEDRALS and IMPROPERS) is done in the TOPOLOGY library or by an AUTOMATIC procedure or explicitly for each specified ATOM. With SELECT the whole SELECTION is used while with the BY ATOMS option only the particular energy term for the specified atoms is added to the list.

It is recommended to use the AUTOMATIC procedure for generation of BOND and ANGLE lists. The AUTOMATIC procedure should be used with caution for generation of DIHEDRAL and IMPROPER lists. Use it for IMPROPER only when creatiing new TOPOLOGY RESIDUES.

Mostly use the BY TOPLOGY procedure. See file in ">utils/def_top_par_19.com".

TOPOLOGY

```
... BY TOPOLOGY ...
```

The BY TOPOLOGY procedure can assign atom CLASSES (types) and atomic charges and on their bases generate lists of BONDS, ANGLES, DIHEDRALS and IMPROPERS.

This option covers most of your needs for CLASSES, CHARGES and DIHEDRALS and IMPROPERS assignment.

AUTOMATIC

```
... BY AUTOMATIC ...
```

The AUTOMATIC procedure generates an ENERGY term for every possible BOND, ANGLE and DIHEDRAL angle in the specified SELECTION. In order to assign IMPROPERS with the AUTOMATIC procedure, the search for the improper angles should be preceded BY the AUTOMATIC definition for atom CLASSES. The IMPROPERS are assigned only to chiral centers (carbon atom with 3 neighbours or to planar groups).

ATOMS

```
... ATOMS 2-4*atom-num
```

ATOMS can be used only with BOND, ANGLE, DIHEDRAL or IMPROPER terms. For BONDS two atoms have to be specified, for ANGLES three and for DIHEDRALS and IMPROPERS four. With the ATOMS the atoms are already specified explicitly. This makes any additional search in TOPOLOGY library as well as explicit RESIDUE reference unneccessary. Used with DELETE ENERGY DIHEDRAL and IMPROPER, combined with the CHECK, it can help to create the desired TOPOLOGY residue. See CLASS and CHARGE as well.

It is assumed, however, that the specified atoms have their ATOM CLASSES already specified, when ATOM CLASSES are not defined no force-constants can be found in the PARAMETER lists of ENERGY terms.

RESIDUE

```
... RESIDUE string
```

When RESIDUE is specified then only the TOPOLOGY residue with the name string is used to DEFINE energy terms for the specified SELECTION. NEIGHBOUR and SYMBOL should be combined with the command RESIDUE.

NEIGHBOR

```
... NEIGHBOR
```

NEIGHBOR is used for the X-PLOR chain patched residues (PEPT) In those residues atom names are preceded by a one letter code (-, +) NEIGHBOR is actually a shortened notation of the SYMBOL command which can be applied to a series of neighbouring residues.

```
MAIN> define residue PEPT neighbour - + select sequence 1H 15 end \
MAIN> dihedral improper
```

SYMBOL

```
... SYMBOL string
```

SYMBOL makes it possible to specify the ENERGY terms for links between two different residues (to use X-PLOR patched residues). The string(s) whow(s) to which SELECTION a certain atom belongs. Up to two different SYMBOLS can be applied. Each SYMBOL definition requires a separate SELECTION.

```
MAIN> define residue DISU symbol 1 select sequence 1 end symbol 2 \
MAIN> select sequence 122 end  dihedral
```

INITIALIZE

```
... INITIALIZE
```

The command word INITIALIZE initializes the BOND, ANGLE, DIHEDRAL or IMPROPER energy terms lists. With CLASS or CHARGE its use is redundant, since the existing CLASS and CHARGE values of the SELECTED atoms are replaced with the new ones anyway.

PAIRS

```
... PAIR FORCE       real
         DISTANCE    real
         CALCULATE
```

The selected PAIRS can be introduced as an additional distance constraint to the energy list. For each selected pair of atoms a FORCE constant can be defined to pull them towards the specified DISTANCE or keep the current one as specified by the CALCULATE command word. The CALCULATE option has to be used for the pair analyses (See ANALYSE PAIR).

CONSTRAINTS

```
...  CONSTRAINTS DIHEDRAL   4*atom-numb real real   COPY
                 INTERACTION  SELECT ... END  SELECT ... END
                 MAP inte SELECT ... END
                 NCS  SELECT ... END
                      FORCE real
                      NEXT_GROUP
                      AUTO_GUESS
                      RMS_GUESS
                      SET_GUESS inte 6*real
```

The MAP, INTERACTION and NCS CONSTRAINTS require one or more selections to be specified. Each selection turns into a KEY so you can check it with a 'SHOW KEY' command. Each KEY includes it string identifier and its group number ('int_ncs__1' is the first NCS interaction key). INITIALIZE preceeding a CONSTRAINT commands sets a group counter to zero and deletes all thereby referred keys.

The DIHEDRAL constraint is the only exeption, it uses the selection that preceeds

DIHEDRAL

```
... DIHEDRAL   4*atom-numb real real   COPY
```

Introduces the dihedral CONSTRAINTS for the specified atoms which are included in a SELECTION. The purpose is to maintain or enforce a particular conformation. The four atoms must be specified by their atom names. When the atom is to be searched in next or previous residue then character + or - has to be attached in front of the atom name. The first real number is the target dihedral angle in degrees and the second the force constant.

The command word COPY shows the program to take the target dihedral value from the INTERNAL COORDINATES table. This option makes possible to invert the direction of a peptide chain by keeping the conformation (secondary structure) of a segment as close as possible to the original one.

INTERACTION

```
... INTERACTION  SELECT ... END  SELECT ... END
```

You can constraint interactions between atoms to avoid inclusion of undesired overlaps by specifying the first ('active') and the second ('passive') selection. The number of INTERACTION groups is not limited. For example when refining equal molecules in two crystal forms that spatially overlap.

By default no INTERACTION group is defined.

WARNING: After modifying the INTERACTION groups, do not forget to reDEFINE the bonding term lists (BOND, ANGLE, DIHEDRAL, IMPROPER) in order to get the desired effects.

MAP

```
... MAP inte SELECT ... END
```

By default atoms interact only with s single map (the last one specified with an ENERGY DENSITY MAP command), the CONSTRAINT MAP command allow you to specify with which MAP a certain atom selection will interact. Each map can have its own selection, and atoms can be in principle included in any number of selections (between none and all). Each MAP has its own force constant (as specified by 'ENERGY DENSITY MAP inte DENSITY SCALE real' command).

NCS

```
... NCS  SELECT ... END
         FORCE real
         NEXT_GROUP
         AUTO_GUESS
         RMS_GUESS
         SET_GUESS inte 6*real
```

NCS energy term is the summ of harmonic FORCES pulling all equivalent atoms within each specified group against their average position. The average atom position is calculated via an RMS fit procedure, which first optimizes the superposition of SELECTIONS within a group to the group first representative and then, after applying the optimized rotation and translation parameters, calculates arithmetic mean of each selected atom coordinates. This averaged model is then transformed by backtransformations to the other NCS GROUP members.

If superposition makes nonsense, try to set and check initial guesses by AUTO_GUESS (performing a RMS fit calculation for the whole group based on the current values, by default all values are zero), RMS_GUESS (result of the RMS COOR ALL calculations) or set your own values (SET_GUESS). The rotations (about X, Y and X axes) are followed by a translation vector.

The FORCE allows you to specify the harmonic FORCE pulling atoms agains their averaged position. Each NCS group can has its own FORCE. When a FORCE constant is a negative number, then the atomic coordinates are simply set to their average value. This is a hard NCS CONSTRAINT, however, it still allows to optimize the NCS rotational and translational parameters during a refinement run.

The NEXT_GROUP means that you are starting with a new NCS group. The number of NCS groups is in principle not limited. After finishing an NCS group, you can not edit it any more. If you have made a mistake, start again with 'DEFINE INIT CONSTRAINT NCS'.

CHECK

```
... IMPROPERS CHECK
```

CHECK is an option that takes care that each chiral center has always a positive value for an IMPROPER angle. It means, that the current chirallity of a center is accepted and preserved during an energy MINIMIZATION procedure. This option makes possible to deal with L and D amino acids on the basis of the same topological description.

DELETE

```
DELETE.TEX       24-OCT-91
```

DELETES the SELECTED ATOMS, BONDS, HYDROGEN bonds, PAIRS, ENERGY terms. The SELECTION is required. There is no default selection.

Syntax

```
DELETE BOND  atom-num1 atom-num2
             SELECT ... END
       HBOND SELECT ... END
       PAIR(S)

       ATOM  SELECT ... END

       ENERGY  BOND        SELECT ... END
               ANGLE
               DIHEDRAL
               IMPROPER
```

BOND

```
DELETE BOND atom-num1 atom-num2
            SELECT ... END
```

DELETE BOND atom-num1 atom-num2 DELETES only the BOND between specified atoms when it exists. When an SELECTION is used instead of an atom pair, then only the bonds connecting atoms within the selection are deleted. A covalent bond between a selected atom and one that is not included in the selection is preserved.

ATOM

```
DELETE ATOM SELECT ... END
```

All the data referring to specified atoms and atoms are deleted. The SELECTION flags for remaining atoms are preserved. The connectivity table (CATBLE) and ZTABLE (connections of internal coordinates) are correspondingly updated as well as the ENERGY term lists.

PAIR

```
DELETE PAIRS SELECT ... END
```

A PAIR of atoms is removed from the PAIR list only when both atoms are SELECTED.

HBOND

```
DELETE HBONDS SELECT ... END
```

A Hydrogen bond is removed from the hydrogen bond list only when both atoms (donor and acceptor) are SELECTED.

ENERGY

```
DELETE ENERGY BOND        SELECT ... END
              ANGLE
              DIHEDRAL
              IMPROPER
              CONSTRAINT
```

DELETES from the specified ENERGY term list the contributins of the SELECTED atoms.

DIFFERENCE

DIFFER.TEX 19-OCT-91

```
Syntax
DIFFERENCE  RESIDUE      SELECT ... END    SELECT ... END
            SEQUENCE
            COORDINATES
            ATOM_NAMES
            CLASS
            CHARGE
            COLOR
            RADII
            TEMPERATURE
            WEIGHT
            INTERNAL  DISTANCE
                      ANGLES
                      DIHEDRALS
                      (ALL)
            POINTS    SURFACE
                      POTENTIAL
```

```
Syntax is the same as by COPY. Only the relation is
different.  Relation is here A := A - B. However, the
results of a string (RESIDUE, SEQUENCE, ATOM) subtraction
is, when the corresponding strings in A and B are the same,
blanks and, when they are different, the string in A is not
modified.  When subtracting RESIDUE names of two
SELECTIONS, are the places of mutations easy to see with a
```

```
MAIN> write sequence residue
```

sentence.

ENERGY

```
File: energy.txt
Last MOdified: 17-mar-1995
```

The ENERGY commands define parameters for energy calculations and can calculate potential energy (including force gradients) of SELECTED ATOMS (or POINTs). They turn individual ENERGY terms ON and OFF, define CUTOFF distance for ELECTROSTATIC and van der Waals (VDW) energy terms and can give detailed information (LIST) about geometry and possible threshold (RANGE) violations of each particular energy term for individual atoms.

```
> ENERGY  SELECT ... END
          EXCLUDE intg
          DIELECTRIC   real
          CUTOFF    real

          ALL        ON / OFF
          BOND       ON / OFF
          ANGLE      ON / OFF
          DIHEDRAL   ON / OFF
          IMPROPER   ON / OFF
          ELECTROS   ON / OFF
                     SCALE   real
          VDW        ON / OFF
                     SCALE   real
          NCS        ON / OFF
                     SCALE   real
          PAIR       ON / OFF
          DENSITY    ON / OFF
                     MAP intg
                     SCALE / RATIO real
                     GRID intg
                     ATOM
                     POINTS
          CONSTRAINT ON / OFF

          TRANSLATE   VECTOR real real real
                      ATOM   iatom
                      POINT  intg
```

```
LIST
RANGE     real real
```

SELECT

```
... SELECT ... END (SELECT ... END)
```

Two SELECTIONS can be specified. The first selection defines atoms on which forces are calculated, the second selection defines the atoms on which the first atom selection interacts. In order to calculate the potential energy of a molecule, its atoms should be defined in both selections.

When only one SELECTION is defined it is assumed that the second selection is equal to the first one. When no SELECTION is specified no ENERGY calculation is perfomed.

EXCLUDE

```
... EXCLUDE intg
```

The EXCLUDE command defines the level of neighboring atoms to the current atom in nonbonding energy (VdW and ELECTROSTATIC) calculations. The level is defined by integer. For example: CA is bound to N, CB and C. Level 1 means that the nonbonding interactions between atom CA and N, CB or C will be scaled with a scaling factor for electrostatics. No atom will be excluded from nonbonding interactions. The interactions with other atoms are not scaled.

Level 2 means that atoms N, CB and C will be excluded from nonbonding interactions, but that the interactions between their neighbors (HN, -C, CG, O, +N) and CA will be scaled with the scaling factor. And so on.

The default level for X-PLOR force fields is 3 and scaling constant is 0.4 for the border atoms interaction (electrostatic scale).

However, level -1 means, that atoms comprising a molecule are interacting only with atoms from the other molecules. (A molecule consist of atoms linked into a covalent bonds network.)

DIELECTRIC

```
... DIELECTRIC   real
```

Defines the dielectric constant. Default value is 1.

CUTOFF

```
... CUTOFF    real
```

Defines CUTOFF distance for nonbonding energy terms. Default value is 8 A.

Energy_terms

```
BOND        ON / OFF
ANGLE       ON / OFF
DIHEDRAL    ON / OFF
IMPROPER    ON / OFF
ELECTRO     ON / OFF
            SCALE real
            DISTANCE ON / OFF
VdW         ON / OFF
            SCALE real
NCS         ON / OFF
            SCALE real
PAIR        ON / OFF
CON_DIHE    ON / OFF
ALL         ON / OFF
```

These commands turn all or separate energy terms ON or OFF. For example ENERGY ALL ON ELECTROSTATIC OFF turns ALL term ON and turns OFF the electrostatic term. The command sentence has the same effect: ENERGY ALL OFF BOND ON ANGLE ON DIHEDRAL ON IMPROPER ON VdW ON For ELECTROSTATIC and VdW term also SCALING constant can be applied. By ELECTROSTATIC term it affects only the exclusion layer 1, while for the VdW term all interactions are affected.

The NCS (Non-Crystallographic-Symmtry) constraints pull the DEFINED groups against their arithmetic middle position with a group force. Here you can specify also additional overall SCALE value.

LIST

The LIST RANGE real real sets the list flag. The meaning is that all interatomic interactions of all energy terms turned on will be written to the terminal. RANGE sets the threshold values. If no real number is specified, the threshold value is set to 0.0. The first real number relates to geometry violations, and the second one to the energy of interaction. Range command has no effect when the LIST flag is not set.

For bonding terms: BOND, ANGLE, DIHEDRAL, IMPROPER

If range is active then only the terms that have a deviation from the ideal value greater than that specified or an energy term larger than specified, will be printed.

For nonbonding terms: ELECTROSTATIC, VdW

If range is active only the pair of atoms with their absolute energies above the specified threshold will be printed.

DENSITY

```
... DENSITY    ON / OFF
               MAP intg
               SCALE real
               GRID  intg
               ATOMS
               POINTS
```

DENSITY energy is kind of correlation between placement of a group of ATOMS or POINTS with a density MAP. This energy term is SCALED (weighted).

ATOMS

```
... DENSIT ATOMS ...
```

Each atom density ENERGY contribution is calculated from three second order polynomials approximation. The coeficients for the second order polynomials are calculated by a least square fit procedure from four density points. The points are laying on the line parallel to an crystall cell axis passing through an atomic center position on grid layers (1, 0, +1, +2), whereas the atomic center defines the 0 grid layer. It is positioned between the 0 and +1 grid layer.

The density values of the four density points are obtained by a linear interpolation from their four neighbor grid points which lay in the layer perpendicular to the line direction.

From these polynomials an atomic density energy is calculated as negative of the averaged summ of all three directions contributions scaled by the DENSITY SCALING factor. Derivatives are calculated along each cell axis direction on the basis from each polynomial approximation.

The DENSITY energy of a POINT selection is the interpolated density from a map to the center position. (The DENSITY energy term is so essentailly a correlation.) The density values are interpolated from the closest GRID intg specified number of grid layers around each selected point position in box (2*2*2=0, 4*4*4=1, 6*6*6=3, 8*8*8=4).

POINTS

```
... DENSITY POINTS
```

In the case of POINTS DENSITY the energy is a product of the interpolated density at the point positions and the value of each particular point. Combined together with SET CENTER, SET MATRIX and TRANSLATE options, it can be used for optimizing local symmetry, Patterson map superposition by rotational searches, and cross peak correlations of a difference Patterson map. The use of loops is recommended.

```
MAIN> energy all off density on density points density scale 1.0
MAIN> set matrix 2 polar 45. 78. 180.
MAIN> set center coordinates 40. 41. 67.
MAIN> energy matrix 2 translate vector 20. 20. 34. select all end
```

GRAPH

`GRAPH.TEX 19-JUN-1990`

GRAPH is a module with prompt: GRAPH>. It is used to displayed text and two dimensional objects (graphs). There are 10 possible GRAPH objects that can be manipulated independently. HIS_RAMA plots the cross of a residue into Ramachandran plot only into object 1. To see the results on the display you must at least once enter the IMAGE DIALOGUE mode.

WARNING: All GRAPH objects are not stored in the program but only transferred to the graphic display. The menu option RE_DRAW will erase them if they are not protected with an IMAGE FROM command. If you want to plot the Ramachandran plot or any other plot, all GRAPH objects must be send to the display when PLOT mode is already ON. When that is not the case, first turn the PLOT mode ON and afterwards repeat the GRAPH commands.

Syntax

```
EXIT
OBJECT  inte
SCALE   real
CHARACTER    SCALE   real

X-AX    real
Y-AX    real
COLOR  inte
TEXT    string
TRANSLATION     real real real

RAMACHANDRAN
     STEP   real
     ENERGY UNIT  inte
     SELECT ... END
     CROSS
     CELL
     SEQUENCE
     RESIDUE

READ FILE file_name
     UNIT int
```

EXIT

EXIT returns command input form GRAPH> to MAIN>.

OBJECT

```
OBJECT inte
```

OBJECT inte defines the current object and resets the translation of the current objects to default position in 3-D space (0.0 0.0 0.0)

SCALE

```
SCALE   real
```

Defines the SCALING of the current OBJECT.

CHARACTER

```
CHARACTER   real
```

Defines the CHARACTER scale of the current OBJECT.

Position

```
X-AX    real
Y-AX    real
Z-AX    real
```

Defines the position for the next TEXT command. It can be changed interactively by using TEXT_TRN mode. The default position is 0.0 0.0 0.0.

COLOR

```
COLOR  inte
```

Sets the color that will be used by displaying the following images.

TEXT

```
TEXT    string
```

Sends the TEXT to the current position on the screen.

TRANSLATION

```
TRANSLATION  3*real
```

Data used for TRANSLATION of the whole GRAPH OBJECT.

RAMACHANDRAN

```
... RAMACHANDRAN   STEP real
                   ENERGY UNIT inte
                   SELECT ... END  CROSS
                                   CELL
                                   SEQUENCE
                                   RESIDUE
```

Displays Ramachandran plot constituents. STEP draws lines in the frame separated for the real. ENERGY plots the contouring vectors that are read from the file accessible under UNIT inte. CROSS, CELL, RESIDUE and SEQUENCE are used to display a CROSS, squared CELL or RESIDUE name or SEQUENCE name of SELECTED residues at their position in the Ramachandran plot. The SELECT command must precede and not follow the kind of image. Otherwise there may be a mass on the display.

IMPORTANT: dihedral angles PHI and PSI should be present in INTERNAL coordinates data and PAIR list should be created. The required condition,however is, that all the selected atoms are correctly covalently bound. Apply the following series of commands

```
MAIN> make ztable
MAIN> calculate internal
MAIN> make pair ramachandran select ... end
```

and then enter the GRAPH module and prepare the plot. The options ENERGY UNIT and STEP are obsolete now, since any GRAPH can be displayed with the READ FILE command. The RAMACHANDRAN plot background images are made with a READ FILE command sentence now. See Examples.

READ

```
READ FILE file.name
READ UNIT int
```

READS the graphical commands from the specified FILE or from the FORTRAN logical UNIT number in the the input format for LWPLOT. This is the way to include any 3-D graphs to the display list. Graphs may consist of vector lists, dots and labels. Each GRAPH structure has a name (DISPLY name).

Format

First 6 characters are for the command field (DISPLY, MOVE ...), followed by 24 characters (3 times 8) for the X, Y Z coordinates and 16 for the COLOR (2 times 8) hue and saturation. The LABEL text continues from the character number 31 (31 = 6 + 3*8 + 1) to the end of the record. The GRAPH FILE should have the following syntax:

```
Syntax:
DISPLY name
COLOR  hue saturation
MOVE   x y z
DRAW   x y z
LABEL  x y z   THE LABEL TEXT
```

HELP

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

HELP is the keyword that can anywhere within the command sentence syntax retrieve information from the MAIN documentation files. You can type it before or after the command word for which you need some information, however if you start with HELP you can only retrieve this file.

(HELP currently works only for UNIX MAIN releases.)

You can get HELP also on Strike window (MENU) items. All you have to do is to enter the MENU DOCUMENTATION mode and then hit menu items. You can enter the documentation mode with the command MENU DOCUMENT ON or by typing 'h'in the MAIN image window. MENU DOCUMENT OFF or another 'h' will take you back to the command mode. Each MENU BLOCK has (or can have) its own documentation file. You are encouraged to write your own menu blocks and their documentation files as well.

Insertion of the HELP utility requires modifications throughout the program, therefore will be subroutines gradually upgraded. I hope to acomplish the task within several month. MAIN 95 release is planned to be fully HELP equiped. Currently only documentation about the 'MENU ...' commands is available.

IMPORTANT: As MAIN works in two modes (command line and dialogue) you should remember that IMAGE DIALOGUE enters the dialogue mode which enables you to use mouse, menu and dials.

IF

```
IF.TEX     20-OCT-91
```

The IF statement is useful when the program runs in loops. To apply loops a loop counter variable should be defined and the IF statement can serve either to repeat the loop or exit from the command file.

MAIN variables as "natom" for the current number of atoms or "npoint" for the current number of points can be used in comparisons.

Syntax

```
IF  number operator  number    a main command sentence

Operators are:
- .LT. less than
- .LE. less or equal than
- .GT. greater than
- .GE. greater or equal than
- .EQ. equal
- .NE. equal

Numbers can be integer or real.

When the expression ( number operator number ) is evaluated
as true, then the following command sentence is interpreted,
otherwise the command input skips to reading next line.
```

Examples

```
The file  MAIN$EXA:[AVER.CS.2HALF.MASK]CELL_LOOP.COM:

> set variable iatom = iatom + 1
> if iatom .gt. natom  return
> set center atom iatom
> show center
```

```
> make point initialize map 1 10 10 10 weigh 0.8 30.  cut
> show point
> if npoin .le. 0 rewind file
> make atom point
> rename select .not. keep end atom OX
> calculate bond distance 1.9 select .not.keep end
> make segment select .not. keep end
> delete atom select segment rang 1 8 .and. .not.keep end
> make atom merge select .not. keep end distance 1.1
> make atom merge select .not. keep end distance 1.3
> make atom merge select .not. keep end distance 1.5
> make atom bond 2.0 select .not. keep end
> make segment select .not. keep end
> if nat_old + 10 .lt. natom write unit 10 -
> select .not. keep end coordinates xplor
> delete atom select .not. keep end
> rewind file
```

IMAGE

```
IMAGE.TEX     1-MAR-93
```

The IMAGE command sentences INITIALIZE the graphical display and prepare images of atoms, bond, labels, points and maps. The DIALOGUE command word transfers the command input to the interactive devices (DIALS and MOUSE).

Picked atoms are stored in the HISTORY list. Only the atoms included in the KEY "image" are pickable. The key "image" is updated each time when an IMAGE of a SELECTION is created, so that the SELECTION is included into the key "image". The key image can, however, be modified interactively with a KEY command.

First an atom must be picked and afterwards a function on the last picked atom(s) is activated and not reverse. Atoms can be sequentially DROPPED from the HISTORY list. The last picked atom is dropped as the first one. Each command picked from the menu is actually translated into one or more command sentences, that could be in principle also typed in from the keyboard.

Syntax

```
SELECT ... END

DIALOG **

ATOM NUMBER
     NAME / SYMBOL
     CROSS
     CLASS
     BALL integer

BOND    [ ]
        DISTANCE
        STICKS  integer

HBOND   [ ]
        DISTANCE
        STICKS  integer
```

```
PAIR    [ ]
        DISTANCE
        STICKS  integer

FORCE real

RESIDUE NUMBER
        NAME / SYMBOL

SEQUENCE

POINTS [integer]
       SURFACE  CONTACT
                REENTRANT
                ALL
       VOLUME
       POTENTIAL STEP real   RANGE real real
                    ( 0.5 )
       DENSITY
       NUMBER   ON / OFF

MARK SELECT .. END
     ON
     OFF

MAP  integer   DENSITY  real  (integer integer integer)
                BOX  integer integer integer
                X-AX
                Y-AX
                Z-AX

STEREO   ON / TRUE
         OFF / FALSE
         CRYSTAL   ON
                   OFF
         XCENTER-DIFFERENCE  integer
         ANGLE   real

VIEW   real
SCREEN   real
CENTER   CALCULATE      SELECT .... END
         ATOM      atom-number
```

```
         COORDINATES  3*real
                   X-AX real
                   Y-AX real

RATIO   real

SCALE   real

TRANSLATE   real real real

STEP
OVER TRUE
     FALSE

CLIP     TRUE
         FALSE
         Z-AX    real

UNIT integer   SELECT ... END   ...
(UNIT 6 )  (SELECT ALL END)

HISTORY  INITIALIZE
         PICK atom-number
         ATOM    NUMBER           ON   / TRUE
                 NAME / SYMBOL    OFF / FALSE
         RESIDUE NUMBER
                 NAME / SYMBOL
         SEQUENCE
         SEGMENT
         DISTANCE
         ANGLE
         DIHEDRAL
         INTERNAL
         DROP
         CONTINUE  TRUE / or/ FALSE
         NAME    TRUE /or/ FALSE

MENU   OFF /TRUE
       ON  /FALSE
       PAGE int
ERASE
INITIALIZE
```

```
DELETE
FROM  (integer)
COLOR integer
SET

PLOTTER ON / OFF

XCENTER   integer
YCENTER   integer
AXCENTER   real
AYCENTER   real

LIGHT  integer    ON
               OFF
               COLOR  3*real
               PHI   real
               PSI   real
               DISTANCE  real
               COORDINATES  3*real
               ANGLE real
               ATTENUATION 2*real
               EXPONENT  real
               AMBIENT
               DIRECTIONAL
               POSITIONAL
               SPOT

SHADOW  integer

REFLEX  BY   integer
        NUMBER integer real
```

Commands

UNIT

```
... UNIT integer
```

The UNIT command words is used to define the FORTRAN unit to which the PLOTTER data are sent. When specified, it should always appear at the beginning of an IMAGE command sentence. The unit remains the same for all following image command sentences until a new unit number is defined via an IMAGE UNIT command sentence.

SELECT

```
... SELECT ... END ...
```

When a SELECT sentence stands before any other command word except UNIT it overrides the default main SELECTION which selects ALL present atoms. When it stands on some other positions the SELECTION (second selection) applies only to the next command word that chooses an atom or point presentation on image. The two SELECTIONS (main and secondary) are related by the logical .AND. operator. The second image selection is the same as SELECT (main image selection) .and. (second image selection) END.

PLOTTER

```
... PLOTTER ON
       OFF
       INITIALIZE
```

Turn the PLOT mode ON or OFF. When the PLOTTER is on, all the following image commands will result in image on the screen and its copy on a file assigned to number under UNIT. The resulting file(s), can be converted using LWPLOT to the postscript language, that can be interpreted by post script laser printer or by plotters. The created plot files can be also read again in GRAPH with the READ FILE command. By default the PLOTTER mode is turned OFF.

STEP

```
... STEP
```

STEP and OVER are two different internal modes of image processing. When the program is in STEP mode, the image appears on the screen and it stays there until it is ERASED. In

STEP mode the program forgets what was drawn after it executes the command sentence so that the IMAGE cane not be redrawn.

OVER

```
... OVER TRUE
         FALSE
```

STEP and OVER are two different internal modes of image processing. When the program is in an OVER mode it remembers what was drawn until the command word ERASE clears image data stored in program's memory. With an IMAGE OVER command the picture is actually REDRAWN (RE_DRAW from the menu). When the OVER flag is set to FALSE, then each time before a new image is displayed the old one is erased from the screen. When the OVER flag is set to true then the old image is not erased.

HISTORY

```
... HISTORY ...
         INITIALIZE
         PICK atom-number
         DROP


         ATOM    NUMBER           ON  / TRUE
                 NAME / SYMBOL    OFF / FALSE
         RESIDUE NUMBER
                 NAME / SYMBOL
         SEQUENCE
         SEGMENT
         NAME    TRUE
                 FALSE


         DISTANCE
         ANGLE
         DIHEDRAL
         INTERNAL
         CONTINUE  TRUE / or/ FALSE
```

HISTORY list is a list of PICKED atoms. The HISTORY list can be INITIALIZED (the count of history atoms is set to 0). The last PICKED atom can always be DROPPED from the list. Up to 200 atoms can be PICKED.

When an atom is picked its HISTORY label appears on the screen. HISTORY label can be composed from ATOM NUMBER and NAME, RESIDUE NUMBER and NAME, SEGMENT name and SEQUENCE name. Flag for each component can be set separately. The visibility of the HISTORY labels can be controlled with the IMAGE HISTORY NAME TRUE or FALSE command sentence.

Projection

XCENTER

`... XCENTER   integer`

Sets the xcenter of the screen relative to the absolute xcenter(axcenter). The default value is 0.0.

YCENTER

`... YCENTER   integer`

Sets the ycenter of the screen relative to the absolute ycenter(aycenter). The default value is 0.0.

AXCENTER

`... AXCENTER   integer`

Sets the absolute xcenter value.

AYCENTER

`... AYCENTER   integer`

Sets the absolute ycenter value.

VIEW

```
... VIEW   real
```

Sets the distance from the viewer to the image center along the Z axes. The default value is 500.0.

SCREEN

```
... SCREEN   real
```

Sets the distance from the viewer to the screen plane along the Z axes. The default value is 2500.0.

CENTER

```
... CENTER
```

CALCULATE

```
... CALCULATE SELECT ... END
```

CALCULATES the CENTER by averaging the coordinates of the given SELECTION. The default SELECTION are ALL atoms.

ATOM

```
... ATOM      atom-number
```

Sets the CENTER to the specified ATOM position.

COORDINATES

```
... COORDINATES  3*real
```

Sets the CENTER to specified COORDINATES.

SEQUENCE

```
... SEQUENCE    string
```

Sets the CENTER to atom CA of residue with SEQUENCE name string. When the residue has no CA atom then the center is set to the position of the first atom in the residue.

MATRIX

```
... MATRIX   integer  Z-AX real X-AX real Y-AX real ...
```

Sets the specified rotation matrix for orientation of the image around specified axes by angle in degrees. Matrix 1 is the default matrix and is used in image processing. See also SET MATRIX.

RATIO

```
... RATIO real
```

Sets the scaling factor for ATOM CROSSES.

STEREO

```
... STEREO  ON  / TRUE
            OFF / FALSE
            CRYSTAL    ON
                       OFF
            ANGLE real
            XCENTER integer
```

There are two modes of stereo: side by side (CRYSTAL OFF) and hardware (CRYSTAL ON). Default value is installation dependent. Sets the stereo flag ON or OFF. ON / TRUE - a pair of stereo images will be generated. With OFF / FALSE only a single image is generated on the screen.

ANGLE sets the difference in view angle (image is rotated along y) between the left and right image. For hardware stereo the ANGLE is actually doubled, since left and right image are rotated into opposite directions. The default value is 3.0 degrees.

XCENTER integer sets the distance from current axcenter value to left and right. The default value is 0.

CLIP

```
... CLIP TRUE / ON
         FALSE / OFF
         Z-AXIS  real
```

When the automatic clipping is ON (set TRUE) then the clipping planes are defined automatically so that the complete IMAGE appears on the screen. The option shouldn't be applied for larger molecules since it slows down the DIAL respond, However, the IMAGE is displayed with optimal depth contrast. The default flag is set to OFF and the default Z-AXIS value is set to 20.0.

SCALE

```
... SCALE real
```

SCALE defines a scaling factor for the image objects. Since PS3X0 have the left handed coordinate system, scaling factor should be negative in order to convert it in the right handed coordinate system. Otherwise the image scaling factor should be positive.

ERASE

```
... ERASE  string
```

ERASES the screen and clears the programs memory from saved images. The default argument is *, which means that all displayed objects will be ERASED. When image object is explicitly defined only the image labeled with the string is deleted. See also IMAGE FROM.

FROM

```
... FROM  integer
```

Protects displayed IMAGES from erasure. The images bellow the integer number can not be deleted with command IMAGE ERASE. When no image object number is specified, as the default value the last image object is taken.

INITIALIZE

```
... INITIALIZE
```

INITIALIZES the graphic device and established connections.

COLOR

```
... COLOR integer
```

Sets the current COLOR for drawing objects on the screen. See IMAGE SET.

SET

```
... SET
```

Disables the current COLOR set by the last COLOR command. The program takes the atomic SET colors as specified in module SET_COLOR.

LINE

```
... LINE integer
```

Defines the line type to be used when drawing vectors. Default is continues line. It doesn't work on PS330.

DELETE

```
... DELETE ...
```

When the DELETE flag is set, the following IMAGE commands do exactly opposite from the usual IMAGE command sentence. The images of selected atoms are deleted from the program's memory and cannot be redrawn any more.

DIALOG

```
... DIALOG (real)
```

Transfers the control from terminals keyboard to the DIALS and mouse. See the Dialog modes (DIAL_PEX and DIAL_PS). A specified real number changes the current DIAL scaling factor by multipling it.

ATOM

```
... ATOM NUMBER
         NAME / SYMBOL
         CROSS
         CLASS
         BALL integer
```

ATOM NUMBERS and NAMES / SYMBOLS can be drawn near the selected atom center. CROSS is drawn through the atomic center. The length of cross lines is specified by the RATIO. CLASS displays atom classes or atom types as specified by an SET CLASS or DEFINE command sentence. It is useful for identifying atom types when building a new residue into topology libraries. The BALL option is not available on E&S PS3nn: ATOM BALLS (spheres) are drawn with the currently valid REFLECTION properties and chosen BALL definition (see SET BALL).

FORCE

```
... FORCE real
```

Draws FORCES acting on atoms as calculated by the last ENERGY or MINIMIZE command sentence. The FORCE IMAGE is a vector with origin at the atom center and is pointing (pushing) the atoms in the direction of the gradient. (Pushing with the positive scaling value and pulling with a negative one.) The FORCE unit is kcal/A. When FORCE scaling factor is 1.0 then is the length of the 1 kcal/Amol force 1Å.

Connections

```
... BONDS   [ ] DISTANCES STICKS integer
    HBONDS
    PAIRS
```

When in COLOR mode is on, all connections between atoms appear in one color, while when the SET mode is on, each connection is divided in 2 parts of equal length, colored according to part's atom color. DISTANCE displays distances of the selected connections. Connections can be displayed also as STICKS (cylinders) with the specified RADIUS and DENSITY of polygons. See SET STICKS ... An integer that can be specified after command word STICKS is a flag that tells whether the polygons are shaded smoothly (more than 0) or not (less or equal 0).

RESIDUES

```
... RESIDUE NUMBER
        NAME / SYMBOL
```

RESIDUE NUMBER and NAMES or SYMBOLS of selected atoms are displayed.

SEQUENCE

```
... SEQUENCE
```

SEQUENCE symbols can be drawn on the place of residue numbers.

SEGMENT

```
SEGMENT NUMBER
        NAME / SYMBOL
```

SEGMENT NUMBER and NAMES or SYMBOLS of selected atoms are displayed.

POINTS

```
... POINTS [integer] ...
```

Since each POINT is related to an atom, they can be also SELECTED with a SELECT ... END sentence. The integer following POINTS is optional. Since on Silicon Graphics machines size of points is not directly adjustable, increasing level from 0 to 1 creates larger spots on screen and slows down dial respond substantially. 1 is recommended to be used for preparing slides.

SURFACE

```
... SURFACE REENTRANT
            CONTACT
            ACCESSIBLE
            ALL
```

Points of REENTRANT, CONTACT or both SURFACES (ALL) are drawn. Colors are taken from the atom_color array (the SET mode) or are defined by the color command.

VOLUME

```
... VOLUME  ATOM
            ACCESSIBLE
```

The use of volume points is now obsolete, because their function is more than replaced with operations on the MAP(s).

NUMBER

```
... NUMBER   ON    / TRUE
             OFF   / FALSE
```

The NUMBER flag can be set ON or OFF. When it is on, the value at a point will be displayed as well. The point values can be either SURFACE, DENSITY, POTENTIAL or VOLUME.

POTENTIAL

```
... POTENTIAL STEP real
              RANGE real real
```

When a POTENTIAL or DENSITY points are selected, then the colors of points will be chosen + and - from the defined color for STEP value. Each STEP the color is increased or decreased by 1. When RANGE is specified then only the points in the range will be colored in specified color and drawn. SET flag for atom coloring is meaningless when STEP or RANGE are activated.

DENSITY

```
... DENSITY STEP real
            RANGE real real
```

When a POTENTIAL or DENSITY points are selected, then the colors of points will be chosen + and - from the defined color for STEP value. Each STEP the color is increased or decreased by 1. When RANGE is specified then only the points in the range will be colored in specified color and drawn. SET flag for atom coloring is meaningless when STEP or RANGE are activated.

MAP

```
... MAP  integer   DENSITY  real  (integer_x integer_y integer_z)
                BOX  integer_x integer_y integer_z
                X-AXIS
                Y-AXIS
                Z-AXIS
```

Displays with integer specified MAP at the DENSITY contouring level in number of grids from current image center by integer_x, integer_y, integer_z to all directions. The BOX size or DENSITY level can be specified separately as well, when only the BOX size or contouring level is suppose to be defined. By default contours are displayed along all 3 cell axes (X,Y and Z), when only one is chosen (X-AX), then contours only in Y,Z planes (along the X-AX) are displayed.

MARK

```
... MARK SELECT ... END
         ON
         OFF
```

MARKS selected atoms with a star. It is usually activated automatically when KEYS active, passive, image and anchor are being modified from the SELECTION menu. The MARKS can be turned ON or OFF.

Examples

```
MAIN> image select pep end bond select atom name CA end  -
MAIN> residue name
```

Displays bonds of the key "pep" and at positions of each CA included in the key "pep" also its residue name

```
MAIN> image color 60 map 3 dens 0.9 5 5 5
```

Displays in color 60 map number 3 at density level 0.9 in a box 5 grids in all directions from the center.

Dialog_mode

The DIALOG mode can be entered only from MAIN> directly and not from a command file. The IMAGE and ATOMIC transformations can be driven by dials and commands picked from menus combined with picked atoms in the HISTORY list.

Menu commands are actually shortened notations for command sentences. Some of resulting command sentences appearing in manual within square brackets [] are written by the program and later on executed. Command interpreter does not distinguish between the sentences typed in from the keyboard and the ones written by the program. The command sentences written by the program itself are also stored into the file INPUT.COP before they are executed. So even if no update of coordinates in a file has been done between the run, all the changes off structural data could be retrieved afterwards. In the case of computer or program crash or a mistake the user's effort is not lost as long data from the file are accessible.

INTERNAL

```
INTCOOR.TXT        23-FEB-1993
```

In INTERNAL module internal coordinates (DISTANCES, ANGLES and DIHEDRAL ANGLES) and internal coordinates connectivity table (ZTABLE) can be edited. Directly by defining values explicitly or indirectly by defining variables and their values. Each internal coordinate may have its own variable name as well as a single variable name may be shared by a group of internal coordinates. ZTABLE, however, consist only of atomic number references.

SYNTAX

```
SET   INTERNAL   VARIABLE  DISTANCE
                 CONSTANT  ANGLE
                           DIHEDRAL
                           (ALL)
                 DISTANCE   real
                 ANGLE      real
                 DIHEDRAL   real
                 (ALL)      3*real

      VARIABLE  STRING real
                       AUTO      DISTANCE
                                 ANGLE
                                 DIHEDRAL
                                 (ALL)

      ZTABLE  ATOM-NUM DISTANCE   atom-num
                       ANGLE      atom-num
                       DIHEDRAL   atom-num  [(0), 1 or -1]
                       (ALL)      3 x atom-num [(0), 1 or -1]
```

SHOW INTERNAL VARIABLE DISTANCE CONSTANT ANGLE DIHEDRAL (ALL) DISTANCE ANGLE DIHEDRAL (ALL)

```
      VARIABLE  string  LIST
```

```
    ZTABLE  atom-num DISTANCE
                     ANGLE
                     DIHEDRAL
                     (ALL)
```

SYMBOL (NUMBER)

VARIABLE (CONSTANT)

IDENTIFY atom-num atom-symbol

EXIT

```
EXIT
```

EXIT exits the INT_COOR modul and returns to MAIN.

SELECT

```
SELECT ... END
```

A command will allways act on the last defined SELECTION. By default all atoms are SELECTED.

SET

```
SET
```

INTERNAL

```
INTERNAL
```

Sets the distance, angle, dihedral or all internal coordinates a real value. Using VARIABLE command word the variable flag for the selected internal coordinates of atoms is set. The CONSTANT unsets the variable flags. The CONSTANCE or VARIABLE ought to be used first otherwise a real value for specified internal coordinate specification is required.

VARIABLE

`VARIABLE`

Connects the selected internal coordinates with a variable name. If a variable name exists (differs from 4 blanks(' ')), a real value can be seted to all the internal coordinates connected with that variable name. If AUTO is specified then the string is a root for automatic assigning of varible name. Each time a variable name is assigned to specified internal coordinate, a number is increased for 1 and added.

ZTABLE

`ZTABLE`

The connections in the table can be overriden by typing in the new connections. When changing the second angle specification into the dihedral angle specification two numbers are required.

SHOW

`SHOW`

Shows the data fields than can be set. VARIABLE shows only the first value of chosen variable. When the user wants to see the list of all the values, that can be different than the command word LIST should be used. While showing the ztable the output can be changed from numbers to atom symbol and vice versa by using the SYMBOL or NUMBER command word.

SYMBOL

NUMBER

SYMBOL and NUMBER commands are used to set the symbol flag (fsymb) that changes from atom-number to atom symbol and vice versa in input and output. By default the numbers are required to identify the atoms. When symbol flag is set then the user shoul type in the atom symbol. The atom with this symbol will be found in the selected range if it is uniquely defined.

When '-' stnands before the atom symbol then the first atom with that identifier, counting from the first atom in the selection down, will be found. When '+' stnands before the atom symbol then the first atom with that identifier, counting from the last atom in the selection up, will be found.

VARIABLE

CONSTANT

VARIABLE and CONSTANT commands are used to set the variable_display flag (fvari). When fvari flag is set then variable names are displayed if they exist on the place of internal coordinate value, if SHOW INTERNAL command sentence is used.

EXAMPLES

```
set var a auto angle
generates variables for angles a1, a2, ... a56, untill the end
of selection.
```

JOIN

`JOIN.TEX   19-OCT-91`

syntax: JOIN atom-number atom-number RESIDUE SELECT ... END SELECT ... END

JOINS atoms by forming covalent bonds or 2 SELECTED RESIDUES into 1. The RESIDUES should follow each other. Joining of two SEGMENTS can be achieved by the RENAME command sentence.

KEY

```
KEY.TEX    19-OCT-91
```

```
Syntax
KEY   string    SELECT ... END
                DROP
                INITIALIZE
```

User can define his own KEY(s) that can be later used in SELECT statements. The KEY name can be up to 10 characters long string. When a key and a MAIN tag have the same name, then the KEY value will prevail. In a SELECT sentence the signs like % and * can be used in order to access more than one KEY at a time.

Keys can be DROPPED of INITIALIZED. By DROPPING only the particular KEY is deleted, while by INITIALIZE all defined KEYS are gone. Also by INITIALIZING a string, as a dummy key, must be typed in.

Use SHOW KEY or SHOW SELECTIONS to see the list of defined KEY(s) and number of SELECTED atoms in each one.

When no atom is SELECTED in the specified KEY, a warning message appears.

MAKE

```
MAKE.TEX     29-MAR-94
```

The command word order is important only for the first 2 command words (MAKE BOND ...). The remaining command words can follow in any order. Something is MADE from something else. For example a covalent BOND list is made from the TOPOLOGY library.

BOND

```
MAKE BOND  FROM RESIDUES
                ZTABLE
                TOPOLOGY
                ATOM  atom-num1 iatom-num2  DROP
                                            APPEND
           APPEND
           INITIALIZE
           SELECT ... END
```

BONDS and CTABLE are only two different ways of the connection table presentation. By make BONDS covalent BONDS are created or their multiplicity (bond order) is modified. MAKE BOND makes or modifies the covalent BONDS of the SELECTED atoms

- from RESIDUES (by connecting CA atoms), or
- from the distance connections in the ZTABLE or
- from the TOPOLOGY library or
- from a pair of ATOMS (atom-num1/2) specified by their atom numbers.

When after an ATOM definition DROP or APPEND is applied, the BOND order of that particular bond can be increased or decreased. The bond list can be INITIALIZED. By default the newly created BONDS are APPENDED to already existing ones.

CTABLE

BONDS and CTABLE are only two different ways of presentation of the connection table. So see MAKE BOND.

ZTABLE

```
MAKE   ZTABLE  FROM   CTABLE / BONDS
                      TOPOLOGY
               (APPEND)
               INITIALIZE
               SELECT ... END (ALL)
```

ZTABLE records are parts of INTERNAL coordinates records. In the ZTABLE the reference atoms for the distance, angle and dihedral angle are stored.

The ZTABLE can be created from the CTABLE by a search through the neighbouring atoms. However, since the reference atoms, should have lower number than the atom they define, the order of the atoms influences the ZTABLE and can result in the "holes" in it. A hole in ZTABLE is, when an atom has less than 3 reference atoms. The holes can be corrected in the INTERNAL_COORDINATE module. The ZTABLE can be INITIALIZED or the new references can be APPENDED to already existing ones. The default SELECTION is the ALL.

PAIR

MAKES a PAIR list by adding a single pair (atom-num1/2) or the whole set of pairs.

Syntax

```
MAKE   PAIR   atom-num1 atom-num2
              INITIALIZE
              APPEND

              SELECT ... END    SELECT ... END
              SEQUENCE
              ATOM
```

```
INVERT

RAMACHANDRAN
```

INITIALIZE

```
... INITIALIZE
```

INITIALIZE the PAIR list (Sets the pair counter to zero).

APPEND

```
... APPEND ...
```

APPEND is the opposite from INITIALIZE. This is the default.

INVERT

```
... ... INVERT
```

INVERTS the second column of the PAIR list, so that the last in the column becomes the first one and so on.

SELECT ... END

```
... SELECT ... END
```

Usually 2 SELECTIONS have to be defined, since the PAIR generation pairs the first atom from the first SELECTION with the first from the second SELECTION, the second from the first selection with the second from the second selection and so on. The pair generation stops when no more atoms are found in the first or in the second selection.

SEQUENCE

```
... SEQUENCE
```

PAIRS only atoms that belong to the residues with the same SEQUENCE name.

ATOM

```
... ATOM
```

PAIRS ATOMS of a residue from the first SELECTION with a residue in the second SELECTION by matching the atoms according to their ATOM NAMES.

RAMACHANDRAN

```
... RAMACHANDRAN
```

Generates PAIRS of atoms so that their INTERNAL dihedral coordinates represent PHI and PSI dihedral angels of the peptide chain. Only one SELECTION is required. So generated pair list is necessary for displaying the RAMACHANDRAN plot with the GRAPH routines.

POINTS

Major purpose of the following conversions is to extract information from electron density MAPs, that can be used either for density maxima analyzes (in a map skeletonization cross vector verification or in identification for solvent sites) for correlation of atomic model with electron density (FROM ATOMS and BONDS).

The MAKE POINTS can serve also as intermediate storage of positions and density in conversions between ATOMS and MAP(S).

Syntax

```
MAKE POINT INITIALIZE
```

```
APPEND
FROM ATOMS MAP inte
           SELECT ... END
     BONDS MAP inte
           SELECT ... END
           DIVISIONS   inte
     MAP inte LOCAL  inte
              PICK   real2 real2  real3
              WEIGHT real1 real2
              RANGE  real1 real2
              CUT
              CENTER  (see SET CENTER)
              RADII  real1 [real2]
              BOX  6*inte
```

INITIALIZE

`... INITIALIZE`

INITIALIZES the POINT list. (Sets the POINT counter to zero.)

APPEND

`... APPEND`

APPENDS newly created points to the present ones. This is the default.

FROM

`... FROM ...`

POINTS will be created either from ATOMS, along covalent BONDS or at grid positions of a MAP. The word FROM is here to increase readability of the syntax.

ATOMS

```
... ATOMS SELECT ... END
          MAP inte
```

When ATOM is specified POINTS are created from the SELECTED atom positions and the density is calculated from the 8 closest MAP grid points by a linear interpolation algorithm. There is no default SELECTION or MAP.

BONDS

```
... BONDS SELECT ... END
          MAP inte
          DIVISON  inte
```

POINTS are calculated along the covalent BONDS between the SELECTED atoms. The 'inte' specifies the number of DIVISIONS (points) generated along each BOND. The density at each point is calculated from the chosen MAP by a linear interpolation algorithm from the 8 closest map grid points. There is no default SELECTION or MAP.

MAP

```
... MAP inte LOCAL  inte
             PICK   real2 real2  real3
             WEIGHT real1 real2
             RANGE  real1 real2
             CUT
             CENTER  (see SET CENTER)
             RADII  real1 [real2]
             BOX  6*inte
             AROUND 3*inte
```

POINTS are extracted from a MAP with a search algorithm. For description see below.

PICK

```
... PICK   real1 real2  real3 MAP ...
```

PICKS POINTS in a chosen MAP with a second order Polinomyal search around each grid point that has higher density than real1. Polinomyal coefficients are defined by a least square fit procedure from the 125 surrounding MAP grid points. POINTS that have lower calculated value than real2 and that are more than real3 of GRID in any direction away from the origin grid point are rejected. (This is a computationally slow procedure. Its use has been replaced by the WEIGHT option.)

WEIGHT

```
... WEIGHT (real1 real2)
```

Applies the WEIGHTING algorithm for the point search. Map grid points, which density values are in the specified range real1 real2 (RANGE can be specified with the RANGE or with the WEIGHT command), are transformed to POINTS so, that first the intervals of grid points laying along the X direction with the density values inside the range are found and then their WEIGHTING CENTER is calculated. Weights are the density values, and the generated point obtains the weighting center coordinates.

RANGE

```
... RANGE  real1 real2
```

From each MAP grid point with the density value in the specified density range, a density POINT is generated.

CUT

...

By default the points are generated anywhere in the space from the current (IMAGE) CENTER for the specified BOX sizes. With the CUT the points can be generated only within the MAP boundaries. The generation of points outside MAP boundaries is not performed.

CENTER

```
... CENTER ...
```

See SET CENTER for the CENTER definitions.

RADII

```
... RADII real1 [real2]
```

Defines the RADIUS of the sphere around the CENTER, inside which points are to be generated. When both RADII are specified then only the grid points at the distances between the specified RADII from the CENTER are chosen.

BOX

```
... BOX 6*int
```

The area for the point generation can be defined also exactly in the grid coordinates by the BOX command. The BOX is defined from the point (int1, int2, int3) to the point (int4, int5, int6). (CUT can modify the boundaries.) The default BOX is the whole map.

AROUND

```
... AROUND 3*int
```

The AROUND redefines the BOX by setting new limits. New BOX expands for specified number of grid points away from the CENTER position in all directions.

LOCAL

```
... LOCAL inte
```

POINTS are created at positions of the LOCAL maxima as found by a MAKE MAP LOCAL sentense, their density value is however taken from the MAP.

ATOMS

```
MAKE  ATOMS SELECT ... END
            MERGE   DISTANCE  real
                    RESIDUE
            FROM  ATOMS
                  BONDS
                  COORDINATES  3*real
                  POINTS  REINDEX
```

MAKES ATOM(S) from POINTS, position (COORDINATES) or modifys the atoms by the ATOM MERGE procedures that on the base of connectivities rearranges the atom arrays. By default all atoms are selected.

POINTS

```
... POINTS   REINDEX
```

Makes ATOMS (as dummies with the ATOM NAME 'X ') in positions of all SELECTED POINTS. All newly created atom are joined within a single residue and segment. WEIGHT of the atom is filled with the point value. REINDEX is an option that, after an atom has been created at the current point position, modifies the point atom index to the newly created atom.

COORDINATES

```
... COORDINATE 3*real
```

Only one atom at position 3*real (x,y,z) is created.

MERGE

```
... MERGE    SELECT ... END
             DISTANCE real
             RESIDUE
```

Reduces the number of atoms by MERGING the SELECTED atoms into each other.

DISTANCE

```
... DISTANCE real
```

When DISTANCE is specified, the atoms forming covalent BOND pairs that are closer than the specified DISTANCE, are MERGED together. The MERGED atom has coordinates of the arithmetic middle of the pair and keeps all covalent BOND connections to the rest of the atoms. Atoms are MERGED in many cycles so that finally there is not a single pair that could be MERGED accoridng to the specified DISTANCE criterion. However, a pair of atoms connected only to each other can not be MERGED.

RESIDUES

```
... RESIDUES
```

All atoms inside a covalent BONDING network are MERGED into a single ATOM placed at their arithmetic middle. No covalent bonds are kept.

MAP

The MAKE MAP inte command acts on the referenced MAP usually by using data present in the FROM map.

Each MAP has a header including cell constants, GRIDS and a BOX (or a layout) and array of density data (grid points). Data are stored in arrays of character*1 (CHARACTER), integer*2 (INTG*2), integer*4 (INTEGER), real*4 (REAL or NUMBER) and complex (COMPLEX) values.

For example, a density value in a CHARACTER map is represented by a character*1 (0 to 255) spanned over a real number range of the map's minimum and maximum density, where a real*4 map contains real*4 values. A grid point is masked when its value is 255 (character*1 MAP) or greater than 9999.0 (of the real*4 MAP). A grid point is assumed to be empty when its value is 0 (character map) or smaller than

- 999.0 (real*4) map. All values in between the masked and empty region are considered as electron density region. Real*4 maps are recommended electron density modifications.

Manual as well as the code do not yet fully support maps in integer*2, integer*4 or complex form so please stick to the examples.

Syntax

```
MAKE MAP  inte   FROM inte
                 INITIALIZE  inte
                 BOX   6 * inte
                 GRID inte inte inte
                 CHARACTER
                 NUMBER
                 LOCAL
                 AROUND inte
                 SET    inte  inte real
                 ZERO
                 COPY
                 ATOM  MASK real
                       CLEAR real
                       DENSITY
                       DISTANCE real
                       HIGHER
                       SYMMETRY  [inte]
                 SELECT ... END
                 FILL  inte
                 REMOVE  inte
                 ROTATE   MATRIX inte
                          RMS
                          CENTER  3*real
                 TRANSLATE    VECTOR   3* real   DISTANCE real
                              RMS
                 CENTER
                 ADD / OVER
                 MULTIPLY
                 SCALE   real
                 RESCALE
                 MERGE  WEIGHTED real1 real2
                        HIGHER
                 CELL
                 CUT / DENSITY   real
                 RADII     real
```

```
                WEIGHT
                ANALYZE  STEP  inte
                         RANGE real
```

SELECT

```
... SELECT ... END
```

A SELECTION is applied by mask or density generation, or when the boundaries (BOX) of the INITIALIZED map are defined indirectly AROUND an atom SELECTION. For the syntax see SELECT.

ATOM

```
... ATOM MASK real   SELECT ... END
```

Defines a mask: sets values of grid points that are closer than the specified real (in Angstroems) to any SELECTED atom. The character MAP grid points are set to 255 and the real MAP grid points to 9999. The minimum and maximum value of a character MAP grid point are set to 0.0 and 1.0 respectively.

```
... ATOM CLEAR real   SELECT ... END
```

CLEARS a map region: sets values of grid points that are closer than the specified real (in Angstroems) to any SELECTED atom. The character MAP grid points are set to 0 and the real MAP grid points to -9999. The minimum and maximum value of a character MAP grid point are set to 0.0 and 1.0 respectively.

```
... ATOM DENSITY  SELECT ... END
```

Adds a gaussian approximation of electron density of an atom to the grid points of a map region. Works only for real*4 maps. Use it in combination with ATOM SYMMETRY [int1 int2]. Consequent usage of MAKE MAP RESCALE is recommended.

```
... ATOM SYMMETRY [int1 int2]
```

Acts only in combination with ATOM DENSITY commands. Spacegroup symmetry operations can be applied to generate electron density throughout the whole unit cell. By default all crystal symmetry operations are applied, however you may select only a particular one or a range of symmetry oparations by specifying only one or a two numbers. Numbers are the consecutive symmetry operations.

```
... ATOM DISTANCE real
```

Creates a distance weighted density around a coordinate system origin within the distance radius. It is used to setup the fast solvent flattening procedure performed via a reciprocal space coeficients multiplication.

BOX

```
... BOX 6* inte
```

BOX defines the new limits of the new map. By default (when no BOX or AROUND SELECTION are specified) the map size is copied from the reference (FROM) map. The first 3 inte define the origin point of the new map in grid coordinates, and the last 3 inte define the final grid point coordinates.

BOX can be used also in combination with the SET command.

GRID

```
... GRID 3*inte
```

In the case when a new map is created FROM 0 MAP (no map), the number of grid points per unit cell length must be defined to build it. BOX has to be defined explicitly as well. The map cell constants are taken from the current MAIN cell constants. By default the cell constants are set to 1.0 A for the lengths and 90.0 degrees for the angles.

CELL

```
... CELL
```

Fills the map by the values of grid points of the reference (FROM) map applying all crystal symmetry operations. The CELL MAP should at the beginning be INITIALIZED to an empty map, since only the points different from 0(character map) and smaller than -9999 in the real map are overwritten by the program.

COPY

```
... COPY
```

Copies the density values from the reference (FROM inte) map to the masked map (MAKE MAP inte) grid points.

FROM

```
... FROM inte
```

Assigns the FROM inte MAP as the reference MAP. When the reference map does not exist (the FROM inte is 0), then a new map can be created only if the GRIDS, BOX or AROUND and INITIALIZE options of the MAKE MAP are specified. It is recommended to have read the CELL constants, since their default values are 1.0 1.0 1.0 and 90.0, 90.0, 90.0.

INITIALIZE

```
... INITIALIZE inte
```

Creates and INITIALIZES a map. The reference (FROM) MAP is required. By default the new map is filled with zeros [0]. If some other value is desired it should be specified by the inte.

MERGE

```
... MERGE WEIGHT real1 real2
          HIGHER
```

MERGES density values at the same grid points of a unit cell FROM the specified MAP and the MAKE MAP together and writes the result into the MAKE MAP. When a grid points in a FROM map is empty or masked, the MAKE MAP is not influenced. When a grid point in a MAKE MAP is empty or masked, the value from a FROM map is copied into the corresponding MAKE MAP grid point. In the case when the MAKE MAP is a CHARACTER*1 map, value of a grid point is simply copied from the FROM map.

The WEIGHTED alternative premultiplies values of each merging points from the FROM (real1) and MAKE MAP (real2) map and then add them together, while by HIGHER option the FROM map replaces the point values of the MAKE MAP only when they both have the same sign and the FROM map has more extreme values. (This is a density combination application.)

RESCALE

```
... RESCALE
```

RESCALE modifies a MAKE MAP first by subtracting its average value from each density grid point and then dividing by its sigma value. A new average value of the grid points that are either not masked or empty becomes zero, and their standard deviation 1.

SET

```
... SET inte inte real
```

SETs all grid points stored inside the specified integer interval to the real value.

When combined with the BOX command it is possible to limit the SET command to a ceratin map region (BOX).

By character maps the integer numbers [0-255] refer to the internal program presentation of density values and not to the real density values themselves.

ZERO

Sets the whole map to ZERO regardles of a map grid point value. This command was added because sometimes intervals specified through a SET command were not enough.

ROTATE

```
... ROTATE   MATRIX inte
         RMS
         CENTER  3*real

... TRANSLATE    VECTOR   3* real   [real]
                 RMS
```

Each masked point is translated and rotated by the specified TRANSLATION and ROTATION parameters as defined below into the FROM map electron density. Density at a masked point is then defined by interpolation from the corresponding 8 surrounding points of the reference map. WAKE UP, this place is a very common source of error, since it appears somehow 'self-evident', that density is rotated into the mask, and not vice versa (as the program actually operates).

The order in which TRANSLATION and ROTATION operators are specified is also important. When TRANSLATION is defined before ROTATION then it is also applied before and vice versa. Points are translated for the specified vector. The fourth real is optional, when it is specified then the vector gives only the direction, the length of translation is specified by the fourth number. RMS takes the translation vector obtained from the RMS fit routine. ROTATION parameter MATRIX inte defines the rotation matrix (1 to 8). RMS takes rotational parameters from the last RMS fit calculation. The CENTER redefines the center of rotation. By default it is set to the origin (0.0, 0.0, 0.0). When there is NO TRANSLATION, the translation vector should be specified anyway by the VECTOR 0.0 0.0 0.0 syntax.

TRANSLATE

```
... TRANSLATE    VECTOR   3* real   [real]
                 RMS
```

See MAKE MAP ROTATE.

ADD

```
... ADD
```

Two maps can be ADDED within MAIN. When a larger set of character*1 maps have to be averaged, the maps should be written as files to a disk and averaged by the program AVEMAP. For real*4 maps there are no limitations. You have to remember that only the density points are ADDED together and that empty and masked points remain unchanged. ADDING of a density point with an empty or masked point results in an empty point, thus removing the inconsistant points from different molecular envelopes.

MULTIPLY

```
... MULTIPLY
```

Two real*4 maps can be MULTIPLIED within MAIN. It should be remembered that only the density points are MULTIPLIED together and that empty and masked points remain unchanged. MULTIPLYING of a density point with an empty or masked grid point results in an empty point.

SCALE

```
... SCALE real
```

SCALES all density points of a MAKE MAP by a real number.

AROUND

```
... AROUND inte
```

Sets the new MAP boundaries AROUND the SELECTED atoms with a boundary of inte grid points. The inte can be also a negative number. It works only when a map is INITIALIZED.

FILL

```
MAKE MAP int1 FROM int2 FILL int3
```

FILLS the holes in the MAKE MAP mask, when the number of grid points from an empty grid point to the masked region along the X, Y or Z axes on both sides is smaller than the specified int3. The MAP int1 and the referenced FROM map are assumed to be equal by size and content at the beginning of the procedure.

It is a kind of contrary of MAKE MAPE REMOVE.

REMOVE

```
MAKE MAP int1 FROM int2 REMOVE int3
```

REMOVES grid points from the MAKE MAP mask, when along the X, Y or Z axes an all sides in the range of int3 grid points an empty grid point in the masked region is found. The MAP int1 and the referenced FROM map are assumed to be equal by size and content at the beginning of the procedure.

It is a kind of contrary of MAKE MAPE FILL.

CHARACTER

```
MAKE MAP 1 FROM 0 CHARACTER ...
```

A new CHARACTER*1 MAP is to be created.

NUMBER

```
MAKE MAP 1 FROM 0 NUMBER ...
```

A new real*4 MAP is to be created. NUMBER is synonym of REAL.

REAL

```
MAKE MAP 1 FROM 0 REAL ...
```

A new real*4 MAP is to be created. REAL is synonym of NUMBER.

COMPLEX

```
MAKE MAP 1 FROM 0 COMPLEX ...
```

A new COMPLEX map is to be created.

INTEGER

```
MAKE MAP 1 FROM 0 INTEGER ...
```

A new integer*4 map is to be created.

INTG*2

```
MAKE MAP 1 FROM 0 INTG2 ...
```

A new integer*2 map is to be created.

CUT

```
MAKE MAP 2 FROM 1 CUT real
```

CUT and DENSITY are synonyms that define the density threshold below which no grid points from the FROM map will contribute to the total density sum in a sphere defined with RADIUS real. The sum of electron density will be WEIGHTED by the distance if required and written to the specified MAP. The WEIGHTED sum corresponds to the standard solvent flattening procedure described by Wang (Wang et. al., 1985). After this the summed map is to be ANALYZED, and afterwards a proper envelope with a specified portions of the density can be chosen.

RADIUS

```
MAKE MAP 2 FROM 1 RADIUS real
```

See MAKE MAP ... CUT.

WEIGHT

```
MAKE MAP 2 FROM 1 ... WEIGHT
```

Sets the distance WEIGHTING summing of density points within a sphere. See MAKE MAP CUT.

ANALYZE

```
MAKE MAP 2 ANALYZE  STEP  inte
                    RANGE real
```

After a map has been ANALYZED with an ANALYZE MAP command sentence, its grid points have been counted for each density interval. This list can be accessed either by the STEP command, where the density values below the STEP are set to a CLEAR area, and values above the STEP are set to a MASKED area. RANGE values can be defined between 0.0 and 1.0, where a STEP closest to the specified RANGE of the map interval histogram is chosen. 0.0 means no points are cut away into the CLEAR area and 1.0 means that all points are CLEARED. See also MAKE MAP CUT.

SEGMENT

```
MAKE SEGMENT SELECT ... END
             FROM    ATOM
                     RESIDUES
```

Reorganizes the SEGMENT structure.

Using the FROM ATOM option (it is the default), each network of covalently bound atoms is reorganized so that they form a new SEGMENT. Each created SEGMENT consist of only one RESIDUE. The residue structure of SELECTIONs is destroyed.

With the FROM RESIDUE option, all residues, connected with the next residue in the row via a covalent BOND are joined within a single SEGMENT name.

MENU

```
File: menu.txt
Last modified: 29-sept-94
> MENU BLOCK  string  ADD / CREATE
                      DELETE / REMOVE
                      DOCUMENT file_name
                      COLOR int
                      INITIALIZE
                      ITEM  string  ADD
                                    MODIFY
                                    REMOVE
                                    RENAME string
                                    SHOW
                                    TEXT "string ..."
                      RENAME string
                      SHOW / LIST
     DEFAULT
     DOCUMENT ON
              OFF
     LIST
     PAGE int  INITIALIZE
               ADD  string
               REMOVE  string
               COPY  int
               LIST
```

MAIN DIALOG mode MENU appears in the window named STRIKES. MENU is organized in PAGES. Only a single MENU PAGE is displayed at a time. EACH MENU PAGE can be composed of MENU BLOCKS. 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, where each ITEM is designed to perform a specific task related to the other ones within a single BLOCK.

With MENU command sentences it is possible to (interactively) edit MAIN menu structures (PAGES, BLOCKS and ITEMS).

PAGE

`... PAGE int ...`

Any PAGE menu command, except LIST, sets the current MENU page ass well.

INITIALIZE

`... INITIALIZE`

INITIALIZES a menu page (removes all BLOCKS entries).

ADD

`... ADD string`

ADDs the specified menu BLOCK to the current menu page.

REMOVE

`... REMOVE string`

REMOVES the specified menu BLOCK from the current page.

LIST

`... LIST`

LISTS all the BLOCKS within the current page.

COPY

`... COPY int`

Copies the BLOCK composition from the COPY page to the current page.

BLOCK

```
...  BLOCK   string  ADD / CREATE
                     DELETE / REMOVE
                     DOCUMENT file_name
                     COLOR
                     INITIALIZE
                     ITEM  string   ...
                     RENAME string
                     SHOW / LIST
```

Each MENU BLOCK has its own COLOR, name, documentation file and can be composed of a reasonable number of ITEMS. Each ITEM has a name which is connected with a single command sentence.

ADD

ADDs another menu BLOCK to already existing ones. BLOCK contains no ITEMS, is not exposed on any PAGE and has COLOR 1 (white). ADD is a synonym for CREATE.

CREATE

CREATES another menu BLOCK. Synonym for ADD.

DELETE

DELETES a menu BLOCK. (Only user created blocks can be deleted.)

DOCUMENT

```
... DOCUMENT file_name
```

The string 'file_name' is the file from which DOCUMENTation of the BLOCK will be retrieved when MENU DOCUMENT mode is ON.

REMOVE

See DELETE.

COLOR

```
... COLOR inte
```

Specifies or changes COLOR of a MENU BLOCK.

INITIALIZE

INITIALIZES the specified BLOCK. (Sets its item count to zero and color to 1 (white).)

ITEM

```
...  ITEM  string   ADD    TEXT ...
                    MODIFY TEXT ...
                    REMOVE
                    RENAME string
                    SHOW
                    ...    TEXT "string(s)"
```

Each ITEM has its own identifier and corresponding command string (TEXT). ITEMs can be ADDed, REMOVED, RENAMED, MODIFIED and viewed (SHOW). The TEXT command must follow an ADD or MODIFY proposal. An ITEM can be viewed (SHOW) as soon as it exist.

```
MAIN> menu block YYY item STR_ON rename STR_OFF
MAIN> menu block YYY item STR_OFF text "<str_off.cmds"
```

RENAME

RENAMES the current BLOCK identifier to something else.

SHOW

SHOWS BLOCKs ITEM composition. It is a synonym for LIST.

LIST

LIST is a synonym for SHOW.

DEFAULT

```
... DEFAULT
```

Restores original composition of MENU PAGES by keeping contents of each USER editable menu BLOCK unchanged.

DOCUMENT

```
... DOCUMENT ON
             OFF
```

Turns the MENU DOCUMENT mode ON or OFF. When the document mode is ON description of each hited menu ITEM and its BLOCK is written to the standard output. No MENU commands are accepted except the page changes. If you want to apply the menu commands you have to turn the document mode OFF again. OFF is the default.

LIST

```
... LIST
```

Displays LIST of available MENU BLOCKs.

Examples

```
MAIN> menu block USER_1 init
```

```
MAIN> menu block USER_1 item AROUND add text "<around.inp"
MAIN> menu block USER_1 item DUMMIES add -
  text "image col 1 select aro .and. weight 0.9 1.1 end atom cros"
MAIN> menu block USER_1 item DELE_RES add text "user_3.inp"
MAIN> menu block USER_1 item SYMMETRY add text "<user_4.inp"
MAIN> menu page 2 add USER_1
```

Initializes the menu BLOCK USER_1 and ADDs four ITEMS (AROUND, DUMMIES, DELE_RES and SYMMETRY) and connects each item with a command file "¡user_1.inp" or a single command sentence and includes the menu menu BLOCK USER_1 to the second menu page.

MINIMIZE

```
File: minimize.txt
Last modified: 13-mar-95
> MINIMIZE  STEP  inte[50]
            WRITE_STEP inte
            IMAGE_STEP inte
            PHASE   CYCLES inte
                    MACRO string
            BY CONJUGATED
               BODY
            SELECT ... END (SELECT ... END)
            KEY (select active end select passive end)
            LIST-GENERATION  ON
                             OFF
            TRANSLATE 3*(real inte)
            POLAR 3*(real inte)
            XYX-AXES 3*(real inte)
            POSITION
            B-VALUES
            RESCALE ON
                    OFF
```

MINIMIZES the potential ENERGY of the SELECTED ATOMS. CONJUGATE gradiend method optimizes positions (or B-values) of each individual atom, while BODY method treats each SELECTED atom GROUP as an rigid-body and optimizes only TRANSLATION and/or orientation (POLAR, XYX-AXES) of each group. (Currently only one SELECTION (GROUP) of atoms can be so optimized.)

B-VALUES are optimized for each defined GROUP. The smallest group can consist of one atom. POSITION optimization is the default.

See DEFINE GROUP.

SELECT

```
... SELECT ... END
```

Usually two SELECTIONS are defined. The first one is allowed to move and the second one serves at the interaction background to the first one. When only one selection is defined program assumes that the second one is equal to the first one.

KEY

```
... KEY
```

Assumes that the SELECTIONS are already defined as KEYs. The first one as the KEY named “active” and the second as the KEY named “passive”. These selection are usually defined through the interactive MENU items. See also MINIMIZE SELECT.

BY

```
... BY CONJUGATED
       BODY
```

With CONJUGATED gradient MINIMIZATION (this is the default) the position of each atom from the first SELECTION is optimized separately, whereas using rigid BODY minimization the placement of the whole SELECTION as a single entity (GROUP) (rigid BODY) is optimized. The placement of POINTS in a map can be optimized only with BODY method.

STEP

```
... STEP inte
```

The starting number of MINIMIZATION STEPS is 50 and can be changed afterwards.

WRITE

```
... WRITE inte
```

With WRITE inte (5 is the default), the number of MINIMIZATION STEPS is defined after which the ENERGY summary is written to the terminal.

PHASE

```
... PHASE   STEPS inte
            MACRO string
```

PHASE STEPS (zero is the default number) is the number of MINIMIZATION steps after which a new structure factor set is calculated. The PHASE step number is meaningless unless the DENSITY ENERGY term is turned ON. Only the first selection (active) contributes to new map generation, the following structure factor calculation and difference map generation. (DENSITY MAP should be properly defined. See ENERGY DENSITY.)

When PHASE MACRO is defined, then the new structure factors are to be calculated within that macro and not as by default, when new structure factors and a difference density map are calculated (Fobs-Fcalc). This is the way how to incorporate density modifications procedures into a refinement procedure and thereby not break continuity of the gradient search by restarting it after each structure factor calculation. WARNING: You should, however, take care that the phasing and the difference map calculation make sense.

IMAGE_STEP

```
... IMAGE_STEP inte
```

The IMAGE defines the number of MINIMIZATION STEPS after the molecular model IMAGE is redrawn (replaced with the new coordiates). The default value is 0, which means that the IMAGE is not updated during the MINIMIZATION. IMAGE is updated after the minimization is done. (This option is currently disabeled.)

POSITION

```
... POSITION
```

POSITION is the switch that turns the B-VALUE optimisation off and truns the POSITION optimisation on. This is the default.

B-VALUES

```
... B-VALUES
```

B-VALUES turns the POSITIONAL optimisation off and truns the B-VALUES optimisation ON. This is not the default. SEE also DEFINE GROUPS. The B-VALUES have no effect when rigid BODY optimisation is requested.

LIST-GENERATION

```
... LIST-GENERATION ON
                    OFF
```

Turns ON/OFF the generation of lists for calculation of nonbonded energy terms (VDW and ELECTROSTATIC), ON is the default. The nonbonded interaction list generation considerably speedes up energy calculation, when the nonbonded energy terms are requested.

RESCALE

```
... RESCALE ON
            OFF
```

RESCALES the generated map before its Fourier transformation in order to introduce a real-space solvent correction. The default is ON.

See MAKE MAP RESCALE.

OBJECT

`OBJECT.TEX 23-nov-91`

Activated OBJECT are defined in order to interactively (by dials) manipulate conformations of models without actually changing the coordinates data. The OBJECTS are supposed to be defined via MENU commands, though they can be changed and also manipulated manually via command sentences. Each OBJECT obtains a KEYED SELECTION. The SELECTIONS can be changed also after the OBJECTS have been already defined. Up to 30 activated OBJECTS are allowed to be set simultaneously. The SYMMETRY OBJECTS have to be defined manually.

Syntax

OBJECT inte SELECT ... END BOND atom-num atom-num (atom-num) DISTANCE atom-num1 atom-num ANGLE atom-num atom-num atom-num DIHEDRAL atom-num atom-num atom-num atom-num TRANSLATE ROTATE atom-num SYMMETRY MATRIX inte TRANSLATION inte inte inte SET TRUE FALSE INITIAL BOND real ANGLE real DISTANCE real DIHEDRAL real TRANSLATION 3*real ROTATION 9*real

```
FROM   int2
       AUTO
```

inte

```
OBJECT inte ...
```

Defines the identity number of the OBJECT on which to following function is activated.

SELECT

```
... SELECT ... END
```

Defines the SELECTION on which the specified function acts. The name of the OBJECT'S KEY is a 4 character string "ob__". The "__" are replaced with the OBJECT identity number.

BOND

```
... BOND atom-num1 atom-num2 [atom-num3]
```

Activates rotation around the BOND atom-num1 atom-num2. The atom-num3 is optional. Usually it is chosen from the neighbours of atom-num2 by the program itself.

DISTANCE

```
...  DISTANCE  atom-num1 atom-num2
```

Activates translation of the SELECTION along the vector atom-num1 atom-num2.

ANGLE

```
... ANGLE  atom-num1 atom-num2 atom-num3
```

Activates rotation of the SELECTION around axes that goes through atom atom-num2 and is perpendicular to the plane defined by the 3 atoms.

DIHEDRAL

```
... DIHEDRAL atom-num1 atom-num2 atom-num3 atom-num4
```

Activates rotation of the SELECTION around bond atom-num2 atom-num3.

TRANSLATE

```
... TRANSLATE
```

Activates TRANSLATION of the SELECTION in X Y and Z components.

ROTATE

```
... ROTATE atom-num
```

Activates ROTATION of the SELECTION around X Y and Z axes. The CENTER of ROTATION is at the position of atom atom-num.

SYMMETRY

```
... SYMMETRY     MATRIX  inte
                 TRANSLATION   inte inte inte
```

Activates crystallographic SYMMETRY operations on the given object. It acts only with a link to an activated parent OBJECT. When the parent is moved (ROT_TRAN) also the children are following its rotations and translations with the chosen SYMMETRY operations plus the additional TRANSLATIONS in whole number fractional coordinates. The SYMMETRY operation MATRIX inte is the sequential number taken from the list of SYMMETRY MATRICES that should be already read before.

FROM

```
OBJECT inte FROM   int0
                   AUTO
```

The changes of the activated OBJECTS can be dependent from each other. The OBJECT int0 is the parent of the OBJECT inte. That means, that whatever happen to the parent OBJECTS, happen to the children as well. The command word AUTO tells the program to find the parents, if they exist, from the SELECTIONS of the activated OBJECTS. An OBJECT is a child, when a parent OBJECT can be found. A parent OBJECT includes the complete SELECTION of its' child.

SET

```
... SET    TRUE
           FALSE
```

```
INITIAL
BOND  real
ANGLE  real
DISTANCE real
DIHEDRAL real
TRANSLATION  3*real
ROTATION    9*real
```

The values of activated OBJECTS' functions are normally defined interactively with DIALS. They can be checked with a SHOW OBJECT command. In the case of restarts or since the user would like to do it manually, The values can be set directly. For BOND, ANGLE, DISTANCE and DIHEDRAL it is enough to specify 1 value, while for the TRANSLATION the whole vector is is required and for ROTATION the whole 3x3 matrix. The values can be any moment INITIALIZED - set to starting point, the current OBJECT definition can be accepted (SET TRUE) (the coordinates are accordingly changed) or rejected (SET FALSE). Either rejection or confirmation of the current OBJECT'S status, eliminates the OBJECT'S definition and the KEY connected to it.

POINT

```
POINT.TEX          20-nov-91
```

Points can be generated on one or more surface levels or in a rectangular box defined by maximum and minimum x, y, and z values.

Syntax:

```
POINTS  INITIALIZE
        APPEND
        SURFACE    REENTRANT
                   CONTACT
                   ( ALL = CONTACT + REENTRANT )
                   ACCESSIBLE
        VOLUME
        PLANE   3*realx/y/z, 3*real (sx/sy/sz), 3*inte (x/y/z)
        SELECT ... END
        RADIUS real (1.4)
        DENSITY real  (4.0)
        RANGE real real
        STEP real
```

SELECT

```
... SELECT ... END
```

Two SELECTIONS are required for generation of a Connolly SURFACE. The first one is the one on which atoms points are generated and the second one serves to cut away the inner points, that wouldn't be generated if the whole molecule would have been chosen. For syntax see SELECT.

SURFACE

```
... SURFACE    REENTRANT
```

```
CONTACT
ALL (= CONTACT + REENTRANT )
ACCESSIBLE
```

Calculates the Connoly surface (by the Connoly algorithm). The atomic radii should be specified by the SET RADII. The 3 kinds of SURFACES can be calculated: CONTACT, REENTRANT and ACCESSIBLE. Points of CONTACT and REENTRANT surfaces lie for the atomic RADII far away from atoms, while points of the solvent ACCESSIBLE surface represent the boundary to which the centers of solvent atoms can still approach. The ACCESSIBLE surface is mathematically the same as the CONTACT surface, only the atomic radii are enlarged for the solvent radius.

RADIUS

```
... RADIUS real
```

Defines the RADIUS of the solvent molecules.

DENSITY

```
... DENSITY
```

Defines the DENSITY of points. Default value is 4.0 point per square A. Higher number means more points. 4.0 is well enough when the protein as whole is suppose to be inspected. For smaller parts it is reasonable to increase it.

RATIO

```
... RATIO real
```

RATIO is the real number with which atomic radii are multiplied.

RANGE

```
... RANGE real1 real2
```

RANGE is the distance from VdW radii of atoms out in space in which the surface points are generated.

STEP

```
... STEP real
```

When surfaces are generated in a RANGE then STEP is the distance between the 2 consecutive layers of SURFACE.

PLANE

```
... PLANE   3*real x/y/z, 3*real sx/sy/sz, 3*inte x/y/z
```

The PLANE command words offers a possibility to generate points in a 3-D lattice. From the origin (3*real x/y,z), step size in each direction (3*real sx/sy/sz) and number of steps (3*inte x/y/z) the 3-D lattice is generated.

VOLUME

The VOLUME points options are more than replaced with the MAP operations.

Examples

```
MAIN> point surface all ratio 1.2 select all end select all end
```

```
MAIN> point surface all select activ_site end -
MAIN> select protein end dens 7.0 initialize
```

```
MAIN> point plane -2. -2. -2. 1. 1. 1. 5 5 5
```

RADII

```
RADII.TEX     21-nov-91


Syntax
SET RADII   SELECT ... END * real
                             INITIAL (0.0)
                             VdW
                             CHARGE
            EXIT
```

To a given selection VdW, CHARGE or nonnegative real value RADII can be set. EXIT should be used to return back to MAIN>.

READ

```
File: read.txt
Last modified: 10-FEB-95
```

When no UNIT number or file is specified, the READ UNIT is the current input, either the terminal or a command file. The number of atoms is changed only when cartesian or internal coordinates are read. The FILES are opened with the READONLY option.

Syntax

```
READ UNIT int
     FILE string
       ATOMS   DEFAULT           ATOM_UNI      INITIALIZE
               CARD         [ANGSTROEM]   APPEND
               PDB          NANOMETER     OVER   SELECT ... END
               XPLOR
               DISCOVER
               AMPAC
               GROMOS
               DIAMOND
        SCATTERI
        ELEMENTS

        BONDS ()       |  INITIALIZE
                NUMBERS  |   APPEND
        CTABLE         |   FIRST   atom-num
        HBONDS         |           SELECT ... END
        ZTABLE         |

        INTERNAL  (GAUSS)   ATOM           INITIALIZE
                   AMPAC     (ANGSTROEM)    (APPEND)
                                            OVERWRITE   FIRST *
        POINTS  ()
                SURFACE          CONNOLLY      INITIALIZE
                VOLUME           GAUSSIAN86    (APPEND)
                POTENTIAL        G80           FIRST *
                DENSITY
        TOPOLOGY   CARD          (APPEND)
```

```
               XPLOR          INITIALIZE
               DISCOVER
               GROMOS
               (MAIN)
      PARAMETERS XPLOR
       SEQUENCE
       CELL
       SYMMETRY
       MAP  (CHARACTER)     OVERWRITE int
            NUMBER
            ALPHA
            PROTEIN
            XPLOR
            CCP4
```

COORDINATES

See READ ATOMS.

ATOMS

```
... ATOMS                        ATOM          INITIALIZE
                    CARD                       APPEND
                    PDB          NANOMETER     OVER      SELECT ... END
                    XPLOR
                    DISCOVER
                    AMPAC
                    GROMOS
                    DIAMOND
```

ATOMIC coordinates can be read in different formats. The program uses angstroems units. INITIALIZE starts reading from zero number of atoms. APPEND adds the atoms to the previously known ones in the program. OVERWRITE finds the FIRST atom number in the SELECTION and replaces the atomic coordinates after the first found atom and leaves the atom and residue structures untouched.

Formats: DEFAULT, CARD, PDB, XPLOR, DISCOVER, AMPAC, GROMOS, DIAMOND

The format without a name is the DEFAULT format. It tries to find an atomic name or atomic element number and 3 coordinates for X, Y, and Z. The format is free and the order of data is not important. When a real number is not found, the program assumes that the coordinate is zero.

CARD is the CHARMM format.

DIAMOND is the format used by FRODO and EREF.

PDB or XPLOR reads Brookhaven Data Bank and XPLOR PDB.

DISCOVER is the format from BIOSYM Inc. (DISCOVER, INSIGHT).

GROMOS is the Groningen package format.

AMPAC and GAUSSIANnn are program packages for quantum mechanical calculations.

Units:

ANGSTROEM units are the default.

NANOMETER accepts that the coordinates in NANOMETERS and multiplies them by 10. In GROMOS format the NANOMETER units are set automatically.

ATOM means that coordinates have to be converted from atomic units to Angstroems. Atom units are quite often used in quantum mechanical calculations.

SCATTERI

SCATTERING factors for each ELEMENT can be read in form of an ELEMENT id (and also as atomic number) followed by 10 or less real numbers (the 5 gaussian presentation as appearing in the International tables.)

ELEMENTS

Each atom has its ATOMIC NUMBER and ELEMENT id. When read each atom gets its ATOMIC NUMBER based on comparison with the ELEMENT id-s table. Each ELEMENT id, which is a string, can be replaced by reading a line consisting of an ATOMIC NUMBER and the new ELEMENT id string. Replacing C with E for example:

```
>read element
> 6 E
>
```

If a new name is not unique, then it can not replace the old one. All characters are converted to capital letters. See also WRITE ELEMENTS.

BONDS

```
... BONDS  NUMBER
```

A file containing only the atom numbers is read when there is the NUMBER command word.

CTABLE

```
... CTABLE
```

A connection table can be read. This make sense only when atoms are in the same order as they were when the CTABLE was written.

ZTABLE

```
... ZTABLE
```

A Z-mat-connection table is used for conversions between the INTERNAL (relative) and cartesian COORDINATES (absolute). Each atom can have a ZTABLE record.

INTERNAL

```
... INTERNAL GAUSSIAN
             AMPAC
```

Reads INTERNAL coordinates and ZTABLE with the INITIALIZE or APPEND options. GAUSSIAN or AMPAC formats can be read.

POINTS

```
... POINTS  ()
    SURFACE          CONNOLLY       INITIALIZE
    VOLUME           GAUSSIAN86    (APPEND)
    POTENTIAL        G80           FIRST *
    DENSITY
```

SURFACE, VOLUME, electrostatic POTENTIAL or DENSITY POINTS can be READ. The default is SURFACE points. When the read points are to be transformed into some other kind (VOLUME, electrostatic POTENTIAL or DENSITY) then the kind should be explicitly specified.

There are three formats of point records available (CONNOLLY, GAUSSIAN86 and G80). Only the CONNOLLY format includes the complete information for each point. The GAUSSIAN86 and G80 formats are only used to READ electrostatic potentials.

The POINT counter can be set to 0 (INITIALIZE) or left unchanged (APPEND). Each point has one or more atomic indices that tell the program to which atom a point belongs. By default they are not changed when using the CONNOLLY format. With GAUSSIAN and G80 all the points in the file are by default assigned to the last atom. The default can be changed by the FIRST option, so that the number of the first atom found in the SELECTION is supposed to be the atomic index 1 from the points. This is achieved simply by adding the difference to each atomic index.

TOPOLOGY

```
... TOPOLOGY  MAIN
              CARD          (APPEND)
              XPLOR          INITIALIZE
              DISCOVER
              GROMOS
```

MAIN format is the default. MAIN topology libaries are the only ones that can be used for model building and energy calculations.

The X-PLOR (XPLOR) TOPOLOGY files can used for energy minimization procedure, however, new residues can not be built from scratch from X-PLOR topology files. The conversion to MAIN topology files is rather simple, so that you should in general try to convert your XPLOR topology files in MAIN format.

The DISCOVER topology file of MOLEDT - DISCOVER format can be used can be used for model building (CLASSES, CHARGES, BONDS and INTERNALS are read).

The GROMOS and CARD (CHARMM) topology files can be used for atom name corrections and partial atomic charges assigneent (only CLASSES and CHARGES are read).

CELL

```
... CELL
```

Cell constants (a, b, c, alpha, beta, gamma) are read in free format. Title line(s) beginning with a '*' is required, when you try to read the cell constants from your terminal.

SYMMETRY

```
... SYMMETRY
```

SYMMETRY operations are read in the form used by the international tables for crystallography. Only a single group of crystallographic symmetry operations can be handeled at once in the program. When MAP files in PROTEIN or MAIN formats are read the symmetry operations are included automatically.

MAPS

```
... MAPS  CHARACTER     OVERWRITE int
          REAL (NUMBER)
          ALPHA
          CCP4
          PROTEIN
          XPLOR
```

Maps can be read by MAIN as character*1 or real*4 maps. The default map format is the CHARACTER. The real*4 maps require the NUMBER format qualifier. PROTEIN, XPLOR and ASCII CCP4 maps are transformed into the real*4 maps. ALPHA maps are a character*1 presentation written hexadecimally. ALPHA, XPLOR and ASCII CCP4 maps are all text files that can be transferred between any hardware.

PROTEIN maps are automatically scaled to 1 sigma.

The OVERWRITE qualifier means, that the map stored under the specified map number will be overwritten and that all maps with higher consecutive numbers are lost.

FIRST

```
... FIRST  atom-num
           SELECT ... END
```

The FIRST atom can be specified directly as an atom number or found as the first atom in the SELECTION.

REFLECTIONS

```
... REFLECTIONS INITIALIZE
                RESOLUTION  real real
                LIMITS
```

Reads a reflections file (with INDEX, FOBS, SIGMA, FCALC, PHASE, COMPLEX). FCALC can be presented as COMPLEX number or with FCALC (amplitude) and PHASE. Format is free. Program interprets an XPLOR reflection file as well. When INITIALIZING the data arrays RESOLUTION limits have to be specified. Also HKL limits are desired, in order to reduce data storage.

Before reading a reflection file the CELL constants must be defined

RENAME

```
RENAME.TEX     19-OCT-91

Syntax
RENAME  SELECT ... END
        ATOM  string
        RESIDUE  string
        SEGMENT   string
        SEQUENCE  string
        INSERT
        DELETE
        APPEND
        REMOVE
```

The atomic character data (ATOM, RESIDUE, SEQUENCE and SEGMENT names) of the SELECTED atoms can be modified using the RENAME command sentence. This can save a lot of effort required to transfer the atomic coordinate files between different programs. The time consuming editor use can be avoided.

The INSERT/DELETE and APPEND/REMOVE are operating only on SEQUENCE names. INSERT inserts a character before the current SEQUENCE name, the DELETE deletes the first character of the sequence names. APPEND appends a character after the current sequence names, REMOVE removes the last character from the sequence names.

EXAMPLES

```
MAIN> rename select atom name CD1 .and. residue name ILE end atom CD


MAIN> rename select residue number 1 end sequence -2


MAIN> rename sequence 33A select residue number 33 end


MAIN> rename select numb segment 1 end sequence A insert
MAIN> rename select numb segment 2 end sequence B insert


MAIN> rename select inhibitor end sequence I append
```

RMS

```
RMS.TEX        6-dec-91
```

RMS = Root Mean Square

With the RMS command sentence it is possible to compare (calculate a RMS deviation) between two different data sets and also optimize the rotational matrix and transformational vector of the two SELECTIONS, so that the RMS of compared coordinates gives a minimum.

```
Syntax
RMS   SELECT ... END         SELECT ... END
      PAIR
      COORDINATES    ()
                     ALL
      CHARGE
      RADII
      INTERNAL  DISTANCE
                ANGLES
                DIHEDRALS
                (ALL)
      POINTS    SURFACE
                POTENTIAL
```

RMS gives a value of root-mean-square differences between PAIRS or 2 different atom SELECTIONS of specified atomic real values data (COORDINATES, CHARGE, RADII, INTERNAL coordinates and POINTS). Points can not be PAIRED by the PAIR command word - 2 SELECTIONS should be specified. Coordinates of atoms can be also matched by a fitting procedure, when ALL follows the COORDINATE command word. The coordinates of atoms are not actually moved. Only the parameters for rotation and translation are found and saved in programs memory. The parameters can be shown with a SHOW RMS sentence. The resulting rotational matrix is the matrix number 8.

The coordinates of the atoms and points can be ROTATED and TRANSLATED into the position found by the RMS fit routine, by first using ROTATION and later TRANSLATION and not vice versa

Examples MAIN> rms coordinates all select atom number 1 29 end - MAIN> select atom number 30 59 end

```
MAIN> rms coordinates pair
```

ROTATE

`ROTATE.TEX     6-dec-91`

A SELECTION of ATOMS or POINTS is ROTATED around a point in space (CENTER). The ROTATION is specified via an MATRIX (in case of ATOM or POINT rotations) or as ROTATION around a BOND.

Syntax

```
ROTATE BOND atom-num1 atom-num2 (atom-num3) -
              (SELECT CUT atom-num1 atom-num2 END )
               SELECT ... END
               ANGLE real

        ATOM  SELECT ... END
              MATRIX inte
              CENTER ATOM atom-num
                     COORDINATE  3*real
                     CALCULATED

        POINTS   SURFACE    SELECT ... END
                 VOLUME     MATRIX inte
                 DENSITY    CENTER ...
                 POTENTIAL
```

BOND

```
...  BOND atom-num1 atom-num2 (atom-num3) -
          SELECT ... END
          ANGLE real
```

The SELECTED atom coordinates are ROTATED around the specified BOND for the specified ANGLE. It is not necessary that atom-num1 and atom-num2 are connected by a covalent bond. When a third atom (atom-num3) is specified it doesn't have to be connected to atom-num2. When the third atom is omitted then the program looks for it in the connection table for a neighbour of atom-num2. The default atom SELECTION is the group of atoms that are on the side of the atom-num2 of the covalent bond atom-num1 atom-num2 (SELECT CUT atom-num1 atom-num2 END).

ATOM

```
... ATOM  SELECT ... END
          MATRIX inte
          RMS
          CENTER ATOM atom-num
                 COORDINATE  3*real
                 CALCULATED
```

ROTATES the SELECTED atoms around the specified CENTER by multiplying atomic coordinates with the specified rotational MATRIX. The ROTATIONAL MATRICES can be specified by the SET MATRIX int ... command sentence. There are 8 matrices available. Using RMS the last RMS fit parameters are used to create the ROTATIONAL MATRIX. The default CENTER for the transformation is the coordinate system origin. Other CENTER positions can be chosen (the current image center - CALCULATED, an ATOM position or some other point in space - COORDINATES).

POINTS

```
... POINTS   SURFACE    SELECT ... END
             VOLUME     MATRIX inte
             DENSITY    RMS
             POTENTIAL  CENTER ...
```

Work on the same way as the ROTATE ATOM command with the only difference, that the points can be selected also by their kind (SURFACE, VOLUME, POTENTIAL, DENSITY).

Examples

```
MAIN> rotate bond 3 4 angle 30.
```

```
MAIN> rotate atom select segment number 3 end -
```

```
MAIN> matrix 3 center atom 4
```

```
MAIN> rotate points potential select number segment 4 end -
MAIN> rms center calculated
```

SECONDARY

```
SECONDARY.TEX   21-nov-91
```

```
Syntax
SECONDARY
       EXIT
       SELECT ... END  ALPHA
                       BETA
                       PARALLEL
                       PHI  real
                       PSI  real
```

The module SECONDARY sets some basic secondary structure elements like ALPHA helix, antiparallel BETA strand and PARALLEL beta strand. Besides PHI and PSI angles can be defined explicitly.

SELECT

```
File: select.txt
Last modified: 17-nov-94
```

The SELECT subsentence can be included in almost any MAIN command sentence. It allows you to perform the desired operations on a limited ATOM or POINT SELECTION. In most cases ALL atoms are selected by default, sometimes (as in a DELETE command) such default is not acceptable, and a selection must be specified.

The SELECT ... END subsentence assigns each atom a value 1 for (true) or 0 for (false).

In general a SELECT sentence looks like this:

```
MAIN> ... SELECT  tag1 .OR. tag2 .AND. ( .NOT. tag3 ...) END
```

The user can combine the tag(s) with logical operators .AND., .OR., .NOT. and brackets (). Up to 10 levels of brackets are allowed. Logical operators .AND. and .OR. act between 2 tags, while .NOT. acts on one only.

Recursive use of the SELECT sentence is possible only indirectly with the help of KEY(s). The SELECT sentence uses the result of a previous one as a tag.

Tags

Tag is a synonym for an atom property or its description. Through tags you can reach particular group of atoms and combine them by applying brackets and logical operations. Tags refer to ATOM NAMES, atomic TEMPERATURE factors, atomic positions regarding to a PLANE or a CENTER, ...

MAIN differentiates between small and capital letters. The star sign '*' and the percent sign '%' have special meaning when atoms are selected according to their NAMES or KEY(s). The star allows any further character, and the percent sign allows any character on that particular place.

Syntax

```
BY    BOND
```

```
      PAIR
      RESIDUE
      SEGMENT
      SEQUENCE

string (KEY(s))

ALL

AROUND   KEY      string                      DISTANCE real
         CENTER   ATOM      atom-num
                  CALCULATED
                  COORDINATES real real real

BOND    PAIR     inte
        NUMBER   inte
        RANGE real1 real2

CHARGE  real real

CLASS   string

COLOR

CUT      atom-num   atom-num

ELEMENTS int1 ...

HISTORY

IMAGE

INTERNAL   DISTANCE   real real
           ANGLE
           DIHEDRAL

MAP   inte(1) real real

MAIN

NEIGHBOUR atom-num inte
```

```
ATOM MODULE  inte  inte [inte]  (*)
     NUMBER  inte [inte]
     NAME    string [strings ...]
     CLASS   string

RESIDUE MODULE  inte  inte [inte]   (*)
        NUMBER  inte [inte]
        NAME    string

SEGMENT MODULE  inte  inte [inte]   (*)
        NUMBER  inte [inte]
        NAME    string [strings ...]
        SIZE    inte inte

PAIR   inte

PLANE  inte real real

SEQUENCE string string

TEMPERATURE  real real

WEIGHT   real real

(*) ATOM NAME is equivalent to NAME ATOM.  Word order is also
not important for combinations of words as RESIDUE and SEGMENT
with words NAME, NUMBER and MODULE.
```

BY

```
... BY   BOND       ...
         PAIR
         RESIDUE
         SEGMENT
         SEQUENCE
```

BY is a special tag operator that can precede any other tag including a KEYED SELECTION. It means that atoms that are covalently bound (BOND), form a PAIR, are in the same RESIDUE or SEGMENT or have the same SEQUENCE name as any of the tagged atoms, will be SELECTED. Operators BY RESIDUE, SEGMENT or SEQUENCE operators SELECT also the tagged atoms, while the BY BOND and PAIR don't.

ALL

```
... ALL ...
```

Selects ALL atoms. In some command sentences (DEFINE, IMAGE, WRITE) it is the default SELECTION so that it doesn't always have to be explicitly specified. In general, ALL atoms are SELECTED, unless a selection is required.

AROUND

```
... AROUND KEY string
           CENTER   ATOM atom-num
                    CALCULATED
                    COORDINATES real real real
           FROM string
           DISTANCE real
```

The AROUND tag selects atoms that are AROUND any atom from the KEY or AROUND a specified point in space (CENTER) for the specified DISTANCE. The CENTER can be defined either by an ATOM position, by the current IMAGE center (CALCULATED) or specified directly with COORDINATES. In order to speed up the calculation, it is reasonable to limit the search only to the atoms FROM the specified key.

CHARGE

```
... CHARGE real real
```

SELECTS atoms with their partial atomic CHARGES in a specified range.

CLASS

```
... CLASS string
```

SELECTS atoms with specified atom CLASSES.

COLOR

```
... COLOR inte
```

SELECT atoms with the specified COLOR.

CUT

```
... CUT  atom-num1   atom-num2
```

SELECTS the atoms, that are included in the network of covalent bonds, starting at the atom-num2 away from the atom-num1. This is a shortcut to the procedure, where you should first cut the bond (atom-num1 - atom-num2), then select all atoms included in the covalent bond network on the side of atom-num2 and at the end join the atoms again.

ELEMENTS

```
... ELEMENTS int1 [int2 ...]
```

SELECTS atoms with the given element number (atomic number). More than one number can be specified at a time.

INTERNAL

```
INTERNAL   DISTANCE   real real
           ANGLE
           DIHEDRAL
```

SELECTS the atoms whose INTERNAL coordinate (DISTANCE, ANGLE or DIHEDRAL angle) is in the specified range. Internal coordinates and Z_TABLE are required.

MAIN

```
MAIN
```

Selects the MAIN chain amino acid residue atoms (C,O,CA,H,N). Its equivalent is ATOM NAME C O CA H N.

ATOM

```
... ATOM MODULE  inte  inte [inte]
         NUMBER  inte [inte]
         NAME    string [strings...]
         CLASS   string
```

Selects ATOMS according to their NAME(S), CLASS, consecutive NUMBER in a range or my a MODULE operator.

RESIDUE

```
... RESIDUE MODULE  inte  inte [inte]
            NUMBER  inte [inte]
            NAME    string [strings...]
```

Selects RESIDUES according to their NAME(S), consecutive NUMBER in a range or my a MODULE operator. See ATOMS for a further description of NAME.

SEGMENT

```
... SEGMENT MODULE  inte  inte [inte]
            NUMBER  inte [inte]
            NAME    string [strings...]
            SIZE    inte inte
```

Selects SEGMENTS according to their NAME(S), consecutive NUMBER in a range or my a MODULE operator. SEGMENT SIZE selects segments that include number of atoms within the specified limits.

MODULE

```
... MODULE ATOM        inte1 inte2  [inte3]
           RESIDUE
           SEGMENT
```

See corresponding ATOM, RESIDUE or SEGMENT equivalents.

MAP

```
... MAP  inte real real
```

Select atoms within the specified (electron) density range. The density at an atom center is calculated from the MAP inte by linear interpolation.

NAME

```
... NAME ATOM      string(s)
         RESIDUE
         SEGMENT
```

See corresponding ATOM, RESIDUE or SEGMENT equivalents.

NEIGHBOUR

```
... NEIGHBOUR atom-num inte
```

SELECTS all the atoms that are within the range of the inte steps form the central atom-num. 1 step is one covalent bond. With 0 only the atom atom-num is selected, with 1 its NEIGHBOURS, with 2 NEIGHBOURS of the NEIGHBOURS and so on. With inte -1 the whole molecule (network of covalent bonds starting at the atom-num) is SELECTED.

NUMBER

```
... NUMBER ATOM        inte1 inte2
```

```
RESIDUE
SEGMENT
```

See corresponding ATOM, RESIDUE or SEGMENT equivalents.

PLANE

```
... PLANE inte real1 real2 ...
```

SELECTS atoms that are located in the specified distance range (real1 and real2) distances from the PLANE inte. Distances are calculated from the scalar product between the atomic position and the plane equation and can be negative. Planes are defined with a SET PLANE command sentence.

SEQUENCE

```
... SEQUENCE string (string) ...
```

SELECTS the residues between the residues with the specified sequence names. When only residues with a single SEQUENCE name are to be found, then the second string is redundant.

TEMPERATURE

```
... TEMPERATURE  real real ...
```

SELECT atoms with TEMPERATURE factors in the specified range.

WEIGHT

```
... WEIGHT real real ...
```

SELECT atoms with crystallographic WEIGHTING factors in the specified range.

Examples:

```
MAIN> write select all end coordinates
```

Selects all atoms and writes their coordinates to the terminal.

```
MAIN> key a select atom name C* N* O* .and. .not.
MAIN> ( main .or. residue -
MAIN>  name A* ) .and. number segment 2 10 end
```

Assigns to key 'a' all atoms, which ATOM NAME starts with C, N or O and are not (the MAIN chain atoms or their RESIDUE NAME doesn't start with an A) and are included in segments with their consecutive numbers from 2 to 10.

```
MAIN> key inhibitor select number segment 4 end
```

Assigns to KEY inhibitor the atoms included in segment number 4.

```
MAIN> key water select symbol residue HOH end
```

Assigns to key water all residues with names HOH

```
MAIN> ... select around key inhib distance 4.5 from water end
```

SELECTS atoms that are closer than 4.5Å to key inhib and belong to key water. (Two solvation shells).

```
MAIN> key bond_to_C  select by bond atom name C* end
```

SELECTS all atoms that are covalently bound to atoms with name starting with C (carbons). When two C* atoms are connected with each other, then they are both SELECTED, since each of them is connected to a C* atom.

SET

```
File set.txt
Last modified: 13-nov-95
```

The SET command sentences are used to SET some values or parameters relevant for atomic records (B_VALUES, WEIGHTS, COLORS, RADII, COORDINATES, SECONDARY - these modules can be entered also from MAIN directly), GEOMETRY relations, they control DIALS assignment and parameters relevant for general MAIN control (VARIABLES, LEVEL, MATRIX, CENTER)...

Syntax

```
SET
    LEVEL       inte
    DIALS .....

    VARIABLE    string   real/inte/string

    MATRIX   int0    INITIALIZE
                     X-AX   real  (in degrees)
                     Y-AX   real
                     Z-AX   real
                     NUMBERED     9 * real
                     * inte
                     \ inte
                     DEORTHOGONAL
                     ORTHOGONAL
                     SYMMETRY inte
                     TRANSPOSE
                     INVERSE
                     COPY
                     RMS
                     POLAR_ANGLES 3*real (psi, phi, kappa) or (phi, psi, kappa)
                     ATOM atom-num atom-num atom-num

     PLANE     ATOM  atom-num1 atom-num2 atom-num3
               NUMBERS 4*real
               SELECT ... END
```

```
          INITIALIZE
          DROP  [inte]

INITIALIZE

RMS   3*real 3*real

CENTER    ATOM          atom-num
          CALCULATE     [SELECT ... END]
          COORDINATES   3*real
          SEQUENCE      string
          POINT         inte

INVERSE/CHANGE   atom-num1 atom-num2

BOND   ATOMS       FORWARD 3*atom-num  BACKWARD
       POINTS

GEOMETRY   DISTANCE       2*atom-num
           ANGLE          3*atom-num
           DIHEDRAL       4*atom-num
           INTERNAL_COOR  4*atom-num
           ALIGN          2*atom-num
           VALUES      real [real real]
           AUTO
           SELECT ... END
```

LEVEL

```
... LEVEL inte
```

Sets the message level (errors, warnings, debugging data). A lower value results in fewer messages and a higher in more. The starting LEVEL value is 0. You can set any number, also only values between -5 and 5 differ in effect.

DIALS

```
... DIALS   inte  TRANSLATION     []
```

```
                X-AX
                Y-AX
                Z-AX
CENTER          ()
                X-AX
                Y-AX
                Z-AX
SCALE
CLIPPING
ROTATION        []
VIEW
SCREEN
STEREO          ANGLE
                XCENTER
COLOR  inte  string
INITIALIZE
CHARACTER
OBJECT  inte    BOND
                ANGLE
                DIHEDRAL
                DISTANCE
                ROTATION
                           X-AX
                           Y-AX
                           Z-AX
                TRANSLATION
                           X-AX
                           Y-AX
                           Z-AX
READ
WRITE
IMAGE_PARAMETERS
DROP
GRAPH     TEXT   string
          OBJECT inte   TRANSLATE   ALL
                                    X-AX
                                    Y-AX
                                    Z-AX
                        SCALE       ALL
                                    X-AX
                                    Y-AX
                                    Z-AX
```

```
                                                CHARACTER
                                                ROTATE      ALL
                                                            X-AX
                                                            Y-AX
                                                            Z-AX
                  FROM inte
```

SETs the DIAL definitions. The DIALS are not set through an IMAGE command sentence to allow the use of a single command word (DIAL) to enter the DIAL-OG mode and to assign functions to DIAL-S. Most dial definitions are governed by the program itself or can be picked from menus when MAIN is in the DIALOG mode. Each DIAL has a label, that tells what is the function of the dial and to which object it is attached (in the case of OBJECT and GRAPH DIALS). Sometimes it is necessary to do DIAL_SAV from menu so as not to lose some dial definitions. Up to 10 different dial sets can be stored and restored. A dial set is a combination of 8 dial functions.

READ

```
... READ
```

It is called using DIAL_RST menu item (dial restore) in DIALOG mode. It READS (restores), the next dial set from the list. So one after another all the saved dial sets can be restored.

WRITE

```
... WRITE
```

It is called using DIAL_SAV menu item (dial save) in DIALOG mode. It WRITES (saves), the current dial set to the list. The dial set is stored as last and the pointer is moved to it. The rule is written last, read first.

DROP

```
... DROP
```

DROPS (forgets) all dial definitions to the consecutive number inte2, that is set by the SET DIAL inte FROM inte2 command. (It sets the list count to inte2. By default this number is equal to 0.) It is called automatically when the current geometry of the active OBJECTS is accepted (OBJ_ACCEP) or rejected (OBJ_REJEC) in DIALOG mode.

FROM

```
... FROM inte2
```

Protects the dial set definitions as saved on the list from deletion, by SETing the lowest value to which the dial set count can be DROPPED. By default it is set to 0, which means none of the dial sets is protected. This command is used for example to protect the Ramachandran plot GRAPH manipulation during a model building session.

TRANSLATION

```
... TRANSLATION     []
                    X-AX
                    Y-AX
                    Z-AX
```

Sets 3 [] or a single DIAL to transfer the translations of the image in X, Y or Z direction. The rotation center of the image remains unchanged and may even move out of the screen.

CENTER

```
... CENTER          []
                    X-AX
                    Y-AX
                    Z-AX
```

Sets 3 [] or a single DIAL to control the translation of the rotation center of the image in X, Y or Z direction. The rotation center remains all the time in the middle of the screen, so the image is shifted. (This is the default.)

SCALE

```
... SCALE
```

Controls SCALING of the IMAGE. The value should be negative for the PSnnn devices, since their coordinate system is left-handed.

CLIPPING

```
... CLIPPING
```

Controls the distance between the two CLIPPING planes. CLIPPING of the image occurs in the Z direction.

ROTATION

```
... ROTATION        []
                    X-AX
                    Y-AX
                    Z-AX
```

Sets 3 [] or a single DIAL to control the rotation of the image around the rotation center in X, Y or Z direction.

VIEW

```
... VIEW
```

Controls distance from the VIEWER eye position to the center of the image. MAIN uses perspective view.

SCREEN

```
... SCREEN
```

Controls the distance between the VIEWER to the imaginary SCREEN on which the image objects are projected. In GL or OpenGL environment this parameter is related to the field of view.

STEREO

```
... STEREO ANGLE
           XCENTER
```

Controls the STEREO ANGLE and separation (XCENTER) of the image rotation centers along the X axes for side by side stereo.

COLOR

```
... COLOR inte  string
```

A dial controls color of an image object. A dial is defined in DIALOG mode by first activating the color mode and then clicking an image object.

INITIALIZE

```
... INITIALIZE
```

Restores the INITIAL definition of the DIALS (X,Y and Z center translations, scaling, X, Y and Z axes rotations and clipping).

CHARACTER

```
... CHARACTER
```

Controls the character size.

OBJECT

```
... OBJECT inte ...
```

The active OBJECTS of MAIN are the SELECTIONS of atoms on which particular functions are activated in order to control the spatial changes of molecules interactively. When an OBJECT is activated from the DIALOG mode the DIALS are assigned to it automatically.

```
... BOND
... ANGLE
... DIHEDRAL
... DISTANCE
... ROTATION []
             X-AX
             Y-AX
             Z-AX
... TRANSLATION []
                X-AX
                Y-AX
                Z-AX
```

The assigned DIAL rotates a BOND, changes an ANGLE, a DIHEDRAL angle, moves along the vector connecting the last twoclicked atoms (DISTANCE). Three DIALS are assigned to ROTATE around all 3 axes or only one DIAL to ROTATE around one (X-AX or Y-AX or Z-AX). Definitions for the TRANSLATION of the OBJECT follow the same rules as the ones for ROTATION.

IMAGE_parameters

```
... IMAGE_parameters
```

SETs the view parameters DIAL set. (1-SCREEN, 2-VIEW, 3-STEREO ANGLE, 4-STEREO XCENTER, 8-CHARACTER scale)

GRAPH

```
... GRAPH ...
```

Controls the GRAPH objects (TEXT - translations inside a GRAPH OBJECT) and a GRAPH OBJECT as a whole. (Its orientation, translation and scaling.)

TEXT

```
... TEXT   string
```

String is a name of an IMAGE object.

OBJECT

```
... OBJECT inte
```

TRANSLATE

```
... TRANSLATE   ALL
                X-AX
                Y-AX
                Z-AX
```

TRANSLATION of a GRAPH OBJECT assigned with ALL, defines 3 DIALS, one for each direction, while the X-AX, Y-AX or Z-AX define 1 DIAL for each separate direction.

SCALE

```
... SCALE       []
                X-AX
                Y-AX
                Z-AX
                ALL
```

SCALING of a GRAPH OBJECT can be coupled (ALL), which means that SCALING in ALL three directions is the same, and is governed with a single DIAL. Each axis can also be scaled independently (X-AX, Y-AX, Z-AX) using one DIAL per axis. With no ([]) explicit specification four DIALS are assigned, one for each of the possible SCALING controls.

CHARACTER

```
... CHARACTER
```

Controls the CHARACTER size of the GRAPH OBJECT. Only works under PHIGS graphics interface (on HP and ESV systems).

ROTATE

```
... ROTATE      ALL
                X-AX
                Y-AX
                Z-AX
```

The ROTATION of a GRAPH OBJECT is controled along each axes (X-AX, Y-AX, Z-AX). If you want to adress rotation about ALL three of them similtaneously use command ALL intstead of three separate dial definition commands.

VARIABLE

```
... VARIABLE string0 = inte/real/string1
```

SETs the VARIABLE string to a value that can be either an integer, a real number or a character string. The program normally recognizes the kind of VARIABLE by itself. Therefore no integer or real numbers should be used for character variable values, however, once a certain variable name is associated with a data type, it can not be modified any more. The variables can be further applied in any command sentence at the place of required input data (integer or real numbers and strings). The only exception is this command sentence, where the string0 is assumed to be the variable name explicitly and not its value. The VARIABLE name string0 can be any string up to 10 characters long. Character variable values can be up to 80 characters long.

BOND

```
... BOND ATOM     FORE atom-num atom-num  atom-num
         POINT    BACK
```

BOND FORE atom-num atom-num transforms the atom coordinates so that the specified BOND is in direction of the X axes and with the origin at the first specified atom. BACK does the opposite transformation. It returns only one level back.

Using two consecutive BOND FORE commands without the BOND BACK command in between, the user can not return to the original coordinate system any more.

MATRIX

```
... MATRIX int0 INITIAL
                X-AX   real  / in degrees
                Y-AX   real
                Z-AX   real
                NUMBERED     9 * real
                * inte
                \ inte
                INVERT
                TRANSPOSE
                DEORTHOGONAL
                ORTHOGONAL
                POLAR_ANGLES phi psi kappa  (or phi psi kappa)
                SYMMETRY inte
                COPY inte
                RMS
                ATOM atom-num atom-num atom-num
```

MATRICES int0 (1 to 8) can be set. MATRIX 1 and 8 are used for the image processing (8 is the stereo pair). MATRIX 6 is the matrix that is used to define a rotation around a single axis (X-AX, Y-AX, Z-AX).

The command

```
MAIN> set mat 3 init x-ax 3. y- 45. z- 90. y- -34. z- 3.45 y- 1890.
```

will result in matrix 3 that is composed of the 6 specified rotations. Matrices can be defined explicitly by NUMBERED input of the 9 consecutive real numbers. MATRICES can be COPIED, INVERTED, TRANSPOSED, multiplied (*), divided (/), INITIALIZED (set to a unit matrix), specified by the POLAR angles or by symmetry operations, or as DE/ORTHOGONALIZATION matrices or calculated from the last RMS fit rotational parameters.

WARNING: Whenever you transfer or interchange matrices between various programs you do always have to check the consistency of matrix definitions. They should be all the same but they are not

INITIAL

Sets all program variables and data to the initial state (ONLY ATOMS AND COVALENT BONDS ARE LEFT). Don't use it unless you are really in trouble because of a bug.

PLANES

```
... PLANES   ATOM  iatom iatom iatom
             NUMBERED  4*real
             SELECT ... END
             INITIALIZE
             DROP  (inte)
```

ATOM creates a plane through the first three SELECTED atoms. NUMBERED requires the normal to the plane (a, b,c) and the d. [$a*X + b*Y + c*Z + d = 0$]

SELECT ... END creates a plane that goes through 3 first atoms in selection. (will be used to calculate the RMS plane)

INITIALIZE the number of planes to 0. 10 is maximum.

DROP (inte) one or more plane from the stack.

- inte .le. 0 : DROPS the last inte planes
- inte .gt. 0 : DROPS the specified plane and fills its place with the last one on the list
- inte not specified : DROPS the last plane from the list

INVERT

```
... INVERT atom-num1 atom-num2
```

Interchanges positions of the two atom chains at a chiral center. (INVERTS the chirality). The chiral center atom is the atom to which both specified atoms (atom-num1 and atom-num2) are attached by a covalent bond. Each atom chain includes all atoms connected via covalent bonds to atoms atom-num1 or atom-num2 apart from the chiral center.

GEOMETRY

```
...  GEOMETRY   DISTANCE     2*atom-num
                ANGLE          3*atom-num
                DIHEDRAL       4*atom-num
                INTERNAL_COOR  4*atom-num
                ALIGN          2*atom-num
                VALUES      real [real real]
                AUTO
                SELECT ... END
```

AUTO

```
... AUTO
```

It is the default option. The desired parameter (DISTANCE or ANGLE) is searched in the forcefield parameter library.

VALEUS

```
... VALUES real [real real]
```

The neccessary number of target values is hereby explicitly defined. One VALUE for BOND, ANGLE, DIHEDRAL and three values for INTERNAL coordinates need to be specified. DISTANCES are in AA and angles in degrees.

SELECT

```
... SELECT ... END
```

By default only the first specified atom is moved, the others are used as reference points only. If you want to move SELECTIONS you have to specify them explicitly.

DISTANCE

```
... DISTANCE     2*atom-num
```

Moves the SELECTION in the direction of the vector going from atom-num1 to atom-num2, for the DISTANCE that is the difference between the specified real and the distance between the atom-num1 and atom-num2. The specified real can also be a negative value. When atom-num1 is a part of the SELECTION the resulting distance between the atoms atom-num1 and atom-num2 is the specified real. When AUTO is chosen instead of an explicitly defined VALUE then the required distance is searched in the list of BOND ENERGY parameters (according to the atom CLASSES).

ANGLE

```
... ANGLE  atom-num1   atom-num2   atom-num3
```

Rotates the SELECTION around the normal to the plane defined by the atoms atom-num1/2/3 and going through atom-num2. The ANGLE of rotation is calculated so that when the atom-num1 is included in the SELECTION, the resulting angle between atoms atom-num1/2/3 is the specified real. When AUTO is chosen instead of an explicitly defined VALUE, the required angle is searched in the list of ANGLE ENERGY parameters (according to the atom CLASSES).

DIHEDRAL

```
... DIHEDRAL atom-num1 atom-num2 atom-num3 atom-num4
```

Rotates the SELECTION around the bond atom-num2 atom-num3. The angle of rotation is calculated so that when the atom-num1 is included in the SELECTION, the resulting DIHEDRAL angle between the atoms atom-num1/2/3/4 becomes equal to the specified real. When AUTO is chosen instead of an explicitly defined VALUE, the required dihedral angle is set to 180°.

INTERNAL_COOR

```
... INTERNAL  atom-num1 atom-num2 atom-num3 atom-num4
```

It combines the translation and rotations of the SET DISTANCE, ANGLE and DIHEDRAL angle into one entity. For description see SET DISTANCE, SET ANGLE and SET DIHEDRAL. Its VALUES parameter however consist of 3 real numbers meaning a distance andgle and dihedral angle.

ALIGN

```
...  ALIGN 2*atom-num
```

ALIGNS two atoms or a SELECTION so that the two appear to each other at the specified (or bond) distance with their attached neighbors at a reasonable geometrical criteria. It as a construction that may not always work.

RMS

```
... RMS 6*real
```

SETs the rotational and translational parameters that are usually obtained via the RMS COORDINATES ALL ... procedure. The first 3 parameters are the rotational angles around the X-axes, Y'-axes and X"-axes and the second 3 parameters are the translational vector.

CENTER

```
...  CENTER    ATOM          atom-num
               CALCULATE     [SELECT ... END]
               COORDINATES   3*real
               SEQUENCE      string
               POINT         inte
```

SETs the CENTER (also IMAGE center) coordinates:

- to the position of an ATOM, specified by its atom-num,
- to the arithmetic mean of the SELECTION,
- to the specified COORDINATES X, Y and Z (3*real),
- to the residue with the SEQUENCE name "string", (the coordinates of the CA atom are chosen. When the residue has no CA atom, then the first atom appearing in the chosen residue),
- to the POINT with the sequential number inte. CENTER coordinates can be SHOWN.

B-VALUES

See under the same keyword directly from MAIN.

TEMPERATURE

See under the same keyword directly from MAIN.

COORDINATES

See under the same keyword directly from MAIN.

RADII

See under the same keyword directly from MAIN.

WEIGHTS

See under the same keyword directly from MAIN.

SECONDARY

See under the same keyword directly from MAIN.

SHOW

SHOW.TEX 14-nov-91

The SHOW command sentence is to be used for interactive control of data (ATOM, BOND, RESIDUE, SEGMENT, SELECTION number, IMAGE parameters ...) and for some data analyses and statistics. Each of the SHOW command group can be continued within the same command sentence by starting a new command group at the end of the previous. Most of the parameters that can be SET can be also SHOWN.

Syntax

```
UNIT int
FILE string

      ALL

      BOX    SELECT ... END
      BOND
      ATOM
      RESIDUE
      SEGMENT

      XCENTER
      YCENTER
      AXCENTER
      AYCENTER
      TEXT
      ALIGHT
      BLIGHT

      VIEW
      SCREEN
      CENTER

      MATRIX

      RATIO
```

```
PLANE  LIST
       ANGLE int int
       DISTANCE atom-num int

POINTS   SURFACE ALL                RESIDUE
                 CONTACT           RANGE  real real
                 REENTRANT          STEP   real
                 ACCESSIBLE

         VOLUME  ALL
                 ATOM
                 ACCESSIBLE

         DENSITY

         POTENTIAL

STEREO_PROJECTION_PARAMETERS

KEY / SELECTION

VARIABLES

TOPOLOGY LIST
         RESIDUE string
                     ATOM string CHARGE CLASS / ALL
                     INTERNAL_COORDINATES
                     ZTABLE_CONNECTIONS
                     VARIABLE_NAMES
                     GROUP_NUMBER
                     BOND
                     DIHEDRAL
                     IMPROPER

PARAMETERS    BOND  string
              ANGLE string
              DIHEDRAL string
              IMPROPER string
              VdW    string

ENERGY
```

```
FORCES         SELECT ... END

DENSITY        SELECT ... END
               RESIDUE

OBJECTS

COLOR SELECT ... END
RADII  SELECT ... END
CHARGE SELECT ... END
CLASS  SELECT ... END
WEIGHT SELECT ... END
TEMPERATURE   SELECT ... END
              RESIDUE
              LIST
              STEP
              RANGE

DISTANCE   atom-num  atom-num
ANGLE atom-num   atom-num   atom-num
DIHEDRAL atom-num   atom-num   atom-num   atom-num
INTERNAL  atom-num   atom-num   atom-num   atom-num
```

UNIT

```
... UNIT int
```

Redirects the SHOW output to the logical UNIT number int.

FILE

```
... FILE string
```

Redirects the SHOW output to the specified FILE.

ALL

```
... ALL
```

SHOWS a variety of parameters.

ATOM

```
... ATOMS
```

SHOWS the number of present ATOMS.

BOX

```
... BOX SELECT ... END
```

SHOWS the BOX limits of the SELECTED atomic coordinates.

RESIDUE

```
... RESIDUE
```

SHOWS the number of present RESIDUES.

SEGMENT

```
... SEGMENT
```

SHOWS the number of present SEGMENTS and lists their names and counts the atoms inside each one.

Projection

```
... VIEW
    SCREEN
    CENTER
```

SHOWS Parameters referring to projection are displayed if required. The parameters are set with an IMAGE command.

RATIO

```
... RATIO
```

SHOWS the VdW ratio for images (acts only the size of the ATOM CROSSES). It can be set with an IMAGE command (IMAGE RATIO real).

PLANES

```
... PLANE  LIST
           ANGLE int int
           DISTANCE atom-num int
```

LISTS currently present planes with their PLANE equations, SHOWS ANGLE between the two specified planes and the DISTANCE of an atom from the plane (int denotes the PLANE number and atom-num an ATOM NUMBER).

POINTS

```
...  POINTS   (SELECT ... END)
               SURFACE ALL                RESIDUE
                       CONTACT           RANGE  real real
                       REENTRANT          STEP   real
                       ACCESSIBLE

               VOLUME  ALL
```

```
                  ATOM
                  ACCESSIBLE

              DENSITY

              POTENTIAL
```

Each point belongs to an atom, so that SELECT statement can be applied. The default SELECTION are ALL atoms.

The 4 kinds of points (SURFACE, VOLUME, map DENSITY, electrostatic POTENTIAL) can be checked and some statistics can be done with their values. The SURFACE points are divided also further in CONTACT, REENTRANT, ACCESSIBLE points and VOLUME points into ATOM and ACCESSIBLE points.

When nothing else is required only the range, sum, average value per point and number of SELECTED atom points are displayed. With RESIDUE, the same data are displayed for each RESIDUE separately and per an averaged ATOM in the residue. With RANGE the points with their values in the specified RANGE are counted. When the STEP is defined, then they are counted for each STEP interval in the specified RANGE.

STEREO

```
... STEREO
```

Shows STEREO projection parameters: angle, separation, status and mode.

CENTER

```
... CENTER
```

SHOWS coordinates of 4 CENTERS. The first one is the current IMAGE center.

MATRIX

```
... MATRIX
```

Shows all (8) 3*3 MATRICES used for rotation transformations.

KEY

```
... KEY / SELECTION
```

Displays the list of KEYED SELECTIONS with the number of atoms included in each one.

SELECTION

```
... KEY / SELECTION
```

Displays the list of KEYED SELECTIONS with the number of atoms included in each one.

VARIABLES

```
... VARIABLES string []
                     NUMBER
```

Displays the list of to the 'string' matching integer, real and character VARIABLES with their values. With no further argument the usual long description is used. With the NUMBER only the variable values without variable names are SHOWN.

TOPOLOGY

```
...   TOPOLOGY LIST
               RESIDUE string1
                           ATOM string2 []
                                        CHARGE
                                        CLASS
                                        COORDINATES
                                        ALL
                           INTERNAL string2
                           ZTABLE string2
                           VARIABLE string2
```

```
                        GROUP string2
                        BOND string2
                        DIHEDRAL string2
                        IMPROPER string2
```

The SHOW TOPOLOGY gives insight into the TOPOLOGY library. With LIST all present RESIDUE names can be listed. With the RESIDUE 'string', only the matching residues are listed. To get the list of ATOMS, INTERNAL coordinates, ZTABLE, BONDS, DIHEDRAL and IMPROPER angles ... of the chosen 'string2' atoms. The ATOM list, can include besides the atom names (without a further argument), also partial atomic CHARGES, atom CLASSES and initial COORDINATES. ALL lists CHARGES, CLASSES and COORDINATES.

PARAMETERS

```
...   PARAMETERS    BOND  string
                    ANGLE string
                    DIHEDRAL string
                    IMPROPER string
```

The SHOW PARAMETER ... lists all force field parameters including the particular atom CLASS.

ENERGY

```
... ENERGY
```

Displays the currently turned on ENERGY terms with the last calculated ENERGIES.

FORCES

```
... FORCES SELECT ... END
```

SHOWS the list of last calculated forces acting on the SELECTED atoms.

DENSITY

```
...   DENSITY       SELECT ... END
                    RESIDUES
```

Calculates the DENSITY energy of the SELECTION. With RESIDUES, it prepares a list of the density energy for each SELECTED RESIDUE and calculates an averaged atom contribution to it. With different weighting factors and density energy options several lists can be prepared (see MAIN$EXA:[DENSITY]).

OBJECTS

```
... OBJECTS
```

Shows the list of the current active OBJECTS with their definitions and their values.

COLOR

```
... COLOR         SELECT ... END
```

Lists COLORS of the SELECTED atoms.

CHARGE

```
... CHARGE        SELECT ... END
```

Lists partial atomic CHARGES of the SELECTED atoms.

CLASS

```
... CLASS         SELECT ... END
```

Lists CLASS of the SELECTED atoms.

RADII

```
... RADII         SELECT ... END
```

Lists atomic RADII of the SELECTED atoms.

WEIGHT

```
... WEIGHT        SELECT ... END
```

Lists crystallographic WEIGHTS of the SELECTED atoms.

TEMPERATURE

```
... TEMPERATURE   SELECT ... END []
                                 LIST
                                 RESIDUE
                                 RANGE  real real
                                 STEP real
```

With no argument [] calculates the average TEMPERATURE factor of the SELECTION. With the LIST writes the list of temperature factors. Per RESIDUE calculates average temperature factor for each RESIDUE and with the RANGE and STEPS it counts all atoms that are in the specified RANGE for each STEP size separately.

DISTANCE

```
... DISTANCE  2*atom-num
```

SHOWS the DISTANCE between the 2 atoms in Angstroems.

ANGLE

```
... ANGLE  3*atom-num
```

SHOWS the ANGLE defined by the 3 specified atoms in degrees.

DIHEDRAL

```
... DIHEDRAL 4*atom-num
```

SHOWS the DIHEDRAL angle defined by the 4 atoms in degrees.

INTERNAL

```
... INTERNAL 4*atom-num
```

SHOWS INTERNAL coordinates as defined by the 4 atoms (DISTANCE, ANGLE and DIHEDRAL angle).

Examples

```
MAIN> show all
MAIN> show bond
MAIN> show color select symbol atom C* .and. number residue 1  5 end
MAIN> show topology residue GL%% atom C* internal ztable
MAIN> show internal 3 \4 100 6789
MAIN> show selections
```

SYMMETRY

SYMMET.TEX 4-JUL-1990

SYMMETRY applies crystal SYMMETRY operations on given SELECTIONS of atoms. The cell constants and symmetry operations in the form of international tables or from a density map should be read before. Each additional SYMMETRY operation applied results in a new segment which name begins with '#'.

Syntax

```
SYMMETRY     SELECT  ... END
             NEIGHBOUR  inte
             RESIDUE
             DISTANCE  real (15.0)
             CUT     real
             MATRIX inte
             TRANSLATION inte inte inte
             CELL
             AROUND   SELECT ... END
                      CENTER *
             DELETE ON / TRUE
                    OFF / FALSE
```

SELECT

```
... SELECT ... END ...
```

CELL

```
... CELL ...
```

CELL applies each SYMMETRY operation only once. The atomic coordinates are afterwards converted so, that they are placed into 1 cell only. (Their fractional coordinates can only have values between 0.0 and 1.0.) However, the resulting coordinates are, as by other options, in cartesian coordinate system.

NEIGHBOUR

```
... NEIGHBOUR inte
```

NEIGHBOUR integer specifies how many neighbour layers (inte) of molecules should be created from each crystal symmetry molecule. Each molecule is translated for inte times for a cell length in the crystal lattice in all 6 directions. All together 26 additional structures are created when integer is 1. Do not use more than 1 for proteins unless you really know what you are doing.

RESIDUE

```
... RESIDUE
```

The RESIDUE command word turns a flag, that disables copying of RESIDUE structure into the newly created SEGMENT, so that each newly created segment is a single RESIDUE only. It should be used for crystal packing studies, otherwise the residue number goes quickly over the array boundaries.

DISTANCE

```
... DISTANCE real
```

The 'DISTANCE real' specifies how close should some the box inside which by symmetry operations generated molecules comes to the AROUND boundaries. When CUT is turned on, then the DISTANCE is explicitly checked for each particular atom. The default value is 15.0Å.

CUT

```
... CUT real
```

CUT is a flag, that enables the DISTANCE checking of each particular atom. Each generated atom should be closer than the specified DISTANCE AROUND the CENTER or any atom in the AROUND SELECTION.

MATRIX

```
... MATRIX inte
```

Applies only the specified crystal rotation MATRIX.

TRANSLATE

```
... TRANSLATE inte inte inte
```

Applies beside the crystal symmetry operation explicitly only the specified TRANSLATION. The NEIGHBOUR option is DISABLED.

AROUND

```
... AROUND  SELECT ... END
... CENTER  *   (see syntax at image center)
```

Creates symmetry related atoms from the first SELECTION around the AROUND SELECTION of atoms.

Specifies the CENTER around which symmetry related atoms will be generated.

The CENTER option defers from the SELECT option since it automaticaly assumes the CUT and DELETE ON option. It is also computationally faster, however it can not generate atoms AROUND a nonspherical shape. The CENTER option is supposed to be used during an interactive model building session. The RESIDUE information can not be suppressed as well.

DELETE

```
...  DELETE ON
            OFF
```

DELETES when the DELETE flag is ON or TRUE, the symmetry related atoms generated by the identity crystal symmetry operation (X,Y,Z) with no additional translation. When the DELETE flag is OFF or FALSE, the atoms are not deleted. OFF is the default. It should be used for generation of symmetry environment while building the residues in to the electron density.

EXAMPLES

```
MAIN> symmetry select all end neigh 1 around select sequence 57 end -
MAIN> distance 20. cut delete on
```

```
MAIN> key old select all end
MAIN> symmetry select numb segment 1 end neigh 1 around select napa end -
MAIN> distance 20. cut delete on
MAIN> key sym1 select .not old end
MAIN> key old select all end
MAIN> symmetry select numb segment 2 end neigh 1 around select napa end -
MAIN> distance 20. cut delete on
MAIN> key sym2 select .not old end
MAIN> key old select all end
MAIN> symmetry select numb segment 3 end neigh 1 around select napa end -
MAIN> distance 20. cut delete on
MAIN> key sym3 select .not old end
MAIN> key old select all end
```

```
MAIN> symmetry select ca end neigh 1 around select ca end -
MAIN> distance 50.0 residue
```

TEMPERATURE

```
TEMP.TEX     21-nov-91
```

```
Syntax
TEMPERATURE
            SELECT ... END real
            EXIT
```

Sets the TEMPERATURE factors to the SELECTED atoms.

The command sentence:

```
MAIN> TEMPERATURE SELECT ALL END 20.0
```

remains in 'MAIN>', while the command sentence:

```
MAIN> TEMPERATURE
```

enters the 'TEMP>' module. EXIT should be used to return back to MAIN>.

TOPOLOGY

```
TOP.TXT        11-DEC-1991


Syntax
TOPOLOGY INITIALIZE
         APPEND  SELECT ... END
                 XPLOR
```

The TOPOLOGY command sentence INITIALIZES the topology library (sets the number of TOPOLOGY residues to 0) or APPENDS new reasidues to already existing ones. If the name of the APPENDING residue matches with the last one in the library then the last one is replaced by the new one.

The newly created TOPOLOGY library residue(s) contain(s) the complete residue description (ATOM NAME, CLASS, partial atomic CHARGE, cartesian (shifted to origin) and INTERNAL COORDINATES, the covalent BOND, DIHEDRAL and IMPROPER angle lists). The required information is extracted form the availabe data attached to the SELECTED residues. More than one residue can be APPENDED with a single TOPOLOGY APPEND sentence.

The XPLOR turns on the XPLOR mode, so that the created residues in the topology library will have no terms (BOND, DIHEDRALS, IMPROPERS) relating to the previous residue in the sequence. By default, the XPLOR mode is turned off, so that ATOM NAMES from the previous residue are preceeded by a hyphen '-'.

TRANSLATE

`TRANSL.TEX     19-OCT-91`

TRANSLATE command sentence moves atom or point selection by the specified vector.

Syntax

TRANSLATE

```
ATOMS
POINTS    SURFACE
          VOLUME
          POTENTIAL
          DENSITY


SELECT ... END


VECTOR    3*real   DISTANCE (abs(3*real))
                             real
RMS


CENTER
```

ATOM

TRANSLATES selected atoms by adding the specified vector. This is the default, it just makes the syntax easier to understand.

POINTS

TRANSLATES the specified kind of points of selected atoms.

VECTOR

The translational vector must be specified by its X Y and Z components. When the DISTANCE is specified than the specified vector is normalized to length 1.0 and each component is multiplied by the specified distance.

RMS

The translational vector is taken from the last RMS fit calculation.

CENTER

The translational vector is calculated from the current image center and the center (arithmetic middle) of the selected coordinates. The selected atoms are translated into the center of the image.

Examples

```
MAIN> translate atom select all end vector 10.0 15. 3. distance 1.0
```

```
MAIN> translate select segment number 1 end vector 10.0 15. 3.
```

```
MAIN> translate atom select all end rms
```

```
MAIN> translate atom select all end center
```

```
MAIN> translate points density select all end vect 10. 0. 3.
```

VLTSET.TXT 4-NOV-87

Purpose: Within Video_Lookup_Table interpreter colours can be defined according to red green and blue real values. 4 different VLT‘s can be loaded into the program. For plotters or monochrome displays is this modul without any sense.

SYNTAX:

BACK inte

CHANGE RED inte inte RED inte GREEN inte inte .... BLUE inte inte ...... COLO inte inte ......

COLOR inte1 inte2 inte3 RED inte4 inte5 GREEN BLUE

COPY inte inte

ERASE

FIRST inte

INITIALIZE

EXIT

MODUL inte

MOVE RED inte inte red inte GREEN inte inte .... BLUE inte inte ...... COLO inte inte ......

RANGE inte inte

SCROLL inte inte

SHOW

VLT int

DESCRIPTION common: Values for colour tables are stored in the 3 field array (VLT,i, RGB).

BACK Defines the background colour. (ussually 0) It is not possible for all terminals.

CHANGE Changes two specified RGB colour in current VLT.

COLOR Sets colour values into the current vlt from inte1 to inte2 by step of colour increas inte. A red gren or blue value of colour inte4 is stored. Inte5 is the step for encreasing the colour value. The colour value is module of maxcol value and current inte4 + n* inte5.

COPY inte inte Copies form first vlt to second.

ERASE Erases the shown colour table rectangle. Fills it with bacground colour.

FIRST The first colour the first line in shown colour table to start.

INITIALIZE Copies the values from the first VLT to the current one.

MODUL inte The length of line in the shown colour table.

MOVE red 16 31 gre 128 Moves one colour into another (RGB) in the current vlt.

RANGE Specifies the minimum and maximim colour addres. 0 255 for tektronix 4115, 0 3 for VISUAL 240 0 15 for TRIGLAV ... SCROLL Rolles the lines of coloure numbers beginning with the first and second integer for the third integer times. Takes the first (top line) and rolls the rest for one line higher and puts the first into the last. Leng of line is current modul.

SHOW Shows an reactangle with terminal current coloures in small rectangles. The number of small reactangles is defined with the modul command. Because small rectangles are of the same size, changing modul valuse affects the general shape of rectangle area where small rectangless are displayed.

VLT Sets the new current vlt. (one of 4 possibilities).

Examples: color 0 255 red 255 -1 gre 0 1 blu 128 change red 16 31 blu 80 move red 16 31 gre 128 range 0 255 scrol 16 128 5 show vlt 3

WEIGHT

```
WEIGHT.TEX     11-dec-1991
```

```
Syntax
WEIGHT
            SELECT ... END * real
            EXIT
```

Sets the crystallographic WEIGHT factors to the SELECTED atoms.

The comand sentence:

```
MAIN> WEIGHT SELECT ... END 1.0
```

remains in MAIN>, while the:

```
MAIN> WEIGHT
```

enters the WEIGHT> module. EXIT should be used to return back to MAIN>.

WRITE

```
WRITE.TEX           19-nov-91
```

The WRITE sentence is used to write data to files or to the terminal. First the FILE or FORTRAN logical UNIT should be specified, then the SELECTION and after that the write object specification (COORDINATES, BONDS, INTERNAL, MAP), format (PDB, DIAMOND ...) and units (ANGSTROM, ATOMIC, NANOMETERS). The FILE, UNIT and SELECT are optional. When the FILE or UNIT are omitted the output comes to the terminal (SYS$OUTOUT). The default SELECTION are all atoms and the default length UNIT is ANGSTROM.

Syntax

```
WRITE UNIT int
      FILE string
      OVER
      APPEND
      SELECT ... END
      ATOM
      NANOMETER
      NUMBER   (inte)
      NAMES

            COORDINATES      NORMAL
                             CARD
                             PDB
                             XPLOR
                             DIAMOND
                             DISCOVER
                             GROMOS
                             GAUSSIAN
            BOND    []
                    NUMBER
            CTABLE  []
                    NUMBER
            HBOND
            PAIR   []
                   NUMBER
```

```
       RAMACHANDRAN
ZTABLE
INTERNAL  (GAUSSIAN)  VARIABLES
           AMPAC

POINT SURFACE   ALL             (CONNOLY)
                REENTRANT       GAUSSIAN
                ACCESSIBLE      G80
      VOLUME    ALL
                ATOM
                ACCESSIBLE
      POTENTIAL
      DENSITY

MAP inte   NUMBER
           CHARACTER
           ALPHA
           FFT
           XPLOR

SYMMETRY

CELL
```

UNIT

`WRITE UNIT inte ...`

WRITES the selected data to the FORTRAN logical UNIT number inte.

FILE

`WRITE FILE string ...`

WRITES the selected data to the FILE string.

APPEND

```
... APPEND
```

Using APPEND it is possible to APPEND information to the end of an already existing file.

OVER

```
... OVER
```

Using OVER it is possible to overwrite an already existing file.

SELECT

```
... SELECT ... END
```

When data related to atoms are WRITTEN a SELECTION can be applied. The SELECT ... END sentence should proceed the command word that specifies the kind of data. The default SELECTION are all atoms.

Units

```
... []
    ATOMIC
    NANOMETER
```

The default length units are Angstroems. When COORDINATES are to be written in NANOMETERS and ATOM units, then the units should be explicitly specified.

NUMBER

```
... NUMBER   (inte)
```

The NUMBER flag is the opposite of the NAMES flag. In common it means that the data are less descriptive and that NAMES are replaced by NUMBERS. In any case, the NAMES or NUMBER specifier must follow the write object specification. The meaning of NUMBER or NAMES has different meanings:

by COORDINATES:

- NORMAL or GAUSSIAN format writes the atomic numbers for the periodic system (this is the default).
- PDB and XPLOR format replaces the SEQUENCE information by the consecutive residue number. A value could however start at the specified 'inte' and then rise by 1 for each next residue.

by BONDS, PAIRS:

This is actually a format to write only the bond list containing only the atomic NUMBERS.

by CTABLE, ZTABLE:

Writes atomic NUMBERS of the reference atoms.

by MAP:

It is the real*4 MAIN MAP format.

NAMES

`... NAMES`

The NAMES flag, is the opposite of the NUMBER flag and has a bit ambiguous meaning. In common it means that the description is more complete and that NUMBERS are replaced by NAMES. In any case, the NAMES or NUMBER specifier must follow the write object specification.

by COORDINATES:

- NORMAL or GAUSSIAN format writes the atom names
- PDB and XPLOR format writes the SEQUENCE names (this is the default).

by BONDS, PAIRS: This is the default form.

by CTABLE, ZTABLE: Writes atomic numbers of the reference atoms.

by MAP: It is the real*4 MAIN MAP format.

COORDINATES

See WRITE ATOMS.

ATOMS

```
... ATOMS  PLAIN
           CARD
           PDB
           XPLOR
           DIAMOND
           DISCOVER
           GROMOS
           GAUSSIAN
           ATOM
           NANOMETER
           NUMBER   inte
           NAMES
```

The length units applied are Angstroems (default for all formats except for GROMOS, where nanometers are used), NANOMETERS and ATOM units. The following formats are available: NORMAL, CARD, PDB, XPLOR, DIAMOND, DISCOVER, GROMOS, GAUSSIAN. The NUMBER and NAMES flag effect only PDB and XPLOR format. The ATOM and NANOMETER units could be applied anywhere.

SCATTERI

Write SCATTERING factors tells you which atomic numbers have their scattering factors defined and what are their Gaussian coeficient values.

ELEMENTS

Writes ATOMIC NUMBERS with ELEMENT IDS. The rule, what is written can be also READ is obeyed.

INTERNAL

```
... INTERNAL  (GAUSSIAN)  VARIABLES
       AMPAC
```

INTERNAL coordinates can be written with VARIABLE names and values too. VARIABLES are used by GAUSSIAN geometry optimization. The default format is the GAUSSIAN.

ZTABLE

```
... ZTABLE
```

WRITES the ZTABLE list either with atomic NUMBERS or names (NAMES).

BONDS

```
... BOND    []
            NUMBER
```

WRITES the BOND list. The default format is NAMES. The outout contains atom, residue, sequence and segment name of each atom included in the covalent bond and its length. When NUMBER is specified, then the BOND list contains only atomic numbers.

CTABLE

```
WRITE       CTABLE  NAMES
                    NUMBER
```

WRITES the connectivity table. The CTABLE contains the complete set of each atom names (atom, residue, sequence and segment NAMES) and its neighbours. The neighbours are written with their atom NUMBER or atom NAMES.

HBONDS

```
WRITE       HBOND
```

WRITES the hydrogen bond (HBOND) list. The list contains the atom, residue, sequence and segment name of each atom included in the hydrogen bond list, its length and angle. Angle is written only when hydrogen atoms are present.

PAIRS

```
WRITE       PAIR   NAMES
                   NUMBER
                   RAMACHANDRAN
```

WRITES the PAIR list. NAMES is the default format. The outout contains atom, residue, sequence and segment name of both PAIRED atoms, the interatomic distance and when the equilibrium distance and force constant are DEFINED also these. With the NUMBER format only atomic NUMBERS are written.

When the PAIR list is defined as the RAMACHANDARN PAIR list then the PHI and PSI angles for each residue are written.

POINTS

```
... POINT SURFACE ALL    (CONNOLY)
                  REENTRANT       GAUSSIAN
                  ACCESSIBLE      G80
          VOLUME ALL
                 ATOM
                 ACCESSIBLE
          POTENTIAL
          DENSITY
```

Points can be chosen according to their kind (SURFACE, VOLUME, DENSITY, POTENTIAL) written in 3 different formats (CONNOLY, GAUSSIAN86, G80). SURFACE and VOLUME points can be also further divided into (REENTRANT, ACCESSIBLE and ATOM, ACCESSIBLE) GAUSSIAN and G80 formats only write point coordinates. G80 is in atom units. So that appropriate programs can read them. Units and NAMES/NUMBER flag have no effect. The CONNOLY format is in Angstroems and the G80 format is in ATOM units.

MAP

```
WRITE MAP inte   NUMBER
                 CHARACTER
                 ALPHA
                 FFT
                 XPLOR
```

The 'inte' tells which MAP to write and is required. When no format is specified the character*1 maps are written with the CHARACTER format and the real*4 maps with the NUMBER format. MAP can be written in 5 different formats (NUMBER, CHARACTER, ALPHA, FFT and XPLOR). The NUMBER, CHARACTER and ALPHA are MAIN formats, while the FFT format is unformatted and is the input for the FFT calculation using P1SF (Lyn Ten Eyck program) or PROTEIN and the XPLOR map is a formatted text file.

SYMMETRY

```
... SYMMETRY
```

WRITES the crystal SYMMETRY operations (matrices and translation vector).

CELL

```
... CELL
```

WRITES the crystal CELL constants.

Examples

```
MAIN> write unit 3 select atom name CA end coordinates pdb
```

```
MAIN> write file int_coor.dat internal variable -
MAIN> first select number residue 2 end
```

```
MAIN> write select pro end point surface accessible
```

```
MAIN> write file cell.fft map 2 fft
```