myPresto 4.2

- cosgene "ANALYSIS" -

USER MANUAL

Version 1.0

About this document

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ACKNOWLEDGEMENT:

The research and development of this software was supported by grants from New Energy and Industrial Technology Development Organization (NEDO) and Ministry of Economy, Trade and Industry (METI), JAPAN.

This software has been developed by the research project promoted by the late Dr. Yoshimasa Kyogoku.

Contents

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1 Overview of cosgene "ANALYSIS"

Cosgene includes the function "ANALYSIS" to analyze energy trajectory file and coordinate trajectory file of MIN and MD.

1.1 Execution

Molecular information such as reference coordinate, topology file and calculation conditions, etc is specified by the control file as the MIN/MD calculation (Later, see the chapter "cosgene" in the user manual)

```
% cosgene < control_file > output
```

1.2 Input data creation

1.2.1 Control file

A control file is comprised of the following groups. Each group is terminated with "QUIT".

- **EXE> INPUTgroup** : The "EXE>INPUT" group designates the primary input file names.
- **EXE> ANAlysisgroup** : The "EXE>ANAlysis" group designates the options of group trajectory analysis.
- **EXE> OUTPUTgroup** : The **"EXE>OUTPUT"** group designates output for final results.
- **EXE> END** : **"EXE>END"** indicates the end of the control file.

```
    EXE> INPUT
         TOPOLOGY=   FORM     NAMETO=    initial.tpl   ; Topology file
         COORDINA=   PDB      NAMECO=    initial.pdb   ; PDB file
         REFCOORD=   PDB      NAMERE=    initial.pdb   ; Reference coordinates
         QUIT
    EXE> ANALYS
         METHOD=     MD
         NAMETR=     traject.cor      ; Coordinate trajectory file for MD calculation
         DATATY=     COR4             ; Designates the types of trajectory files
         LOGFOR=     DETAIL           ; Designates standard output
         INTERV=     1                ; Analysis step interval
         STARTT=     0.0              ; Analysis start time (PSEC)
         ENDTIM=     20.0             ; Analysis end time (PSEC)
         UNITBS=     61               ; I/O unit number of NAMEBS
         NAMEBS=      setbst_1.bst     ; Atom designation used for superimposing coordinates
BESTFI=     YES              ; Superimposes coordinates.
         FLUCTU=     YES              ; Calculates fluctuation.
         NAMEPL=     rmsd_plot.data   ; Plot data of RMSD.
         QUIT
    EXE> OUTPUT
         COORDINATE=  PDB     NAMECO=    mean.pdb   ; Average structure to output.
         QUIT
    EXE> END
```

Example of control files in the case of trajectory analysis

1.2.1.1 EXE> INPUT group

As the MIN/MD calculation, The INPUT group designates external files like the topology, initial coordinates, and files designating atoms to be restrained or monitored (Refer to A Input/Output file at the end of the user manual). ANALISIS can perform the following designations.

Items designated in the INPUT group :

(1) Designation of topology of system
(2) Designation of coordinates of system
(3) Designation of fixed atoms and free atoms
(4) Designation of CAP potential
(5) Designation for RMSD calculation
(6) Designation of position restraint
(7) Designation of restraint distance between atoms
(8) Designation of dihedral angle restraint
(9) QUIT

(1) Designation of topology of system

```
TOPOLOgy : Format of topology file (◎)
    =NOREad        ; No topology file input (Default)
    =FORMAtted     ; Formatted ASCII file
    =BINAry        ; Binary file
UNITTOpology : IO unit of topology file (△)
    =10            ; (Default)
NAMETOpology=(Topology name, 80 chars. max. When TOPOLOgy=[FORMIBINA])
```

(2) Designation of coordinates of system

```
COORDInate: Format of 3-dimensional coordinate file in PDB format (◎)
    =NOREad        ; No coordinate input (Default)
    =PDB           ; PDB file format
    =BINAry        ; Binary file
UNITCOordiante : UNITCOordinate: IO unit of coordinate file (△)
    =11            ; (Default)
NAMECOordinate=(Coordinate file name, 80 chars. max. When COORD=[PDBIBINA])
```

(3) Designation of fixed atoms and free atoms

With fixed atom designation, the designated atom is not subject to MIN/MD calculation, and is handled as a point where a force field is applied. Free atoms are those atoms subject to the normal MIN/MD calculation. You can designate the nos.

of atoms to be fixed, or designate radii R1 and R2 relative to a specific center, or designate atoms so the distance R from the center satisfies R1 < R < R2. A control file is necessary to do this. Free atom designation is done in the same way. If no designation is made, all atoms in the system are handled as free atoms.

```
SETVARiables=:Format of fixed/free atom designation file (△)
    =NOREad  ; No fixed atom designation (Default)
    =READ    ; Designate fixed atoms
UNITVAribles : IO unit of fixed atom designation file (△)
    =13      ; (Default)
NAMEVAriables =(Name of file designating fixed atoms, 80 chars. max.).)
```

(4) Designation of CAP potentialAP

This designates the atoms to which CAP potential is applied, coordinates of the CAP center, and constants for radius and force. You can designate atoms in the CAP designation file, and information like center coordinates can be designated either in the CAP designation file, or in the control file. However, control file input will take priority.

```
SETBOUndary : Designates atoms for applying CAP potential, and CAP radius and force
              constants (○)
    =NOREad         ; Do not use CAP
    =READ           ; Use CAP
UNITBOundary : IO unit of CAP designation file (△)
    =14             ; (Default)
NAMEBOundary=(Name of CAP designation file, 80 chars. max. (○) )
```

(5) Designation for RMSD calculation (when using MIN or MD)

```
REFCOOrdinate : Reference file. The coordinate file in PDB format which serves as the basis.
    =NOREad       ; Do not use (Default)
    =PDB          ; Use
UNITREfcoordi : IO unit of reference file (△)
    =15           ; (Default)
NAMEREFcoordi=(Reference file name, 80 chars. max.)
```

(6) Designation of position restrain

You must prepare the following two files in order to use position restraint.

- A restraint designation file which designates the atoms to be restrained and information about the force constant
- Reference file in PDB format listing coordinates to be restrained

REFCOOrdinate : Reference file, same as for RMSD (○)
=NOREad ; Do not use (Default)
=PDB ; Use
UNITREfcoordi : IO Unit of reference file (△)
=15 ; Default
NAMEREFcoordi=(Reference file name, 80 chars. max. (○))
POSITIonrestrain : Designation of applicable atoms and force constant etc. (○)
=NOREad ; Do not use (Default)
=READ ; Use
UNITPOsition : IO unit of file designating atoms to be constrained
=16 ; (Default) (△)
NAMEPOsition=(Name of file designating atoms to be constrained, 80 chars. max. (○)

(7) Designation of restraint distance between atoms

Prepare a file designating the distance restraint between atoms.

DISTANcerestrain : Use restraint distance between atoms
=NOREad ; Do not apply (Default)
=READ ; Apply
UNITDIstance : IO unit of distance designation file
=17 ; (Default) (△)
NAMEDIstance=(Name of file for designating distance between atoms, 80 chars. max.)

(8) Designation of dihedral angle restraints

DIHEDRalrestrain : Use dihedral angle restraints
=NOREad ; Do not apply (Default)
=READ ; Apply
UNITDH : IO unit of dihedral angle restraint designation file
=18 ; (Default) (△)
NAMEDH=(Name of dihedral angle restraint designation file, 80 chars. max.)

(9) QUIT

Indicates end of EXE> group input.

1.2.1.2 EXE> ANAlysis group

Here, you designate the method, convergence conditions, calculation result output, energy terms used in calculation, and the boundary/restraint conditions which are needed for energy minimization.

Almost all designations relating to energy calculation are the same as those for the EXE>MD group.

(1) Analysis method

(1－1) Method to analyze a single structure

It analyzes the coordinate file designated by the INPUTgroup.

VIOLATioncheck :Test the abnormalgene-associated length, abnormal binding angle and van der Waals contact.

=NO ; (Default)

=YES

FORCEAnalysis : Output the force applied to each atom in the atom data file. It is required to designate the energy parameter as MIN/MD. FMM/PME is not supported.

=NO ; (Default)

=YES

ELECTRostatic :Calculate 1-5 electrostatic interaction applied to each atom and output to the atom data file.

A dielectric constant must be designated.

=NO ; (Default)

=YES

【Caution】 Prepare a trajectory file that is empty now. It is required to perform an input designation "NAMETR" of trajectory file (after-mentioned) formally. .

(1－2) A method to analyze a trajectory file

ENERGYtrajectory :Calculate the energy trajectory and calculate and output the average and standard deviation in the plot-data file.

=NO ; (Default)

=YES

DISTANceanalysis :This calculates a trajectory of an atomic distance from a trajectory file of coordinate and outputs to a plot-data file. It is required

to load a control file of a distance restraint.
=NO ; (Default)
=YES

DIHEDRalanalysis : This calculates a dihedral angle trajectory from a trajectory file of coordinates. It is required to load a control file of a dihedral angle restraint.
=NO ; (Default)
=YES

FLUCTUation : This calculates a fluctuation of an average structure, RMSD and coordinates from a coordinate trajectory file and outputs it to a plot-data file. An average structure is output in the OUTPUT section.
=NO ; (Default)
=YES

(2) Calculation result output designation

LOGFORmat : Format of standard input (△)
=SHORt ; Simple output within 80 chars. in 1 line (Default)
=DETAil ; Detailed output within 80 chars. in 1 line. Add each energy.

(3) Structure superimposing calculation designation

BESTFIt : This superimposess the 1st chain of the system relative to the reference structure or atoms designated by a coordinate superimposing designation file. This is designated when fluctuation of average structure, coordinate or RMSD is calculated (FLUCTUation=YES) .
=NO ; Do not calculate. (Default)
=YES ; Calculate.

【Caution】 For the reference structure, you must designate "REFCOORD" and "NAMERE" in the EXE>INPUT phase. (△)

(4) Analysis data input

(4－1) Trajectory file

NAMETR = (Name of a trajectory file)

UNITRA : IO Unit of a trajectory file
=60 ; (Default)
DATATYpe = (Types of trajectory file)
= ENER ; Energy trajectory file (Default)
= COR4 ; Single-precision coordinate trajectory file
= COR8 ; Double-precision coordinate trajectory file

(4－2) Coordinate superimposing designation file

When calculating an average structure, fluctuation of coordinates or RMSD, (FLUCTUation=YES) , this designate atoms used by superimposing coordinates to the reference coordinates.

NAMEBS = (Name of an atom name designation file)
UNITBS : IO Unit of atom name designation file
=0 ; (Default)

【Caution】 If "UNITBS" is 0 or a negative number, a file designated by "NAMEBS"is not loaded and, all atoms of the 1st chain the 1st chain are used. If a positive number (=61) is designated, thefile is loaded and atoms of multiple chains can be designated. However, a designated atom must include an atom of the 1st chain.

(5) Analysis data output

NAMEPL = (Name of a plot data file)
UNITPL : IO Unit of a plot data file
=62 ; (Default)

NAMEAT = (Name of an atom data file)
UNITAT : IO Unit of atom data file
=63 ; (Default)

(6) Designation of energy trajectory calculation

METHOD : This designates types of energy trajectory.
= MINI ; Energy trajectory analysis of the result of minimization (Default)
= MD ; Energy trajectory analysis of MD result

The following is enabled only when METHOD=MINI.

STARTLoop : Loop number to start an analysis
=0 ; (Default)

ENDLOOp : Loop number to end an analysis
=10000 ; (Default)

The following is enabled only when METHOD=MD.

INTERVal : Step interval to perform an analysis
=1 ; (Default)

STARTTime : Time to start an analysis (PSEC)
=0 ; (Default)

ENDTIMe : Time to end an analysis (PSEC)
=10000 ; (Default)

(7) Control parameter for "FORCEAnalysis=YES"

Designate the same parameter as generating trajectory.

(7－1) Interaction CUTOFF method

CUTMEThod : Interaction CUTOFF method
=RESC ; Residue base cutoff (Default)
Calculates the interactions between all atoms included in residues if the distance between the residue centers of mass is at or below the CUTOFF distance.
=ATOM ; Atom base cutoff
Calculates the interactions between atoms if the distance between the atom centers of mass is less than the CUTOFF distance.
=RESA ; Residue base cutoff
Calculates interaction between all atoms included in residues if the minimum distance between two atoms of a residue is less than the CUTOFF distance.

CUTLENgth : Cutoff length (Å)
=8.0 ; (Default)

DIEFUNction : Format of relative dielectric function in space
=CONS ; Dielectric function is constant (Default)
=DIST ; Dielectric constant is proportional to the distance. ε=DIEVAL*Distance (Å)

DIEVALue : Dielectric constant of space
=1.0 ; (Default)

(7－2) Interaction calculation switch

Use the following switch to calculate (or not calculate) a specific interaction.

(7－2－1) 1-2, 1-3 and 1-4 interaction switches

All default values are used in ordinary MIN/MD calculation. Although it is extremely rare, this is used only when you do not wish to calculate a certain interaction.

CALBONd : 1-2 interaction calculation
=CALC ; Calculate (Default)
=NOCAlc ; Do not calculate
CALANGle : 1-3 interaction calculation
=CALC ; Calculate (Default)
=NOCAlc ; Do not calculate
CALTORsion : Torsion interaction calculation
=CALC ; Calculate (Default)
=NOCAlc ; Do not calculate
CALIMProper : Improper torsion calculation
=CALC ; Calculate (Default)
=NOCAlc ; Do not calculate
CALV14 : 1-4 van der Waals calculation
=CALC ; Calculate (Default)
=NOCAlc ; Do not calculate
CALE14 : 1-4 electrostatic interaction calculation
=CALC ; Calculate (Default)
=NOCAlc ; Do not calculate

(7－2－2) 1-5 interaction switch

This changes the switch designation when calculating using CUTOFF (calculation using an interaction table), and when calculating all 1-5 interactions for all atoms without using CUTOFF (direct calculation). The default setting is to use CUTOFF. Normally (default), all of the following are calculated: van der Waals, 1-5 electrostatic interaction, and hydrogen bonding. Although it is extremely rare, please use this only when you do not wish to calculate a certain interaction. If you use a force field which does not include hydrogen bonds (12-10 Potential), hydrogen bonds are not calculated, regardless of the value of the switch CALHYD.

When using an interaction table (using CUTOFF)

The following CALV15, CLAE15 and CALHYD are set to =CALC, and CALV5N, CALE5N and CALH5N are set to =NOCALC. (Default)

CALV15 : 1-5 van der Waals
=CALC ; Calculate(Default)
=NOCAlc ; Do not calculate
CALE15 : 1-5 electrostatic interaction calculation
=CALC ; Calculate(Default) ※Mandatory with *PME/FMM
=NOCAlc ; Do not calculate
CALHYD : Hydrogen bonds
=CALC ; Calculate(Default)
=NOCAlc ; Do not calculate

When not using an interaction table

The above CALV15, CLAE15 and CALHYD are set to =NOCALC, and CALV5N, CALE5N and CALH5N are set to =CALC.

CALV5N : 1-5 van der Waals
=NOCAlc ; Do not directly calculate 1-5 van der Waals (Default)
=CALC ; Calculate
CALE5N : 1-5 electrostatic interaction
=NOCAlc ; Do not directly calculate 1-5 electrostatic interaction (Default)
=CALC ; Calculate
CALH5N : Hydrogen bonds
=NOCAlc ; Do not directly calculate hydrogen bonds (Default)
=CALC ; Calculate

(7－2－3) Restraint potential

Restraint potential settings are all set to NOCALC (no calculation) by default.

Please set the corresponding energy calculation term when using soft core (soft repulsion) for CAP restraint, position restraint, distance/angle/torsion restraint or van der Waals repulsion etc. In addition, ordinarily you should designate the applicable atoms for these potentials (see the section on EXE>INPUT), and input parameters where they are required for force constants etc.

All of these restraint potentials are added to the potential energy term of the entire system.

CALPSR : Position restraint
=NOCAlc ; Do not calculate(Default)
=CALC ; Calculate
Designate the following in the EXE>INPUT phase.
POSITION=READ
NAMEPO= (Position restraint designation file)
REFCOORD=PDB
NAMERE= (Reference coordinate file)
CALDSR : distance-restraint
=NOCAlc ; Do not calculate(Default)
=CALC ; Calculate
Designate the following in the EXE>INPUT phase.
DISTANcerestrain =READ
NAMEDIstance= (Distance restraint designation file)
CALDHR : dihedral-restraint
=NOCAlc ; Do not calculate(Default)
=CALC ; Calculate
Designate the following in the EXE>INPUT phase.
DIHEDRalrestrain =READ
NAMEDH= (Dihedral restraint designation file)
CALREP : simple repulsion
=NOCAlc ; Do not calculate(Default)
=CALC ; Calculate
CALCAP : CAP restraint
=NOCAlc ; Do not calculate(Default)
=CALC ; Calculate
Designate the following in the EXE>INPUT phase.
SETBOUndary =READ
NAMEBOundary = (CAP boundary designation file)

Parameters necessary for restraint potential

TEMPERature: Temperature used for restraint (K) (Position, Distance, Repulsion, Dihedral).
=300.0 ; (Default) (△)
WETDSR : Distance restraint weight

=1.0 ; (Default)

WETPSR : Position restraint weight

=5.0 ; (Default)

WETDHR : Dihedral restraint weight

=10.0 ; (Default)

Simple repulsion parameters

WETREP : Simple repulsion weight

=1.0 ; (Default)

REPSCAle : Van der Waals radius scale factor

=1.0 ; (Default)

REPDELta : Permissible tolerance

=1.0 ; (Default)

CAP restraint parameters

With CAP restraint, you must designate the CAP center, radius and the repulsion type and force coefficient which form the walls of CAP. This is in addition to the file designating atoms subject to CAP restraint (see the chapter on EXE>INPUT), and designation of "CALCAP=CALC". There are default values, but the user usually designates parameters other than the force constant (FORCAP).

RADCAP : Radius of CAP restraint(Å).

Within this radius, the restraint force is 0, and outside of it, restraint is determined by the potential.

=20.0 : (Default)

FORCAP : Force constant of repulsion potential forming the CAP wall

=150.0 : (Default)

FUNCAP : Form of repulsion potential of the CAP wall

=HARMonic : Quadratic parabola potential (Default)

F = 0.5 * FORCAP * (R - RADCAP) **2

R = # (MASS-CENTER OF CHAIN) - (CAP-CENTER) .

=BIQUadratic : Biquadratic potential

F = 0.25 * FORCAP * (R**2 - RADCAP**2) **2

R = # (MASS-CENTER OF CHAIN) - (CAP-CENTER) .

(8) Boundary conditions

The boundary conditions which can be used in myPresto are a sphere/ellipsoid, or periodic boundary conditions (a cell with the 6 faces of a rectangular parallelepiped). A rigid wall which provides elastic collision is used in a sphere or ellipsoid. Common names are used for some variables (like designation of the center). When using periodic boundary conditions, be sure not to forget to designate the cycle (UPDATE) for returning coordinates to the unit cell. In contrast with CAP restraint, there is no need for a file designating applicable atoms.

```
BOUNDAry : Boundary condition type
    =NO          ; No boundary (Default)
    =PERI        ; Periodic boundary conditions
    =ELLIPSoid   ; Ellipsoid boundary

    =SPHERE      ; Sphere boundary
```

(8－1) Boundary condition size setting

For periodic boundary conditions :
This sets the length along the X, Y and Z axes of the unit cell

```
    LXCELL=          40.0     ; (Default)
    LYCELL=          40.0     ; (Default)
    LZCELL=          40.0     ; (Default)
```

For an ellipsoid :
This designates the radius in the X, Y and Z directions, assuming the major and minor axes of the ellipsoid are aligned with the XYZ coordination directions.

```
    ELLIPA=          30.0     ; (Default)
    ELLIPB=          30.0     ; (Default)
    ELLIPC=          30.0     ; (Default)
```

For a sphere :
This designates the radius of the sphere.

```
    RADIUS=          30.0     ; (Default)
```

(9) LIST

If you add the command "LIST", current parameter settings will be displayed. No parameters.

(10) QUIT

This indicates the end of EXE> group input. No parameters.

(Blank space)

2 Sample calculations

■Control file (md.inp)

```
    EXE> INPUT
         TOPOLOGY= FORM     NAMETO=  initial.tpl
         COORDINA= PDB      NAMECO=  initial.pdb
         POSITION= READ     NAMEPO=  M_all.res
         REFCOORD= PDB      NAMERE=  initia0.pdb
         SETBOU=   READ     NAMEBO=  M_dock.capbc
         SETSHAKE= READ     NAMESH=  initial.shk
         QUIT
    EXE> MD
         LOOPLI=   10000
         SETTIM=   5000.0D0  CPUTIM= 3600000.0D0
         UPDATE=   20
         TIMEST=   2.0D0
         OUTLOG=    200      LOGFOR=   DETA
         STOPCE=   NO

         OUTCOO=    100
         NAMECO=    traject.cor   ; Coordinates trajectory file
         MNTRCO=    SING

         OUTENE=    200
         NAMEEN=    traject.ene   ; Energy trajectory file
         MNTREN=    ASCI

         NAMETO=    traject.eto
         MNTRTO=    ASCI

         METHOD=   CANONICAL
         SETTEM=   300.0D0   INITIA=   SET
         STARTT=   300.0D0   RANDOM=   654321
         SHAKEM=   ALLB
         CALCAP=   CALC      RADCAP=   22.0
         FORCAP=   100.0     FUNCAP=   HARMonic
         SETCEN=   NO
         CALPSR=   CALC      WETPSR=   10.00
         BESTFI=   YES
         CUTMET=   RESA      CUTLEN=   10.0D0
         DIEFUN=   CONS      DIEVAL=   1.0D0
         CALV15=   CALC      CALE15=   CALC
         CALHYD=   NOCALC    CALV5N=   NOCALC
         CALE5N=   NOCALC    CALH5N=   NOCALC
         QUIT
    EXE> OUTPUT
         COORDINATE= PDB     NAMECO=   final.pdb
         QUIT
    EXE> END
```

A part of protein fixed by position restraint and a system including metal atoms and ligand coordinated to it surrounded by CAP water are calculated. With regard to

the system, the 1st chain is protein, the 2nd to 4th chain is Ca ion, the 5th chain is Zn ion, the 6th chain is ligand, the 7th chain or later is water molecule. MD of the system performs the md.inp as a control file.

Position restraint fileM_all.res is designated as follows. The ligand molecule and water molecule can move freely in CAP potential.

■Position restraint designation file (M_all.res)

```
GROUP> LIST
     1    1    1  137    CA   *      1.0    MASS   YES
     1    1    1  137    N    *      1.0    MASS   YES
     1    1    1  137    C    *      1.0    MASS   YES
     1    1    1  137    0    *      1.0    MASS   YES
     2    5    1    1    *    *      1.0    MASS   YES
END
GROUP> STOP
```

This coordinate trajectory file is analyzed. Transitions of deviations (RMSD) from the reference coordinates of coordinates trajectory at each step and average structure are obtained. Transitions of RMSD are output to the standard output and plot data. The average structure is output to a file designated by NAMECO.

■Control file ana_1.inp

```
    EXE> INPUT
         TOPOLOGY=   FORM     NAMETO=    initial.tpl   ; Topology file of the system
         COORDINA=   PDB      NAMECO=    initial.pdb   ; PDB file of the system
         REFCOORD=   PDB      NAMERE=    initial.pdb   ; Reference coordinates
         QUIT
    EXE> ANALYS
         METHOD=     MD
         NAMETR=     traject.cor      ; Coordinates trajectory file calculating MD
         DATATY=     COR4             ; Designation of types of trajectory file
         LOGFOR=     DETAIL           ; Designation of standard output
         INTERV=     1                ; Step interval of analysis
         STARTT=     0.0              ; Start time of analysis (PSEC)
         ENDTIM=     20.0             ; End time of analysis (PSEC)
         UNITBS=     61               ;  IO unit number of NAMEBS
         NAMEBS=     setbst_1.bst     ; Atom designation used for superimposing coordinates
         BESTFI=     YES              ; Superimposes the coordinates.
         FLUCTU=     YES              ; Calculates the fluctuation.
         NAMEPL=     rmsd_plot.data   ; Plot data of RMSD.
         QUIT
    EXE> OUTPUT
         COORDINATE=  PDB     NAMECO=     mean.pdb   ;  Average structure to be output
         QUIT
    EXE> END
```

RMSD is calculated by superimposing the reference coordinate to the coordinates of the trajectory file. If no superimposing of atoms is designated, all toms of the 1st chain are designated. It is preferable to designate so that hydrogen atom is not designated for superimposing and metalatoms from the 2nd to 5th chain are used for superimposing. Therefore, prepare the following atom designation file to designate. In the second line, cancel the designation of all atoms by FIX temporarily, and newly designate atoms with the lines after that. Atoms of the 1st chain must be included in the designation.

■Atom designation file (setbst_1.bst)

```
SETBST> LIST
FIX   1  1  1 137  *   YES   ; Release atom designation.
FREE  1  1  1 137  C*  YES   ; Designate all atoms with an atom name starting from C.
FREE  1  1  1 137  N*  YES   ; Designate all atoms with an atom name starting from N.
FREE  1  1  1 137  O*  YES   ; Designate all atoms with an atom name starting from O.
FREE  1  1  1 137  S*  YES   ; Designate all atoms with an atom name starting from S.
FREE  2  5  1   1  *   YES   ; Designate all atoms of from the 2nd to 5th chain.
SETBST> END
```

Transition of RMSD, average structure, RMSD of each atom and x, y and z components of RMSD, etc are output to the standard output file.

■Standard output file (ana_1.out)

```
INFORMATION> ANALYS
     CALCULATE AVERAGE AND FLUCTUATION
        NUMBER OF SELECTED DATA   :  100

     RMSD DATA
     NUMBER OF ATOMS OF FIRST CHAIN :  2008
     NUMBER OF ATOMS FOR BEST-FIT   :  1049
     1) AVERAGE
        ALL ATOM       :  4.2578762709675724
        SELCTED ATOM   :  0.41109270952623123
     2) SD
        ALL ATOM       :  1.3583200792547043
        SELCTED ATOM   :  3.94575716745282287E-2

     EACH ATOM DATA   ; x, y and z coordinates of average structure, RMSD, x, y and z components
of RMSD
        1 N       GLY        1     1  1 -16.58385   5.37864  14.14423   0.12539
  0.7546969E-01  0.8198197E-01  0.5748686E-01
        2 H1      GLY        1     1  1 -16.96925   5.08163  14.94453   0.04053
  0.1919956E-01  0.3203947E-01  0.1574088E-01
```

Transition of RMSD is output to the plot data. The 1st column shows the elapsed time (PSEC) , the 2nd column shows RMSD(Å).At first, superimpose the coordinates of trajectory of an atom designated by the designation of superimposing atom on the reference coordinate, and calculate and output RMSD of all atoms. Then, after #RMSD, PART, superimpose the trajectory coordinates of an atom designated by the superimposing atom and output the value of RMSD of only the atom designated. Normally, the values after #RMSD PART are used for analyses.

■Plot data (rmsd_plot.data)

```
# RMSD ALL       ; RMSD of all atoms
      0.2000000           0.7820804
      0.4000000           1.1031598
      0.6000000           1.3053278
      0.8000000           1.4847158
        :
        :
        :
     19.7999992           6.1756648
     20.0000000           6.2183821
# RMSD PART      ; RMSD of designated atoms
      0.2000000           0.2947671
      0.4000000           0.3071040
      0.6000000           0.3031894
      0.8000000           0.3269165
        :
        :
        :
```

(Blank space)

***myPresto* 4.2**

- cosgene "ANALYSIS" -