1. Anal

Usage:

```
anal [-O] -i analin -o analout -p prmtop -c inpcrd [-ref refc ]
```

−O Overwrite output files if they exist.

1.1. Introduction

This is the energy analysis module of AMBER. Its purpose is to do energetic analyses of individual structures. The key function of this program is decomposition of the energy among different groups of atoms in order to find the interaction energies between different parts of the system. The program puts those atoms which are not in explicitly defined groups into a separate group. In the case of a belly or partial minimization the unfrozen part of the system can be defined as the desired groups and the frozen part will be automatically taken by the program as an additional group.

1.2. Files

```
analin    5     Input control data for the analysis run
analout   6     Output results
prmtop   20     Input Molecular topology file from PARM
inpcrd   21     Input Coordinates to be analyzed
refc     24     Input positional constraint coordinates
```

1.3. Input description

```
- 1 -       TITLE

           FORMAT(20A4)

TITLE       Title for identification.
```

```
- 2 -      NTX , NTXO , NRC , NRCX , NGRPX , KFORM,    FORMAT(6I)

NTX        Format of coordinates.

 = 1  Formatted (inpcrd, unit 21)
 = 2  Unformatted (inpcrd, unit 21)
```

```
NTXO       Read but not used

NRC        Option to read position constraints.

 = 0  no constraints
 = 1  constrained minimization

      The atoms to be constrained are read as groups with
      different harmonic force constants for each group.
      Consult the section on GROUP in the Appendices for
      group specification format.
      When using positional constraints, the constrained
      groups are given first in the group input followed
      by the groups for energy analysis.

NRCX       Format of constraint coordinates.   The constraint
      coordinate file has the same organization as the structure
      coordinates.

 = 0  Formatted (refc, unit 24)
 = 1  Binary (refc, Unit 24)

NGRPX      Maximum number of groups that the structure can be
      divided into for analysis. Note that if any atoms are not
      explicitly included in a group, they will automatically
      be put in an additional group.

 = 0  Default = 70
 = N  Structure may be partitioned into N different groups

KFORM      The Flag for the type of Topology File
 = 0  Binary    (prmtop, unit 20)
 = 1  Formatted (prmtop, unit 20)
```

```
- 3 -      NTB , BOX(1) , BOX(2) , BOX(3) , BETA

          FORMAT(I,4F)

NTB        Flag for periodic boundary conditions.
      ( not yet operational )

 =-n  Periodicity is applied.  Box is truncated octahedron
      (BETA = 90)
 = 0  No periodicity is applied
 =+n  Periodicity is applied.  Box is rectangular or monoclinic
      depending on the value of BETA

BOX(1..3)  Lengths of the edges of the periodic box
```

BETA Angle between the X- and Z- axes of the box in degrees. the Y- axis is assumed to be orthogonal to the other axes. (0 < BETA < 180)

\- 4 - NTF , NTID , NTN , NTNB , NSNB , IDIEL, FORMAT(6I)

NTF Flag for force evaluation.

= 1 complete interaction is calculated

= 2 bond interactions involving H-atoms omitted

= 3 all the bond interactions are omitted

= 4 angle involving H-atoms and all bonds are omitted

= 5 all bond and angle interactions are omitted

= 6 dihedrals involving H-atoms and all bonds and all angle interactions are omitted

= 7 all bond, angle and dihedral interactions are omitted

= 8 all bond, angle, dihedral and non-bonded interactions are omitted

NTID Flag for improper dihedral contribution (read but not used).

NTN Read but not used

Note: non-bonded interactions are now always calculated using a residue based cutoff. The nb pairs are stored as residue pairs. This uses substantially less memory than the atom pairlist in the minimizer.

NTNB Read but not used

NSNB Read but not used

IDIEL Flag for the type of dielectric function to be used in calculating the electrostatic energy.

= 0 distance dependent dielectric function
= 1 constant dielectric function

\- 5 - CUT , SCNB , SCEE , DIELC, FORMAT(4F)

```
CUT        The cutoff distance for the non-bonded pairs.


SCNB       1-4 vdw interactions are divided by SCNB.
      if SCNB .le. 0.0 then SCNB = 2.0

SCEE       1-4 electrostatic interactions are divided by SCEE
      if SCEE .le. 0.0 then SCEE = 2.0

DIELC      Dielectric multiplicative constant for the electrostatic
      interactions.  If DIELC .le. 0.0 then DIELC = 1.0.  DIELC
      and IDIEL are coupled.  For example to obtain a dielectric
      'constant' of 4rij set DIELC=4 and IDIEL=0.
```

```
- 6 -      Printout of energies beyond specified values.  You
      must use the ENERGY keyword to obtain output.

      IMAX , EMAX(I) , I = 1, 9,       FORMAT(I,9F)

IMAX       Flag for printing the energy contributions.

 = 0  no printing
 = 1  energy contributions will be printed

EMAX(1)    All the bonds whose energy contribution is greater
      than EMAX(1) will be printed.

EMAX(2)    All the angles whose energy contribution is greater
      than EMAX(2) will be printed.

EMAX(3)    All the dihedrals whose energy contribution is
      greater than EMAX(3) will be printed.

EMAX(4)    All the 1-4 vdw whose energy contribution is greater
      than EMAX(4) will be printed.

EMAX(5)    All the 1-4 eel whose energy contribution is greater
      than EMAX(5) will be printed.

EMAX(6)    All the vdw nb pairs whose energy contribution is
      greater than EMAX(6) will be printed.

EMAX(7)    All the eel nb-pairs with absolute value of energy
      greater than EMAX(7) will be printed.

EMAX(8)    All the H-bond pairs whose energy contribution is
      greater than EMAX(8) will be printed.
```

EMAX(9)   All the constrained atoms whose energy contribution is greater than EMAX(9) will be printed.

\- 7 -   The control for doing the desired options. The only currently-supported control word is ENERGY.

IOPT,   FORMAT(A)

IOPT   The control word for the option.

'ENERGY' Energy decomposition into groups

'STOP'   Control to terminate the run

ENERGY

Parts of the molecule for which interaction energies are to be calculated are entered in GROUP format. See the section on GROUP in the Appendices for details. Groups are read sequentially in any order. Each group is terminated by an "END" card.

The ENERGY option is terminated by another "END" card.