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SSH Secure Shell 3.2.9 (Build 283)
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This copy of SSH Secure Shell is a non-commercial version.
This version does not include PKI and PKCS #11 functionality.


Last login: Mon Oct 27 10:29:57 2008 from phys9569.phys.tue.nl
-bash: Sample: command not found
andrea@nanopol:~> ls
:   bin         fftw-3.0.1.tar.gz  gromacs-3.3.3.tar.gz  lesstif-0.95.0.tar.gz  PS           tutor
:.  fftw-3.0.1  gromacs-3.3.3      lesstif-0.95.0        PDB                    public_html
andrea@nanopol:~> cd PS
andrea@nanopol:~/PS> ls
32x80_equil_540_out.gro  dimer.gro    ffG43a1bon.itp     ffG43a1.hdb      ffG43a1-n_new.tdb
monomer.top    trimer.gro      #trimer.top.1#
32x80_equil_540_out.pdb  dimer.pdb    ffG43a1-c_new.tdb  ffG43a1.itp      ffG43a1-n.tdb
pdb2gmx.log    #trimer.gro.1#
32x80_equil_540_out.top  dimer.top    ffG43a1-c.tdb      ffG43a1nb.itp    ffG43a1.rtp        posre.itp
     trimer.pdb
chain.pdb                ffG43a1.atp  ffG43a1.ddb        ffG43a1_new.hdb  monomer.pdb
#posre.itp.1#  trimer.top
andrea@nanopol:~/PS> less trimer.top




;
;       File 'trimer.top' was generated
;       By user: onbekend (0)
;       On host: onbekend
;       At date: Mon Oct 27 15:42:15 2008
;
;       This is your topology file
;       "Good Music Saves your Soul" (Lemmy)
;
; Include forcefield parameters
#include "ffG43a1.itp"

[ moleculetype ]
; Name            nrexcl
Protein             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB      massB
     1        CH3      1    PS1    CH3      1          0     15.035   ; qtot 0
     2        CH1      1    PS1     CH      1          0     13.019   ; qtot 0
     3          C      1    PS1     CB      1          0     12.011   ; qtot 0
     4        CR1      1    PS1    CG1      1          0     13.019   ; qtot 0
     5        CR1      1    PS1    CG2      1          0     13.019   ; qtot 0
     6        CR1      1    PS1    CG3      1          0     13.019   ; qtot 0
     7        CR1      1    PS1    CG4      1          0     13.019   ; qtot 0
     8        CR1      1    PS1    CG5      1          0     13.019   ; qtot 0
     9        CH2      2     PS    CH2      2          0     14.027   ; qtot 0
    10        CH1      2     PS     CH      2          0     13.019   ; qtot 0
    11          C      2     PS     CB      2          0     12.011   ; qtot 0
    12        CR1      2     PS    CG1      2          0     13.019   ; qtot 0
    13        CR1      2     PS    CG2      2          0     13.019   ; qtot 0
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    14        CR1      2     PS    CG3      2          0     13.019   ; qtot 0
    15        CR1      2     PS    CG4      2          0     13.019   ; qtot 0
    16        CR1      2     PS    CG5      2          0     13.019   ; qtot 0
    17        CH2      3    PSN    CH2      3          0     14.027   ; qtot 0
    18        CH1      3    PSN     CH      3          0     13.019   ; qtot 0
    19          C      3    PSN     CB      3          0     12.011   ; qtot 0
    20        CR1      3    PSN    CG1      3          0     13.019   ; qtot 0
    21        CR1      3    PSN    CG2      3          0     13.019   ; qtot 0
    22        CR1      3    PSN    CG3      3          0     13.019   ; qtot 0
    23        CR1      3    PSN    CG4      3          0     13.019   ; qtot 0
    24        CR1      3    PSN    CG5      3          0     13.019   ; qtot 0
    25        CH3      3    PSN    CH3      3          0     15.035   ; qtot 0

[ bonds ]
;  ai    aj funct            c0            c1            c2            c3
    1     2     2    gb_26
    2     3     2    gb_26
    2     9     2    gb_26
    3     4     2    gb_15
    3     8     2    gb_15
    4     5     2    gb_15
    5     6     2    gb_15
    6     7     2    gb_15
    7     8     2    gb_15
    9    10     2    gb_26
   10    11     2    gb_26
   10    17     2    gb_26
   11    12     2    gb_15
   11    16     2    gb_15
   12    13     2    gb_15
   13    14     2    gb_15
   14    15     2    gb_15
   15    16     2    gb_15
   17    18     2    gb_26
   18    19     2    gb_26
   18    25     2    gb_26
   19    20     2    gb_15
   19    24     2    gb_15
   20    21     2    gb_15
   21    22     2    gb_15
   22    23     2    gb_15
   23    24     2    gb_15

[ pairs ]
;  ai    aj funct            c0            c1            c2            c3
    1     4     1
    1     8     1
    1    10     1
    2     5     1
    2     7     1
    2    11     1
    2    17     1
    3     6     1
    3    10     1
    4     7     1
    4     9     1
    5     8     1
    8     9     1
    9    12     1
    9    16     1
    9    18     1
   10    13     1
   10    15     1
   10    19     1
   10    25     1
   11    14     1
   11    18     1
   12    15     1
   12    17     1
   13    16     1
   16    17     1
   17    20     1
   17    24     1
   18    21     1
```

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   18    23     1
   19    22     1
   20    23     1
   20    25     1
   21    24     1
   24    25     1

[ angles ]
;  ai    aj    ak funct            c0            c1            c2            c3
    1     2     3     2    ga_12
    1     2     9     2    ga_12
    3     2     9     2    ga_12
    2     3     4     2    ga_26
    2     3     8     2    ga_26
    4     3     8     2    ga_26
    3     4     5     2    ga_26
    4     5     6     2    ga_26
    5     6     7     2    ga_26
    6     7     8     2    ga_26
    3     8     7     2    ga_26
    2     9    10     2    ga_12
    9    10    11     2    ga_12
    9    10    17     2    ga_12
   11    10    17     2    ga_12
   10    11    12     2    ga_26
   10    11    16     2    ga_26
   12    11    16     2    ga_26
   11    12    13     2    ga_26
   12    13    14     2    ga_26
   13    14    15     2    ga_26
   14    15    16     2    ga_26
   11    16    15     2    ga_26
   10    17    18     2    ga_12
   17    18    19     2    ga_12
   17    18    25     2    ga_12
   19    18    25     2    ga_12
   18    19    20     2    ga_26
   18    19    24     2    ga_26
   20    19    24     2    ga_26
   19    20    21     2    ga_26
   20    21    22     2    ga_26
   21    22    23     2    ga_26
   22    23    24     2    ga_26
   19    24    23     2    ga_26

[ dihedrals ]
;  ai    aj    ak    al funct            c0            c1            c2            c3            c4
        c5
    1     2     3     4     1    gd_1
    1     2     3     8     1    gd_1
    9     2     3     4     1    gd_1
    9     2     3     8     1    gd_1
    1     2     9    10     1    gd_16
    3     2     9    10     1    gd_16
    2     3     4     5     1
    2     3     8     7     1
    2     9    10    11     1    gd_16
    9    10    11    12     1    gd_1
    9    10    11    16     1    gd_1
   17    10    11    12     1    gd_1
   17    10    11    16     1    gd_1
    9    10    17    18     1    gd_16
   11    10    17    18     1    gd_16
   10    11    12    13     1
   10    11    16    15     1
   10    17    18    19     1    gd_16
   10    17    18    25     1    gd_16
   17    18    19    20     1    gd_1
   17    18    19    24     1    gd_1
   25    18    19    20     1    gd_1
   25    18    19    24     1    gd_1
   18    19    20    21     1
   18    19    24    23     1
```

```
[ dihedrals ]
;  ai    aj    ak    al funct            c0            c1            c2            c3
    1     9     3     2     2    gi_1
    2     8     4     3     2    gi_1
    2     9     1     3     2    gi_1
    2     1     3     9     2    gi_1
    3     8     2     4     2    gi_1
    3     4     5     6     2    gi_1
    3     8     7     6     2    gi_1
    3     2     4     8     2    gi_1
    4     3     8     7     2    gi_1
    4     5     6     7     2    gi_1
    5     4     3     8     2    gi_1
    5     6     7     8     2    gi_1
    9    17    11    10     2    gi_1
   10    16    12    11     2    gi_1
   10    17     9    11     2    gi_1
   10     9    11    17     2    gi_1
   11    16    10    12     2    gi_1
   11    12    13    14     2    gi_1
   11    16    15    14     2    gi_1
   11    10    12    16     2    gi_1
   12    11    16    15     2    gi_1
   12    13    14    15     2    gi_1
   13    12    11    16     2    gi_1
   13    14    15    16     2    gi_1
   17    25    19    18     2    gi_1
   18    24    20    19     2    gi_1
   18    25    17    19     2    gi_1
   18    17    19    25     2    gi_1
   19    24    18    20     2    gi_1
   19    20    21    22     2    gi_1
   19    24    23    22     2    gi_1
   19    18    20    24     2    gi_1
   20    19    24    23     2    gi_1
   20    21    22    23     2    gi_1
   21    20    19    24     2    gi_1
   21    22    23    24     2    gi_1

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif

; Include water topology
#include "spc.itp"

#ifdef POSRES_WATER
; Position restraint for each water oxygen
[ position_restraints ]
;  i funct       fcx        fcy        fcz
   1    1       1000       1000       1000
#endif

; Include generic topology for ions
#include "ions.itp"

[ system ]
; Name
Protein

[ molecules ]
; Compound        #mols
Protein             1
trimer.top lines 204-242/242 (END)
```