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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 03:49:48 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 ffG43a1.rtp




[ bondedtypes ]
; Col 1: Type of bond
; Col 2: Type of angles
; Col 3: Type of proper dihedrals
; Col 4: Type of improper dihedrals
; Col 5: Generate all dihedrals if 1, only heavy atoms of 0.
; Col 6: Number of excluded neighbors for nonbonded interactions
; Col 7: Generate 1,4 interactions between pairs of hydrogens if 1
; Col 8: Remove propers over the same bond as an improper if it is 1
; bonds  angles  dihedrals  impropers all_dihedrals nrexcl HH14 RemoveDih
     2      2         1          2         0           3     0     1

;start editing by Andrea

[PS1]
[atoms]
CH3     CH3     0       0
CH      CH1     0       0
CB      C       0       0
CG1     CR1     0       0
CG2     CR1     0       0
CG3     CR1     0       0
CG4     CR1     0       0
CG5     CR1     0       0

[bonds]
CH3     CH      gb_26
CH      CB      gb_26
CB      CG1     gb_15
CG1     CG2     gb_15
CG2     CG3     gb_15
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```
CG3     CG4     gb_15
CG4     CG5     gb_15
CG5     CB      gb_15
CH      +CH2    gb_26

[angles]
;109,5 angle
CH3     CH      +CH2    ga_12
CH3     CH      CB      ga_12
CB      CH      +CH2    ga_12
;120 angle
CH      CB      CG1     ga_26
CH      CB      CG5     ga_26
CG1     CB      CG5     ga_26
CB      CG1     CG2     ga_26
CG1     CG2     CG3     ga_26
CG2     CG3     CG4     ga_26
CG3     CG4     CG5     ga_26
CG4     CG5     CB      ga_26

[impropers]
;keep the planarity of the ring
CB      CG1     CG2     CG3     gi_1
CG1     CG2     CG3     CG4     gi_1
CG2     CG3     CG4     CG5     gi_1
CG3     CG4     CG5     CB      gi_1
CG4     CG5     CB      CG1     gi_1
CG5     CB      CG1     CG2     gi_1
;around CB
CB      CG1     CG5     CH      gi_1
CB      CG5     CH      CG1     gi_1
CB      CH      CG1     CG5     gi_1
;around CH
CH      CB      +CH2    CH3     gi_1
CH      +CH2    CH3     CB      gi_1
CH      CH3     CB      +CH2    gi_1

[dihedrals]
;in the chain - 3-fold (n=3)
CH3     CH      +CH2    +CH     gd_16
CB      CH      +CH2    +CH     gd_16
;around CH-CB - 2-fold (n=2)
CH3     CH      CB      CG5     gd_1
CH3     CH      CB      CG1     gd_1
+CH2    CH      CB      CG5     gd_1
+CH2    CH      CB      CG1     gd_1
;around CB-CG - 2-fold?,do we need them?
CH      CB      CG1     CG2
CH      CB      CG5     CG4


[PS]
[atoms]
CH2     CH2     0       0
CH      CH1     0       0
CB      C       0       0
CG1     CR1     0       0
CG2     CR1     0       0
CG3     CR1     0       0
CG4     CR1     0       0
CG5     CR1     0       0

[bonds]
-CH     CH2     gb_26
CH2     CH      gb_26
CH      CB      gb_26
CB      CG1     gb_15
CG1     CG2     gb_15
CG2     CG3     gb_15
CG3     CG4     gb_15
CG4     CG5     gb_15
CG5     CB      gb_15
CH      +CH2    gb_26
```

```
[angles]
;109,5 angle
-CH     CH2     CH      ga_12
CH2     CH      +CH2    ga_12
CH2     CH      CB      ga_12
CB      CH      +CH2    ga_12
;120 angle
CH      CB      CG1     ga_26
CH      CB      CG5     ga_26
CG1     CB      CG5     ga_26
CB      CG1     CG2     ga_26
CG1     CG2     CG3     ga_26
CG2     CG3     CG4     ga_26
CG3     CG4     CG5     ga_26
CG4     CG5     CB      ga_26

[impropers]
;keep the planarity of the ring
CB      CG1     CG2     CG3     gi_1
CG1     CG2     CG3     CG4     gi_1
CG2     CG3     CG4     CG5     gi_1
CG3     CG4     CG5     CB      gi_1
CG4     CG5     CB      CG1     gi_1
CG5     CB      CG1     CG2     gi_1
;around CB
CB      CG1     CG5     CH      gi_1
CB      CG5     CH      CG1     gi_1
CB      CH      CG1     CG5     gi_1
;around CH
CH      CB      +CH2    CH2     gi_1
CH      +CH2    CH2     CB      gi_1
CH      CH2     CB      +CH2    gi_1

[dihedrals]
;in the chain - 3-fold
CH2     CH      +CH2    +CH     gd_16
CB      CH      +CH2    +CH     gd_16
-CH     CH2     CH      CB      gd_16
-CH     CH2     CH      +CH2    gd_16
;around CH-CB - 2-fold
CH2     CH      CB      CG5     gd_1
CH2     CH      CB      CG1     gd_1
+CH2    CH      CB      CG5     gd_1
+CH2    CH      CB      CG1     gd_1
;around CB-CG - 2-fold?,do we need them?
CH      CB      CG1     CG2
CH      CB      CG5     CG4

[ PSN ]
[atoms]
CH2     CH2     0       0
CH      CH1     0       0
CB      C       0       0
CG1     CR1     0       0
CG2     CR1     0       0
CG3     CR1     0       0
CG4     CR1     0       0
CG5     CR1     0       0
CH3     CH3     0       0

[bonds]
-CH     CH2     gb_26
CH2     CH      gb_26
CH      CB      gb_26
CB      CG1     gb_15
CG1     CG2     gb_15
CG2     CG3     gb_15
CG3     CG4     gb_15
CG4     CG5     gb_15
CG5     CB      gb_15
CH      CH3     gb_26

[angles]
-CH     CH2     CH      ga_12
```

```
CH2     CH      CH3     ga_12
CH2     CH      CB      ga_12
CB      CH      CH3     ga_12
CH      CB      CG1     ga_26
CH      CB      CG5     ga_26
CG1     CB      CG5     ga_26
CB      CG1     CG2     ga_26
CG1     CG2     CG3     ga_26
CG2     CG3     CG4     ga_26
CG3     CG4     CG5     ga_26
CG4     CG5     CB      ga_26

[impropers]
;keep the planarity of the ring
CB      CG1     CG2     CG3     gi_1
CG1     CG2     CG3     CG4     gi_1
CG2     CG3     CG4     CG5     gi_1
CG3     CG4     CG5     CB      gi_1
CG4     CG5     CB      CG1     gi_1
CG5     CB      CG1     CG2     gi_1
;around CB
CB      CG1     CG5     CH      gi_1
CB      CG5     CH      CG1     gi_1
CB      CH      CG1     CG5     gi_1
;around CH
CH      CB      CH3    CH2     gi_1
CH      CH3     CH2    CB      gi_1
CH      CH2     CB     CH3     gi_1

[dihedrals]
;in the chain - 3-fold (n=3)
-CH     CH2     CH      CB      gd_16
-CH     CH2     CH      CH3     gd_16
;around CH-CB - 2-fold (n=2)
CH2     CH      CB      CG5     gd_1
CH2     CH      CB      CG1     gd_1
CH3     CH      CB      CG5     gd_1
CH3     CH      CB      CG1     gd_1
;around CB-CG - 2-fold?,do we need them?
CH      CB      CG1     CG2
CH      CB      CG5     CG4

;end of editing by Andrea

[ ACE ]
 [ atoms ]
    CA   CH3   0.000     0
     C     C   0.380     1
     O     O  -0.380     1
 [ bonds ]
     C    CA   gb_26
     C     O   gb_4
     C    +N   gb_9
 [ angles ]
   CA     C    +N    ga_18
ffG43a1.rtp lines 196-234/9540 1%
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