GROMACS - Bug #6

genbox remove protein from system

09/02/2005 06:34 PM - junmin-quan empty

Status:	Closed		
Priority:	High		
Assignee:	Erik Lindahl		
Category:	analysis tools		
Target version:	3.3_rc1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

genbox ~~cp CD81-dimer.gro -cs spc216.gro -p CD81-dimer.top -o CD81-dimer~~
b4em.gro
:-) G R O M A C S (-:

```
Grunge ROck MAChoS

:-)  VERSION 3.3_rc1  (-:

Written by David van der Spoel, Erik Lindahl, Berk Hess, and others.
       Copyright (c) 1991-2000, University of Groningen, The Netherlands.
             Copyright (c) 2001-2004, The GROMACS development team,
            check out http://www.gromacs.org for more information.

This program is free software; you can redistribute it and/or
          modify it under the terms of the GNU General Public License
         as published by the Free Software Foundation; either version 2
             of the License, or (at your option) any later version.

:-)  genbox  (-:
```

Option Filename Type Description

-cp CD81-dimer.gro Input, Opt! Generic structure: gro g96 pdb tpr tpb tpa xml
-cs spc216.gro Input, Opt!, Lib. Generic structure: gro g96 pdb tpr tpb tpa xml
-ci insert.gro Input, Opt. Generic structure: gro g96 pdb tpr tpb tpa xml
-o CD81-dimer-b4em.gro Output Generic structure: gro g96 pdb xml
-p CD81-dimer.top In/Out, Opt! Topology file

```
Option    Type  Value  Description
------------------------------------------------------
      -[no]h    bool     no  Print help info and quit
       -nice     int     19  Set the nicelevel
        -box vector  0 0 0  box size
       -nmol     int      0  no of extra molecules to insert
        -try     int     10  try inserting -nmol*-try times
       -seed     int   1997  random generator seed
       -vdwd    real  0.105  default vdwaals distance
      -shell    real      0  thickness of optional water layer around solute
```

WARNING: masses will be determined based on residue and atom names,
this can deviate from the real mass of the atom type
In case you use free energy of solvation predictions:

+++ PLEASE READ AND CITE THE FOLLOWING REFERENCE +++
D. Eisenberg and A. D. McLachlan

```
Solvation energy in protein folding and binding
Nature 319 (1986) pp. 199-203
-------- -------- --- Thank You --- -------- --------

Opening library file /usr/local/gromacs/share/top/aminoacids.dat
Opening library file /usr/local/gromacs/share/top/atommass.dat
Opening library file /usr/local/gromacs/share/top/vdwradii.dat
Opening library file /usr/local/gromacs/share/top/dgsolv.dat
#Entries in atommass.dat: 82 vdwradii.dat: 26 dgsolv.dat: 7
Reading solute configuration
?
Containing 1770 atoms in 180 residues
Initialising van der waals distances...
Reading solvent configuration
"216H2O,WATJP01,SPC216,SPC-MODEL,300K,BOX=1.86206NM,WFVG,MAR. 1984"
solvent configuration contains 648 atoms in 216 residues

Initialising van der waals distances...
Will generate new solvent configuration of 3x4x4 boxes
Generating configuration
Sorting configuration
Found 1 molecule type:
SOL (   3 atoms): 10368 residues
Calculating Overlap...
box_margin = 0.315
Removed 6309 atoms that were outside the box
Segmentation fault
```

History

#1 - 09/05/2005 05:28 PM - Erik Lindahl

This bug seems to have been fixed as a side-effect of the QM group bug David corrected in the TPR format.