GROMACS - Bug #25

g_hbonds+Gromacs version 3.3

10/24/2005 04:31 PM - Isabella Daidone

Status:	Closed		
Priority:	High		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:	3.3		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

I experienced the following problems in using g_hbond of Gromacs 3.3:
1) option -sel gives a core (I was previously able with version 3.1.4 to use this option)
2) options -acflen and -fitfn do not work (i.e. my oputput files do not change)
3) When I use options -b and -e (with -b different from 0.0) the program might either give a core or get stuck.

History

#1 - 04/01/2006 10:16 PM - David van der Spoel

-sel is disfunctional for now. Sorry
-b and -e work fine with the -ac flag
-acflen has no effect. Is that of concern?
-fitfn doesn't work either...

I've investigated all this stuff in a recent paper which you might want to check out:

David van der Spoel, Paul J. van Maaren, Per Larsson and Nicusor Timneanu:
Thermodynamics of hydrogen bonding in hydrophilic and hydrophobic media
Accepted, J. Phys. Chem. B 110, 4393-4398