

GROMACS - Bug #183

system grompps fine in 3.3.1 but fails with a cryptic error in 3.3.2

01/04/2008 12:36 AM - David Mobley

Status:	Closed	
Priority:	Normal	
Assignee:	Erik Lindahl	
Category:	mdrun	
Target version:	3.3.1	
Affected version - extra info:		Difficulty: uncategorized
Affected version:		

Description

I'm attaching a tarball of a peptide/TFE/water system that grompps fine in 3.3.1 for me, but fails with a cryptic error in 3.3.2. As far as I can tell my setup is fine (as evidenced by the fact it works fine in 3.3.1) so I suspect a bug, although it could also be that something about the topology format has changed without me being aware of it.

History

#1 - 01/04/2008 12:38 AM - David Mobley

Created an attachment (id=270)
tarball to reproduce

tarball to reproduce

#2 - 01/04/2008 09:46 AM - David van der Spoel

I can confirm this bug, and simultaneously say that it has been fixed a while ago in 3.3.3 CVS. We should really release this version. You could try the attached src/kernel/splitter.c in 3.3.2 if you wish.

#3 - 01/04/2008 09:48 AM - David van der Spoel

Created an attachment (id=271)
splitter.c source filee

Alternatively, you could use 3.3.1 for making topologies. Anyway, if you patch the source please compare the resulting tpr files with the 3.3.1 tpr using gmxcheck.

Files

bug.tar.gz	276 KB	01/03/2008	David Mobley
splitter.c	19.3 KB	01/04/2008	David van der Spoel