GROMACS - Bug #8

g_covar SegFaults with -debug in gmx 3.1.4

09/03/2005 12:26 PM - Dmytro Kovalskyy

Status:	Closed		
Priority:	High		
Assignee:	Erik Lindahl		
Category:	analysis tools		
Target version:	3.2.1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

[root@violet r1000]# g_covar f
~~g_covar/4vcc/filt_filt_double_10n_r1000_fit_Ca1v4.xtc -s~~
~~g_covar/4vcc/average.pdb -debug~~
:-) G R O M A C S (-:

```
God Rules Over Mankind, Animals, Cosmos and Such
```

```
:-)  VERSION 3.2.1  (-:
```

<skip>

+~~++++~~+ PLEASE 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/share/gromacs/top/aminoacids.dat
Opening library file /usr/local/share/gromacs/top/atommass.dat
Segmentation fault

In GMX 3.1.4 everything was Ok

History

#1 - 12/08/2005 10:26 PM - Erik Lindahl

Dmytro,

Sorry for letting this linger, but due to the subject it looked like a bug report against a deprecated release (3.1.4).

Could you possibly check if it still fails in 3.3 with your system?

#2 - 02/22/2006 10:16 PM - David van der Spoel

This was due to printing NULL variables. Resolved in 3.3. and 4.0