

GROMACS - Bug #295

editconf -f some.tpr -mead segfaults

02/11/2009 05:31 PM - Carsten Kutzner

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: analysis tools	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
<p>When using editconf with the -mead option, it will segfault with any tpr input file.</p> <p>The reason is that read_stx_conf makes a new atoms pointer and thus loses the atoms.pdbinfo[] pointer: In gmh_mtop_global_atoms the init_t_atoms routine is always called with bool bPdbInfo = FALSE, though it should be TRUE when -mead is set.</p> <p>A quick fix is to add the line</p> <pre>snew(atoms.pdbinfo, top->atoms.nr);</pre> <p>after line 619 of gmh_editconf.c (if bMead { ...}).</p>	

History

#1 - 02/12/2009 11:35 AM - Carsten Kutzner

Oops, the snew(atoms.pdbinfo, ...) has to go in front of the loop over atoms (line 597) of course.

A quick fix is to add the line

```
snew(atoms.pdbinfo, top->atoms.nr);
```

after line 619 of gmh_editconf.c (if bMead { ...}).

#2 - 02/12/2009 05:48 PM - Berk Hess

The line should not be added in the loop, but before, around line 592.

I fixed it for 4.0.4.

Berk