GROMACS - Bug #283

g_traj crashes with -mol option

01/28/2009 09:26 AM - Alexey Anikeenko

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	analysis tools		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Created an attachment (id=346)
fix

g_traj crashes with -mol option

fix:

--- a/gmx_traj.c 2009-01-28 14:12:38.000000000 0600
±+ b/gmx_traj.c 2009-01-28 14:12:49.000000000 0600
@ -601,7 +601,7 @@
snew(isize,ngroups);
snew(index,ngroups);
for (i=0; i<ngroups; i+) {
- if (index0[0][i] < 0 || index[0][i] >= mols->nr)
+ if (index0[0][i] < 0 || index0[0][i] >= mols->nr)
gmx_fatal(FARGS,"Molecule index (%d) is out of range (%d-%d)",
index0[0][i]+1,1,mols->nr);
isize[i] = atndx[index0[0][i]+1] - atndx[index0[0][i]];

History

#1 - 01/28/2009 12:00 PM - Berk Hess

I fixed it for 4.0.4.

Thanks for reporting this with the fix,

Berk

Files

gmx_traj_2009-01-28.patch	485 Bytes	01/28/2009	Alexey Anikeenko