GROMACS - Bug #116

FEP: Proton of OH-Group falls on the oxygen, even if just state A is of interest

11/08/2006 11:43 AM - Maik Goette

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

Description

I tried to FEP a TYR to PHE by morphing OH-Proton to dummy and OH-Oxygen to hydrogen. In EM/PR-Run/MD the proton of the OH-group falls upon the oxygen.
Tested: OPLS/AMBER-FFs, PME/CO, SOL/Vacuo. 3.2.1-tpr with 3.3.1 mdrun.
The error occured in every test with 3.3.1. It was ok with 3.2.1. It seems to be a problem with the bonds/angles.
I set up a tripeptide in vacuo for you to make debugging easier.

History

#1 - 11/08/2006 11:45 AM - Maik Goette

Created an attachment (id=98)
Small debugging testsystem

Tripeptide in vacuo with THR-FEP to artificial ALA/LEU-Intermediate. ;)

#2 - 11/08/2006 06:07 PM - Berk Hess

This seems to me like a bug in grompp that I have fixed for 3.3.1.
Did you make the tpr file with 3.3 and not 3.3.1?

You probably got warnings when running grompp.
In grompp of 3.3 when the A-state parameters can be found in the defaults and the B-state not, it gives a warning, but then uses zeros for all parameters.

#3 - 11/08/2006 06:28 PM - Berk Hess

I just compiled 3.3.1 and grompp indeed gives the correct constraint distances.

This was a bug.
But the user should also check all warnings and get rid of all warnings about topology stuff.
Maybe we should make grompp stop on topology warnings by default and add a switch to continue.

Files

bugreport.tar.gz	935 KB	11/08/2006	Maik Goette