GROMACS - Bug #339

all-bonds option not constraining all bonds?

07/13/2009 04:37 PM - Jussi Lehtola

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

Description

Hi,

IIUC setting
constraints = all-bonds
in the run .mdp file results in all bond lengths being constrained to the equilibrium value defined by the force field. Does this require some extra magic in the .top file?

My OPLS-AA alcohol simulations with "constraints = all-bonds" have resulted in largely the same results as for "constraints = h-bonds". Now having had a look at the bond length distributions it seems that the H bond lengths are correctly constrained, but the C-C bond lengths are not.

I've used Gromacs 4.0.3 for the simulations.

History

#1 - 07/14/2009 10:20 AM - Berk Hess

Please provide all the input files required to reproduce this problem.

Berk

#2 - 07/14/2009 12:45 PM - Jussi Lehtola

This is a bit odd.

When I look at the C-C bond in ethanol with an index file I see that it is constrained with all-bonds (normal distribution with std 0.000410457, compared to 0.00326475 with 'none' and 0.00330772 with 'h-bonds').

However the distribution in bonds.xvg given by g_bond is identical for 'h-bonds' and 'all-bonds': there are sharp peaks at 0.95 Å and 1.1 Å and a bell curve at roughly 1.77Å with a standard deviation of 0.6 Å.

#3 - 07/14/2009 12:47 PM - Jussi Lehtola

Created an attachment (id=384)
CA-CB bond length distributions in liquid ethanol as obtained by g_bond

#4 - 07/14/2009 01:09 PM - Berk Hess

Can it be that you have a mistake in your index file forr g_bond?
A distance of 0.177 nm is far too long for a C-C bond.
I suspect you are looking at an H-C distance.

Berk

#5 - 07/14/2009 01:45 PM - Jussi Lehtola

(In reply to comment #4)

> Can it be that you have a mistake in your index file forr g_bond?
> A distance of 0.177 nm is far too long for a C-C bond.
> I suspect you are looking at an H-C distance.

Yes, that is what I would think too.

It just came to me that g_hbond has a mandatory index file input. In the run folder I had the file index.ndx that contained the default groups System and EtOH. When run on either of these groups g_hbond produces the distances of all sorts of combinations of pairs.

It would be nice if g_bond gave some warning (or an error, even) about nonexisting bonds if the atoms don't have a bond in the topology..

Thanks for your help, and sorry for the trouble!

#6 - 07/14/2009 02:05 PM - Berk Hess

The problem is more in the name of the program.
g_bond simply determines distance distributions, not bond distributions.
One can use it for any pair of atoms.

Berk

Files

bonddists.tar.bz2	6.69 KB	07/14/2009	Jussi Lehtola