

## GROMACS - Bug #61

### dihedral restraint force constant not converted from degrees

03/30/2006 11:21 PM - David Mobley

<b>Status:</b> Closed	
<b>Priority:</b> High	
<b>Assignee:</b> David van der Spoel	
<b>Category:</b> mdrun	
<b>Target version:</b> 3.3	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	

#### Description

The function of the dihedral restraints is currently a bit odd, and probably should be considered a bug:  $\phi_0$  and  $d\phi$  are read from the topology file in degrees and converted internally to radians, but the force constant ( $k_{\text{fac}}$ ) is used as read. In other words, to get the expected behavior, one would need to specify  $\phi$  and  $d\phi$  in the topology file in units of degrees, but the force constant in units of  $\text{kJ}/\text{rad}^2$  (rather than the expected  $\text{kJ}/\text{degree}^2$ ).

Probably this should be fixed so that expected input units are consistent. The relevant lines are in `dihres.c`:

```
phi0 = ip[type].dihres.phi*d2r;  
dphi = ip[type].dihres.dphi*d2r;  
kfac = ip[type].dihres.kfac*fc;
```

Sorry, I should have caught this before. I finally figured it out because I realized I was using units of  $\text{kJ}/\text{rad}^2$  for my input force constants but the input angles were in degrees. I had adjusted the force constant to get the restraint energy I was expecting, so I didn't notice before.

#### History

##### #1 - 03/31/2006 09:07 AM - David van der Spoel

This is by design, and is the same for all other angle and dihedral forces. Hence it is not a bug. I agree that it is not very elegant, it would be very messy to change it however, because it would imply reading interpreting the force constants in another way. I added a small remark in the manual in the relevant sections.

##### #2 - 03/31/2006 05:23 PM - David Mobley

OK, great. I realized after I submitted it that the angle force constant has the same units, so I can see why it is a bit confusing. Fixing the documentation should solve the problem, since essentially the problem was just that the 3.2 manual doesn't even mention dihedral restraints, so it's not clear what units one should expect things to be in.

##### #3 - 08/15/2007 03:17 PM - Ruby Lutz

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