

GROMACS - Bug #210

when `g_order` is used for tetrahedrality order, but all outputing results is zero.

09/20/2008 05:52 PM - tuyusong empty

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: analysis tools	
Target version: 3.3_rc2	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
when <code>g_order</code> is used for tetrahedrality order, but all outputing results is zero.	
1. checking the src file: <code>src/tools/gmx_order.c</code>	
2. the problem is	
The key code lines have been annotated:	
The 170-171 lines of the src file look like:	
<pre>/* sgmol[i] += 3*cost2/32; sgmol[i] += cost2; /</pre>	
3. the possible modification	
<pre>/ sgmol[i] += 3*cost2/32; */ sgmol[i] += cost2;</pre>	
This is a trivial bug.	
Yusong Tu.	

History

#1 - 11/09/2008 09:27 AM - Erik Lindahl

Sorry for not seeing this; apparently my search filter doesn't show "unconfirmed" bugs by default...

I'm not 100% what this fix actually does, but it makes sense that *something* should go in `sgmol[i]`, so I've committed it.