

GROMACS - Bug #53

Angle definitions maybe wrong in g_chi

03/03/2006 09:18 AM - David van der Spoel

Status: Closed	
Priority: High	
Assignee: David van der Spoel	
Category: analysis tools	
Target version: 3.3	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
<p>David, I saw the discussion about the omega angle calculated by by the g_chi program and you pointed out that the omega definition is wrong in 3.3. I think the phi and psi angles are wrongly definied as well. Compare the angles given by g_rama and by g_chi -rama. In the result given by the latter program the phi psi are also wrong.</p> <p>bye, Sandor Lovas (from the mailing list)</p>	

History

#1 - 04/02/2006 05:11 PM - Erik Lindahl

Fixed angle definitions in g_chi, so that Phi/Psi angles are defined correctly whenever possible instead of using faked angles involving O. (This is still done for the first and last residues). The phase is now also correct for Omega dihedrals, and ramachandran values should agree with those from g_rama.