GROMACS - Bug #67

g_rdf has GROMOS atom names hardocoded

04/09/2006 04:53 PM - David van der Spoel

Status:	Closed		
Priority:	High		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:	3.3.1		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Summary says it all, this is in the structure factor calculation

History

#1 - 04/18/2006 08:28 AM - David van der Spoel

Created an attachment (id=37)
Patched version of gmd_rdf.c

This version does not check on the atom type but on the atom name.

#2 - 08/21/2006 01:28 PM - David van der Spoel

The proposed version has been adopted in 3.3.1 and 4.0.

Files

gmx_rdf.c	34.2 KB	04/18/2006	David van der Spoel