GROMACS - Bug #66

graph problem with distance restraints

04/08/2006 12:56 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

Analysis tools will bail out upon reading a tpr file with distance restraints
with the following error:

Fatal error:
More than 8 graph edges per atom (atom 19)

History

#1 - 06/12/2006 11:47 AM - no name

Although the bug can be partially resolved changing the peroidic boundary
conditions to pbc = full and using the LINCS constraint algorithm, the problem
remains to be resolved...

#2 - 04/14/2007 03:24 PM - David van der Spoel

Fixed in CVS for 3.3 and 4.0. The number of bonds is now unlimited, but this
does mean one can get inconsisten shift messages when a distance is larger than
half the box size.