GROMACS - Bug #327

g_mindist in 4.0.4 produces weird results

05/20/2009 01:03 PM - Martin Hoefling

Status:	Closed		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	analysis tools		
Target version:	4.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:			

Description

Analyzing a transient protein complex (chain A with residue 1-110 and B resid 111-199), I get weird results:

I am using option -or: "With -or, minimum distances to each
residue in the first group are determined and plotted as a function of
residue number."

echo -e "chA\nchB\n"|g_mindist -or chAbyres.xvg
echo -e "chB\nchA\n"|g_mindist -or chBbyres.xvg

The last residue of chB always has a very low distance (0.09nm) which I can't observe in the simulation e.g. with vmd, and from how I understand this tool - there should be a residue on the other chain with the same (minimum) distance.

Here's what I did to check:

g_mindist of chain A / B / r_199 with -pi (periodic images). Looks fine, distances are > 3nm

chain A vs r_199 gives me the same results as chA vs chB

Any ideas what could be wrong?

History

#1 - 05/20/2009 01:23 PM - Martin Hoefling

Created an attachment (id=374)
Tarball with traj / tpr / input pdb / ndx file and g_mindist -or output

#2 - 05/21/2009 02:20 PM - Martin Hoefling

I double checked the distance lists and couldn't find residues in chA and chB with the same distance. Maybe I misinterpret the documentation of -or?

#3 - 09/04/2009 04:58 PM - Berk Hess

The residue index for -or was not built correctly for the last residue.
I fixed it for 4.0.6.

Berk

Files

mindistbyres.tar.gz	5.14 MB	05/20/2009	Martin Hoefling