

GROMACS - Bug #62

g_hbond problem

04/03/2006 08:13 AM - Jonathan Moore

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 I created a hydrogen bond map using g_hbond of version 3.3. The manual indicates that for the hbmap the "Ordering is identical to that in -hbn index file." However, in my case, the hbmap file contains 13 hydrogen bond indices, but the hbond.ndx file lists 20 sets of donors and acceptors. Thus, I don't know how to determine which specific hydrogen bonds are represented in the hbmap data. Another user suggested that the hbonds that actually occur are listed in the log file, but I could not get a log file to write (see other g_hbond bug submission by me).	

History

#1 - 04/03/2006 09:51 AM - David van der Spoel

Please upload trajectory (short) tpr and command line to reproduce the problem.

#2 - 04/04/2006 09:46 PM - Jonathan Moore

(In reply to comment [#1](#))

I figured out what the difficulty is. I used a command like:
g_hbond -f filename -s filename -num -hbn -hbm -n index.ndx

Thus, I was using the default -merge option. For the particular case I was running, there are 41 hbonds listed in the outputted hbond.ndx file but only 30 listed in the outputted hbmap file. I just noticed in the g_hbond output that 30 is the number of hbonds that result after merging hbonds with donor and acceptor swapped. So, I guess I could go through the 41 hbonds listed in hbond.ndx and throw out each of the second occurrences with donor and acceptor swapped, and that should then leave the identities of the hbonds listed in the hbmap file. However, I think it would be preferable to have a more straightforward method to determine the hbond identities. Maybe include in hbond.ndx a listing of hbonds after merging hbonds with donor and acceptor swapped and leaving off the index number of the H? Or, I could use the -nomerge option and handle the merging myself later.

#3 - 06/15/2006 02:25 PM - Erik Marklund

Fixed this problem, along with -contact functionality and bugs in -ac -life -hbm.

/Erik Marklund, June 15