GROMACS - Feature #1028

Tool to calculate fraction of native contacts during simulation

11/01/2012 06:46 PM - bipin singh

Status:	New	
Priority:	Normal	
Assignee:		
Category:	analysis tools	
Target version:		
Difficulty:	uncategorized	

Description

Currently there is no way to calculate fraction of native contacts during the simulation in GROMACS. It would be a nice feature if one could modify the existing tools to get this feature as most of the popular MD packages contains this analysis script (Also fraction of native contacts is being widely used as reaction coordinate in protein folding/unfolding studies).
As suggested by Justin and Eric, one could modify the g_mindist code or modify the the g_hbond code to get the -sel option to work again then one would get such information with -contact option.

History

#1 - 11/01/2012 10:05 PM - Szilárd Páll

- Target version deleted (4.5.6)

No features request for 4.x, new features have to go into 5.x.

#2 - 11/01/2012 10:27 PM - David van der Spoel

- Assignee deleted (David van der Spoel)

- Priority changed from High to Normal

g_hbond will probable be modularized to some extent based on the new analysis framework in 5.0. I definitely don't have time for this. Priority set to normal since this is not a crucial issue.