

GROMACS - Bug #1668

Incorrect PBC removal in gmx hbond

01/07/2015 11:28 PM - Erik Marklund

Status:	Rejected	
Priority:	Normal	
Assignee:	Erik Marklund	
Category:	analysis tools	
Target version:	5.0.5	
Affected version - extra info:	Has been around for some time so many versions affected.	Difficulty: uncategorized
Affected version:	5.0	

Description

The PBC removal in gmx hbond appears to be done along the box vectors instead of orthogonal vectors. pbc_correct_gem() is to blame

History

#1 - 01/13/2015 04:08 PM - Erik Marklund

- Status changed from New to Rejected

The description is incorrect. PBC removal should be along box vectors. This issue furthermore only arose in a now abandoned patch.