Remove support for generation of virtual sites to replace aromatic rings in standard residues

12/19/2019 11:57 AM - Eric Irrgang

Status: New
Priority: Normal
Assignee: 
Category: core library
Target version: 
Difficulty: uncategorized

Description
Deprecated in GROMACS 2019

These are thought to produce artefacts under some circumstances (unpublished results), were never well tested, are not widely used, and we need to simplify pdb2gmx.

History
#1 - 12/19/2019 12:13 PM - Eric Irrgang
- Private changed from Yes to No