Currently TNG is prohibitive slow for very large systems. I gave up waiting after ~10min to write a file for a system containing 2M atoms. The problem is that several functions search large tables for every atom in the system. E.g. tng_chain_residue_find (O(N^2), N: residues) or tng_residue_atom_w_id_add (O(NM) N: total number of atoms, M:atoms per residue). It seems, TNG needs to be profiled for a large system, and those searches need to be replaced with hash-table lookups.
- Status changed from Accepted to Fix uploaded

#10 - 06/24/2014 09:58 PM - Magnus Lundborg
- Status changed from Fix uploaded to Resolved

#11 - 06/26/2014 10:15 PM - Erik Lindahl
- Status changed from Resolved to Closed

#12 - 07/15/2014 06:48 AM - Teemu Murtola
- Tracker changed from Feature to Bug
- Category set to core library
- Target version changed from 5.x to 5.0
- Affected version set to 5.0