

## Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2979	GROMACS	Task	Accepted	Normal	Reconsider default 1 OpenMP thread per thread-MPI rank	Berk Hess	11/01/2019 03:24 PM	2020-rc1
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	08/26/2019 03:47 PM	2020
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 AM	
2391	GROMACS	Task	Accepted	Normal	re-enable TPI test	Berk Hess	01/09/2019 05:17 PM	2020
2822	GROMACS	Task	Accepted	Normal	Make nbxnm a module	Berk Hess	01/03/2019 03:07 PM	2020
2798	GROMACS	Bug	New	Normal	Default mpi rank number fails when there are 16 cores and 3 gpus	Berk Hess	12/11/2018 10:11 PM	2020
2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	12/03/2018 01:15 PM	2020
1880	GROMACS	Bug	Feedback wanted	Normal	PP-PME load balancing issue	Berk Hess	10/03/2018 09:45 PM	future
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 PM	
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
1843	GROMACS	Bug	In Progress	Normal	pbc=xy with 2 walls floating point exception with the verlet scheme	Berk Hess	10/31/2016 11:35 AM	
1192	GROMACS	Feature	Accepted	Normal	Add support for Verlet scheme with Buckingham	Berk Hess	07/11/2016 08:19 PM	
1658	GROMACS	Feature	New	Normal	Electrostatics treatment for multiple lambda sites	Berk Hess	07/11/2016 08:05 PM	
1162	GROMACS	Feature	New	Normal	Implement gb_saltconc	Berk Hess	02/26/2013 05:33 PM	future
1053	GROMACS	Feature	In Progress	Normal	L-BFGS doesn't use constraints or call do_em_step	Berk Hess	01/18/2013 11:00 AM	future
2192	GROMACS	Bug	Accepted	Low	grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error	Berk Hess	12/03/2018 01:25 PM	2020
760	GROMACS	Feature	New	Low	Implement rigid body groups	Berk Hess	12/30/2012 06:04 AM	future