

## Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3274	GROMACS	Bug	New	Normal	Remove ARM NEON SIMD		12/28/2019 07:53 AM	2021-infrastructure-stable
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	12/20/2019 08:20 AM	2021-infrastructure-stable
3112	GROMACS	Bug	Closed	Normal	CG minimization with DD broken by recent refactoring	Berk Hess	10/02/2019 11:38 AM	2020-beta2
3111	GROMACS	Bug	Closed	Low	sample_restraint testing should not download files	Eric Irrgang	10/31/2019 03:35 PM	2020-beta2
3097	GROMACS	Bug	Closed	Normal	nbnxm grid issue with regressiontest complex/nbnxn_rzero with gpubufferops path		12/02/2019 01:12 PM	2020-beta3
3091	GROMACS	Bug	Closed	Normal	simulator comparison test failing in gpucomm matrix	Mark Abraham	09/18/2019 01:41 PM	2020-beta1
3090	GROMACS	Bug	Closed	Normal	virtual site reference manual docs need care with subscripts	Paul Bauer	09/17/2019 11:02 AM	2020-beta2
3089	GROMACS	Task	Closed	Normal	relax dlb scaling limit when that would suit GPU halo exchange	Berk Hess	10/14/2019 01:32 PM	2020-beta2
3084	GROMACS	Bug	Closed	Normal	gmx report-methods test unstable	Paul Bauer	10/14/2019 01:31 PM	2020-beta2
3065	GROMACS	Task	Closed	Normal	Agree and implement version support for GROMACS 2021		08/24/2019 05:25 PM	
2981	GROMACS	Bug	New	Normal	segfault in opencl build		06/18/2019 03:30 AM	
2921	GROMACS	Bug	Closed	Normal	hwloc test makes invalid assumptions	Mark Abraham	04/15/2019 08:16 AM	2019.2
2917	GROMACS	Bug	Closed	Low	do_steep segfaults with non-interacting system	Mark Abraham	05/03/2019 11:18 AM	2019.3
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 PM	2021-infrastructure-stable
2913	GROMACS	Task	Closed	Low	remove GMX_HAVE_WINSOCK	Mark Abraham	04/10/2019 05:10 PM	2020-beta1
2908	GROMACS	Task	New	Normal	Renaming things in nbnxm	Berk Hess	03/28/2019 10:10 AM	
2899	GROMACS	Task	Closed	Normal	Update testing matrix versions for GROMACS 2020 release	Mark Abraham	10/29/2019 05:41 PM	2020-infrastructure-update-post-beta1
2897	GROMACS	Bug	New	Normal	rotation/flex2 can still fail on cpu-only run on OpenCL build		04/04/2019 06:24 PM	
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	12/27/2019 04:38 PM	future
2877	GROMACS	Task	New	Normal	use gmx::Options more	Mark Abraham	12/20/2019 01:22 PM	2021
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2861	GROMACS	Task	Closed	Normal	import an implementation of c++17 std::optional	Mark Abraham	04/29/2019 11:47 AM	future
2839	GROMACS	Task	New	Normal	make module and file naming consistent		01/16/2020 05:11 PM	2021
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	12/28/2019 10:40 AM	2021
2831	GROMACS	Task	Closed	Normal	Bump required version numbers of infrastructure for 2020	Mark Abraham	10/29/2019 05:40 PM	2020-infrastructure-update-post-beta1
2826	GROMACS	Task	Closed	Low	introduce ssize free function		02/27/2019 05:43 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2797	GROMACS	Task	Rejected	Low	document whether fourier-nx/y/z mdp options disable PME tuning		12/10/2018 01:07 PM	
2796	GROMACS	Task	New	Low	clarify what mdrun -cpt means		01/03/2019 02:09 PM	
2784	GROMACS	Task	Closed	Low	update parallel lincs reference manual section for update groups	Berk Hess	12/05/2018 05:15 PM	2019
2783	GROMACS	Bug	Closed	Normal	PDF reference manual suggestions	Paul Bauer	12/10/2018 04:15 AM	2019-rc1
2782	GROMACS	Bug	Closed	Normal	dd flowchart image loses resolution in HTML sphinx output	Paul Bauer	11/30/2018 02:39 PM	2019-rc1
2775	GROMACS	Bug	Closed	Normal	number of ranks reporting was wrong		12/10/2018 03:05 AM	2019
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		12/20/2019 01:09 PM	2021
2772	GROMACS	Task	Rejected	Normal	check performance on POWER9		04/05/2019 04:50 PM	2019.2
2770	GROMACS	Task	New	Normal	change branch maintenance policy		01/16/2020 05:09 PM	2021
2767	GROMACS	Bug	Closed	Normal	grompp warns about md + FEP even for fully coupled states	Berk Hess	12/20/2019 08:17 AM	2020-rc1
2761	GROMACS	Feature	New	Low	lincs-order 4 is too conservative for some force fields		11/16/2018 09:55 AM	
2751	GROMACS	Task	Closed	Normal	checking for Sphinx executable version needs improvement	Mark Abraham	11/16/2018 09:19 AM	2019
2750	GROMACS	Task	Closed	Normal	Jenkins FPE should be disabled for 2018 branch	Mark Abraham	11/11/2018 03:08 AM	2018.4
2728	GROMACS	Bug	Closed	Normal	Fix NB kernel picking		02/28/2020 09:13 AM	2020.1
2726	GROMACS	Bug	Closed	Normal	FP exception in cufft 7.0		12/13/2018 11:41 AM	2019
2724	GROMACS	Task	Closed	Normal	Clean up organization of bonded cuda module	Mark Abraham	11/29/2018 10:41 AM	2019
2723	GROMACS	Task	New	Normal	Update mdrun-performance.rst to clearly express the nature of task	Joe Jordan	02/27/2020 11:07 AM	2020.2
2722	GROMACS	Bug	Closed	Normal	gmxapi may over-manage RPATH	Mark Abraham	12/20/2019 08:22 AM	2020-rc1
2704	GROMACS	Bug	Closed	Normal	investigate change to log file	Mark Abraham	10/21/2018 11:07 AM	2019
2699	GROMACS	Task	New	Normal	Test POWER9		12/04/2019 03:29 PM	2021-infrastructure-stable
2692	GROMACS	Bug	Closed	Normal	docs should not have unused files	Paul Bauer	10/29/2018 11:01 AM	2019
2691	GROMACS	Feature	Closed	Normal	MiMiC needs reference documentation		12/03/2018 12:06 PM	2019
2690	GROMACS	Task	Closed	Normal	relax new dependency cycle		10/15/2018 05:13 PM	2019
2689	GROMACS	Bug	Rejected	Normal	gpu timer state not cleaned up		02/08/2019 06:51 AM	2019.1
2671	GROMACS	Task	New	Normal	replace constants like M_PI		12/20/2019 01:17 PM	future
2665	GROMACS	Task	Closed	Normal	remove fermi support	Szilárd Páll	10/22/2018 12:23 PM	2019
2664	GROMACS	Bug	Closed	Low	gmxapi tests using gmx to make a .tpr needs to be quieter	Paul Bauer	11/23/2018 02:17 PM	2019
2655	GROMACS	Task	Closed	Normal	Remove NVML support	Mark Abraham	10/01/2018 11:46 AM	2019

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2654	GROMACS	Task	Closed	Normal	make more symbols always defined		01/08/2019 05:27 PM	2020
2651	GROMACS	Feature	Closed	Normal	clean up mdrun log file handling	Mark Abraham	10/11/2018 10:15 PM	2019
2648	GROMACS	Bug	Closed	Normal	icc 18 post-submit fails to compile not_null tests		11/28/2018 03:39 PM	2019
2646	GROMACS	Bug	Closed	Normal	gmxapi uses major() and minor() which clashes with deprecated glibc macros	Eric Irrgang	09/19/2018 03:03 PM	2019
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/24/2018 05:51 PM	future
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2636	GROMACS	Bug	Closed	Low	DD code writes to terminals too much	Mark Abraham	10/03/2018 11:33 PM	2019
2635	GROMACS	Bug	Closed	Normal	Failing to detect GPUs should not write to terminals	Mark Abraham	12/21/2018 09:20 AM	2019
2629	GROMACS	Task	Closed	Normal	stabilise testing matrices for GROMACS 2019		01/21/2019 01:22 PM	2019.1
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2578	GROMACS	Bug	Closed	Normal	with PME on GPU, EM setup does not propagate state->x pinning settings	Mark Abraham	08/23/2018 10:47 AM	2018.3
2571	GROMACS	Bug	Closed	Normal	clang-tidy cmake needs improvement	Roland Schulz	07/13/2018 07:20 AM	2019
2569	GROMACS	Task	Closed	Normal	announce deprecations in GROMACS 2019	Mark Abraham	12/17/2018 01:45 PM	2019
2558	GROMACS	Bug	Rejected	Normal	gmx polystat mis-uses nmol	Mark Abraham	06/21/2018 03:13 PM	2018.3
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 PM	
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		09/23/2018 11:47 PM	future
2518	GROMACS	Task	New	Normal	redesign task-assignment code for OpenCL		12/20/2019 12:19 PM	future
2508	GROMACS	Bug	Closed	Low	gmx enemat segment faults	Mark Abraham	06/05/2018 04:26 PM	2018.2
2505	GROMACS	Task	Closed	Normal	increase cmake requirement for GROMACS 2020	Mark Abraham	01/28/2019 11:56 AM	2020
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	
2495	GROMACS	Task	Accepted	Normal	replace -noconfout with mdp option	Mark Abraham	12/28/2019 10:39 AM	2021
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 PM	future
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		12/02/2019 01:22 PM	2021-infrastructure-stable
2478	GROMACS	Task	New	Low	avoid use of getenv in static initialization		04/13/2018 11:57 AM	
2434	GROMACS	Bug	Closed	Normal	wrong values accumulated to dvdlambda in SHAKE with FE calcs	Mark Abraham	03/06/2018 04:31 PM	2018.1
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	12/20/2019 12:13 PM	2021

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2423	GROMACS	Task	New	Normal	modernize constraints code	Mark Abraham	09/19/2018 03:01 PM	future
2422	GROMACS	Task	New	Normal	write C kernel for tables in Verlet scheme		02/26/2018 01:38 PM	
2405	GROMACS	Bug	Closed	Normal	improve gpu_utils-test	Mark Abraham	03/02/2018 03:52 PM	2018.1
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	12/15/2019 11:51 AM	2021-infrastructure-stable
2394	GROMACS	Bug	Closed	Low	energy average printing segfaults when no data sets are recorded	Mark Abraham	02/06/2018 04:34 PM	2018.1
2392	GROMACS	Bug	Closed	Normal	mdp field 'define' does not correctly handle inputs that used to work	Mark Abraham	03/02/2018 03:52 PM	2018.1
2390	GROMACS	Bug	Feedback wanted	Normal	GROMACS build system should check for valid nvcc flags before use		12/20/2019 12:13 PM	2021
2376	GROMACS	Task	New	Normal	max_mpi_ranks has wrong name		02/10/2018 11:03 AM	
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
2371	GROMACS	Task	New	Normal	mtop searching needs reconsideration		01/04/2018 11:54 AM	future
2370	GROMACS	Bug	Closed	Normal	pdb2gmx does not report why chains of residues are terminated		02/28/2018 11:27 PM	
2368	GROMACS	Task	In Progress	Normal	update implementation of gmx msd	Kevin Boyd	11/03/2018 07:43 PM	future
2367	GROMACS	Task	New	Normal	construct pbc_simd less often		09/24/2018 11:02 PM	future
2355	GROMACS	Task	Closed	Normal	update bundled googletest	Mark Abraham	02/23/2018 05:51 PM	2019
2354	GROMACS	Feature	New	Normal	develop configuration file support for control of task layout		09/19/2018 03:01 PM	future
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		12/20/2019 12:12 PM	2021
2346	GROMACS	Bug	Closed	Normal	inconsistent behavior of mdrun -nt 1 with mdrun -nt 3 when both are undersubscribed	Mark Abraham	12/19/2017 02:29 AM	2018-beta3
2345	GROMACS	Bug	Closed	Normal	Avoid duplicate over-subscription note+warning	Mark Abraham	12/19/2017 02:37 AM	2018-beta3
2340	GROMACS	Bug	Closed	Normal	avx512fma test code warning with icpc		12/11/2017 01:23 PM	2018
2339	GROMACS	Feature	Closed	Low	sum of two largest charge group is enormous and bigger than rlist		12/15/2017 11:40 AM	2018-beta3
2332	GROMACS	Bug	Closed	Normal	verlet + pme-user should give grompp and mdrun fatal error	Mark Abraham	12/12/2017 11:50 AM	2016.5
2326	GROMACS	Bug	Closed	Normal	double precision avx(2)_128_fma and sse4.1 broken		12/14/2017 01:18 AM	2018-beta2
2325	GROMACS	Bug	Closed	Normal	avx512 double precision simd failure		12/14/2017 10:17 AM	2018
2323	GROMACS	Bug	Closed	Normal	avx512 implementation of operator << requires immediate with gcc 6.4		12/11/2017 11:54 AM	
2273	GROMACS	Bug	Closed	Normal	CUDA CC 2.0 issue		11/28/2017 05:59 PM	2018
2269	GROMACS	Feature	Rejected	Low	support some latest-1 versions in Jenkins testing		01/07/2019 01:48 AM	
2241	GROMACS	Bug	New	Low	refdata can segfault when reading		09/07/2017 11:57 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2225	GROMACS	Bug	Closed	Low	gmx trjcat -o pdb doesn't work		12/12/2017 10:37 PM	
2223	GROMACS	Bug	Closed	Normal	Orientation restraints broken with OpenMP	David van der Spoel	08/15/2017 04:55 PM	2016.4
2220	GROMACS	Feature	New	Normal	report relevant env var behaviour to console		07/31/2017 09:40 PM	
2217	GROMACS	Bug	New	Low	GPU emulation and separate PME ranks doesn't work properly		12/12/2017 11:50 AM	
2204	GROMACS	Bug	Closed	Low	mismangement of npme variable	Mark Abraham	12/21/2017 03:20 PM	2018-rc1
2199	GROMACS	Bug	Closed	Normal	continuations can report double the initial temperature	Berk Hess	06/27/2017 07:22 PM	2016.4
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	12/20/2019 12:11 PM	2021
2182	GROMACS	Task	New	Low	de-duplicate code in densorder and hydorder		05/16/2017 11:29 AM	
2180	Support Platforms	Feature	Fix uploaded	Low	releng matrices would work better with a hint for execution		05/19/2017 01:02 AM	
2178	GROMACS	Task	New	Normal	Move checks for specific warnings to source repo		05/12/2017 03:57 PM	
2175	GROMACS	Task	New	Normal	improve clang static analyzer docs further		01/04/2018 04:13 PM	future
2174	GROMACS	Bug	Closed	Normal	LJPME should not accept VDW modifiers it does not support	Berk Hess	05/31/2017 08:39 PM	2016.4
2173	GROMACS	Bug	Closed	Low	checkpoint restart with missing restart file is too verbose	Mark Abraham	12/11/2017 09:19 PM	2016.5
2172	GROMACS	Bug	Closed	Normal	EM run does give valid reason for not printing performance report	Mark Abraham	12/17/2017 07:12 AM	2016.5
2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		12/29/2019 10:31 AM	2021
2164	GROMACS	Bug	Closed	Normal	SIMD sqrt in double-precision build does not work correctly		10/25/2017 04:57 PM	2018
2161	GROMACS	Task	Closed	Normal	update the way testing matrices are specified	Mark Abraham	10/15/2018 05:16 PM	2019
2146	GROMACS	Task	Closed	Normal	salvage documentation from old webpage		12/28/2018 12:35 PM	2019
2135	GROMACS	Task	Closed	Normal	check non-Jenkins compilers work	Mark Abraham	01/04/2018 04:20 PM	2018
2134	GROMACS	Task	Closed	Normal	assess whether Jenkins is testing multi-rank runs appropriately		01/04/2018 02:24 PM	2018
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2123	GROMACS	Task	Closed	Normal	Use RAll for file-static data	Mark Abraham	04/24/2017 09:12 AM	2018
2122	GROMACS	Task	Closed	Low	Stop using where()	Mark Abraham	04/13/2018 01:21 PM	2019
2115	GROMACS	Task	New	Normal	trjconv does too many things, and combinations of them work poorly		10/02/2018 09:04 AM	
2112	GROMACS	Bug	Closed	Normal	Rerun tests with MSVC may expose existing bug		04/05/2018 11:04 AM	
2105	GROMACS	Bug	Closed	Normal	multi-domain rerun broken	Mark Abraham	02/06/2017 04:10 PM	2016.2

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2101	GROMACS	Feature	New	Low	warning could print the offending line, as well as its number		01/20/2017 03:06 PM	
2098	GROMACS	Bug	Closed	Low	NVML linking fails	Mark Abraham	03/15/2017 05:56 PM	2018
2093	GROMACS	Bug	Closed	Normal	possible unstable listedforces-test BondedTest.IfncBondsPbcNo		12/12/2017 10:56 PM	
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2072	GROMACS	Feature	Closed	Low	target hardware description is silent about the result	Mark Abraham	10/03/2018 09:38 PM	2019
2066	Support Platforms	Feature	Closed	Normal	possible release workflow enhancements		05/31/2017 07:48 PM	
2050	GROMACS	Bug	Closed	Normal	amber03 HIP charges are wrong	Mark Abraham	09/07/2016 03:06 PM	5.1.4
2049	GROMACS	Bug	Closed	Normal	remove duplicate amino-acid definitions	Mark Abraham	11/17/2016 03:35 PM	5.1.4
2039	GROMACS	Bug	New	Normal	mrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
2021	GROMACS	Bug	Rejected	Normal	mrun -multidir should not have default		12/12/2017 03:27 PM	
2016	GROMACS	Bug	Rejected	Normal	DD setup may sometimes use wrong periodic images		08/08/2016 03:09 PM	
2012	GROMACS	Task	Closed	Normal	Bump required version numbers of infrastructure for 2018	Mark Abraham	11/01/2018 10:06 AM	2018
2009	GROMACS	Task	New	Normal	improve command-line reporting of useful things		07/26/2016 12:54 PM	
2006	GROMACS	Bug	Closed	Normal	issues with not using 64-bit step numbers everywhere		07/30/2016 08:38 PM	
2004	GROMACS	Bug	Closed	Low	parallelism selection code needs work		03/17/2018 12:32 AM	
2003	GROMACS	Task	New	Normal	reconsider various simd flags		07/07/2016 11:23 PM	
2002	GROMACS	Feature	Closed	Normal	extend cmake/gmxDetectTargetArchitecture.cmake for ARM and POWER		01/07/2019 01:52 AM	
2000	GROMACS	Bug	Closed	Low	cmake 3.5.1 + ninja not quite happy with dev-guide build system	Teemu Murtola	07/08/2016 03:21 PM	2016
1998	GROMACS	Bug	Closed	Normal	membed is apparently broken		07/11/2016 09:12 PM	2016
1997	GROMACS	Bug	Closed	Low	big-endian power7 testbits is broken		07/05/2016 01:46 AM	2016
1993	GROMACS	Bug	Closed	Normal	calc_verlet_buffer_size can't handle nstlist==1	Berk Hess	06/27/2016 07:28 PM	2016
1992	GROMACS	Task	Closed	Low	mrun should not advise users of things that don't matter	Berk Hess	06/22/2016 05:43 PM	2016
1989	GROMACS	Bug	Closed	Low	simple distance restraints should work with REMD and multiple ranks per simulation	Mark Abraham	08/10/2016 12:31 PM	5.1.3
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		12/20/2019 12:07 PM	2021
1975	GROMACS	Feature	Closed	Normal	grompp should warn if .mdp define does nothing	Kevin Boyd	06/02/2019 09:07 PM	2020
1973	GROMACS	Task	New	Normal	OpenCL implementation wish list		05/27/2016 03:42 PM	
1963	GROMACS	Task	New	Low	collect examples of systems where users tried to do something that performed badly	Mark Abraham	08/09/2016 07:30 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1953	GROMACS	Feature	New	Low	use more regular polymorphism for GPU code		05/06/2016 10:06 PM	future
1947	GROMACS	Task	New	Normal	Consider fixing corner case in TinyXML2	Mark Abraham	04/19/2016 01:40 AM	
1937	GROMACS	Task	New	Low	stop supporting changing CUDA host compiler	Mark Abraham	10/15/2018 05:19 PM	future
1936	GROMACS	Task	New	Normal	treat default-able mdp fields as strings		04/02/2016 10:32 PM	future
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		12/29/2019 10:35 AM	2021
1913	GROMACS	Bug	Closed	Normal	tabulated bonded interaction files cannot be read	Mark Abraham	06/08/2016 10:26 AM	5.1.3
1908	GROMACS	Task	Closed	Normal	remove external dependencies that are sometimes problematic	Mark Abraham	06/27/2017 11:17 PM	2018
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	
1897	GROMACS	Bug	Rejected	Normal	Memory leak in mdrun		03/15/2016 03:09 PM	
1893	GROMACS	Bug	Closed	Normal	grompp fails to warn about .mdp values with the wrong type	Mark Abraham	02/02/2017 10:35 PM	5.1.2
1883	GROMACS	Bug	Closed	Normal	many velocity-verlet combinations do not produce exact restarts		05/08/2016 11:55 AM	
1882	GROMACS	Bug	Closed	Normal	issue with DD missing impossible exclusions	Mark Abraham	02/03/2016 01:52 PM	2016
1872	GROMACS	Bug	Closed	Normal	md-vv with NPT and more than one temperature-coupling group was broken	Mark Abraham	01/12/2016 04:24 PM	5.0.8
1868	GROMACS	Task	Closed	Normal	implement mdrun -rerun better, simplifying do_md	Mark Abraham	10/03/2018 09:40 PM	2019
1867	GROMACS	Feature	New	Normal	make coupling implementations reversible		12/02/2015 07:43 AM	
1858	GROMACS	Bug	Closed	Normal	compute globals should not have logic about which integrator is in use		01/12/2016 04:23 PM	5.1.2
1855	GROMACS	Task	New	Normal	Convert preprocessor use so that symbols are always defined		06/28/2016 02:17 PM	
1852	GROMACS	Task	New	Normal	Remove group scheme		03/03/2020 09:03 PM	future
1823	GROMACS	Bug	Closed	Low	checks for mdrun rerun with energy groups and possible GPUs not working correctly	Mark Abraham	11/23/2015 05:47 PM	5.1.1
1822	GROMACS	Bug	Closed	Low	mdrun writes broken energy group values to .edr file	Erik Lindahl	01/03/2018 03:47 PM	2018
1815	Support Platforms	Task	In Progress	Normal	implement and execute plan for new releng machinery		10/15/2016 05:37 PM	
1795	GROMACS	Bug	Closed	Normal	limit test binaries to only one MPI rank where necessary/appropriate	Teemu Murtola	05/03/2016 07:37 PM	2016
1793	GROMACS	Task	New	Normal	cleanup of integration loop	Mark Abraham	10/31/2018 10:49 PM	future
1785	GROMACS	Task	New	Low	no pV term written to energy file when pressure coupling is anisotropic		07/26/2015 01:47 PM	future
1777	GROMACS	Bug	Closed	Low	Teach mdrun about explicit -append		07/11/2016 05:09 PM	2016
1768	GROMACS	Task	New	Normal	decide future of command-line options vs env vars		11/03/2016 05:51 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1767	GROMACS	Bug	Closed	Normal	Coulomb energy sometimes wrong in complex/nbxxn_vsite	Berk Hess	10/14/2015 06:02 PM	4.6.8
1758	GROMACS	Task	New	Normal	Verlet scheme reorganization / modularization	Mark Abraham	07/20/2015 06:33 PM	future
1749	GROMACS	Bug	Closed	Normal	pairs_nb is unknown directive in grompp		06/16/2015 10:30 PM	5.0.6
1740	GROMACS	Bug	Closed	Normal	invalid use of gmx_simd_check_and_reset_overflow	Mark Abraham	06/04/2015 02:00 PM	5.0.6
1730	GROMACS	Bug	New	Normal	gmx compare does not compare all fields of a .tpr		06/12/2015 09:33 PM	future
1729	GROMACS	Task	New	Normal	Resolve whether and how to resolve "state" variables stored in .tpr		05/13/2015 10:48 AM	future
1724	GROMACS	Bug	Closed	Low	membed docs missing		06/16/2015 11:41 PM	5.1
1720	GROMACS	Feature	Rejected	Low	Manage GROMACS JIT caching		08/03/2016 12:25 PM	future
1706	GROMACS	Bug	Closed	Low	NVML message reports wrong version	Szilárd Páll	06/16/2015 11:40 PM	5.1
1703	GROMACS	Bug	Closed	Normal	be less vocal about affinity where it is not relevant		06/16/2015 12:55 PM	5.1
1701	GROMACS	Bug	Closed	Low	arrayref doesn't always work on BlueGene/Q xlc	Mark Abraham	06/16/2015 12:55 PM	5.1
1700	GROMACS	Bug	Closed	Normal	tarball man pages are too deep in the file hierarchy		04/09/2015 11:19 AM	5.1
1699	GROMACS	Task	Closed	Low	document change in andersen thermostat behaviour in the code		07/11/2016 08:03 PM	5.1
1697	GROMACS	Bug	Closed	Normal	rare replica-exchange problem	Michael Shirts	05/06/2015 04:52 PM	5.0.5
1696	GROMACS	Task	Closed	Normal	FFTW auto-build and advice is no longer generally applicable		06/16/2015 10:25 PM	5.1
1695	GROMACS	Bug	Closed	Normal	Andersen thermostats wrong in 5.0	Mark Abraham	04/09/2015 10:57 AM	5.0.5
1683	GROMACS	Bug	Closed	Normal	mdrun-only build does not link correctly	Mark Abraham	03/05/2015 10:25 AM	5.1
1681	GROMACS	Bug	Closed	Normal	use of incorrect initial value of variable	Mark Abraham	04/09/2015 11:07 AM	5.1
1677	GROMACS	Bug	Closed	Low	floating-point exceptions found	Erik Lindahl	06/16/2015 10:28 PM	5.1
1673	GROMACS	Bug	Closed	Normal	mis-use of simd.h after refactoring	Mark Abraham	11/16/2015 06:11 PM	5.1.1
1666	GROMACS	Feature	New	Normal	new approach for Verlet-scheme kernel generation	Erik Lindahl	10/08/2018 07:04 PM	future
1659	GROMACS	Bug	Closed	Low	DD error message writes ncells pointer value, not value pointed to		01/12/2015 06:34 PM	5.0.5
1647	GROMACS	Bug	Closed	High	race condition with lincs + openmp + free-energy	Mark Abraham	12/09/2014 04:18 PM	5.0.3
1633	GROMACS	Bug	Closed	Low	mdrun -nsteps -1 reports silly numbers	Szilárd Páll	12/15/2014 09:45 PM	5.0.4
1617	GROMACS	Bug	Closed	Normal	uncrustify indenting strangely		07/11/2016 09:08 PM	
1616	GROMACS	Bug	Closed	Normal	configuration should check that the compiler will work with nvcc	Mark Abraham	01/10/2019 10:18 AM	2018
1615	GROMACS	Bug	Closed	Normal	possible bug in shell code		07/11/2016 07:44 PM	5.1
1614	GROMACS	Bug	Rejected	Low	thread-MPI has broken support for operations on MPI_INT		05/21/2016 04:54 PM	



#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1612	GROMACS	Feature	Closed	Normal	generating SIMD code		06/23/2016 11:14 AM	2016
1597	GROMACS	Feature	Closed	High	OpenCL port	Mark Abraham	07/05/2015 10:39 AM	5.1
1593	GROMACS	Bug	Closed	Low	step-size scaling in lbfgs doesn't work as intended		06/22/2015 12:42 PM	
1554	GROMACS	Bug	Closed	Low	build of template.cpp is broken	Teemu Murtola	10/01/2014 06:48 PM	5.1
1550	GROMACS	Bug	Closed	Low	GMX_MAX_MPI_THREADS has no implementation		06/22/2015 12:43 PM	
1535	GROMACS	Bug	Closed	Low	osx C++ symbol visibility warnings		08/18/2014 02:42 AM	
1531	GROMACS	Bug	Closed	Low	gmx bar fatal errors write garbage values		06/16/2015 11:46 PM	
1520	GROMACS	Bug	Closed	Normal	tng include/library/linking problems	Mark Abraham	06/29/2014 10:03 AM	5.0
1505	GROMACS	Task	New	Normal	improve handling of logging	Mark Abraham	01/02/2019 06:06 PM	
1500	GROMACS	Feature	New	Normal	Post-5.0 feature clean-up plan	Mark Abraham	08/26/2019 03:47 PM	
1487	GROMACS	Bug	Closed	Normal	do_cpt_enerhist sets variables that are not used	Berk Hess	07/11/2016 07:48 PM	
1472	GROMACS	Feature	Closed	Normal	complete removal of libgsl support	David van der Spoel	10/14/2015 06:10 PM	5.1.1
1459	GROMACS	Bug	Closed	Normal	clean up naming in pme code	Mark Abraham	07/15/2014 06:49 AM	5.0
1455	GROMACS	Task	Closed	Normal	fix regressiontests to correctly rerun and report the mdrun usage	Mark Abraham	07/11/2016 08:12 PM	5.1
1438	GROMACS	Bug	Closed	Normal	gmx mdrun -h broken	Teemu Murtola	02/24/2014 10:59 AM	5.0
1431	GROMACS	Bug	Closed	Normal	rotation/flex-t regressiontest failing on BG/Q	Carsten Kutzner	01/10/2019 03:50 PM	4.6.x
1429	GROMACS	Bug	Closed	Normal	shell code issues (broken with DD+grid; broken with Verlet scheme)	Berk Hess	06/20/2014 07:35 AM	4.6.6
1423	GROMACS	Bug	Closed	Normal	Using xtc-grps with a subset leaks memory	Mark Abraham	02/06/2014 10:38 PM	5.0
1397	GROMACS	Feature	New	Normal	gmx eneconv -offset 1.998 -dt 2 is broken for large times	Mark Abraham	06/12/2014 01:31 AM	future
1390	GROMACS	Task	Closed	Normal	manage C+11 support and CUDA better		06/27/2016 08:28 PM	2016
1378	GROMACS	Bug	Closed	Normal	Problem with interactions longer than pair-list range with NBNxN kernels	Berk Hess	12/03/2013 04:11 PM	4.6.4
1359	GROMACS	Bug	Closed	Normal	race condition(s) in hardware detection(?)	Mark Abraham	12/03/2013 04:14 PM	4.6.4
1347	GROMACS	Feature	New	Normal	future of tables	Berk Hess	01/09/2020 02:37 PM	future
1327	GROMACS	Bug	Closed	Normal	CMake bugs with set(var value PARENT_SCOPE)	Mark Abraham	10/16/2013 03:28 PM	4.6.4
1325	GROMACS	Bug	Closed	Normal	"Core t" time is wrong with separate PME nodes	Mark Abraham	10/16/2013 03:33 PM	4.6.4
1323	GROMACS	Task	New	Normal	determine future of existing tools for	David van der Spoel	12/04/2018 11:53 AM	
1320	GROMACS	Task	Closed	Normal	renaming of MPI-related conditional-compilation machinery	Mark Abraham	07/11/2016 08:18 PM	5.1
1319	GROMACS	Bug	Closed	Normal	g_tune_pme assumes an MPI environment is available	Mark Abraham	10/16/2013 01:49 PM	4.6.4

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1310	GROMACS	Task	Closed	Normal	update bundled threading support for GMock	Teemu Murtola	08/14/2013 08:03 AM	5.0
1298	GROMACS	Feature	Closed	Low	g_traj -f file.xtc -ov writes an empty file (silently?)		06/23/2014 02:16 PM	5.0
1297	GROMACS	Bug	Closed	Normal	infinite relative permittivity is incompletely implemented	Mark Abraham	06/22/2015 12:43 PM	
1295	GROMACS	Feature	Closed	Low	improve method for disabling use of GPU		12/03/2013 04:24 PM	4.6.4
1292	GROMACS	Feature	Closed	Normal	mddrun features to deprecate for 5.0	Mark Abraham	08/26/2019 03:47 PM	5.0
1291	GROMACS	Bug	Closed	Low	GPU/CPU force evaluation time ratio seems wrong	Szilárd Páll	07/11/2016 08:38 PM	2016
1290	GROMACS	Task	Closed	Low	OpenMPI 1.4.3 in Ubuntu 12.04 can produce simulation crashes with any version of GROMACS		12/03/2013 04:19 PM	
1289	GROMACS	Bug	Closed	Low	EEL_USER is true when eelPMESWITCH is true	Mark Abraham	10/16/2013 03:36 PM	4.6.4
1287	GROMACS	Feature	Closed	Normal	bump cmake requirement for 5.0	Mark Abraham	12/03/2013 04:17 PM	5.0
1271	GROMACS	Bug	Closed	Normal	GMXRC install is broken in master	Teemu Murtola	01/24/2014 07:16 PM	5.0
1269	GROMACS	Feature	Closed	Normal	create CMake variable for x86	Mark Abraham	10/31/2013 12:15 PM	4.6.4
1260	Support Platforms	Feature	Closed	Normal	create 4.6.x target		06/10/2014 02:02 PM	
1259	GROMACS	Bug	Closed	Normal	gcc-4.6.1 is buggy for AVX_256	Mark Abraham	05/13/2014 09:03 PM	4.6.x
1248	GROMACS	Bug	Closed	Low	nvcc host compiler sanity checks break with cmake >=2.8.10	Szilárd Páll	05/08/2016 12:50 PM	2016
1247	GROMACS	Feature	New	Normal	fix hardcoded references to atom names in analysis tools	Mark Abraham	06/12/2014 01:20 AM	future
1246	GROMACS	Task	New	Normal	expanded ensemble .tpr cannot be rerun	Michael Shirts	06/19/2015 01:56 PM	
1242	GROMACS	Feature	Closed	Normal	Documentation reorganization	Mark Abraham	01/07/2019 02:02 AM	
1241	GROMACS	Bug	Closed	Normal	gmx_system_xdr.[ch] files cite Sun's license, but COPYING does not	Mark Abraham	12/16/2013 05:41 PM	5.0
1236	GROMACS	Feature	Closed	Low	deprecate genion non-random insertion of ions	Mark Abraham	12/16/2013 05:40 PM	4.6.3
1235	GROMACS	Bug	New	Normal	peptide dihedral angle definitions violate IUPAC	David van der Spoel	06/19/2015 12:24 AM	future
1231	GROMACS	Feature	Closed	Low	single-point energies	Erik Lindahl	07/15/2014 06:44 AM	5.0
1228	GROMACS	Bug	Closed	Normal	various install guide (etc.) improvements noted on gmx-users	Mark Abraham	10/01/2014 06:55 PM	
1226	GROMACS	Bug	Closed	Low	make install installs .cvsignore files	Mark Abraham	02/10/2014 09:40 PM	4.5.8
1223	GROMACS	Bug	Closed	Normal	assert in 4.6	Mark Abraham	07/23/2016 03:32 PM	
1209	GROMACS	Feature	Closed	Normal	Reduce tools verbosity	Teemu Murtola	01/10/2014 11:37 PM	5.0
1208	GROMACS	Bug	Closed	Low	genion should treat a combination of -nn (or -np) with -conc better		07/05/2013 06:35 PM	4.6.3
1204	GROMACS	Feature	Closed	Normal	multi simulations should report that they are multi simulations	Erik Lindahl	04/27/2015 09:37 AM	5.0
1193	GROMACS	Feature	Rejected	Normal	planning for new trajectory file reading component	Mark Abraham	06/23/2016 04:05 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1190	GROMACS	Bug	New	Normal	Use of FORCE in setting cached variables	Mark Abraham	06/17/2014 06:09 AM	
1189	GROMACS	Bug	Closed	Normal	g_mindist and PBC	Rossen Apostolov	06/20/2014 04:27 PM	4.6.6
1186	GROMACS	Bug	Closed	Normal	install guide should mention how to configure blas and lapack	Mark Abraham	05/31/2013 10:44 AM	4.6.2
1182	GROMACS	Feature	New	Normal	improve trajectory writing to support parallel I/O		05/13/2014 10:42 AM	future
1177	GROMACS	Task	Closed	Normal	Moving manual repo into source repo	Mark Abraham	01/01/2014 06:51 AM	5.0
1164	GROMACS	Bug	Closed	Normal	rlistlong seems not to work correctly for grompp warning	Berk Hess	12/16/2013 05:39 PM	4.6.3
1159	GROMACS	Bug	Closed	Normal	Shell completions are partly broken	Teemu Murtola	02/08/2014 06:52 AM	5.0
1149	GROMACS	Bug	Closed	Normal	changes to dihedral restraints need corresponding changes to the manual	Rossen Apostolov	06/20/2014 10:39 AM	
1135	GROMACS	Bug	Closed	Normal	various detection and -multi don't work well enough together	Mark Abraham	07/05/2016 12:40 AM	2016
1124	GROMACS	Bug	Rejected	Normal	g_tool -hidden is broken - prints some binary rubbish	Mark Abraham	02/08/2013 01:08 PM	4.5.7
1123	GROMACS	Feature	Rejected	Normal	binary incompatibility		01/07/2019 02:05 AM	
1119	GROMACS	Bug	Closed	Normal	g_tune_pme needs work for GPUs and/or OpenMP	Mark Abraham	07/11/2016 07:59 PM	
1117	GROMACS	Bug	Closed	Low	ensemble-averaged distance restraints is probably broken		12/11/2017 12:19 PM	future
1111	GROMACS	Feature	Closed	Normal	use of rsqrt()	Mark Abraham	11/17/2016 03:46 PM	5.1
1108	GROMACS	Task	Closed	Normal	for releases, regenerate shell completion files in scripts directory	Mark Abraham	01/18/2013 03:26 PM	4.6
1107	GROMACS	Task	Closed	Normal	update online manual when releasing	Mark Abraham	07/11/2016 09:10 PM	5.1.3
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	
1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
1094	GROMACS	Bug	Closed	Normal	remove g_dih	Mark Abraham	01/07/2013 09:55 PM	4.6
1075	GROMACS	Bug	Closed	Normal	mdrun doesn't build on non-x86	Mark Abraham	12/28/2012 08:48 PM	4.6
1066	GROMACS	Bug	Rejected	Normal	FMA and icc	Mark Abraham	01/10/2013 02:52 AM	4.6
1063	GROMACS	Task	Closed	Normal	update documentation to correct "single" precision	Mark Abraham	06/29/2014 05:56 PM	5.0
1058	GROMACS	Task	Closed	High	gcc 4.4.something up to at least 4.6.0 can't compile AVX256 kernels	Erik Lindahl	12/29/2012 12:24 AM	4.6
1057	GROMACS	Bug	Closed	Normal	Remove acml vestiges	Mark Abraham	02/15/2014 07:10 PM	5.0
1056	GROMACS	Task	Accepted	Normal	status of fft5d_threads and fftw3_threads functionality	Mark Abraham	07/11/2016 08:21 PM	
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
1049	GROMACS	Bug	Closed	High	pick_nbnxn_kernel needs reworking	Berk Hess	01/18/2013 11:00 AM	4.6
1047	GROMACS	Feature	Closed	Normal	CMake configuration summary	Mark Abraham	07/11/2016 08:42 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1039	GROMACS	Task	Rejected	Low	investigate whether clang 3.0 really is buggy for the 4.6 group kernels	Mark Abraham	11/29/2013 12:26 AM	4.6.x
1024	GROMACS	Bug	Closed	Normal	REMD and Verlet lists	Berk Hess	01/14/2013 08:54 AM	4.6
1019	GROMACS	Bug	Closed	Normal	Timing stats broken	Berk Hess	01/14/2013 08:56 AM	4.6
1018	GROMACS	Bug	Closed	Normal	cmake and gpu acceleration	Szilárd Páll	01/01/2013 12:35 PM	4.6
1001	GROMACS	Bug	Closed	Normal	REMD statistics not collected properly any more	Michael Shirts	12/28/2012 08:34 PM	4.6
1000	GROMACS	Bug	Closed	Normal	Possible bug with v-rescale thermostat and md-vv	Michael Shirts	12/16/2013 05:38 PM	4.5.7
974	GROMACS	Task	Closed	Normal	Document use of environment variables		05/23/2014 02:02 PM	4.6
954	GROMACS	Bug	Closed	Low	calc_fluctuation_props output	David van der Spoel	10/21/2012 12:40 PM	4.5.6
886	GROMACS	Bug	Closed	Normal	pdb2gmx -cmap needs some mention in manual section 5.6	Rossen Apostolov	06/18/2014 02:11 PM	4.6.x
884	GROMACS	Bug	Closed	High	Don't allow mixed-precision appending	Berk Hess	04/16/2012 03:35 PM	4.6
862	GROMACS	Bug	Closed	Normal	g_hbond -r2 needs more documentation	David van der Spoel	05/23/2014 02:02 PM	
853	GROMACS	Task	Closed	Normal	Fix FAHCORE because it can no longer use -DMPI in CMakeLists.	Michael Shirts	12/28/2012 08:49 PM	4.6
843	GROMACS	Feature	New	Low	g_helixorient could benefit from more documentation	Erik Lindahl	05/23/2014 02:02 PM	
834	GROMACS	Bug	Closed	Normal	g_bond and PBC	Mark Abraham	06/13/2014 02:34 PM	
833	GROMACS	Bug	Closed	Normal	NUMA should probably not be used under Cygwin	Mark Abraham	04/16/2012 01:48 PM	4.5.6
820	GROMACS	Bug	Closed	Normal	dihedral restraints need more documentation	Erik Lindahl	06/20/2014 10:39 AM	5.0
816	GROMACS	Bug	Closed	Low	clarification of documentation of surface-tension coupling	Rossen Apostolov	06/20/2014 08:29 AM	5.0
813	GROMACS	Bug	Closed	Normal	pairs_nb needs documentation		05/23/2014 02:02 PM	5.0
812	GROMACS	Bug	Closed	Normal	g_sham needs more documentation	David van der Spoel	07/15/2014 06:43 AM	5.0
807	GROMACS	Bug	Closed	Normal	Use of [cmap]	Erik Lindahl	05/23/2014 02:02 PM	
781	GROMACS	Bug	Closed	Low	Reading .g96 trajectories is broken	Sander Pronk	09/06/2012 07:06 PM	4.5.6
776	GROMACS	Bug	Closed	Low	Typo in description of BD parameters	Berk Hess	05/23/2014 02:02 PM	
775	GROMACS	Bug	Closed	Low	Possible comment wrong in do_update_bd()	Berk Hess	04/26/2012 09:37 PM	4.5.6
765	GROMACS	Task	New	Normal	Improving serialization of data structures prior to communication	Mark Abraham	05/13/2014 10:04 AM	future
764	GROMACS	Bug	Closed	Normal	md = steep calculates and reports pressure and virial	Berk Hess	06/22/2011 11:12 AM	4.5.5
755	GROMACS	Bug	Closed	Normal	pdb2gmx -debug 1 writes *_new.hdb and new*.tdb files		01/09/2014 01:58 PM	
753	GROMACS	Feature	Closed	Normal	Use of GB in parallel and/or with all-vs-all kernels needs a mention in the manual	Mark Abraham	07/11/2016 08:45 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
752	GROMACS	Bug	Closed	Normal	With PD, non-master processes allocate state twice	Berk Hess	05/17/2011 12:06 PM	4.5.5
738	GROMACS	Task	Closed	Normal	Remove code duplication from various places	Mark Abraham	09/21/2011 11:08 AM	
736	GROMACS	Feature	Closed	Normal	BlueGene kernel upgrade	Mark Abraham	04/19/2013 03:53 PM	
735	GROMACS	Task	Closed	Normal	conversion of manual build system to CMake	Mark Abraham	05/23/2014 02:02 PM	
731	GROMACS	Feature	New	Normal	pdb2gmx should warn about missing residues when bonds are too long		06/22/2014 10:55 AM	
729	GROMACS	Bug	Closed	Normal	With GMX_THREADS on, cmake blindly sets GMX_MPI=1	Sander Pronk	06/08/2011 01:52 PM	git master
723	GROMACS	Bug	Closed	Normal	Need 4.5.4 manual release	Rossen Apostolov	05/23/2014 02:02 PM	
702	GROMACS	Feature	Rejected	Normal	Introducing gmx_cmdline_t	Mark Abraham	04/19/2013 08:57 PM	5.0
695	GROMACS	Bug	Closed	Low	replica exchange can occur when energies are not current	Mark Abraham	12/29/2012 03:59 PM	4.5.6
690	GROMACS	Bug	Closed	Low	options program needs to be built by default	Mark Abraham	12/29/2012 02:06 PM	4.5.6
684	GROMACS	Bug	Closed	Low	Nonsense sentence		05/23/2014 02:02 PM	
683	GROMACS	Feature	Closed	Low	do_dssp could be improved	Mark Abraham	06/17/2014 03:11 PM	
679	GROMACS	Task	Closed	Normal	g_select documentation should be included in the manual	Teemu Murtola	06/05/2015 07:30 PM	5.1
678	GROMACS	Bug	Closed	Normal	regularize status of g_kinetics		06/08/2011 04:45 PM	
677	GROMACS	Task	New	Normal	Make sure manual uses consistent style throughout		06/19/2014 11:49 AM	
675	GROMACS	Feature	Closed	Low	pdb2gmx should issue a warning when applying non-zwitterionic termini to single-residue molecules		12/29/2012 08:55 PM	
674	GROMACS	Bug	Closed	Normal	Use of specbond.dat is not documented	Justin Lemkul	05/23/2014 02:02 PM	
667	GROMACS	Feature	Rejected	Low	check_bonds_timestep() only reports the first suspicious bond	Mark Abraham	07/11/2016 08:29 PM	
664	GROMACS	Task	Closed	Low	Update code formatting to follow coding conventions		12/29/2012 12:54 PM	
648	Support Platforms	Task	Closed	Normal	Use of commit hook scripts		05/31/2017 05:40 PM	
647	Support Platforms	Bug	Closed	Normal	redmine repository hasn't picked up commits to release-4-5-patches for a few days		01/12/2011 03:45 PM	
636	GROMACS	Task	Closed	Low	check for updates to FindMPI.cmake	Mark Abraham	01/17/2012 01:51 PM	
633	Support Platforms	Task	Closed	Normal	Expand range of versions available when reporting bugs	Rossen Apostolov	05/31/2017 05:50 PM	
632	GROMACS	Feature	Closed	Normal	Implementation of periodic improper dihedrals is incomplete	Erik Lindahl	01/11/2013 12:36 PM	4.6
631	GROMACS	Task	Rejected	Low	Check that CMake default compiler options are mutually consistent		05/01/2013 12:50 AM	