

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 | |

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| 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 |

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| 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 dvlambdas 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 |

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| 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 | |

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| 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 | releing 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 |

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| 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 | mdrun -pinstride defaults are too confusing | | 12/13/2017 04:14 AM | |
| 2021 | GROMACS | Bug | Rejected | Normal | mdrun -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 | mdrun 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 | |

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| 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 | |