

Issues

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|------------------------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 2573 | GROMACS | Bug | New | High | Different mdp files describing the same change yield different free energy on the same trajectory | | 07/19/2018 06:52 PM | |
| 2600 | GROMACS | Bug | New | High | coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype | | 08/07/2018 06:50 PM | |
| 2637 | GROMACS | Bug | New | High | gmx solvate tears apart molecules | | 09/11/2018 07:43 PM | |
| 3210 | GROMACS | Bug | New | High | rerun does not reproduce dVcoul/dl | | 12/27/2019 10:45 AM | |
| 3266 | GROMACS | Bug | New | High | gmx density show wrong symmetrize density profile using -symm? | Super duper | 02/28/2020 08:24 AM | 2020.2 |
| 2935 | Support Platforms | Bug | New | High | redmine issue updates about gerrit uploads stopped working | | 06/11/2019 01:42 PM | current |
| 2229 | GROMACS | Feature | New | High | Full Object Oriented Modularization of GROMACS MDRUN Codebase | Mark Abraham | 08/22/2018 05:03 PM | future |
| 2099 | Support Platforms | Feature | New | High | sharing accounts/credentials | | 12/06/2017 08:11 PM | |
| 2519 | GROMACS | Task | New | High | Improve/remove PME OpenCL kernel barriers | | 02/15/2019 06:34 PM | |
| 2792 | GROMACS | Task | New | High | Improvement of PME gather and spread CUDA kernels | | 03/18/2020 03:57 PM | |
| 3082 | GROMACS | Task | New | High | move launch/synchronization points to clarify task dependencies | | 12/27/2019 04:21 PM | 2021 |
| 3262 | GROMACS | Task | New | High | Trjconv - dimer protein-ligand | | 12/20/2019 09:26 PM | |
| 3370 | GROMACS | Task | New | High | Further improvements to GPU Buffer Ops and Comms | | 03/04/2020 01:38 PM | |
| 2054 | GROMACS | Feature | Accepted | High | PME on GPU | Aleksei lupinov | 12/20/2019 12:18 PM | future |
| 2915 | GROMACS | Feature | In Progress | High | GPU direct communications | | 02/14/2020 12:48 PM | |
| 2071 | GROMACS | Task | In Progress | High | Low accuracy default settings yield incorrect liquid densities | Berk Hess | 01/05/2018 03:32 PM | |
| 3093 | GROMACS | Task | In Progress | High | rework GPU direct halo-exchange related force reduction complexities | | 02/14/2020 11:35 AM | 2021-infrastructure-stable |
| 3189 | GROMACS | Task | In Progress | High | implement heuristics for switching between different spread/gather kernel layouts | Jonathan Vincent | 01/29/2020 04:18 PM | 2021-infrastructure-stable |
| 3160 | GROMACS | Feature | Fix uploaded | High | implement direct comm for different src/target memory spaces | Alan Gray | 02/14/2020 11:28 AM | 2021-infrastructure-stable |
| 2188 | TNG trajectory library | Feature | Resolved | High | Masses missing from TNG specification | Magnus Lundborg | 06/13/2017 05:08 PM | |
| 2453 | GROMACS | Task | Resolved | High | PME OpenCL porting effort | Aleksei lupinov | 12/20/2019 12:18 PM | 2021 |
| 2580 | GROMACS | Bug | Feedback wanted | High | sc-coul option yields different free energy estimate on a ligand with zero partial charge | | 09/11/2018 08:10 AM | |
| 1190 | GROMACS | Bug | New | Normal | Use of FORCE in setting cached variables | Mark Abraham | 06/17/2014 06:09 AM | |
| 1235 | GROMACS | Bug | New | Normal | peptide dihedral angle definitions violate IUPAC | David van der Spoel | 06/19/2015 12:24 AM | future |
| 1339 | GROMACS | Bug | New | Normal | Center of mass drift with Nose-Hoover, MTTK and md-vv | Michael Shirts | 06/18/2015 08:53 PM | future |
| 1354 | GROMACS | Bug | New | Normal | Constant acceleration NEMD is broken. | David van der Spoel | 01/09/2019 04:42 PM | |

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| 1448 | GROMACS | Bug | New | Normal | multiple successive crashes during REMD can lead to .log files that do not represent the actual replica exchanges to match the .xtc files (complicating demultiplexing) | Mark Abraham | 06/23/2016 03:15 PM | |
| 1583 | GROMACS | Bug | New | Normal | gmx msd with mol flag requires excessive memory | | 12/18/2017 03:34 PM | |
| 1655 | GROMACS | Bug | New | Normal | g_membed and box type | | 12/09/2014 01:33 PM | |
| 1667 | GROMACS | Bug | New | Normal | gmx convert-tpr writes wrong number of mol in output tpr | David van der Spoel | 06/27/2016 08:29 PM | |
| 1730 | GROMACS | Bug | New | Normal | gmx compare does not compare all fields of a .tpr | | 06/12/2015 09:33 PM | future |
| 1770 | GROMACS | Bug | New | Normal | segmentation fault with free energy changes and multiple GPU's | | 07/14/2015 03:24 AM | |
| 1811 | GROMACS | Bug | New | Normal | Extrae build issues | | 12/13/2017 03:43 AM | |
| 1934 | GROMACS | Bug | New | Normal | QMMM with ORCA: memory leaks, buffer overflows and much more | | 07/10/2016 09:26 AM | |
| 2020 | GROMACS | Bug | New | Normal | Possible issue with md-vv integrator | Mark Abraham | 03/11/2017 08:30 AM | |
| 2039 | GROMACS | Bug | New | Normal | mddrun -pinstride defaults are too confusing | | 12/13/2017 04:14 AM | |
| 2065 | GROMACS | Bug | New | Normal | thread-MPI internal errors | | 11/08/2018 03:43 PM | |
| 2094 | GROMACS | Bug | New | Normal | Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size | | 01/20/2017 04:56 PM | |
| 2113 | GROMACS | Bug | New | Normal | Google tests and execution order | | 03/05/2018 02:05 PM | |
| 2208 | GROMACS | Bug | New | Normal | cuFFT linking | | 06/30/2017 01:58 PM | |
| 2231 | GROMACS | Bug | New | Normal | convert-tpr aborts when saving subset of the system | | 01/12/2018 03:52 PM | |
| 2232 | GROMACS | Bug | New | Normal | pdb2gmx can't form special bonds with terminal patched atoms | | 12/03/2017 01:35 PM | |
| 2255 | GROMACS | Bug | New | Normal | nstlist override stopped affecting the input parameter listing | | 12/17/2017 08:05 AM | |
| 2393 | GROMACS | Bug | New | Normal | incorrect error message with omitted command line flag before its argument | | 01/24/2018 11:24 PM | |
| 2427 | GROMACS | Bug | New | Normal | gmx select gives syntax error for selection involving evaluating simple arithmetic expression | | 02/27/2018 05:15 PM | |
| 2460 | GROMACS | Bug | New | Normal | Allow inclusion of user libraries through CMake cache variables | | 03/28/2018 08:47 PM | |
| 2473 | GROMACS | Bug | New | Normal | mddrun sometimes stalls due to large coordinates with no constraints | | 04/04/2018 10:15 PM | |
| 2480 | GROMACS | Bug | New | Normal | pdb2gmx does not protonate correctly for united-atom Gromos | Mark Abraham | 12/20/2019 12:17 PM | 2021 |
| 2526 | GROMACS | Bug | New | Normal | Bug of gmx hbond | | 05/30/2018 03:12 PM | |
| 2544 | GROMACS | Bug | New | Normal | gmx rmsf does not fix periodicity in reference structure | David van der Spoel | 08/21/2018 10:36 AM | future |
| 2563 | GROMACS | Bug | New | Normal | Windows 7 Compilation with GPU support | | 07/02/2018 09:58 AM | |
| 2564 | GROMACS | Bug | New | Normal | Result Summary Different For Jobs With Different Numbers of Nodes | | 07/05/2018 02:39 PM | |

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| 2567 | GROMACS | Bug | New | Normal | make check fails at test 23 SIMD errors | | 07/10/2018 09:35 AM | |
| 2576 | GROMACS | Bug | New | Normal | gmx potential -correct outputs the wrong potential | | 07/25/2018 02:58 PM | |
| 2598 | GROMACS | Bug | New | Normal | Tools using read_next_x cannot read TNG files with sanitizers | | 10/15/2018 01:16 PM | future |
| 2606 | GROMACS | Bug | New | Normal | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert | | 08/10/2018 01:48 AM | |
| 2607 | GROMACS | Bug | New | Normal | Grompp becomes extremely slow when many pull groups are present | | 08/11/2018 08:54 AM | |
| 2611 | GROMACS | Bug | New | Normal | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX | | 08/14/2018 07:03 PM | |
| 2624 | GROMACS | Bug | New | Normal | GPU build system not robust enough | | 09/05/2018 02:00 AM | |
| 2645 | GROMACS | Bug | New | Normal | Security | | 09/28/2018 01:16 PM | |
| 2649 | GROMACS | Bug | New | Normal | Virial calculation necessary for correct energy calculation on GPU | | 12/17/2018 02:32 PM | future |
| 2657 | GROMACS | Bug | New | Normal | Biphasic tutorial | | 09/28/2018 10:02 AM | |
| 2693 | GROMACS | Bug | New | Normal | Several memory leaks in mdrun | | 12/18/2018 04:22 AM | future |
| 2707 | GROMACS | Bug | New | Normal | Installed OpenCL files include clh file from gpu_utils directory | | 10/30/2018 04:02 AM | |
| 2740 | GROMACS | Bug | New | Normal | mdrun reports incorrect error with -bonded gpu without gpu | Mark Abraham | 11/07/2018 01:59 PM | |
| 2754 | GROMACS | Bug | New | Normal | Simulated Tempering seems to be broken | Michael Shirts | 02/05/2019 03:58 PM | |
| 2763 | GROMACS | Bug | New | Normal | GMXAPI layout / grouping in development docs "modules" page | | 12/14/2018 12:49 PM | future |
| 2785 | GROMACS | Bug | New | Normal | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG | | 11/30/2018 02:36 PM | |
| 2788 | GROMACS | Bug | New | Normal | PME will not run on AMD GPU with NVidia GPU present | | 01/03/2019 02:24 PM | |
| 2848 | GROMACS | Bug | New | Normal | gmx make_ndx ignores last residue in case only CA's are present in GRO file | | 01/30/2019 06:16 AM | |
| 2853 | GROMACS | Bug | New | Normal | EwaldUnitTests segfault on armv7hl with gcc-9.0.1 | Paul Bauer | 02/04/2019 05:34 PM | |
| 2854 | GROMACS | Bug | New | Normal | OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1 | Paul Bauer | 02/04/2019 11:17 AM | |
| 2869 | GROMACS | Bug | New | Normal | GPU detection error only issued as a note to the log | | 03/05/2019 04:09 PM | |
| 2870 | GROMACS | Bug | New | Normal | GPU detection error message missing from the output | | 03/05/2019 03:55 PM | |
| 2872 | GROMACS | Bug | New | Normal | gmx solvate and genion topology update | | 02/27/2019 10:18 AM | |
| 2873 | GROMACS | Bug | New | Normal | Simple way to get last frame from trajectory | | 02/28/2019 11:14 PM | |
| 2876 | GROMACS | Bug | New | Normal | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3) | Erik Lindahl | 03/08/2019 10:32 AM | |
| 2883 | GROMACS | Bug | New | Normal | essentialedynamics fail with Intel MPI | | 03/08/2019 03:10 AM | |
| 2897 | GROMACS | Bug | New | Normal | rotation/flex2 can still fail on cpu-only run on OpenCL build | | 04/04/2019 06:24 PM | |
| 2902 | GROMACS | Bug | New | Normal | 2019.1 equilibration issue? (Intel 2018u3) | | 04/30/2019 08:17 AM | |
| 2907 | GROMACS | Bug | New | Normal | Gromacs autocompletion appears to be broken with ZSH | | 07/16/2019 04:46 AM | |

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| 2924 | GROMACS | Bug | New | Normal | Failing version check when reading new tpr file with older gromacs version | | 04/12/2019 10:52 AM | |
| 2948 | GROMACS | Bug | New | Normal | SIMD support detected as none on AMD R5 2500U | | 05/21/2019 12:58 PM | |
| 2949 | GROMACS | Bug | New | Normal | cmake fails when building mdrun only | | 07/08/2019 10:04 AM | |
| 2954 | GROMACS | Bug | New | Normal | genion changes residue numbering | | 05/26/2019 12:08 AM | |
| 2958 | GROMACS | Bug | New | Normal | Compiling master (to become 2020) using CUDA 9.0 | | 03/02/2020 03:57 PM | 2020.2 |
| 2974 | GROMACS | Bug | New | Normal | position-restraints regressiontest fails on intel GPU with OpenCL | | 02/25/2020 03:52 PM | 2020.2 |
| 2978 | GROMACS | Bug | New | Normal | Some suggestions about the gmx current tool | | 06/13/2019 12:41 PM | |
| 2980 | GROMACS | Bug | New | Normal | taskassignment fails with unit tests when GPUs and custom number of ranks is used | | 06/17/2019 05:28 PM | |
| 2981 | GROMACS | Bug | New | Normal | segfault in opencl build | | 06/18/2019 03:30 AM | |
| 2987 | GROMACS | Bug | New | Normal | assess the bonded GPU task assignment default | | 12/20/2019 01:06 PM | 2021 |
| 3000 | GROMACS | Bug | New | Normal | CMake "webpage" target does not fail when it should | | 06/25/2019 02:43 PM | |
| 3042 | GROMACS | Bug | New | Normal | core dump error in grompp command | | 10/09/2019 07:30 PM | |
| 3048 | GROMACS | Bug | New | Normal | Dihedral parameters for N-terminal in gromos53a6 force field in the aminoacids.n.tdb file with different values in versions 4.6.7 and gromacs 2019/2016/5.1.5 | | 07/29/2019 10:41 AM | |
| 3054 | GROMACS | Bug | New | Normal | Missing dihedral define | | 08/02/2019 05:47 PM | |
| 3066 | GROMACS | Bug | New | Normal | Gauss transform and density fit classes should operate on real values instead of float | Christian Blau | 08/26/2019 11:53 AM | |
| 3068 | GROMACS | Bug | New | Normal | Misleading warning on rerun | | 08/26/2019 03:44 PM | |
| 3073 | GROMACS | Bug | New | Normal | Total potential energy goes crazy, but I don't know why this happens. | | 09/04/2019 07:25 PM | |
| 3075 | GROMACS | Bug | New | Normal | Frozen atoms are moving | Erik Lindahl | 12/27/2019 10:51 AM | |
| 3083 | GROMACS | Bug | New | Normal | Listed forces tests failing on ICC19 with AVX2_256 nightly build | | 09/10/2019 11:56 AM | |
| 3086 | GROMACS | Bug | New | Normal | gmxapi fails with MPI build of GROMACS 2020 | | 09/25/2019 04:18 PM | |
| 3088 | GROMACS | Bug | New | Normal | Reference to theory needed for cylindrical pull geometry | | 09/13/2019 11:26 AM | |
| 3116 | GROMACS | Bug | New | Normal | regressiontests/freeenergy core dumps on ppc64le | Paul Bauer | 10/04/2019 10:52 PM | |
| 3124 | GROMACS | Bug | New | Normal | significant performance loss due to DLB auto-off when PP/PME load >1 | | 01/28/2020 02:44 PM | 2021 |
| 3127 | GROMACS | Bug | New | Normal | mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia | | 10/09/2019 05:33 PM | |
| 3136 | GROMACS | Bug | New | Normal | gmxapi.operation data flow topology unclear or incomplete | Eric Irrgang | 12/11/2019 11:25 AM | 2021-infrastructure-stable |
| 3141 | GROMACS | Bug | New | Normal | gmxapi File placeholders missing from beta release | Eric Irrgang | 12/10/2019 02:02 PM | 2021-infrastructure-stable |
| 3150 | GROMACS | Bug | New | Normal | gmxapi data type annotations are confusing and inadequate | Eric Irrgang | 10/22/2019 03:08 PM | 2021-infrastructure-stable |
| 3165 | GROMACS | Bug | New | Normal | task assignment silent abort | | 10/18/2019 07:46 PM | |

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|------|---------|---------|--------|----------|---|----------------|---------------------|----------------------------|
| 3166 | GROMACS | Bug | New | Normal | Compilation failing on Ubuntu 19.04 with Cuda 10.1 | | 10/19/2019 09:13 PM | |
| 3196 | GROMACS | Bug | New | Normal | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing | | 11/01/2019 11:28 PM | |
| 3197 | GROMACS | Bug | New | Normal | Rework usage of gitattributes and filter in source code formatting scripts | | 11/04/2019 12:50 PM | 2021-infrastructure-stable |
| 3198 | GROMACS | Bug | New | Normal | Fails to build on FreeBSD with Clang since f7940fa01e8b6ef0703236b53721cca2d81b40d3 Use gmock and gtest targets from googletest-release-1.8.0 | | 11/06/2019 12:20 PM | |
| 3209 | GROMACS | Bug | New | Normal | Interactive molecular dynamics with VMD becomes stuttering after reconnecting | | 11/19/2019 11:36 AM | |
| 3213 | GROMACS | Bug | New | Normal | Having a local residuetypes.dat for custom force field | | 11/21/2019 09:18 PM | |
| 3214 | GROMACS | Bug | New | Normal | Out-of-bounds, overflow and incorrect outputs in gmx spatial | | 11/25/2019 04:11 PM | |
| 3223 | GROMACS | Bug | New | Normal | unit test failures give verify -1 | | 12/02/2019 11:58 AM | |
| 3227 | GROMACS | Bug | New | Normal | solvate does not check return status of gmx_file_rename | | 12/04/2019 01:43 PM | |
| 3228 | GROMACS | Bug | New | Normal | gmxapi.commandline_operation should gracefully handle input/output file arguments | Eric Irrgang | 12/04/2019 03:27 PM | 2021-infrastructure-stable |
| 3233 | GROMACS | Bug | New | Normal | clang-format incorrectly aligning altered function arguments | | 12/13/2019 12:41 PM | |
| 3239 | GROMACS | Bug | New | Normal | GPU DD direct communication with GPU update error with RF | | 12/14/2019 05:15 PM | |
| 3240 | GROMACS | Bug | New | Normal | segv with GPU DD direct communication with GPU update and -dlb off | | 01/15/2020 06:16 PM | |
| 3273 | GROMACS | Bug | New | Normal | gmxapi setup.py complains too much | | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3274 | GROMACS | Bug | New | Normal | Remove ARM NEON SIMD | | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3281 | GROMACS | Bug | New | Normal | Test data directory GMX_RELEASE_ASSERT triggers | | 01/06/2020 08:07 PM | |
| 3284 | GROMACS | Bug | New | Normal | gmx msd cannot output two xvg files as suggested by command line option | Christian Blau | 01/08/2020 04:50 PM | 2021-infrastructure-stable |
| 3294 | GROMACS | Bug | New | Normal | multiple tests fail on fedora 31 | Paul Bauer | 02/28/2020 03:12 PM | 2020.2 |
| 3301 | GROMACS | Bug | New | Normal | pdb2gmx adding hydrogen | | 01/15/2020 10:17 PM | |
| 3304 | GROMACS | Bug | New | Normal | Failure in Log Output for Expanded Ensemble Weights using Simulated Tempering in GROMACS 2019.5 | Michael Shirts | 03/01/2020 03:23 PM | 2020.2 |
| 3305 | GROMACS | Bug | New | Normal | Case gives FPE with Debug build when GPU update is enabled | | 01/21/2020 05:44 PM | |
| 3309 | GROMACS | Bug | New | Normal | -reprod: checkpoint reading bug and general considerations | | 02/27/2020 10:45 PM | |
| 3333 | GROMACS | Bug | New | Normal | Assertion failure when trying to get unit test help | Paul Bauer | 02/25/2020 10:16 AM | 2021-infrastructure-stable |
| 3334 | GROMACS | Bug | New | Normal | Check for DD when increasing rlist is broken | Berk Hess | 02/25/2020 03:28 PM | 2020.2 |
| 3368 | GROMACS | Bug | New | Normal | Erroneous interplay between gmx rms command and atommass.dat: Can not find mass in database for atom MG in residue | Vedat Durmaz | 02/05/2020 04:51 PM | future |
| 3385 | GROMACS | Bug | New | Normal | FindLibStdCpp.cmake - wrong sanity check for clang | | 03/04/2020 06:59 PM | |

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| 3387 | GROMACS | Bug | New | Normal | Death test bug | | 02/20/2020 05:39 PM | |
| 3398 | GROMACS | Bug | New | Normal | Intermittent failure of non-bonded kernels when run using nvprof | | 02/25/2020 12:14 PM | |
| 3411 | GROMACS | Bug | New | Normal | Nightly master release build failure | | 03/06/2020 11:44 AM | 2021-infrastructure-stable |
| 3412 | GROMACS | Bug | New | Normal | Domain decomposition problems with Gromacs >2018 | | 03/06/2020 04:10 PM | |
| 3440 | GROMACS | Bug | New | Normal | Multi-nodes run exits with error with openmpi/4.0.0 | | 03/23/2020 02:10 PM | |
| 3443 | GROMACS | Bug | New | Normal | Bonded GPU kernel performance regression with 2020 | | 03/15/2020 08:15 PM | |
| 3448 | GROMACS | Bug | New | Normal | GMX 2020.1 - Multidir simulations can stop at different times when killed by job manager | | 03/23/2020 02:50 PM | |
| 1732 | Support Platforms | Bug | New | Normal | review and extend jenkins tests setups, coverage | | 05/03/2016 05:30 AM | |
| 1836 | Support Platforms | Bug | New | Normal | Support a way to retrigger part of matrix job | | 07/22/2017 12:30 AM | |
| 2096 | Support Platforms | Bug | New | Normal | Redmine internal error with special characters | | 05/31/2017 08:48 PM | |
| 2149 | Support Platforms | Bug | New | Normal | gerrit server excessive CPU usage | | 04/05/2017 07:25 PM | |
| 1536 | TNG trajectory library | Bug | New | Normal | TNG uses incorrect format for size_t on 32bit | | 06/28/2014 03:56 AM | |
| 2362 | TNG trajectory library | Bug | New | Normal | tng_*_of_particle_nr_get() functions return wrong result for structures with multiple molecule types | | 12/21/2017 11:51 AM | |
| 2937 | TNG trajectory library | Bug | New | Normal | tng_num_frames_get reports incorrect num frames | | 04/29/2019 11:30 AM | |
| 731 | GROMACS | Feature | New | Normal | pdb2gmx should warn about missing residues when bonds are too long | | 06/22/2014 10:55 AM | |
| 742 | GROMACS | Feature | New | Normal | Enhancing the performance of the free energy code | | 08/26/2019 04:55 PM | future |
| 950 | GROMACS | Feature | New | Normal | Path/directory/filename handling in Gromacs | | 07/11/2016 08:24 PM | |
| 951 | GROMACS | Feature | New | Normal | Multiple versions of Gromacs (e.g., single and double) in the same library/binary | | 01/07/2019 02:10 AM | future |
| 1028 | GROMACS | Feature | New | Normal | Tool to calculate fraction of native contacts during simulation | | 11/01/2012 10:27 PM | |
| 1102 | GROMACS | Feature | New | Normal | Detect incompletely written itp files | | 06/19/2014 03:23 PM | |
| 1137 | GROMACS | Feature | New | Normal | Proposal for integrator framework (do_md) in future GROMACS | Michael Shirts | 02/21/2017 12:48 AM | future |
| 1139 | GROMACS | Feature | New | Normal | Adding the possibility to arbitrarily evaluate different components in the energy/force term when the energy/force is calculated | | 07/11/2016 08:19 PM | |
| 1162 | GROMACS | Feature | New | Normal | Implement gb_saltconc | Berk Hess | 02/26/2013 05:33 PM | future |
| 1182 | GROMACS | Feature | New | Normal | improve trajectory writing to support parallel I/O | | 05/13/2014 10:42 AM | future |
| 1247 | GROMACS | Feature | New | Normal | fix hardcoded references to atom names in analysis tools | Mark Abraham | 06/12/2014 01:20 AM | future |
| 1303 | GROMACS | Feature | New | Normal | Adding lambda dependent distance for pull code | Michael Shirts | 07/11/2016 08:18 PM | |
| 1335 | GROMACS | Feature | New | Normal | Improved interaction of free energies with pull code to better support Hamiltonian replica exchange with umbrella sampling | Michael Shirts | 05/13/2014 10:38 AM | future |
| 1347 | GROMACS | Feature | New | Normal | future of tables | Berk Hess | 01/09/2020 02:37 PM | future |

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| 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 |
| 1422 | GROMACS | Feature | New | Normal | CSH angle incorrect with GROMOS force field and virtual sites | David van der Spoel | 06/12/2014 12:01 AM | |
| 1437 | GROMACS | Feature | New | Normal | Online help formatting improvements | | 06/04/2015 09:20 PM | future |
| 1464 | GROMACS | Feature | New | Normal | implement PP-PME re-balancing | Szilárd Páll | 10/16/2015 08:34 AM | future |
| 1489 | GROMACS | Feature | New | Normal | Don't solely rely on filename extension | | 04/30/2014 05:23 AM | |
| 1500 | GROMACS | Feature | New | Normal | Post-5.0 feature clean-up plan | Mark Abraham | 08/26/2019 03:47 PM | |
| 1562 | GROMACS | Feature | New | Normal | introducing a Monte Carlo framework (first application: MC barostat) | Michael Shirts | 07/11/2016 08:08 PM | |
| 1625 | GROMACS | Feature | New | Normal | Gromacs Python API | | 03/02/2019 01:44 AM | future |
| 1634 | GROMACS | Feature | New | Normal | Boxed Molecular Dynamics | | 11/04/2014 04:40 PM | |
| 1635 | GROMACS | Feature | New | Normal | Proper Unicode support | | 06/18/2015 08:34 PM | |
| 1641 | GROMACS | Feature | New | Normal | Add toolchain file for Cray systems | | 06/06/2015 11:24 PM | |
| 1652 | GROMACS | Feature | New | Normal | Decide how to represent multiple lambda states internally | Michael Shirts | 06/05/2018 03:58 PM | |
| 1653 | GROMACS | Feature | New | Normal | Decide how to represent multiple lambda states in the .top file and how to parse them | Michael Shirts | 06/05/2018 03:58 PM | |
| 1654 | GROMACS | Feature | New | Normal | How to carry out movement between chemical end states in a multiple end state framework? | Michael Shirts | 07/11/2016 08:05 PM | |
| 1658 | GROMACS | Feature | New | Normal | Electrostatics treatment for multiple lambda sites | Berk Hess | 07/11/2016 08:05 PM | |
| 1665 | GROMACS | Feature | New | Normal | improve free energy non-bonded kernel performance | | 08/26/2019 03:47 PM | future |
| 1666 | GROMACS | Feature | New | Normal | new approach for Verlet-scheme kernel generation | Erik Lindahl | 10/08/2018 07:04 PM | future |
| 1670 | GROMACS | Feature | New | Normal | create mdrun option checking mini-tool | | 06/23/2016 04:06 PM | |
| 1842 | GROMACS | Feature | New | Normal | Replace XML with JSON | | 01/18/2018 05:12 PM | |
| 1849 | GROMACS | Feature | New | Normal | expanded ensemble -- Adaptive Integration Method | Christopher Mirabzadeh | 07/11/2016 08:01 PM | |
| 1854 | GROMACS | Feature | New | Normal | Remove all cyclic dependencies | | 05/25/2017 08:34 AM | |
| 1864 | GROMACS | Feature | New | Normal | write tng files with energies | Magnus Lundborg | 07/11/2016 08:00 PM | |
| 1867 | GROMACS | Feature | New | Normal | make coupling implementations reversible | | 12/02/2015 07:43 AM | |
| 1885 | GROMACS | Feature | New | Normal | DPD Thermostat | | 01/26/2016 10:17 AM | |
| 1900 | GROMACS | Feature | New | Normal | Implement some new errors in grompp | | 06/22/2016 05:20 PM | |
| 1972 | GROMACS | Feature | New | Normal | external potential modules for refinement against experimental data | | 08/22/2018 05:03 PM | future |
| 1974 | GROMACS | Feature | New | Normal | Report atom numbers and types in the error message about missed parameters | | 05/30/2016 09:24 AM | |
| 2001 | GROMACS | Feature | New | Normal | add MPI info to the mdrun log header | | 07/06/2016 05:21 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 2005 | GROMACS | Feature | New | Normal | Full Correlation Analysis (FCA) as Trajectory Analysis Module | Christian Blau | 02/07/2018 02:19 PM | future |
| 2015 | GROMACS | Feature | New | Normal | Auto recovery from dd communication error | | 07/28/2016 03:17 PM | |
| 2018 | GROMACS | Feature | New | Normal | Pulling along a line between given points | | 07/27/2016 09:59 AM | |
| 2034 | GROMACS | Feature | New | Normal | Unit tests for bonded forces | David van der Spoel | 06/29/2019 10:22 AM | future |
| 2060 | GROMACS | Feature | New | Normal | Convert enum to enum class | | 10/17/2016 05:27 PM | |
| 2068 | GROMACS | Feature | New | Normal | Access to low level classes | | 03/02/2019 01:37 AM | future |
| 2080 | GROMACS | Feature | New | Normal | add grompp warning for suitability for domain decomposition | | 11/23/2016 03:03 PM | |
| 2090 | GROMACS | Feature | New | Normal | redirecting stdout or stderr for testing | Mark Abraham | 12/15/2016 03:15 AM | |
| 2126 | GROMACS | Feature | New | Normal | implement native CUDA support in CMake | | 10/29/2019 09:03 PM | |
| 2132 | GROMACS | Feature | New | Normal | Intermediate code for xvg handling | | 03/08/2017 05:12 PM | future |
| 2137 | GROMACS | Feature | New | Normal | Preliminary refactoring of constraints and update machinery. | Michael Shirts | 03/11/2017 08:32 AM | future |
| 2139 | GROMACS | Feature | New | Normal | More precise/explicit documentation conventions | | 01/07/2018 11:54 PM | |
| 2207 | GROMACS | Feature | New | Normal | solvent excluded volume of large molecule with periodic boundary condition | | 06/16/2017 10:37 AM | |
| 2220 | GROMACS | Feature | New | Normal | report relevant env var behaviour to console | | 07/31/2017 09:40 PM | |
| 2224 | GROMACS | Feature | New | Normal | Proposed feature: conditional stop | Vedran Miletic | 12/20/2019 12:11 PM | 2021 |
| 2226 | GROMACS | Feature | New | Normal | Harmonise commands for exit in make_ndx and distance | | 08/04/2017 12:24 PM | |
| 2239 | GROMACS | Feature | New | Normal | split libgromacs into base and full | | 01/07/2019 01:47 AM | |
| 2248 | GROMACS | Feature | New | Normal | Label all SIMD functions as pure/nodiscard | | 02/04/2019 04:49 AM | |
| 2282 | GROMACS | Feature | New | Normal | Density map toolset | Christian Blau | 03/21/2019 06:08 PM | future |
| 2283 | GROMACS | Feature | New | Normal | Force distribution analysis | Bernd Doser | 10/27/2017 11:44 AM | |
| 2289 | GROMACS | Feature | New | Normal | gmx spatial add ability to perform over multiple reference structures | | 11/08/2017 12:31 AM | |
| 2354 | GROMACS | Feature | New | Normal | develop configuration file support for control of task layout | | 09/19/2018 03:01 PM | future |
| 2428 | GROMACS | Feature | New | Normal | Add way of selecting interactive arguments of pdb2gmx by string rather than an index | | 02/27/2018 06:28 PM | |
| 2429 | GROMACS | Feature | New | Normal | Add option of periodic chain topology to pdb2gmx | | 03/10/2018 01:01 PM | |
| 2545 | GROMACS | Feature | New | Normal | Should grompp fix periodicity of input files? | David van der Spoel | 10/03/2018 11:32 PM | future |
| 2556 | GROMACS | Feature | New | Normal | make default selections suitable for DNA and RNA | Mark Abraham | 06/20/2018 01:48 PM | |
| 2570 | GROMACS | Feature | New | Normal | Better string formatting and printing | | 05/02/2019 12:20 PM | |
| 2574 | GROMACS | Feature | New | Normal | iForceSchedule Abstraction | Prashanth Kanduri | 03/29/2019 05:20 PM | future |
| 2579 | GROMACS | Feature | New | Normal | Add dimensionality option to gmx trjconv -center | | 07/19/2018 04:53 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------------------|
| 2594 | GROMACS | Feature | New | Normal | Multi-level GMX API | Prashanth Kanduri | 02/22/2019 03:48 PM | future |
| 2596 | GROMACS | Feature | New | Normal | Constant potential method | Benson Muite | 05/10/2019 09:54 AM | |
| 2601 | GROMACS | Feature | New | Normal | Free energy calculations, soft-core potential | Vytautas Gapsys | 02/10/2020 11:29 AM | future |
| 2667 | GROMACS | Feature | New | Normal | Suggested steps for calculating entropy in solution and binding | David van der Spoel | 03/01/2020 01:35 PM | 2020.2 |
| 2710 | GROMACS | Feature | New | Normal | Separate dvdI for each molecule (of couple-moltype) when running FEP | | 12/27/2019 04:41 PM | 2021 |
| 2713 | GROMACS | Feature | New | Normal | Constant offset for external electric fields | | 10/28/2018 12:57 AM | |
| 2715 | GROMACS | Feature | New | Normal | Avoid requesting the user to recompile gromacs for Intel OpenCL support | | 12/27/2019 04:06 PM | future |
| 2739 | GROMACS | Feature | New | Normal | Parallel continuous tempering and enhanced sampling feature | | 11/13/2018 11:36 PM | |
| 2774 | GROMACS | Feature | New | Normal | Refactor shell code into its own integrator | David van der Spoel | 12/27/2019 04:05 PM | 2021 |
| 2806 | GROMACS | Feature | New | Normal | SIMD algorithms for ARM SVE // nobonded cluster and others | | 12/27/2019 03:59 PM | 2021 |
| 2840 | GROMACS | Feature | New | Normal | Test that functionality does not compile that is not supposed to. | | 01/25/2019 02:35 PM | future |
| 2860 | GROMACS | Feature | New | Normal | Option for outputting min/max coordinates in gmx traj | | 02/08/2019 12:35 AM | |
| 2866 | GROMACS | Feature | New | Normal | Alternative non-bonded potentials | David van der Spoel | 03/05/2019 03:50 PM | future |
| 2910 | GROMACS | Feature | New | Normal | Mixed scaling for 1-4 interactions | | 04/10/2019 10:13 PM | |
| 2928 | GROMACS | Feature | New | Normal | Add ability to use expression "count of ATOM_EXPR" in selection statements. | | 04/16/2019 04:52 PM | |
| 2930 | GROMACS | Feature | New | Normal | Limited range for reference group detection in cylinder pulling | | 04/26/2019 05:17 PM | |
| 2931 | GROMACS | Feature | New | Normal | Tables in Verlet kernels | | 04/29/2019 12:01 PM | |
| 2944 | GROMACS | Feature | New | Normal | Roadmap for thermostats / barostats in new propagation/integration scheme | Michael Shirts | 12/27/2019 04:00 PM | 2021 |
| 2956 | GROMACS | Feature | New | Normal | SAXS resolution | | 05/17/2019 09:58 AM | |
| 2961 | GROMACS | Feature | New | Normal | How should Python package find GROMACS resources under various circumstances? | | 12/09/2019 10:47 AM | |
| 2967 | GROMACS | Feature | New | Normal | GPU reallocateDeviceBuffer improvements | | 01/23/2020 12:15 PM | 2021-refactoring |
| 2975 | GROMACS | Feature | New | Normal | LJ PME calculations on GPUs | | 06/12/2019 01:17 PM | |
| 2977 | GROMACS | Feature | New | Normal | print DD load balancing improvement | | 06/13/2019 10:56 AM | |
| 2984 | GROMACS | Feature | New | Normal | More Extensive Selections Examples | Dallas Warren | 06/18/2019 11:50 PM | |
| 2993 | GROMACS | Feature | New | Normal | Scalar and structured type expression and definitions for API | Eric Irrgang | 10/17/2019 09:55 AM | |
| 2994 | GROMACS | Feature | New | Normal | Data flow topology in gmxapi 2020 | | 12/11/2019 11:33 AM | 2021-infrastructure-stable |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|-----------------|---------------------|----------------------------|
| 3030 | GROMACS | Feature | New | Normal | RST style guidelines | | 07/09/2019 03:38 PM | |
| 3038 | GROMACS | Feature | New | Normal | Improvements to MD plugin development environment | Eric Irrgang | 12/10/2019 01:58 PM | 2021-infrastructure-stable |
| 3114 | GROMACS | Feature | New | Normal | Improve GPU update-constraints module | Artem Zhmurov | 02/10/2020 04:30 PM | 2021 |
| 3115 | GROMACS | Feature | New | Normal | Device stream manager | | 10/04/2019 09:00 AM | |
| 3117 | GROMACS | Feature | New | Normal | Coulomb FEP PME on GPU | Magnus Lundborg | 02/17/2020 03:58 PM | 2021-infrastructure-stable |
| 3126 | GROMACS | Feature | New | Normal | State propagator GPU data manager | | 10/09/2019 02:42 PM | |
| 3135 | GROMACS | Feature | New | Normal | Make GPU traits ino opaque types | | 10/14/2019 10:24 AM | |
| 3138 | GROMACS | Feature | New | Normal | Improve ensemble support in Context specification. | | 10/15/2019 03:56 PM | |
| 3140 | GROMACS | Feature | New | Normal | Allow explicit input definition for gmxapi.operation function wrapper | Eric Irrgang | 12/10/2019 02:00 PM | 2021-infrastructure-stable |
| 3147 | GROMACS | Feature | New | Normal | gmxapi workflow checkpointing | Eric Irrgang | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 3148 | GROMACS | Feature | New | Normal | Roadmap for gmxapi filesystem interactions. | Eric Irrgang | 10/15/2019 06:23 PM | 2021-infrastructure-stable |
| 3149 | GROMACS | Feature | New | Normal | Python user interface for obtaining simulation artifacts as files. | Eric Irrgang | 10/15/2019 06:21 PM | |
| 3152 | GROMACS | Feature | New | Normal | Infrastructure and patterns for expressing public interfaces | | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 3172 | GROMACS | Feature | New | Normal | QM/MM Interface with CP2K | Dmitry Morozov | 01/17/2020 12:18 PM | future |
| 3177 | GROMACS | Feature | New | Normal | Spack package management support | | 11/06/2019 06:37 PM | |
| 3179 | GROMACS | Feature | New | Normal | Clarify access to parallel data outputs | Eric Irrgang | 10/26/2019 12:23 PM | |
| 3242 | GROMACS | Feature | New | Normal | Please do not remove the -nsteps flag | | 03/01/2020 01:59 PM | |
| 3277 | GROMACS | Feature | New | Normal | Allow testing feature that is partly implemented | | 12/31/2019 12:44 PM | 2021 |
| 3288 | GROMACS | Feature | New | Normal | Use build system infrastructure instead of custom scripts to manage API levels. | | 02/26/2020 04:16 PM | 2021-infrastructure-stable |
| 3295 | GROMACS | Feature | New | Normal | Expand gmxapi.modify_input use cases. | Eric Irrgang | 01/16/2020 05:13 PM | 2021-refactoring |
| 3298 | GROMACS | Feature | New | Normal | start early PP work for first dimension of halo exchange | | 03/01/2020 01:36 PM | |
| 3307 | GROMACS | Feature | New | Normal | General interface for communication between simulation ranks | | 01/22/2020 03:22 PM | 2021-refactoring |
| 3328 | GROMACS | Feature | New | Normal | Testing framework for task assignment | | 01/22/2020 09:48 AM | 2021-refactoring |
| 3332 | GROMACS | Feature | New | Normal | gmx helixorient doesn't have a -tu option to change time unit | | 01/22/2020 11:57 AM | |
| 3350 | GROMACS | Feature | New | Normal | GPU update-constraints performance | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3351 | GROMACS | Feature | New | Normal | GPU update-constraints code organization and integration | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3352 | GROMACS | Feature | New | Normal | GPU update-constraints feature support | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3362 | GROMACS | Feature | New | Normal | gmx traj: add an option to plot each component in a separate file | | 01/29/2020 06:18 PM | |
| 3363 | GROMACS | Feature | New | Normal | Improve FEP testing | Pascal Merz | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3369 | GROMACS | Feature | New | Normal | Add quote about "the truth" | | 02/05/2020 05:08 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|------------------------|---------|--------|----------|--|-----------------|---------------------|----------------------------|
| 3371 | GROMACS | Feature | New | Normal | Control FEP using AWH | Magnus Lundborg | 02/06/2020 02:20 PM | 2021 |
| 3374 | GROMACS | Feature | New | Normal | SimulationInput abstraction | | 03/03/2020 05:32 PM | 2021-refactoring |
| 3378 | GROMACS | Feature | New | Normal | genion usage without stdin (facilitates use in gmx python api) | | 02/13/2020 12:04 PM | |
| 3379 | GROMACS | Feature | New | Normal | C++ API for simulation input and output | | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3394 | GROMACS | Feature | New | Normal | improve gmxapi error handling | Eric Irrgang | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 3401 | GROMACS | Feature | New | Normal | Policy and procedure for installed headers (public API) | | 02/26/2020 04:17 PM | 2021-infrastructure-stable |
| 3402 | GROMACS | Feature | New | Normal | Clarify distinction between public API documentation and developer docs. | | 02/26/2020 04:16 PM | 2021-infrastructure-stable |
| 3410 | GROMACS | Feature | New | Normal | Random Acceleration Molecular Dynamics (RAMD) | Bernd Doser | 03/05/2020 03:22 PM | 2021 |
| 3417 | GROMACS | Feature | New | Normal | Make modular simulator feature-complete | Pascal Merz | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 3423 | GROMACS | Feature | New | Normal | Implement additional temperature and pressure control algorithms for modular simulator | Pascal Merz | 03/10/2020 11:22 PM | 2021-infrastructure-stable |
| 3424 | GROMACS | Feature | New | Normal | Implement stochastic dynamics / langevin integrator in modular simulator | Pascal Merz | 03/10/2020 11:48 PM | 2021-infrastructure-stable |
| 3425 | GROMACS | Feature | New | Normal | Implement rerun for the modular simulator | Pascal Merz | 03/10/2020 11:57 PM | 2021-infrastructure-stable |
| 3426 | GROMACS | Feature | New | Normal | Support acceleration in modular simulator | Pascal Merz | 03/11/2020 04:09 PM | 2021-infrastructure-stable |
| 3427 | GROMACS | Feature | New | Normal | Support freeze groups in modular simulator | Pascal Merz | 03/11/2020 12:07 AM | 2021-infrastructure-stable |
| 3428 | GROMACS | Feature | New | Normal | Implement SIMD version of modular simulator propagators | Pascal Merz | 03/11/2020 12:12 AM | 2021-infrastructure-stable |
| 3430 | GROMACS | Feature | New | Normal | Implement NMR restraints for modular simulator | Pascal Merz | 03/11/2020 12:28 AM | 2021-infrastructure-stable |
| 3431 | GROMACS | Feature | New | Normal | Implement virtual sites for modular simulator | Pascal Merz | 03/11/2020 12:33 AM | 2021-infrastructure-stable |
| 3432 | GROMACS | Feature | New | Normal | Implement essential dynamics for modular simulator | Pascal Merz | 03/11/2020 12:38 AM | 2021-infrastructure-stable |
| 3433 | GROMACS | Feature | New | Normal | Decide how to handle multisim with modular simulator | Pascal Merz | 03/11/2020 06:42 AM | 2021-infrastructure-stable |
| 3434 | GROMACS | Feature | New | Normal | Support box deformation in modular simulator | Pascal Merz | 03/11/2020 12:50 AM | 2021-infrastructure-stable |
| 3435 | GROMACS | Feature | New | Normal | Implement pull for modular simulator | Pascal Merz | 03/11/2020 06:31 AM | 2021-infrastructure-stable |
| 3436 | GROMACS | Feature | New | Normal | Implement AWH for modular simulator | Pascal Merz | 03/11/2020 06:32 AM | 2021-infrastructure-stable |
| 3439 | GROMACS | Feature | New | Normal | Optimize successive simulation segments | | 03/11/2020 01:42 PM | |
| 687 | Support Platforms | Feature | New | Normal | Add content on the front page | | 09/02/2019 01:08 PM | |
| 987 | Support Platforms | Feature | New | Normal | Feature wishlist should be moved to Redmine | | 08/03/2012 12:22 PM | |
| 1601 | Support Platforms | Feature | New | Normal | use Git for Jenkins Config | | 05/24/2015 10:59 AM | |
| 1105 | Benchmark suite | Feature | New | Normal | produce a benchmark suite | | 09/13/2016 10:31 PM | |
| 1106 | Benchmark suite | Feature | New | Normal | publish benchmark numbers | | 06/19/2014 12:08 PM | |
| 1197 | TNG trajectory library | Feature | New | Normal | Rework the molecule descriptions | | 03/18/2013 04:16 PM | version 2 |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|------------------------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 1199 | TNG trajectory library | Feature | New | Normal | residue numbering | Magnus Lundborg | 04/24/2013 09:33 AM | version 2 |
| 1200 | TNG trajectory library | Feature | New | Normal | Field for the PDB format 'segment identifier' | Magnus Lundborg | 04/24/2013 09:32 AM | version 2 |
| 1202 | TNG trajectory library | Feature | New | Normal | Other hash types | | 06/25/2013 10:02 PM | version 2 |
| 665 | GROMACS | Task | New | Normal | Port existing trajectory analysis tools to use the new framework | | 07/14/2014 11:29 AM | future |
| 677 | GROMACS | Task | New | Normal | Make sure manual uses consistent style throughout | | 06/19/2014 11:49 AM | |
| 701 | GROMACS | Task | New | Normal | Add symbol visibility macros | | 03/02/2019 01:46 AM | future |
| 765 | GROMACS | Task | New | Normal | Improving serialization of data structures prior to communication | Mark Abraham | 05/13/2014 10:04 AM | future |
| 838 | GROMACS | Task | New | Normal | Improve generic error reporting routines | | 07/11/2016 08:29 PM | |
| 909 | GROMACS | Task | New | Normal | Reimplement displacement calculation module | | 07/14/2014 11:30 AM | future |
| 948 | GROMACS | Task | New | Normal | C++ thread synchronization primitives | Sander Pronk | 07/11/2016 08:24 PM | |
| 986 | GROMACS | Task | New | Normal | Handling C++ out-of-memory errors | | 12/24/2014 08:42 PM | future |
| 988 | GROMACS | Task | New | Normal | Definition of "public API" | | 08/28/2019 02:50 PM | future |
| 996 | GROMACS | Task | New | Normal | C++ MPI Framework | Roland Schulz | 07/14/2014 11:53 AM | future |
| 1017 | GROMACS | Task | New | Normal | C++ Vector/Matrix classes | | 07/11/2016 08:23 PM | |
| 1140 | GROMACS | Task | New | Normal | Class design for passing options and data | | 07/11/2016 08:19 PM | |
| 1170 | GROMACS | Task | New | Normal | mdlib reorganization | | 11/17/2016 03:47 PM | future |
| 1214 | GROMACS | Task | New | Normal | Keep track of important changes for Changelog | Mark Abraham | 06/26/2013 11:24 AM | |
| 1246 | GROMACS | Task | New | Normal | expanded ensemble .tpr cannot be rerun | Michael Shirts | 06/19/2015 01:56 PM | |
| 1323 | GROMACS | Task | New | Normal | determine future of existing tools for | David van der Spoel | 12/04/2018 11:53 AM | |
| 1411 | GROMACS | Task | New | Normal | Future of thread_mpi | Mark Abraham | 02/26/2018 04:56 PM | future |
| 1490 | GROMACS | Task | New | Normal | Usage of forward declarations vs typedef vs #include | Mark Abraham | 01/21/2015 10:23 AM | |
| 1505 | GROMACS | Task | New | Normal | improve handling of logging | Mark Abraham | 01/02/2019 06:06 PM | |
| 1515 | GROMACS | Task | New | Normal | improve g_bar output | Szilárd Páll | 07/11/2016 08:10 PM | |
| 1523 | GROMACS | Task | New | Normal | add missing code-paths to CUDA emulation kernel | | 07/11/2016 08:09 PM | |
| 1587 | GROMACS | Task | New | Normal | improve the configurability of regression tests | | 12/20/2019 12:02 PM | 2021 |
| 1729 | GROMACS | Task | New | Normal | Resolve whether and how to resolve "state" variables stored in .tpr | | 05/13/2015 10:48 AM | future |
| 1745 | GROMACS | Task | New | Normal | Moving to C++11 after Gromacs-5.1 | | 06/01/2016 03:01 PM | |
| 1758 | GROMACS | Task | New | Normal | Verlet scheme reorganization / modularization | Mark Abraham | 07/20/2015 06:33 PM | future |
| 1768 | GROMACS | Task | New | Normal | decide future of command-line options vs env vars | | 11/03/2016 05:51 PM | future |
| 1786 | GROMACS | Task | New | Normal | Python style standards in developer docs | Peter Kasson | 12/26/2019 03:15 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|--|--------------|---------------------|----------------|
| 1793 | GROMACS | Task | New | Normal | cleanup of integration loop | Mark Abraham | 10/31/2018 10:49 PM | future |
| 1826 | GROMACS | Task | New | Normal | investigate non-optimal results with CPU-GPU balancing on AMD | Szilárd Páll | 12/20/2019 12:04 PM | future |
| 1828 | GROMACS | Task | New | Normal | Exception handling in mdrun | | 10/07/2015 11:36 AM | |
| 1829 | GROMACS | Task | New | Normal | Future of thread level parallelism | | 11/18/2016 05:29 PM | |
| 1852 | GROMACS | Task | New | Normal | Remove group scheme | | 03/03/2020 09:03 PM | future |
| 1855 | GROMACS | Task | New | Normal | Convert preprocessor use so that symbols are always defined | | 06/28/2016 02:17 PM | |
| 1862 | GROMACS | Task | New | Normal | Fully replace t_topology by gmx_mtop_t | | 02/13/2019 04:53 PM | |
| 1876 | GROMACS | Task | New | Normal | Reorganize vector input passed to core MD routines | | 06/01/2016 01:59 PM | future |
| 1936 | GROMACS | Task | New | Normal | treat default-able mdp fields as strings | | 04/02/2016 10:32 PM | future |
| 1947 | GROMACS | Task | New | Normal | Consider fixing corner case in TinyXML2 | Mark Abraham | 04/19/2016 01:40 AM | |
| 1971 | GROMACS | Task | New | Normal | Removing buggy features vs. keeping workflows | | 01/19/2018 01:36 PM | future |
| 1973 | GROMACS | Task | New | Normal | OpenCL implementation wish list | | 05/27/2016 03:42 PM | |
| 2003 | GROMACS | Task | New | Normal | reconsider various simd flags | | 07/07/2016 11:23 PM | |
| 2009 | GROMACS | Task | New | Normal | improve command-line reporting of useful things | | 07/26/2016 12:54 PM | |
| 2010 | GROMACS | Task | New | Normal | Use size_t instead of int for indexing | | 07/01/2018 07:57 AM | |
| 2035 | GROMACS | Task | New | Normal | A common trajectory analysis data exchange format | | 03/15/2017 05:46 PM | future |
| 2045 | GROMACS | Task | New | Normal | API design and language bindings | Peter Kasson | 01/29/2020 03:59 PM | |
| 2048 | GROMACS | Task | New | Normal | C++11: CUDA dependency on general headers | | 09/07/2016 10:30 PM | |
| 2053 | GROMACS | Task | New | Normal | refine notation in GPU code | | 12/20/2019 01:04 PM | 2021 |
| 2089 | GROMACS | Task | New | Normal | Encourage code review | | 01/10/2017 12:03 AM | |
| 2092 | GROMACS | Task | New | Normal | Tests running on GPU, and hardware assignment | | 12/19/2017 05:27 PM | future |
| 2115 | GROMACS | Task | New | Normal | trjconv does too many things, and combinations of them work poorly | | 10/02/2018 09:04 AM | |
| 2158 | GROMACS | Task | New | Normal | consider adding post-submit test that runs PME with 2xNN kernels | | 04/19/2017 08:04 PM | |
| 2169 | GROMACS | Task | New | Normal | remove 'continuation' mdp option | | 12/29/2019 10:31 AM | 2021 |
| 2175 | GROMACS | Task | New | Normal | improve clang static analyzer docs further | | 01/04/2018 04:13 PM | future |
| 2178 | GROMACS | Task | New | Normal | Move checks for specific warnings to source repo | | 05/12/2017 03:57 PM | |
| 2185 | GROMACS | Task | New | Normal | add docs on MPI + CUDA w/wo MPS | | 05/24/2017 05:17 PM | |
| 2216 | GROMACS | Task | New | Normal | GROMACS SIMD acceleration: generation 3 | Erik Lindahl | 07/17/2017 06:57 PM | future |
| 2221 | GROMACS | Task | New | Normal | Avoid preprocessor for SIMD functions | | 02/21/2018 01:43 PM | |
| 2294 | GROMACS | Task | New | Normal | Require identical hardware on nodes on parallel runs | | 11/19/2017 08:54 PM | |
| 2304 | GROMACS | Task | New | Normal | Document and propose tracking mdrun heuristics | | 10/03/2018 09:39 PM | future |
| 2351 | GROMACS | Task | New | Normal | Avoid the SIMD module depending on non-trivial parts of Gromacs | | 12/14/2017 02:47 AM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|--------------|---------------------|----------------------------|
| 2353 | GROMACS | Task | New | Normal | improve on relative tolerance for constructing tables | | 12/20/2019 12:12 PM | 2021 |
| 2367 | GROMACS | Task | New | Normal | construct pbc_simd less often | | 09/24/2018 11:02 PM | future |
| 2371 | GROMACS | Task | New | Normal | mtop searching needs reconsideration | | 01/04/2018 11:54 AM | future |
| 2375 | GROMACS | Task | New | Normal | Clarify execution phases for MD simulation | | 04/30/2019 12:59 PM | |
| 2376 | GROMACS | Task | New | Normal | max_mpi_ranks has wrong name | | 02/10/2018 11:03 AM | |
| 2379 | GROMACS | Task | New | Normal | check leftover FIXMEs in r2018 | Szilárd Páll | 12/31/2018 11:16 AM | future |
| 2382 | GROMACS | Task | New | Normal | Simplify Doxygen guidelines | | 01/13/2018 12:40 AM | |
| 2383 | GROMACS | Task | New | Normal | Add JSON interface to write and read files | Paul Bauer | 01/16/2018 02:01 PM | future |
| 2396 | GROMACS | Task | New | Normal | Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation | Paul Bauer | 12/02/2019 01:24 PM | 2021-infrastructure-stable |
| 2402 | GROMACS | Task | New | Normal | PME kernels general performance improvements | | 03/26/2018 10:41 AM | future |
| 2412 | GROMACS | Task | New | Normal | attempt to do better FFTW planning | | 03/15/2018 05:01 PM | |
| 2422 | GROMACS | Task | New | Normal | write C kernel for tables in Verlet scheme | | 02/26/2018 01:38 PM | |
| 2423 | GROMACS | Task | New | Normal | modernize constraints code | Mark Abraham | 09/19/2018 03:01 PM | future |
| 2425 | GROMACS | Task | New | Normal | testing multisim with multiple ranks per simulation | Mark Abraham | 12/20/2019 12:13 PM | 2021 |
| 2435 | GROMACS | Task | New | Normal | identify and note about/tune task offload in GPU-bound runs | | 03/02/2018 04:08 PM | |
| 2442 | GROMACS | Task | New | Normal | Port gmx saxs and gmx sans to c++ | Joe Jordan | 06/28/2018 10:06 PM | future |
| 2445 | GROMACS | Task | New | Normal | Decide if/how to check for incompatible user input to mdrun for bonds and vsites | | 03/13/2018 02:02 PM | |
| 2456 | GROMACS | Task | New | Normal | Add a pull module external potential tests | | 03/15/2018 03:02 PM | |
| 2462 | GROMACS | Task | New | Normal | consider adding STL misuse tests | | 03/23/2018 01:23 AM | |
| 2464 | GROMACS | Task | New | Normal | GPU performance goals overview | | 03/26/2018 10:42 AM | |
| 2469 | GROMACS | Task | New | Normal | implement GPU timer reduction for reporting | | 03/27/2018 05:08 PM | |
| 2475 | GROMACS | Task | New | Normal | make OpenCL 1st class-citizen in the build system | | 12/20/2019 12:14 PM | 2021 |
| 2488 | GROMACS | Task | New | Normal | use MPI non-blocking collectives to overlap pull comm | | 04/25/2018 04:19 PM | |
| 2490 | GROMACS | Task | New | Normal | evaluate two-step communicators | Szilárd Páll | 10/03/2018 09:47 PM | future |
| 2492 | GROMACS | Task | New | Normal | implement force calculation via ForceProviders containing collections of IForceProvider | Mark Abraham | 09/19/2018 03:13 PM | future |
| 2498 | GROMACS | Task | New | Normal | OpenCL memory pinning/mapping | | 12/20/2019 12:18 PM | future |
| 2501 | GROMACS | Task | New | Normal | Documentation section on log file contents | Kevin Boyd | 10/03/2018 09:48 PM | future |
| 2514 | GROMACS | Task | New | Normal | PME OpenCL reductions with intrinsics | | 05/31/2018 12:27 AM | future |
| 2518 | GROMACS | Task | New | Normal | redesign task-assignment code for OpenCL | | 12/20/2019 12:19 PM | future |
| 2520 | GROMACS | Task | New | Normal | Treat OpenCL kernel width more diligently | | 05/24/2018 06:21 PM | |
| 2521 | GROMACS | Task | New | Normal | Implement alternating PME/NB wait for OpenCL | | 10/15/2018 12:39 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|--|-------------------|---------------------|----------------------------|
| 2524 | GROMACS | Task | New | Normal | struct alignment/packing for OpenCL host & device code | | 12/20/2019 12:20 PM | future |
| 2527 | GROMACS | Task | New | Normal | Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL) | | 10/30/2018 04:06 AM | future |
| 2528 | GROMACS | Task | New | Normal | PME GPU tuning | | 12/31/2018 11:18 AM | future |
| 2530 | GROMACS | Task | New | Normal | consider using CUDA Driver API | | 09/23/2018 11:47 PM | future |
| 2532 | GROMACS | Task | New | Normal | enable queue priorities in OpenCL | | 05/29/2018 02:29 PM | |
| 2535 | GROMACS | Task | New | Normal | consider compiling opencl fft kernels once | | 05/31/2018 01:33 PM | |
| 2537 | GROMACS | Task | New | Normal | Simplify PME solve reduction | Aleksei lupinov | 12/20/2019 12:21 PM | future |
| 2538 | GROMACS | Task | New | Normal | organize more of the PME GPU code along task-specific lines | Mark Abraham | 05/31/2018 05:41 PM | |
| 2546 | GROMACS | Task | New | Normal | Add more assertions to AWH code | Viveca Lindahl | 06/06/2018 11:20 AM | future |
| 2590 | GROMACS | Task | New | Normal | Essential Dynamics as module providing forces | Christian Blau | 08/22/2018 05:03 PM | future |
| 2595 | GROMACS | Task | New | Normal | Reusable Utilities for Schedules | Prashanth Kanduri | 02/22/2019 03:48 PM | future |
| 2603 | GROMACS | Task | New | Normal | Add ability to properly check coordinate files during testing | Paul Bauer | 10/15/2018 01:16 PM | future |
| 2608 | GROMACS | Task | New | Normal | Remove code duplication between OpenCL and CUDA | | 09/24/2018 12:47 PM | |
| 2616 | GROMACS | Task | New | Normal | Model for MD state | | 09/14/2018 05:12 PM | |
| 2621 | GROMACS | Task | New | Normal | Fine-Grained API to Describe Force Calculation and Neighbourhood Search | Prashanth Kanduri | 08/22/2018 11:36 AM | future |
| 2644 | GROMACS | Task | New | Normal | Replace compute_globals | Mark Abraham | 09/24/2018 05:51 PM | future |
| 2650 | GROMACS | Task | New | Normal | revise OpenCL stack recommendations | | 12/31/2018 11:19 AM | future |
| 2658 | GROMACS | Task | New | Normal | Secondary structure assignment via DSSP as native gromacs code | Christian Blau | 10/09/2018 04:51 PM | future |
| 2671 | GROMACS | Task | New | Normal | replace constants like M_PI | | 12/20/2019 01:17 PM | future |
| 2672 | GROMACS | Task | New | Normal | check & document execution width requirements in OpenCL | | 12/31/2018 11:20 AM | future |
| 2682 | GROMACS | Task | New | Normal | Add MSAN configuration | | 10/09/2018 06:28 PM | |
| 2686 | GROMACS | Task | New | Normal | add tests for gpu bonded interactions | | 12/27/2019 04:40 PM | 2021 |
| 2697 | GROMACS | Task | New | Normal | improve FFT library flavor/version reporting | | 12/27/2019 04:40 PM | future |
| 2699 | GROMACS | Task | New | Normal | Test POWER9 | | 12/04/2019 03:29 PM | 2021-infrastructure-stable |
| 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 |
| 2735 | GROMACS | Task | New | Normal | Allow gmx_genrestr to write correct position restraints for molecules after the first molecule | Joe Jordan | 12/11/2019 09:26 AM | future |
| 2764 | GROMACS | Task | New | Normal | gmxapi version updates for post release-2019 | Eric Irrgang | 11/21/2018 12:53 PM | |
| 2770 | GROMACS | Task | New | Normal | change branch maintenance policy | | 01/16/2020 05:09 PM | 2021 |
| 2771 | GROMACS | Task | New | Normal | Size independent Hessian for normal mode analysis | | 12/28/2019 10:50 AM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|--|----------------|---------------------|----------------------------|
| 2773 | GROMACS | Task | New | Normal | improve GPU error handling and make such handling uniform across modules | | 12/20/2019 01:09 PM | 2021 |
| 2787 | GROMACS | Task | New | Normal | allow passing flags to allocateDeviceBuffer | | 12/03/2018 01:54 PM | |
| 2795 | GROMACS | Task | New | Normal | Incorporate regressiontests into core gromacs | | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2833 | GROMACS | Task | New | Normal | Update topology datastructures | Paul Bauer | 12/02/2019 01:43 PM | 2021-infrastructure-stable |
| 2835 | GROMACS | Task | New | Normal | Matrix class constraint to upper or lower triangle | | 02/07/2019 02:44 PM | |
| 2839 | GROMACS | Task | New | Normal | make module and file naming consistent | | 01/16/2020 05:11 PM | 2021 |
| 2855 | GROMACS | Task | New | Normal | Allow compiling GROMACS without C compiler | | 01/10/2020 12:06 PM | |
| 2857 | GROMACS | Task | New | Normal | Clarify recommended function specifies (constexpr, noexcept, pure) | | 02/04/2019 04:48 AM | |
| 2863 | GROMACS | Task | New | Normal | improve PBC handling | | 03/11/2019 04:28 PM | |
| 2864 | GROMACS | Task | New | Normal | Building incompatibilities | Benson Muite | 02/19/2019 02:00 PM | |
| 2874 | GROMACS | Task | New | Normal | Refactor Gromacs (cluster) neighborlist into separate module | Erik Lindahl | 02/28/2019 11:36 AM | |
| 2877 | GROMACS | Task | New | Normal | use gm::Options more | Mark Abraham | 12/20/2019 01:22 PM | 2021 |
| 2882 | GROMACS | Task | New | Normal | evaluate different storage layouts for GPU coordinates/changes/forces | Szilárd Páll | 03/07/2019 06:21 PM | |
| 2889 | GROMACS | Task | New | Normal | update grompp warnings for brevity, usefulness and actionability | Mark Abraham | 12/27/2019 04:38 PM | future |
| 2905 | GROMACS | Task | New | Normal | Add a Jenkins configuration with std library assert | | 08/24/2019 05:22 PM | |
| 2908 | GROMACS | Task | New | Normal | Renaming things in nbnxm | Berk Hess | 03/28/2019 10:10 AM | |
| 2909 | GROMACS | Task | New | Normal | consider implementing mechanisms to ensure pair lists are not used past their max lifetime | | 04/03/2019 05:14 PM | |
| 2916 | GROMACS | Task | New | Normal | Decide future of symtab | Paul Bauer | 09/06/2019 02:35 PM | 2021-infrastructure-stable |
| 2919 | GROMACS | Task | New | Normal | C++ style guidelines for namespace use | | 04/15/2019 01:21 PM | |
| 2925 | GROMACS | Task | New | Normal | BasicVector addition operator yields unexpected result when adding scalar | Christian Blau | 12/17/2019 10:04 AM | 2021-infrastructure-stable |
| 2933 | GROMACS | Task | New | Normal | Convert walls to a ForceProvider | | 04/25/2019 02:43 PM | |
| 2936 | GROMACS | Task | New | Normal | introduce check that CPU-GPU transfers/assignments are made between compatible types | | 02/05/2020 03:57 PM | 2021 |
| 2976 | GROMACS | Task | New | Normal | Basic math for Multidimensional arrays | | 12/27/2019 04:37 PM | 2021 |
| 2983 | GROMACS | Task | New | Normal | better suited data-types for bonded GPU kernels | | 07/11/2019 04:32 PM | |
| 2992 | GROMACS | Task | New | Normal | Split hw_opt in const user options and dynamic settings | | 12/27/2019 04:31 PM | future |
| 2997 | GROMACS | Task | New | Normal | improve performance of alchemical free energy calculations | | 12/27/2019 04:31 PM | 2021 |
| 2999 | GROMACS | Task | New | Normal | Move all logging in core library and tools to use MDLogger | | 09/06/2019 02:36 PM | 2021-infrastructure-stable |
| 3001 | GROMACS | Task | New | Normal | explore simplifying virial and shift force reduction | | 12/27/2019 04:30 PM | 2021 |
| 3002 | GROMACS | Task | New | Normal | consider splitting bonded work into local/nonlocal | | 06/25/2019 04:06 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|----------------|---------------------|----------------------------|
| 3003 | GROMACS | Task | New | Normal | implement heuristic fallback to CPU when there is too little work for GPU offload | | 06/25/2019 04:10 PM | |
| 3004 | GROMACS | Task | New | Normal | Move trajectory analysis logging to MDLogger | | 06/26/2019 09:59 AM | |
| 3005 | GROMACS | Task | New | Normal | Move logging in gmx preprocess to MDLogger | | 06/26/2019 10:01 AM | |
| 3008 | GROMACS | Task | New | Normal | verify block size choice of CUDA bonded kernel | | 12/27/2019 04:30 PM | 2021 |
| 3013 | GROMACS | Task | New | Normal | Extend logging levels in MDLogger | | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3015 | GROMACS | Task | New | Normal | Create central log handle for calls to gmx_fatal | | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3016 | GROMACS | Task | New | Normal | intermittent failure of essentialdynamics test | | 07/18/2019 05:23 PM | |
| 3031 | GROMACS | Task | New | Normal | evaluate the impact of particle order on PME | | 12/27/2019 04:29 PM | 2021 |
| 3035 | GROMACS | Task | New | Normal | Provide central logger in wrapper binary | Paul Bauer | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3040 | GROMACS | Task | New | Normal | Refactor Restraint module | | 07/18/2019 03:59 PM | |
| 3057 | GROMACS | Task | New | Normal | re-enable fusion on Power8/9 | Szilárd Páll | 12/27/2019 04:22 PM | 2021 |
| 3062 | GROMACS | Task | New | Normal | add twin cut-off mdrun test | | 12/27/2019 04:22 PM | 2021 |
| 3064 | GROMACS | Task | New | Normal | add test for perturbed bonded forces | | 12/27/2019 04:22 PM | 2021 |
| 3072 | GROMACS | Task | New | Normal | Use gmx::index for indexing instead of int | Christian Blau | 09/03/2019 04:23 PM | 2021-infrastructure-stable |
| 3076 | GROMACS | Task | New | Normal | Selectively activate MdModules during simulation instead of instantiating all of them | Christian Blau | 01/17/2020 02:40 PM | 2021-infrastructure-stable |
| 3078 | GROMACS | Task | New | Normal | Allow MD modules to register energy output fields themselves | | 09/06/2019 11:36 AM | |
| 3096 | GROMACS | Task | New | Normal | Multiple time-stepping: correct coupling algorithms, virial calculation and energy output | Christian Blau | 09/18/2019 02:18 PM | 2021-infrastructure-stable |
| 3104 | GROMACS | Task | New | Normal | implement GPU DD cycle counting | | 12/27/2019 04:21 PM | 2021 |
| 3105 | GROMACS | Task | New | Normal | implement GPU PME/PP comm cycle counting | | 12/27/2019 04:20 PM | 2021 |
| 3119 | GROMACS | Task | New | Normal | clang-tidy coverage of parallelization codepaths | | 12/27/2019 04:20 PM | 2021 |
| 3123 | GROMACS | Task | New | Normal | address sanitizer coverage of parallelization code-paths | | 10/05/2019 12:32 AM | |
| 3130 | GROMACS | Task | New | Normal | Interim handling of gmxapi data references. | Eric Irrgang | 12/11/2019 11:26 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 |
| 3132 | GROMACS | Task | New | Normal | gmxapi testing support tools | | 10/31/2019 03:35 PM | |
| 3139 | GROMACS | Task | New | Normal | gmxapi Futures should be subscribable | Eric Irrgang | 10/15/2019 03:56 PM | |
| 3143 | GROMACS | Task | New | Normal | move the non-force accumulation/accounting tasks out of the GPU wait functions | Szilárd Páll | 12/27/2019 04:16 PM | 2021 |
| 3145 | GROMACS | Task | New | Normal | gmxapi.mdrun needs improved (and public) interface for attaching an MD extension. | Eric Irrgang | 01/16/2020 04:31 PM | 2021-refactoring |
| 3162 | GROMACS | Task | New | Normal | Add virtual site support to GPU version of update-constraints. | Artem Zhmurov | 01/23/2020 11:52 AM | 2021-infrastructure-stable |
| 3171 | GROMACS | Task | New | Normal | schedule CPU H2D force contribution in separate stream | | 12/20/2019 08:33 AM | 2021-infrastructure-stable |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|----------------|---------------------|----------------------------|
| 3180 | GROMACS | Task | New | Normal | Remove extra D2H and H2D copies of coordinates when the COM motion is compensated. | Artem Zhmurov | 02/14/2020 12:45 PM | 2021-infrastructure-stable |
| 3181 | GROMACS | Task | New | Normal | consolidate task assignment and workload data initialization | | 10/28/2019 02:53 PM | |
| 3185 | GROMACS | Task | New | Normal | Update PME CUDA kernels to allow a different number of threads per atom in the gather and spread kernels. | | 10/30/2019 11:18 AM | |
| 3187 | GROMACS | Task | New | Normal | Template updated PME kernels using threads per atom | | 10/30/2019 11:33 AM | |
| 3194 | GROMACS | Task | New | Normal | consider passing GPU dependency list to both dependency producers and consumers | | 11/01/2019 07:10 PM | |
| 3212 | GROMACS | Task | New | Normal | Update regression tests for new kernel flavours | | 11/21/2019 11:50 AM | |
| 3216 | GROMACS | Task | New | Normal | improve CPU force reductions | Szilárd Páll | 12/04/2019 09:24 PM | |
| 3220 | GROMACS | Task | New | Normal | change rolling pruning scheduling with GPU update | | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3224 | GROMACS | Task | New | Normal | add regression test case large enough to miscalculated GPU grid launch cases | | 12/20/2019 01:18 PM | 2021 |
| 3229 | GROMACS | Task | New | Normal | Move checkpointing to the beginning of the MD step | | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 3235 | GROMACS | Task | New | Normal | Run mdrun-test in parallel and make sure they tests test critical quantities like energy conservation | Christian Blau | 12/12/2019 03:46 PM | 2021-infrastructure-stable |
| 3236 | GROMACS | Task | New | Normal | GPU update-constraints: Pulling support | Artem Zhmurov | 01/23/2020 11:53 AM | 2021-infrastructure-stable |
| 3252 | GROMACS | Task | New | Normal | Remove support for 32 bit architectures | | 03/01/2020 02:05 PM | |
| 3254 | GROMACS | Task | New | Normal | Remove support for generation of virtual sites to replace aromatic rings in standard residues | | 12/19/2019 12:13 PM | |
| 3255 | GROMACS | Task | New | Normal | Move benchmarking options from mdrun to a dedicated tool | | 12/19/2019 01:21 PM | |

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