

Issues

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|-----------------|---------|-----------------|----------|--|----------|---------------------|----------------------------|
| 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 | |
| 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 | |
| 3443 | GROMACS | Bug | New | Normal | Bonded GPU kernel performance regression with 2020 | | 03/15/2020 08:15 PM | |
| 3442 | GROMACS | Bug | Accepted | Normal | continuing mdrun with -deffnm and pulling does not work | | 03/15/2020 08:33 AM | |
| 3440 | GROMACS | Bug | New | Normal | Multi-nodes run exits with error with openmpi/4.0.0 | | 03/23/2020 02:10 PM | |
| 3439 | GROMACS | Feature | New | Normal | Optimize successive simulation segments | | 03/11/2020 01:42 PM | |
| 3413 | GROMACS | Bug | Feedback wanted | Normal | COMM Removal Failure in GROMACS 2020.1 | | 03/12/2020 02:31 PM | |
| 3412 | GROMACS | Bug | New | Normal | Domain decomposition problems with Gromacs >2018 | | 03/06/2020 04:10 PM | |
| 3411 | GROMACS | Bug | New | Normal | Nightly master release build failure | | 03/06/2020 11:44 AM | 2021-infrastructure-stable |
| 3405 | GROMACS | Bug | Accepted | Normal | intermittent OpenCL regressiontest failures | | 03/02/2020 11:01 AM | |
| 3403 | GROMACS | Bug | Resolved | Normal | solvation free energy with couple-intramol set to no | | 12/10/2020 02:45 PM | |
| 3402 | GROMACS | Feature | New | Normal | Clarify distinction between public API documentation and developer docs. | | 02/26/2020 04:16 PM | 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 |
| 3398 | GROMACS | Bug | New | Normal | Intermittent failure of non-bonded kernels when run using nvprof | | 02/25/2020 12:14 PM | |
| 3395 | GROMACS | Feature | Feedback wanted | Normal | Consider scripted composition of Dockerfiles | | 03/16/2020 12:16 PM | |
| 3387 | GROMACS | Bug | New | Normal | Death test bug | | 02/20/2020 05:39 PM | |
| 3385 | GROMACS | Bug | New | Normal | FindLibStdCpp.cmake - wrong sanity check for clang | | 03/04/2020 06:59 PM | |
| 3382 | GROMACS | Task | Accepted | Normal | Split up t_inputrec | | 02/17/2020 05:28 PM | |
| 3379 | GROMACS | Feature | New | Normal | C++ API for simulation input and output | | 02/28/2020 10:38 AM | 2021-infrastructure-stable |
| 3378 | GROMACS | Feature | New | Normal | genion usage without stdin (facilitates use in gmx python api) | | 02/13/2020 12:04 PM | |
| 3374 | GROMACS | Feature | New | Normal | SimulationInput abstraction | | 03/03/2020 05:32 PM | 2021-refactoring |
| 3370 | GROMACS | Task | New | High | Further improvements to GPU Buffer Ops and Comms | | 03/04/2020 01:38 PM | |
| 3369 | GROMACS | Feature | New | Normal | Add quote about "the truth" | | 02/05/2020 05:08 PM | |
| 3366 | GROMACS | Task | New | Normal | Enforce compability of MdModules | | 02/28/2020 11:20 AM | |
| 3365 | GROMACS | Task | New | Low | consider making GPU bonded work independent from nonbonded | | 03/01/2020 01:11 PM | |
| 3362 | GROMACS | Feature | New | Normal | gmx traj: add an option to plot each component in a separate file | | 01/29/2020 06:18 PM | |
| 3360 | GROMACS | Task | New | Normal | investigate the future of DD dynamic load balancing with GPU offload | | 01/29/2020 11:23 AM | |

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| 3357 | GROMACS | Task | New | Normal | Make sure "colvars" interoperates stably and smoothly with gromacs | | 03/04/2020 11:25 AM | |
| 3356 | GROMACS | Task | New | Normal | Expose setting of random seed to API | | 01/29/2020 06:16 PM | 2021 |
| 3353 | GROMACS | Task | New | Normal | Document gmx densmap output | | 01/23/2020 12:52 PM | |
| 3332 | GROMACS | Feature | New | Normal | gmx helixorient doesn't have a -tu option to change time unit | | 01/22/2020 11:57 AM | |
| 3330 | GROMACS | Task | New | Normal | Compile list of codepaths for testing task assignment | | 01/22/2020 10:03 AM | 2021-refactoring |
| 3329 | GROMACS | Task | New | Normal | Extend energy comparison testing framework | | 01/22/2020 09:51 AM | 2021-refactoring |
| 3328 | GROMACS | Feature | New | Normal | Testing framework for task assignment | | 01/22/2020 09:48 AM | 2021-refactoring |
| 3327 | GROMACS | Task | New | Normal | Refactor workload flags | | 01/22/2020 09:45 AM | 2021-refactoring |
| 3326 | GROMACS | Task | New | Normal | Allow changing task assignment | | 01/22/2020 09:44 AM | 2021-refactoring |
| 3325 | GROMACS | Task | New | Normal | Allow complete re-initialization of a simulation | | 01/29/2020 05:13 PM | 2021-refactoring |
| 3324 | GROMACS | Task | New | Normal | Rework CMake handling of GPU code | | 01/22/2020 09:52 AM | 2021-refactoring |
| 3311 | GROMACS | Feature | In Progress | Normal | GPU infrastructure development | | 03/20/2020 09:54 AM | 2021-refactoring |
| 3310 | GROMACS | Bug | Blocked, need info | Low | Thread affinity on Mac OS | | 02/27/2020 11:10 PM | |
| 3309 | GROMACS | Bug | New | Normal | -reprod: checkpoint reading bug and general considerations | | 02/27/2020 10:45 PM | |
| 3308 | GROMACS | Task | New | Normal | GPU update-constraints: Cycle counting for GPU launches | | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 3307 | GROMACS | Feature | New | Normal | General interface for communication between simulation ranks | | 01/22/2020 03:22 PM | 2021-refactoring |
| 3305 | GROMACS | Bug | New | Normal | Case gives FPE with Debug build when GPU update is enabled | | 01/21/2020 05:44 PM | |
| 3301 | GROMACS | Bug | New | Normal | pdb2gmx adding hydrogen | | 01/15/2020 10:17 PM | |
| 3300 | GROMACS | Task | New | Normal | Abandon docs/OpenCLTODOList.txt? | | 01/15/2020 02:46 PM | |
| 3298 | GROMACS | Feature | New | Normal | start early PP work for first dimension of halo exchange | | 03/01/2020 01:36 PM | |
| 3297 | GROMACS | Task | Resolved | Normal | Require gcc > 5 | | 04/30/2020 11:00 AM | 2021-infrastructure-stable |
| 3290 | GROMACS | Task | Resolved | Normal | Require CMake >= 3.12 | | 04/14/2020 02:45 PM | 2021-refactoring |
| 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 |
| 3287 | GROMACS | Task | New | Normal | Deprecate make_ndx, use select instead | | 01/23/2020 01:16 PM | |
| 3285 | GROMACS | Feature | Resolved | Normal | Run simulations from the same tpr file with different random seeds | | 02/27/2020 11:22 PM | future |
| 3283 | GROMACS | Feature | Resolved | Normal | Support for the string method with swarms of trajectories in GROMACS | | 03/01/2020 01:16 PM | 2021 |
| 3281 | GROMACS | Bug | New | Normal | Test data directory GMX_RELEASE_ASSERT triggers | | 01/06/2020 08:07 PM | |
| 3279 | GROMACS | Task | New | Low | Provide more advice for building client software | | 03/02/2020 11:54 AM | |
| 3277 | GROMACS | Feature | New | Normal | Allow testing feature that is partly implemented | | 12/31/2019 12:44 PM | 2021 |
| 3274 | GROMACS | Bug | New | Normal | Remove ARM NEON SIMD | | 12/28/2019 07:53 AM | 2021-infrastructure-stable |
| 3273 | GROMACS | Bug | New | Normal | gmxapi setup.py complains too much | | 12/27/2019 06:42 PM | 2021-infrastructure-stable |

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| 3271 | GROMACS | Task | Resolved | Normal | Adopt PEP-518 for Python package build system configuration. | | 04/09/2020 10:15 PM | 2021-infrastructure-stable |
| 3268 | GROMACS | Task | New | Normal | add more Intel driver recommendations | | 12/26/2019 04:39 PM | |
| 3267 | GROMACS | Task | New | Normal | Document tools | | 12/26/2019 03:20 PM | future |
| 3262 | GROMACS | Task | New | High | Trjconv - dimer protein-ligand | | 12/20/2019 09:26 PM | |
| 3256 | GROMACS | Task | New | Normal | Remove -nsteps option from mdrun | | 12/19/2019 12:12 PM | |
| 3255 | GROMACS | Task | New | Normal | Move benchmarking options from mdrun to a dedicated tool | | 12/19/2019 01:21 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 | |
| 3252 | GROMACS | Task | New | Normal | Remove support for 32 bit architectures | | 03/01/2020 02:05 PM | |
| 3243 | GROMACS | Bug | Feedback wanted | Normal | Convert GROMACS 1 OpenMP thread per rank fatal error into a warning | | 12/27/2019 10:31 AM | |
| 3242 | GROMACS | Feature | New | Normal | Please do not remove the -nsteps flag | | 03/01/2020 01:59 PM | |
| 3240 | GROMACS | Bug | New | Normal | segv with GPU DD direct communication with GPU update and -dlb off | | 01/15/2020 06:16 PM | |
| 3239 | GROMACS | Bug | New | Normal | GPU DD direct communication with GPU update error with RF | | 12/14/2019 05:15 PM | |
| 3233 | GROMACS | Bug | New | Normal | clang-format incorrectly aligning altered function arguments | | 12/13/2019 12:41 PM | |
| 3229 | GROMACS | Task | New | Normal | Move checkpointing to the beginning of the MD step | | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 3227 | GROMACS | Bug | New | Normal | solvate does not check return status of gmx_file_rename | | 12/04/2019 01:43 PM | |
| 3224 | GROMACS | Task | New | Normal | add regression test case large enough to miscalculated GPU grid launch cases | | 12/20/2019 01:18 PM | 2021 |
| 3223 | GROMACS | Bug | New | Normal | unit test failures give verify -1 | | 12/02/2019 11:58 AM | |
| 3220 | GROMACS | Task | New | Normal | change rolling pruning scheduling with GPU update | | 02/25/2020 03:41 PM | 2021-infrastructure-stable |
| 3219 | GROMACS | Bug | Resolved | Normal | MANPATH setting is fragile | | 11/02/2020 11:45 AM | |
| 3214 | GROMACS | Bug | New | Normal | Out-of-bounds, overflow and incorrect outputs in gmx spatial | | 11/25/2019 04:11 PM | |
| 3213 | GROMACS | Bug | New | Normal | Having a local residuetypes.dat for custom force field | | 11/21/2019 09:18 PM | |
| 3212 | GROMACS | Task | New | Normal | Update regression tests for new kernel flavours | | 11/21/2019 11:50 AM | |
| 3210 | GROMACS | Bug | New | High | rerun does not reproduce dVcoul/dl | | 12/27/2019 10:45 AM | |
| 3209 | GROMACS | Bug | New | Normal | Interactive molecular dynamics with VMD becomes stuttering after reconnecting | | 11/19/2019 11:36 AM | |
| 3202 | GROMACS | Bug | New | Low | gmx solvate fails to overwrite topology file | | 11/13/2019 02:44 PM | |
| 3201 | GROMACS | Task | In Progress | Normal | Convert mdp parameters to key value tree | | 11/06/2019 06:06 PM | |
| 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 | |
| 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 |

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| 3196 | GROMACS | Bug | New | Normal | ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing | | 11/01/2019 11:28 PM | |
| 3194 | GROMACS | Task | New | Normal | consider passing GPU dependency list to both dependency producers and consumers | | 11/01/2019 07:10 PM | |
| 3187 | GROMACS | Task | New | Normal | Template updated PME kernels using threads per atom | | 10/30/2019 11:33 AM | |
| 3186 | GROMACS | Task | In Progress | Normal | Update Constant/Variable naming in the PME GPU kernels. | | 10/30/2019 11:23 AM | |
| 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 | |
| 3183 | GROMACS | Task | Accepted | Normal | enable bonded interactions on GPU | | 12/20/2019 08:32 AM | 2021-infrastructure-stable |
| 3181 | GROMACS | Task | New | Normal | consolidate task assignment and workload data initialization | | 10/28/2019 02:53 PM | |
| 3177 | GROMACS | Feature | New | Normal | Spack package management support | | 11/06/2019 06:37 PM | |
| 3171 | GROMACS | Task | New | Normal | schedule CPU H2D force contribution in separate stream | | 12/20/2019 08:33 AM | 2021-infrastructure-stable |
| 3166 | GROMACS | Bug | New | Normal | Compilation failing on Ubuntu 19.04 with Cuda 10.1 | | 10/19/2019 09:13 PM | |
| 3165 | GROMACS | Bug | New | Normal | task assignment silent abort | | 10/18/2019 07:46 PM | |
| 3154 | GROMACS | Task | Resolved | Low | Update use of Python subprocess for >=3.5 | | 04/09/2020 10:15 PM | |
| 3153 | GROMACS | Task | New | Low | Let CMake process module directories earlier to support more modern CMake idioms. | | 10/17/2019 10:40 AM | 2021-infrastructure-stable |
| 3152 | GROMACS | Feature | New | Normal | Infrastructure and patterns for expressing public interfaces | | 01/09/2020 05:19 PM | 2021-infrastructure-stable |
| 3138 | GROMACS | Feature | New | Normal | Improve ensemble support in Context specification. | | 10/15/2019 03:56 PM | |
| 3135 | GROMACS | Feature | New | Normal | Make GPU traits into opaque types | | 10/14/2019 10:24 AM | |
| 3132 | GROMACS | Task | New | Normal | gmxapi testing support tools | | 10/31/2019 03:35 PM | |
| 3127 | GROMACS | Bug | New | Normal | mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia | | 10/09/2019 05:33 PM | |
| 3126 | GROMACS | Feature | New | Normal | State propagator GPU data manager | | 10/09/2019 02:42 PM | |
| 3125 | GROMACS | Bug | Resolved | Normal | OpenCL on Volta and Turing broken | | 02/27/2020 11:01 AM | 2020.2 |
| 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 |
| 3123 | GROMACS | Task | New | Normal | address sanitizer coverage of parallelization code-paths | | 10/05/2019 12:32 AM | |
| 3119 | GROMACS | Task | New | Normal | clang-tidy coverage of parallelization codepaths | | 12/27/2019 04:20 PM | 2021 |
| 3115 | GROMACS | Feature | New | Normal | Device stream manager | | 10/04/2019 09:00 AM | |
| 3105 | GROMACS | Task | New | Normal | implement GPU PME/PP comm cycle counting | | 12/27/2019 04:20 PM | 2021 |
| 3104 | GROMACS | Task | New | Normal | implement GPU DD cycle counting | | 12/27/2019 04:21 PM | 2021 |
| 3093 | GROMACS | Task | In Progress | High | rework GPU direct halo-exchange related force reduction complexities | | 02/14/2020 11:35 AM | 2021-infrastructure-stable |
| 3088 | GROMACS | Bug | New | Normal | Reference to theory needed for cylindrical pull geometry | | 09/13/2019 11:26 AM | |
| 3086 | GROMACS | Bug | New | Normal | gmxapi fails with MPI build of GROMACS 2020 | | 09/25/2019 04:18 PM | |
| 3083 | GROMACS | Bug | New | Normal | Listed forces tests failing on ICC19 with AVX2_256 nightly build | | 09/10/2019 11:56 AM | |

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|------|---------|---------|-----------------|----------|---|----------|---------------------|----------------------------|
| 3082 | GROMACS | Task | New | High | move launch/synchronization points to clarify task dependencies | | 12/27/2019 04:21 PM | 2021 |
| 3078 | GROMACS | Task | New | Normal | Allow MD modules to register energy output fields themselves | | 09/06/2019 11:36 AM | |
| 3077 | GROMACS | Task | Feedback wanted | Normal | PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor | | 11/01/2019 06:56 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 | |
| 3068 | GROMACS | Bug | New | Normal | Misleading warning on rerun | | 08/26/2019 03:44 PM | |
| 3064 | GROMACS | Task | New | Normal | add test for perturbed bonded forces | | 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 |
| 3058 | GROMACS | Bug | Feedback wanted | Normal | Error when using a large PME grid on a GPU | | 09/04/2019 07:26 PM | |
| 3055 | GROMACS | Bug | Feedback wanted | Normal | Error in gmx xpm2ps | | 08/22/2019 03:27 PM | |
| 3054 | GROMACS | Bug | New | Normal | Missing dihedral define | | 08/02/2019 05:47 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 | |
| 3047 | GROMACS | Task | Feedback wanted | Normal | Set required versions for GROMACS 2021 | | 02/20/2020 11:42 AM | |
| 3045 | GROMACS | Feature | New | Low | Option to remove v-sites in trjconv? | | 07/19/2019 04:42 PM | |
| 3042 | GROMACS | Bug | New | Normal | core dump error in grompp command | | 10/09/2019 07:30 PM | |
| 3041 | GROMACS | Task | Resolved | Normal | Remove workaround for gcc bug 58265 | | 06/19/2020 04:45 PM | |
| 3040 | GROMACS | Task | New | Normal | Refactor Restraint module | | 07/18/2019 03:59 PM | |
| 3033 | GROMACS | Task | In Progress | Normal | Clean up and modernize googletest bundling and usage | | 01/16/2020 04:50 PM | 2021-refactoring |
| 3032 | GROMACS | Feature | Feedback wanted | Normal | Clean up dev-manual structure | | 12/11/2019 11:27 AM | 2021-infrastructure-stable |
| 3031 | GROMACS | Task | New | Normal | evaluate the impact of particle order on PME | | 12/27/2019 04:29 PM | 2021 |
| 3030 | GROMACS | Feature | New | Normal | RST style guidelines | | 07/09/2019 03:38 PM | |
| 3028 | GROMACS | Bug | Feedback wanted | Normal | install fail on Centos 6 | | 07/15/2019 12:32 PM | |
| 3021 | GROMACS | Feature | Feedback wanted | Normal | Completion of docs for GPU developments | | 03/02/2020 03:58 PM | 2020.2 |
| 3020 | GROMACS | Feature | New | Low | modernize DeviceBuffer and GPU memory management | | 08/13/2019 06:01 PM | |
| 3016 | GROMACS | Task | New | Normal | intermittent failure of essentialdynamics test | | 07/18/2019 05:23 PM | |
| 3015 | GROMACS | Task | New | Normal | Create central log handle for calls to gmx_fatal | | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3014 | GROMACS | Task | In Progress | Normal | gmxapi example Python scripts | | 01/03/2020 11:00 AM | 2021-infrastructure-stable |

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| 3013 | GROMACS | Task | New | Normal | Extend logging levels in MDLogger | | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3010 | GROMACS | Task | In Progress | Normal | upgrade OpenCL stack on bs-gpu01 | | 12/20/2019 08:25 AM | 2021-infrastructure-stable |
| 3008 | GROMACS | Task | New | Normal | verify block size choice of CUDA bonded kernel | | 12/27/2019 04:30 PM | 2021 |
| 3005 | GROMACS | Task | New | Normal | Move logging in gmx preprocess to MDLogger | | 06/26/2019 10:01 AM | |
| 3004 | GROMACS | Task | New | Normal | Move trajectory analysis logging to MDLogger | | 06/26/2019 09:59 AM | |
| 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 | |
| 3002 | GROMACS | Task | New | Normal | consider splitting bonded work into local/nonlocal | | 06/25/2019 04:06 PM | |
| 3001 | GROMACS | Task | New | Normal | explore simplifying virial and shift force reduction | | 12/27/2019 04:30 PM | 2021 |
| 3000 | GROMACS | Bug | New | Normal | CMake "webpage" target does not fail when it should | | 06/25/2019 02:43 PM | |
| 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 |
| 2998 | GROMACS | Task | Resolved | Normal | Update Python detection | | 04/23/2020 04:45 PM | 2021-infrastructure-stable |
| 2997 | GROMACS | Task | New | Normal | improve performance of alchemical free energy calculations | | 12/27/2019 04:31 PM | 2021 |
| 2994 | GROMACS | Feature | New | Normal | Data flow topology in gmxapi 2020 | | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 2992 | GROMACS | Task | New | Normal | Split hw_opt in const user options and dynamic settings | | 12/27/2019 04:31 PM | future |
| 2988 | GROMACS | Task | In Progress | Low | clean up and refactor code to modern standards | | 12/27/2019 04:37 PM | future |
| 2987 | GROMACS | Bug | New | Normal | assess the bonded GPU task assignment default | | 12/20/2019 01:06 PM | 2021 |
| 2983 | GROMACS | Task | New | Normal | better suited data-types for bonded GPU kernels | | 07/11/2019 04:32 PM | |
| 2981 | GROMACS | Bug | New | Normal | segfault in opencl build | | 06/18/2019 03:30 AM | |
| 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 | |
| 2978 | GROMACS | Bug | New | Normal | Some suggestions about the gmx current tool | | 06/13/2019 12:41 PM | |
| 2977 | GROMACS | Feature | New | Normal | print DD load balancing improvement | | 06/13/2019 10:56 AM | |
| 2976 | GROMACS | Task | New | Normal | Basic math for Multidimensional arrays | | 12/27/2019 04:37 PM | 2021 |
| 2975 | GROMACS | Feature | New | Normal | LJ PME calculations on GPUs | | 06/12/2019 01:17 PM | |
| 2974 | GROMACS | Bug | New | Normal | position-restraints regressiontest fails on intel GPU with OpenCL | | 02/25/2020 03:52 PM | 2020.2 |
| 2967 | GROMACS | Feature | New | Normal | GPU reallocateDeviceBuffer improvements | | 01/23/2020 12:15 PM | 2021-refactoring |
| 2965 | GROMACS | Task | In Progress | Normal | Performance of GPU direct communications | | 02/14/2020 12:38 PM | 2021 |
| 2961 | GROMACS | Feature | New | Normal | How should Python package find GROMACS resources under various circumstances? | | 12/09/2019 10:47 AM | |
| 2958 | GROMACS | Bug | New | Normal | Compiling master (to become 2020) using CUDA 9.0 | | 03/02/2020 03:57 PM | 2020.2 |
| 2956 | GROMACS | Feature | New | Normal | SAXS resolution | | 05/17/2019 09:58 AM | |
| 2954 | GROMACS | Bug | New | Normal | genion changes residue numbering | | 05/26/2019 12:08 AM | |
| 2949 | GROMACS | Bug | New | Normal | cmake fails when building mdrun only | | 07/08/2019 10:04 AM | |

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| 2948 | GROMACS | Bug | New | Normal | SIMD support detected as none on AMD R5 2500U | | 05/21/2019 12:58 PM | |
| 2947 | GROMACS | Task | Accepted | Normal | make an end to end test for membed | | 09/24/2019 03:22 PM | future |
| 2936 | GROMACS | Task | New | Normal | introduce check that CPU-GPU transfers/assignments are made between compatible types | | 02/05/2020 03:57 PM | 2021 |
| 2933 | GROMACS | Task | New | Normal | Convert walls to a ForceProvider | | 04/25/2019 02:43 PM | |
| 2931 | GROMACS | Feature | New | Normal | Tables in Verlet kernels | | 04/29/2019 12:01 PM | |
| 2930 | GROMACS | Feature | New | Normal | Limited range for reference group detection in cylinder pulling | | 04/26/2019 05:17 PM | |
| 2928 | GROMACS | Feature | New | Normal | Add ability to use expression "count of ATOM_EXPR" in selection statements. | | 04/16/2019 04:52 PM | |
| 2924 | GROMACS | Bug | New | Normal | Failing version check when reading new tpr file with older gromacs version | | 04/12/2019 10:52 AM | |
| 2919 | GROMACS | Task | New | Normal | C++ style guidelines for namespace use | | 04/15/2019 01:21 PM | |
| 2915 | GROMACS | Feature | In Progress | High | GPU direct communications | | 02/14/2020 12:48 PM | |
| 2910 | GROMACS | Feature | New | Normal | Mixed scaling for 1-4 interactions | | 04/10/2019 10:13 PM | |
| 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 | |
| 2907 | GROMACS | Bug | New | Normal | Gromacs autocompletion appears to be broken with ZSH | | 07/16/2019 04:46 AM | |
| 2905 | GROMACS | Task | New | Normal | Add a Jenkins configuration with std library assert | | 08/24/2019 05:22 PM | |
| 2902 | GROMACS | Bug | New | Normal | 2019.1 equilibration issue? (Intel 2018u3) | | 04/30/2019 08:17 AM | |
| 2898 | GROMACS | Task | New | Low | Naming common variables | | 03/26/2019 11:46 PM | |
| 2897 | GROMACS | Bug | New | Normal | rotation/flex2 can still fail on cpu-only run on OpenCL build | | 04/04/2019 06:24 PM | |
| 2896 | GROMACS | Feature | Feedback wanted | Normal | Python packaging | | 01/16/2020 07:11 PM | 2021-refactoring |
| 2891 | GROMACS | Feature | In Progress | Normal | PME/PP GPU communications | | 02/14/2020 12:40 PM | |
| 2890 | GROMACS | Feature | In Progress | Normal | GPU Halo Exchange | | 02/14/2020 12:41 PM | 2021 |
| 2883 | GROMACS | Bug | New | Normal | essentialdynamics fail with Intel MPI | | 03/08/2019 03:10 AM | |
| 2873 | GROMACS | Bug | New | Normal | Simple way to get last frame from trajectory | | 02/28/2019 11:14 PM | |
| 2872 | GROMACS | Bug | New | Normal | gmx solvate and genion topology update | | 02/27/2019 10:18 AM | |
| 2870 | GROMACS | Bug | New | Normal | GPU detection error message missing from the output | | 03/05/2019 03:55 PM | |
| 2869 | GROMACS | Bug | New | Normal | GPU detection error only issued as a note to the log | | 03/05/2019 04:09 PM | |
| 2863 | GROMACS | Task | New | Normal | improve PBC handling | | 03/11/2019 04:28 PM | |
| 2860 | GROMACS | Feature | New | Normal | Option for outputting min/max coordinates in gmx traj | | 02/08/2019 12:35 AM | |
| 2859 | GROMACS | Task | Resolved | Normal | Change ArrayRef iterator type from pointer to std::iterator | | 06/26/2020 06:15 PM | |
| 2857 | GROMACS | Task | New | Normal | Clarify recommended function specifies (constexpr, noexcept, pure) | | 02/04/2019 04:48 AM | |
| 2855 | GROMACS | Task | New | Normal | Allow compiling GROMACS without C compiler | | 01/10/2020 12:06 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------------------|----------|---|----------|---------------------|----------------------------|
| 2852 | GROMACS | Bug | New | Low | the in-tree regressiontest download can get out of sync with code | | 01/30/2019 03:58 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 | |
| 2846 | GROMACS | Feature | New | Low | Set rpath in FindLibStdCpp.cmake | | 02/02/2019 08:09 AM | |
| 2840 | GROMACS | Feature | New | Normal | Test that functionality does not compile that is not supposed to. | | 01/25/2019 02:35 PM | future |
| 2839 | GROMACS | Task | New | Normal | make module and file naming consistent | | 01/16/2020 05:11 PM | 2021 |
| 2835 | GROMACS | Task | New | Normal | Matrix class constraint to upper or lower triangle | | 02/07/2019 02:44 PM | |
| 2828 | GROMACS | Bug | Feedback wanted | Normal | Installation issue on Power 9 system with SIMD support | | 01/18/2019 11:54 AM | |
| 2806 | GROMACS | Feature | New | Normal | SIMD algorithms for ARM SVE // nobnoded cluster and others | | 12/27/2019 03:59 PM | 2021 |
| 2796 | GROMACS | Task | New | Low | clarify what mdrun -cpt means | | 01/03/2019 02:09 PM | |
| 2795 | GROMACS | Task | New | Normal | Incorporate regressiontests into core gromacs | | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2792 | GROMACS | Task | New | High | Improvement of PME gather and spread CUDA kernels | | 03/18/2020 03:57 PM | |
| 2788 | GROMACS | Bug | New | Normal | PME will not run on AMD GPU with NVidia GPU present | | 01/03/2019 02:24 PM | |
| 2787 | GROMACS | Task | New | Normal | allow passing flags to allocateDeviceBuffer | | 12/03/2018 01:54 PM | |
| 2785 | GROMACS | Bug | New | Normal | Inconsistent and erroneous behaviour of trjconv when writing a partial TNG | | 11/30/2018 02:36 PM | |
| 2773 | GROMACS | Task | New | Normal | improve GPU error handling and make such handling uniform across modules | | 12/20/2019 01:09 PM | 2021 |
| 2771 | GROMACS | Task | New | Normal | Size independent Hessian for normal mode analysis | | 12/28/2019 10:50 AM | future |
| 2770 | GROMACS | Task | New | Normal | change branch maintenance policy | | 01/16/2020 05:09 PM | 2021 |
| 2763 | GROMACS | Bug | New | Normal | GMXAPI layout / grouping in development docs "modules" page | | 12/14/2018 12:49 PM | future |
| 2762 | GROMACS | Bug | Blocked, need info | Normal | incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads | | 07/01/2019 11:26 PM | |
| 2761 | GROMACS | Feature | New | Low | lincs-order 4 is too conservative for some force fields | | 11/16/2018 09:55 AM | |
| 2758 | GROMACS | Task | New | Low | Modernize genconf | | 11/15/2018 07:38 AM | future |
| 2756 | GROMACS | Task | In Progress | Normal | gmxapi integration testing | | 01/16/2020 05:12 PM | 2021-refactoring |
| 2739 | GROMACS | Feature | New | Normal | Parallel continuous tempering and enhanced sampling feature | | 11/13/2018 11:36 PM | |
| 2715 | GROMACS | Feature | New | Normal | Avoid requesting the user to recompile gromacs for Intel OpenCL support | | 12/27/2019 04:06 PM | future |
| 2713 | GROMACS | Feature | New | Normal | Constant offset for external electric fields | | 10/28/2018 12:57 AM | |
| 2710 | GROMACS | Feature | New | Normal | Separate dvl for each molecule (of couple-moltype) when running FEP | | 12/27/2019 04:41 PM | 2021 |
| 2707 | GROMACS | Bug | New | Normal | Installed OpenCL files include clh file from gpu_utils directory | | 10/30/2018 04:02 AM | |
| 2706 | GROMACS | Task | Accepted | Normal | Rework classic QM/MM interface | | 12/02/2019 01:45 PM | 2021-infrastructure-stable |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-------------|----------|---|----------|---------------------|----------------------------|
| 2702 | GROMACS | Bug | Accepted | Normal | PME gather reduction race in OpenCL (and CUDA) | | 03/28/2019 03:14 PM | |
| 2699 | GROMACS | Task | New | Normal | Test POWER9 | | 12/04/2019 03:29 PM | 2021-infrastructure-stable |
| 2698 | GROMACS | Task | In Progress | Normal | gmxapi documentation integration | | 01/29/2020 03:59 PM | 2021-infrastructure-stable |
| 2697 | GROMACS | Task | New | Normal | improve FFT library flavor/version reporting | | 12/27/2019 04:40 PM | future |
| 2695 | GROMACS | Task | New | Low | bonded GPU module timing | | 12/27/2019 04:40 PM | 2021 |
| 2693 | GROMACS | Bug | New | Normal | Several memory leaks in mdrun | | 12/18/2018 04:22 AM | future |
| 2686 | GROMACS | Task | New | Normal | add tests for gpu bonded interactions | | 12/27/2019 04:40 PM | 2021 |
| 2682 | GROMACS | Task | New | Normal | Add MSAN configuration | | 10/09/2018 06:28 PM | |
| 2675 | GROMACS | Task | In Progress | Normal | bonded CUDA offload task | | 02/12/2020 05:54 PM | 2021 |
| 2674 | GROMACS | Task | Accepted | Normal | Improve domain decomposition for bilayer systems | | 12/07/2018 04:03 PM | future |
| 2672 | GROMACS | Task | New | Normal | check & document execution width requirements in OpenCL | | 12/31/2018 11:20 AM | future |
| 2671 | GROMACS | Task | New | Normal | replace constants like M_PI | | 12/20/2019 01:17 PM | future |
| 2670 | GROMACS | Task | New | Low | remove old/backward compatibility OpenCL support from releng | | 10/04/2018 06:06 PM | |
| 2657 | GROMACS | Bug | New | Normal | Biphasic tutorial | | 09/28/2018 10:02 AM | |
| 2650 | GROMACS | Task | New | Normal | revise OpenCL stack recommendations | | 12/31/2018 11:19 AM | future |
| 2649 | GROMACS | Bug | New | Normal | Virial calculation necessary for correct energy calculation on GPU | | 12/17/2018 02:32 PM | future |
| 2645 | GROMACS | Bug | New | Normal | Security | | 09/28/2018 01:16 PM | |
| 2643 | GROMACS | Feature | New | Low | mdp options and/or docs for anisotropic aspects of implementations | | 09/12/2018 02:23 PM | |
| 2637 | GROMACS | Bug | New | High | gmx solvate tears apart molecules | | 09/11/2018 07:43 PM | |
| 2632 | GROMACS | Task | New | Low | make sure cmake defines proper hwloc versionc with cross-compilation enabled | | 12/03/2018 01:35 PM | future |
| 2628 | GROMACS | Bug | Resolved | Normal | GMXRC removes trailing colon from existing MANPATH | | 11/02/2020 11:45 AM | |
| 2624 | GROMACS | Bug | New | Normal | GPU build system not robust enough | | 09/05/2018 02:00 AM | |
| 2622 | GROMACS | Feature | New | Low | Reduce severity of Berendsen warning | | 08/23/2018 11:16 PM | future |
| 2616 | GROMACS | Task | New | Normal | Model for MD state | | 09/14/2018 05:12 PM | |
| 2611 | GROMACS | Bug | New | Normal | issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX | | 08/14/2018 07:03 PM | |
| 2608 | GROMACS | Task | New | Normal | Remove code duplication between OpenCL and CUDA | | 09/24/2018 12:47 PM | |
| 2607 | GROMACS | Bug | New | Normal | Grompp becomes extremely slow when many pull groups are present | | 08/11/2018 08:54 AM | |
| 2606 | GROMACS | Bug | New | Normal | Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert | | 08/10/2018 01:48 AM | |
| 2602 | GROMACS | Bug | New | Low | build information gets outdated if build tree is reused | | 08/13/2018 09:04 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 | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|----------|---------------------|----------------|
| 2598 | GROMACS | Bug | New | Normal | Tools using read_next_x cannot read TNG files with sanitizers | | 10/15/2018 01:16 PM | future |
| 2587 | GROMACS | Feature | In Progress | Normal | Provide Context (e.g. to runner code) to manage client and runtime environment | | 10/15/2018 03:34 PM | |
| 2585 | GROMACS | Feature | Resolved | Normal | Infrastructure supporting external API | | 12/11/2019 12:39 PM | |
| 2581 | GROMACS | Feature | Accepted | Normal | User interface for hybrid Monte Carlo | | 12/20/2019 12:24 PM | future |
| 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 | |
| 2579 | GROMACS | Feature | New | Normal | Add dimensionality option to gmx trjconv -center | | 07/19/2018 04:53 PM | future |
| 2576 | GROMACS | Bug | New | Normal | gmx potential -correct outputs the wrong potential | | 07/25/2018 02:58 PM | |
| 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 | |
| 2570 | GROMACS | Feature | New | Normal | Better string formatting and printing | | 05/02/2019 12:20 PM | |
| 2568 | GROMACS | Bug | New | Low | gmx editconf -rotate does not rotate the box | | 07/10/2018 10:27 AM | future |
| 2567 | GROMACS | Bug | New | Normal | make check fails at test 23 SIMD errors | | 07/10/2018 09:35 AM | |
| 2564 | GROMACS | Bug | New | Normal | Result Summary Different For Jobs With Different Numbers of Nodes | | 07/05/2018 02:39 PM | |
| 2563 | GROMACS | Bug | New | Normal | Windows 7 Compilation with GPU support | | 07/02/2018 09:58 AM | |
| 2555 | GROMACS | Bug | New | Low | building GROMACS 2018.2 | | 07/03/2018 11:41 PM | |
| 2535 | GROMACS | Task | New | Normal | consider compiling opencl fft kernels once | | 05/31/2018 01:33 PM | |
| 2532 | GROMACS | Task | New | Normal | enable queue priorities in OpenCL | | 05/29/2018 02:29 PM | |
| 2531 | GROMACS | Task | New | Low | Consider optimizing tabulated data access on GPU | | 07/30/2018 12:31 PM | |
| 2530 | GROMACS | Task | New | Normal | consider using CUDA Driver API | | 09/23/2018 11:47 PM | future |
| 2528 | GROMACS | Task | New | Normal | PME GPU tuning | | 12/31/2018 11:18 AM | future |
| 2527 | GROMACS | Task | New | Normal | Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL) | | 10/30/2018 04:06 AM | future |
| 2526 | GROMACS | Bug | New | Normal | Bug of gmx hbond | | 05/30/2018 03:12 PM | |
| 2524 | GROMACS | Task | New | Normal | struct alignment/packing for OpenCL host & device code | | 12/20/2019 12:20 PM | future |
| 2522 | GROMACS | Task | Resolved | Normal | OpenCL context duplication | | 03/11/2020 04:15 PM | future |
| 2521 | GROMACS | Task | New | Normal | Implement alternating PME/NB wait for OpenCL | | 10/15/2018 12:39 PM | |
| 2520 | GROMACS | Task | New | Normal | Treat OpenCL kernel width more diligently | | 05/24/2018 06:21 PM | |
| 2519 | GROMACS | Task | New | High | Improve/remove PME OpenCL kernel barriers | | 02/15/2019 06:34 PM | |
| 2518 | GROMACS | Task | New | Normal | redesign task-assignment code for OpenCL | | 12/20/2019 12:19 PM | future |
| 2514 | GROMACS | Task | New | Normal | PME OpenCL reductions with intrinsics | | 05/31/2018 12:27 AM | future |
| 2498 | GROMACS | Task | New | Normal | OpenCL memory pinning/mapping | | 12/20/2019 12:18 PM | future |
| 2496 | GROMACS | Task | New | Low | find system xdr properly | | 05/02/2018 02:19 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|--|----------|---------------------|----------------------------|
| 2488 | GROMACS | Task | New | Normal | use MPI non-blocking collectives to overlap pull comm | | 04/25/2018 04:19 PM | |
| 2482 | GROMACS | Bug | Feedback wanted | Normal | Atoms/molecules in freezegrps move and system crashes | | 05/18/2018 07:13 PM | |
| 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 | |
| 2475 | GROMACS | Task | New | Normal | make OpenCL 1st class-citizen in the build system | | 12/20/2019 12:14 PM | 2021 |
| 2473 | GROMACS | Bug | New | Normal | mdrun sometimes stalls due to large coordinates with no constraints | | 04/04/2018 10:15 PM | |
| 2469 | GROMACS | Task | New | Normal | implement GPU timer reduction for reporting | | 03/27/2018 05:08 PM | |
| 2468 | GROMACS | Bug | New | Low | incorrect GPU timing reported with OpenCL and domain decomposition | | 12/17/2018 01:28 PM | future |
| 2464 | GROMACS | Task | New | Normal | GPU performance goals overview | | 03/26/2018 10:42 AM | |
| 2463 | GROMACS | Task | New | Low | PME GPU decomposition | | 03/26/2018 10:42 AM | |
| 2462 | GROMACS | Task | New | Normal | consider adding STL misuse tests | | 03/23/2018 01:23 AM | |
| 2460 | GROMACS | Bug | New | Normal | Allow inclusion of user libraries through CMake cache variables | | 03/28/2018 08:47 PM | |
| 2456 | GROMACS | Task | New | Normal | Add a pull module external potential tests | | 03/15/2018 03:02 PM | |
| 2448 | GROMACS | Task | Accepted | Normal | should mdrun -multidir permit only one directory? | | 03/21/2018 12:10 PM | |
| 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 | |
| 2435 | GROMACS | Task | New | Normal | identify and note about/tune task offload in GPU-bound runs | | 03/02/2018 04:08 PM | |
| 2429 | GROMACS | Feature | New | Normal | Add option of periodic chain topology to pdb2gmx | | 03/10/2018 01:01 PM | |
| 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 | |
| 2427 | GROMACS | Bug | New | Normal | gmx select gives syntax error for selection involving evaluating simple arithmetic expression | | 02/27/2018 05:15 PM | |
| 2426 | GROMACS | Feature | In Progress | Normal | Trajectory analysis tool for functional mode analysis by partial least squares fitting (PLS-FMA) | | 10/03/2018 11:31 PM | future |
| 2422 | GROMACS | Task | New | Normal | write C kernel for tables in Verlet scheme | | 02/26/2018 01:38 PM | |
| 2412 | GROMACS | Task | New | Normal | attempt to do better FFTW planning | | 03/15/2018 05:01 PM | |
| 2402 | GROMACS | Task | New | Normal | PME kernels general performance improvements | | 03/26/2018 10:41 AM | future |
| 2393 | GROMACS | Bug | New | Normal | incorrect error message with omitted command line flag before its argument | | 01/24/2018 11:24 PM | |
| 2390 | GROMACS | Bug | Feedback wanted | Normal | GROMACS build system should check for valid nvcc flags before use | | 12/20/2019 12:13 PM | 2021 |
| 2382 | GROMACS | Task | New | Normal | Simplify Doxygen guidelines | | 01/13/2018 12:40 AM | |
| 2380 | GROMACS | Bug | New | Low | cycle counter issues with separate PME rank + GPUs | | 01/16/2018 10:21 PM | |
| 2376 | GROMACS | Task | New | Normal | max_mpi_ranks has wrong name | | 02/10/2018 11:03 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|--|----------|---------------------|----------------|
| 2375 | GROMACS | Task | New | Normal | Clarify execution phases for MD simulation | | 04/30/2019 12:59 PM | |
| 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 |
| 2367 | GROMACS | Task | New | Normal | construct pbc_simd less often | | 09/24/2018 11:02 PM | future |
| 2360 | GROMACS | Bug | New | Low | error at counter reset with PME-only rank | | 01/05/2018 12:43 PM | future |
| 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 |
| 2351 | GROMACS | Task | New | Normal | Avoid the SIMD module depending on non-trivial parts of Gromacs | | 12/14/2017 02:47 AM | future |
| 2341 | GROMACS | Task | New | Low | assess the state of building and using GROMACS on Windows | | 07/29/2019 11:09 PM | future |
| 2310 | GROMACS | Feature | Accepted | Low | Let mdrun dump coordinates with non-finite energy | | 10/03/2018 09:47 PM | future |
| 2304 | GROMACS | Task | New | Normal | Document and propose tracking mdrun heuristics | | 10/03/2018 09:39 PM | future |
| 2294 | GROMACS | Task | New | Normal | Require identical hardware on nodes on parallel runs | | 11/19/2017 08:54 PM | |
| 2289 | GROMACS | Feature | New | Normal | gmx spatial add ability to perform over multiple reference structures | | 11/08/2017 12:31 AM | |
| 2288 | GROMACS | Feature | Accepted | Low | gmx msd doesn't optimally handle missing input trajectory frames | | 11/10/2017 11:03 AM | |
| 2255 | GROMACS | Bug | New | Normal | nstlist override stopped affecting the input parameter listing | | 12/17/2017 08:05 AM | |
| 2254 | GROMACS | Feature | Resolved | Normal | GPU extensions for Google Tests | | 10/06/2020 12:15 PM | |
| 2252 | GROMACS | Bug | New | Low | Memory allocation failures with large page sizes during PME tuning | | 12/14/2017 04:27 AM | |
| 2248 | GROMACS | Feature | New | Normal | Label all SIMD functions as pure/nodiscard | | 02/04/2019 04:49 AM | |
| 2241 | GROMACS | Bug | New | Low | refdata can segfault when reading | | 09/07/2017 11:57 AM | |
| 2240 | GROMACS | Task | Accepted | Low | GPU emulation mode support for PME missing | | 09/16/2017 10:02 PM | |
| 2239 | GROMACS | Feature | New | Normal | split libgromacs into base and full | | 01/07/2019 01:47 AM | |
| 2233 | GROMACS | Bug | Accepted | Normal | replica exchange and -append bugged? | | 03/05/2018 01:38 PM | |
| 2232 | GROMACS | Bug | New | Normal | pdb2gmx can't form special bonds with terminal patched atoms | | 12/03/2017 01:35 PM | |
| 2231 | GROMACS | Bug | New | Normal | convert-tpr aborts when saving subset of the system | | 01/12/2018 03:52 PM | |
| 2226 | GROMACS | Feature | New | Normal | Harmonise commands for exit in make_ndx and distance | | 08/04/2017 12:24 PM | |
| 2221 | GROMACS | Task | New | Normal | Avoid preprocessor for SIMD functions | | 02/21/2018 01:43 PM | |
| 2220 | GROMACS | Feature | New | Normal | report relevant env var behaviour to console | | 07/31/2017 09:40 PM | |
| 2218 | GROMACS | Feature | Feedback wanted | Normal | A tiny feature: damping for umbrella pull | | 08/16/2017 07:20 PM | |
| 2217 | GROMACS | Bug | New | Low | GPU emulation and separate PME ranks doesn't work properly | | 12/12/2017 11:50 AM | |
| 2211 | GROMACS | Bug | New | Low | gmx writes normal output to stderr | | 03/05/2018 02:00 PM | future |
| 2208 | GROMACS | Bug | New | Normal | cuFFT linking | | 06/30/2017 01:58 PM | |
| 2207 | GROMACS | Feature | New | Normal | solvent excluded volume of large molecule with periodic boundary condition | | 06/16/2017 10:37 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|--|----------|---------------------|----------------|
| 2194 | GROMACS | Feature | Accepted | Low | xvg output requested as an output option in place of xpm files | | 05/31/2017 04:26 PM | |
| 2185 | GROMACS | Task | New | Normal | add docs on MPI + CUDA w/wo MPS | | 05/24/2017 05:17 PM | |
| 2182 | GROMACS | Task | New | Low | de-duplicate code in densorder and hydorder | | 05/16/2017 11:29 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 |
| 2169 | GROMACS | Task | New | Normal | remove 'continuation' mdp option | | 12/29/2019 10:31 AM | 2021 |
| 2168 | GROMACS | Task | Feedback wanted | Normal | Design for multiple comparisons against same test reference data | | 05/08/2017 02:45 PM | future |
| 2166 | GROMACS | Task | Accepted | Normal | gmx trjconv functionality should check for mismatch between the tpr and the trajectory | | 05/05/2017 04:32 PM | |
| 2158 | GROMACS | Task | New | Normal | consider adding post-submit test that runs PME with 2xNN kernels | | 04/19/2017 08:04 PM | |
| 2147 | GROMACS | Bug | Feedback wanted | Normal | Parrinello-Rahman barostat not properly working | | 06/06/2017 07:53 AM | |
| 2139 | GROMACS | Feature | New | Normal | More precise/explicit documentation conventions | | 01/07/2018 11:54 PM | |
| 2133 | GROMACS | Task | New | Low | gmx traj needs reform | | 03/07/2017 02:02 PM | |
| 2132 | GROMACS | Feature | New | Normal | Intermediate code for xvg handling | | 03/08/2017 05:12 PM | future |
| 2126 | GROMACS | Feature | New | Normal | implement native CUDA support in CMake | | 10/29/2019 09:03 PM | |
| 2118 | GROMACS | Feature | New | Low | More verbose comments requested in header of gmx distance -oxyz | | 02/08/2017 05:46 AM | |
| 2115 | GROMACS | Task | New | Normal | trjconv does too many things, and combinations of them work poorly | | 10/02/2018 09:04 AM | |
| 2113 | GROMACS | Bug | New | Normal | Google tests and execution order | | 03/05/2018 02:05 PM | |
| 2111 | GROMACS | Feature | In Progress | Normal | Implement Gaussian screening of electrostatics | | 02/23/2019 12:33 PM | |
| 2101 | GROMACS | Feature | New | Low | warninp could print the offending line, as well as its number | | 01/20/2017 03:06 PM | |
| 2097 | GROMACS | Feature | New | Low | Move output of dhdl file entirely to edr, rather than having a separate text dhdl file | | 01/05/2017 05:21 PM | future |
| 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 | |
| 2092 | GROMACS | Task | New | Normal | Tests running on GPU, and hardware assignment | | 12/19/2017 05:27 PM | future |
| 2089 | GROMACS | Task | New | Normal | Encourage code review | | 01/10/2017 12:03 AM | |
| 2084 | GROMACS | Task | New | Low | MPI and stderr/log output | | 11/28/2016 06:37 PM | |
| 2080 | GROMACS | Feature | New | Normal | add grompp warning for suitability for domain decomposition | | 11/23/2016 03:03 PM | |
| 2069 | GROMACS | Task | New | Low | Simple thread-parallelism inside routines | | 11/09/2016 06:06 PM | |
| 2068 | GROMACS | Feature | New | Normal | Access to low level classes | | 03/02/2019 01:37 AM | future |
| 2065 | GROMACS | Bug | New | Normal | thread-MPI internal errors | | 11/08/2018 03:43 PM | |
| 2060 | GROMACS | Feature | New | Normal | Convert enum to enum class | | 10/17/2016 05:27 PM | |
| 2059 | GROMACS | Task | In Progress | Normal | Separate different types of data in t_state | | 12/27/2019 04:42 PM | 2021 |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------------|----------|--|----------|---------------------|----------------|
| 2056 | GROMACS | Feature | New | Low | rename "gmx select" | | 10/03/2016 08:24 PM | |
| 2055 | GROMACS | Task | New | Low | Wiki registration is broken | | 01/20/2017 11:31 AM | |
| 2053 | GROMACS | Task | New | Normal | refine notation in GPU code | | 12/20/2019 01:04 PM | 2021 |
| 2048 | GROMACS | Task | New | Normal | C++11: CUDA dependency on general headers | | 09/07/2016 10:30 PM | |
| 2039 | GROMACS | Bug | New | Normal | mdrun -pinstride defaults are too confusing | | 12/13/2017 04:14 AM | |
| 2035 | GROMACS | Task | New | Normal | A common trajectory analysis data exchange format | | 03/15/2017 05:46 PM | future |
| 2018 | GROMACS | Feature | New | Normal | Pulling along a line between given points | | 07/27/2016 09:59 AM | |
| 2015 | GROMACS | Feature | New | Normal | Auto recovery from dd communication error | | 07/28/2016 03:17 PM | |
| 2010 | GROMACS | Task | New | Normal | Use size_t instead of int for indexing | | 07/01/2018 07:57 AM | |
| 2009 | GROMACS | Task | New | Normal | improve command-line reporting of useful things | | 07/26/2016 12:54 PM | |
| 2003 | GROMACS | Task | New | Normal | reconsider various simd flags | | 07/07/2016 11:23 PM | |
| 2001 | GROMACS | Feature | New | Normal | add MPI info to the mdrun log header | | 07/06/2016 05:21 PM | |
| 1994 | GROMACS | Feature | New | Low | explore using JIT for CUDA | | 07/11/2016 10:20 PM | future |
| 1985 | GROMACS | Bug | Fix uploaded | Low | CUDA build system refactoring awaiting review | | 12/20/2019 12:07 PM | 2021 |
| 1974 | GROMACS | Feature | New | Normal | Report atom numbers and types in the error message about missed parameters | | 05/30/2016 09:24 AM | |
| 1973 | GROMACS | Task | New | Normal | OpenCL implementation wish list | | 05/27/2016 03:42 PM | |
| 1972 | GROMACS | Feature | New | Normal | external potential modules for refinement against experimental data | | 08/22/2018 05:03 PM | future |
| 1971 | GROMACS | Task | New | Normal | Removing buggy features vs. keeping workflows | | 01/19/2018 01:36 PM | future |
| 1966 | GROMACS | Feature | New | Low | Hydrogen mass repartiniog | | 05/25/2016 06:04 PM | future |
| 1964 | GROMACS | Feature | Accepted | Normal | "pull=no" should not produce warnings about "unknown" pull keywords | | 05/20/2016 02:37 PM | |
| 1953 | GROMACS | Feature | New | Low | use more regular polymorphism for GPU code | | 05/06/2016 10:06 PM | future |
| 1948 | GROMACS | Feature | New | Low | add warning when non-identical GPUs are used | | 06/12/2017 08:45 PM | |
| 1936 | GROMACS | Task | New | Normal | treat default-able mdp fields as strings | | 04/02/2016 10:32 PM | future |
| 1934 | GROMACS | Bug | New | Normal | QMMM with ORCA: memory leaks, buffer overflows and much more | | 07/10/2016 09:26 AM | |
| 1925 | GROMACS | Task | In Progress | Normal | remove concept of unilateral global communication | | 12/29/2019 10:35 AM | 2021 |
| 1919 | GROMACS | Bug | Accepted | Normal | static linking issues cause by hwloc support | | 10/12/2018 10:49 PM | future |
| 1907 | GROMACS | Task | Accepted | Low | keeping compile- and run-time CPU/arch detection consistent | | 08/01/2016 10:09 PM | |
| 1902 | GROMACS | Feature | Accepted | Low | Add grompp check that non-excluded atoms are not too close to each other in the starting structure | | 02/15/2016 01:34 PM | |
| 1900 | GROMACS | Feature | New | Normal | Implement some new errors in grompp | | 06/22/2016 05:20 PM | |
| 1885 | GROMACS | Feature | New | Normal | DPD Thermostat | | 01/26/2016 10:17 AM | |
| 1879 | GROMACS | Task | In Progress | Low | make the GROMACS OpenCL kernel work on Gallium | | 11/30/2018 05:46 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-------------|----------|---|----------|---------------------|----------------|
| 1876 | GROMACS | Task | New | Normal | Reorganize vector input passed to core MD routines | | 06/01/2016 01:59 PM | future |
| 1867 | GROMACS | Feature | New | Normal | make coupling implementations reversible | | 12/02/2015 07:43 AM | |
| 1862 | GROMACS | Task | New | Normal | Fully replace t_topology by gmx_mtop_t | | 02/13/2019 04:53 PM | |
| 1855 | GROMACS | Task | New | Normal | Convert preprocessor use so that symbols are always defined | | 06/28/2016 02:17 PM | |
| 1854 | GROMACS | Feature | New | Normal | Remove all cyclic dependencies | | 05/25/2017 08:34 AM | |
| 1852 | GROMACS | Task | New | Normal | Remove group scheme | | 03/03/2020 09:03 PM | future |
| 1842 | GROMACS | Feature | New | Normal | Replace XML with JSON | | 01/18/2018 05:12 PM | |
| 1839 | GROMACS | Bug | Accepted | Low | pdb2gmx: Failure to rename non-standard hydrogen atom names after generating missing hydrogens in pdb2gmx | | 07/09/2016 07:27 PM | future |
| 1829 | GROMACS | Task | New | Normal | Future of thread level parallelism | | 11/18/2016 05:29 PM | |
| 1828 | GROMACS | Task | New | Normal | Exception handling in mdrun | | 10/07/2015 11:36 AM | |
| 1827 | GROMACS | Bug | New | Low | cmake multi-configuration generator support partly broken | | 12/11/2017 05:20 PM | future |
| 1811 | GROMACS | Bug | New | Normal | Extrae build issues | | 12/13/2017 03:43 AM | |
| 1785 | GROMACS | Task | New | Low | no pV term written to energy file when pressure coupling is anisotropic | | 07/26/2015 01:47 PM | future |
| 1770 | GROMACS | Bug | New | Normal | segmentation fault with free energy changes and multiple GPU's | | 07/14/2015 03:24 AM | |
| 1768 | GROMACS | Task | New | Normal | decide future of command-line options vs env vars | | 11/03/2016 05:51 PM | future |
| 1745 | GROMACS | Task | New | Normal | Moving to C++11 after Gromacs-5.1 | | 06/01/2016 03:01 PM | |
| 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 |
| 1715 | GROMACS | Feature | New | Low | improve cycle counting GPU sharing and multi-sim | | 08/03/2016 12:32 PM | future |
| 1688 | GROMACS | Feature | New | Low | g_cluster "middle" is not exactly the same as the definition in the cited paper | | 04/01/2015 05:53 AM | |
| 1670 | GROMACS | Feature | New | Normal | create mdrun option checking mini-tool | | 06/23/2016 04:06 PM | |
| 1665 | GROMACS | Feature | New | Normal | improve free energy non-bonded kernel performance | | 08/26/2019 03:47 PM | future |
| 1655 | GROMACS | Bug | New | Normal | g_membed and box type | | 12/09/2014 01:33 PM | |
| 1641 | GROMACS | Feature | New | Normal | Add toolchain file for Cray systems | | 06/06/2015 11:24 PM | |
| 1635 | GROMACS | Feature | New | Normal | Proper Unicode support | | 06/18/2015 08:34 PM | |
| 1634 | GROMACS | Feature | New | Normal | Boxed Molecular Dynamics | | 11/04/2014 04:40 PM | |
| 1627 | GROMACS | Feature | In Progress | Normal | DPD integrator | | 07/11/2016 08:08 PM | |
| 1625 | GROMACS | Feature | New | Normal | Gromacs Python API | | 03/02/2019 01:44 AM | future |
| 1602 | GROMACS | Feature | New | Low | gmx order S per slice along all 3 axes | | 09/22/2014 07:25 AM | |
| 1587 | GROMACS | Task | New | Normal | improve the configurability of regression tests | | 12/20/2019 12:02 PM | 2021 |
| 1583 | GROMACS | Bug | New | Normal | gmx msd with mol flag requires excessive memory | | 12/18/2017 03:34 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------------------|----------|--|----------|---------------------|----------------|
| 1568 | GROMACS | Bug | New | Low | inconsistent/incorrect threading checks and reporting in mdrun | | 05/25/2016 02:01 AM | |
| 1530 | GROMACS | Task | New | Low | Offer binary downloads | | 06/29/2014 02:58 PM | |
| 1523 | GROMACS | Task | New | Normal | add missing code-paths to CUDA emulation kernel | | 07/11/2016 08:09 PM | |
| 1511 | GROMACS | Feature | Accepted | Normal | add PDBx (ie mmcif) support | | 10/05/2018 07:14 PM | |
| 1489 | GROMACS | Feature | New | Normal | Don't solely rely on filename extension | | 04/30/2014 05:23 AM | |
| 1476 | GROMACS | Bug | New | Low | Odd behavior with verlet-buffer-drift | | 05/25/2016 01:45 AM | future |
| 1437 | GROMACS | Feature | New | Normal | Online help formatting improvements | | 06/04/2015 09:20 PM | future |
| 1328 | GROMACS | Feature | Accepted | Normal | Names for selection positions | | 07/11/2016 08:15 PM | |
| 1221 | GROMACS | Feature | Accepted | Normal | More generic position mapping for selections | | 06/10/2014 02:58 PM | future |
| 1182 | GROMACS | Feature | New | Normal | improve trajectory writing to support parallel I/O | | 05/13/2014 10:42 AM | future |
| 1170 | GROMACS | Task | New | Normal | mdlib reorganization | | 11/17/2016 03:47 PM | future |
| 1165 | GROMACS | Feature | Accepted | Low | Multi-SIMD binaries | | 12/20/2019 12:00 PM | future |
| 1140 | GROMACS | Task | New | Normal | Class design for passing options and data | | 07/11/2016 08:19 PM | |
| 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 | |
| 1120 | GROMACS | Feature | New | Low | Make build work with multi-cofiguration generators | | 06/03/2014 03:04 PM | future |
| 1104 | GROMACS | Feature | New | Low | Implement dihedral restraints | | 02/06/2013 07:04 PM | future |
| 1102 | GROMACS | Feature | New | Normal | Detect incompletely written itp files | | 06/19/2014 03:23 PM | |
| 1083 | GROMACS | Feature | In Progress | Normal | Improve collective error/warning/note handling in mdrun | | 07/11/2016 08:21 PM | |
| 1028 | GROMACS | Feature | New | Normal | Tool to calculate fraction of native contacts during simulation | | 11/01/2012 10:27 PM | |
| 1026 | GROMACS | Feature | New | Low | request for gen_vel to work with multiple temperature coupling groups at different temperatures | | 11/17/2016 04:39 PM | |
| 1017 | GROMACS | Task | New | Normal | C++ Vector/Matrix classes | | 07/11/2016 08:23 PM | |
| 988 | GROMACS | Task | New | Normal | Definition of "public API" | | 08/28/2019 02:50 PM | future |
| 986 | GROMACS | Task | New | Normal | Handling C++ out-of-memory errors | | 12/24/2014 08:42 PM | future |
| 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 |
| 950 | GROMACS | Feature | New | Normal | Path/directory/filename handling in Gromacs | | 07/11/2016 08:24 PM | |
| 921 | GROMACS | Feature | Blocked, need info | Normal | Default index groups and selections | | 07/11/2016 08:27 PM | |
| 909 | GROMACS | Task | New | Normal | Reimplement displacement calculation module | | 07/14/2014 11:30 AM | future |
| 907 | GROMACS | Feature | Accepted | Normal | Add tests for verifying installed headers | | 03/11/2014 09:15 PM | future |
| 895 | GROMACS | Feature | In Progress | Normal | g_rmsf previous frame as reference | | 04/29/2013 07:39 PM | future |
| 838 | GROMACS | Task | New | Normal | Improve generic error reporting routines | | 07/11/2016 08:29 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------------------|----------|--|-----------------|---------------------|----------------------------|
| 742 | GROMACS | Feature | New | Normal | Enhancing the performance of the free energy code | | 08/26/2019 04:55 PM | future |
| 731 | GROMACS | Feature | New | Normal | pdb2gmx should warn about missing residues when bonds are too long | | 06/22/2014 10:55 AM | |
| 720 | GROMACS | Feature | Accepted | Low | permit pdb2gmx to choose a kind of HIS based on proton position | | 11/17/2016 03:51 PM | future |
| 701 | GROMACS | Task | New | Normal | Add symbol visibility macros | | 03/02/2019 01:46 AM | future |
| 677 | GROMACS | Task | New | Normal | Make sure manual uses consistent style throughout | | 06/19/2014 11:49 AM | |
| 665 | GROMACS | Task | New | Normal | Port existing trajectory analysis tools to use the new framework | | 07/14/2014 11:29 AM | future |
| 652 | GROMACS | Task | Blocked, need info | Normal | Change selection method implementation to use C++ | | 04/23/2017 08:05 PM | future |
| 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 |
| 2537 | GROMACS | Task | New | Normal | Simplify PME solve reduction | Aleksei lupinov | 12/20/2019 12:21 PM | future |
| 2516 | GROMACS | Task | New | Low | Support PME OpenCL execution width < 16 | Aleksei lupinov | 06/05/2019 05:32 PM | |
| 2453 | GROMACS | Task | Resolved | High | PME OpenCL porting effort | Aleksei lupinov | 12/20/2019 12:18 PM | 2021 |
| 2054 | GROMACS | Feature | Accepted | High | PME on GPU | Aleksei lupinov | 12/20/2019 12:18 PM | future |
| 438 | GROMACS | Feature | In Progress | Low | New tool: g_correl | Alexey Shvetsov | 06/20/2014 10:38 AM | future |
| 3352 | GROMACS | Feature | New | Normal | GPU update-constraints feature support | 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 |
| 3350 | GROMACS | Feature | New | Normal | GPU update-constraints performance | Artem Zhmurov | 01/23/2020 11:59 AM | 2021 |
| 3348 | GROMACS | Task | New | Normal | GPU LINCS and SETTLE: unify virial reduction | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3346 | GROMACS | Task | New | Normal | GPU SETTLE: Use the same parameters and parameters initialization in GPU and CPU versions of SETTLE. | Artem Zhmurov | 01/23/2020 11:58 AM | 2021-infrastructure-stable |
| 3345 | GROMACS | Task | New | Normal | GPU update-constraints: Reconsider the naming of coordinates buffer in constraints. | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3344 | GROMACS | Task | New | Normal | GPU update-constraints: Better virial reduction. | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3343 | GROMACS | Task | New | Normal | GPU SETTLE: Use different ordering for matrices. | Artem Zhmurov | 01/23/2020 11:57 AM | 2021-infrastructure-stable |
| 3342 | GROMACS | Task | New | Normal | GPU SETTLE: Read only one index per water molecule. | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------|----------|---|---------------|---------------------|----------------------------|
| 3341 | GROMACS | Task | New | Normal | GPU LINCS: Use analytical solution for the matrix A inversion. | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3340 | GROMACS | Task | New | Normal | GPU LINCS: Move more data to local/shared memory | Artem Zhmurov | 01/23/2020 11:56 AM | 2021-infrastructure-stable |
| 3339 | GROMACS | Task | New | Normal | GPU LINCS: Warp-level synchronization for coupled constraints | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |
| 3338 | GROMACS | Task | New | Normal | GPU update-constraints: Do not save intermediate coordinates if there is no constraints | Artem Zhmurov | 01/23/2020 11:55 AM | 2021-infrastructure-stable |

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