

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 | |
| 3446 | GROMACS | Task | New | Normal | apply maintainability updates across all GPU kernels | Jonathan Vincent | 03/19/2020 03:31 PM | |
| 3445 | GROMACS | Task | New | Normal | create heuristic for c_skipNeutralAtoms | Jonathan Vincent | 03/17/2020 12:12 PM | |
| 3444 | GROMACS | Bug | Resolved | Normal | do_dssp does not work(gmx 2020 and 2020.1) | Christian Blau | 06/10/2020 02:45 PM | 2020.2 |
| 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 | |
| 3441 | GROMACS | Bug | Resolved | Normal | Ewald surface-epsilon is incorrect | Berk Hess | 03/18/2020 11:15 PM | 2020.2 |
| 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 | |
| 3437 | GROMACS | Task | New | Normal | Use builders to prepare modules | Pascal Merz | 03/11/2020 07:05 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 |
| 3435 | GROMACS | Feature | New | Normal | Implement pull for modular simulator | Pascal Merz | 03/11/2020 06:31 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 |
| 3433 | GROMACS | Feature | New | Normal | Decide how to handle multisim with modular simulator | Pascal Merz | 03/11/2020 06:42 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 |
| 3431 | GROMACS | Feature | New | Normal | Implement virtual sites for modular simulator | Pascal Merz | 03/11/2020 12:33 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 |
| 3428 | GROMACS | Feature | New | Normal | Implement SIMD version of modular simulator propagators | Pascal Merz | 03/11/2020 12:12 AM | 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 |
| 3426 | GROMACS | Feature | New | Normal | Support acceleration in modular simulator | Pascal Merz | 03/11/2020 04:09 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 |
| 3424 | GROMACS | Feature | New | Normal | Implement stochastic dynamics / langevin integrator in modular simulator | Pascal Merz | 03/10/2020 11:48 PM | 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 |
| 3422 | GROMACS | Task | Resolved | Normal | Implement modular checkpointing for modular simulator | Pascal Merz | 09/16/2020 09:45 AM | 2021-infrastructure-stable |
| 3421 | GROMACS | Task | New | Normal | Implement client system for global reduction | Pascal Merz | 03/11/2020 03:31 PM | 2021-infrastructure-stable |
| 3420 | GROMACS | Task | New | Normal | Unify force and shellfc elements for modular simulator | Pascal Merz | 03/10/2020 09:50 PM | 2021-infrastructure-stable |

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|------|---------|---------|-----------------|----------|--|-----------------|---------------------|----------------------------|
| 3419 | GROMACS | Task | New | Normal | Reduce / remove use of legacy t_state objects throughout modular simulator | Pascal Merz | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 3418 | GROMACS | Task | New | Normal | Infrastructure improvements for modular simulator | Pascal Merz | 03/10/2020 10:24 PM | 2021-infrastructure-stable |
| 3417 | GROMACS | Feature | New | Normal | Make modular simulator feature-complete | Pascal Merz | 03/23/2020 03:57 AM | 2021-infrastructure-stable |
| 3416 | GROMACS | Task | New | Normal | Port post-submit matrix to Gitlab CI | Joe Jordan | 03/16/2020 05:50 PM | 2021-refactoring |
| 3415 | GROMACS | Task | New | Normal | Port Pre-submit matrix to Gitlab CI | Szilárd Páll | 03/23/2020 10:09 AM | 2021-refactoring |
| 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 |
| 3410 | GROMACS | Feature | New | Normal | Random Acceleration Molecular Dynamics (RAMD) | Bernd Doser | 03/05/2020 03:22 PM | 2021 |
| 3408 | GROMACS | Bug | Fix uploaded | Normal | Gmxapi* tests segfault in rpmbuild | Eric Irrgang | 03/23/2020 01:27 PM | 2020.2 |
| 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 | |
| 3394 | GROMACS | Feature | New | Normal | improve gmxapi error handling | Eric Irrgang | 02/24/2020 11:45 AM | 2021-infrastructure-stable |
| 3393 | GROMACS | Feature | Resolved | Normal | Allow gmxapi.commandline_operation to use STDIN | Eric Irrgang | 02/25/2020 05:15 PM | 2021-infrastructure-stable |
| 3392 | GROMACS | Task | New | Low | Unify box correction for modular simulator | Pascal Merz | 03/11/2020 05:20 PM | 2021-infrastructure-stable |
| 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 | |
| 3380 | GROMACS | Bug | Resolved | Low | IBM VSX checks fail with gcc-10 | Erik Lindahl | 04/30/2020 01:30 PM | 2020.2 |
| 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 |
| 3371 | GROMACS | Feature | New | Normal | Control FEP using AWH | Magnus Lundborg | 02/06/2020 02:20 PM | 2021 |
| 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 | |

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| 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 |
| 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 | |
| 3363 | GROMACS | Feature | New | Normal | Improve FEP testing | Pascal Merz | 03/01/2020 03:22 PM | 2021-infrastructure-stable |
| 3362 | GROMACS | Feature | New | Normal | gmx traj: add an option to plot each component in a separate file | | 01/29/2020 06:18 PM | |
| 3361 | GROMACS | Task | New | Normal | Gitlab source archive contains files from build directory | Paul Bauer | 02/25/2020 10:13 AM | 2020.2 |
| 3360 | GROMACS | Task | New | Normal | investigate the future of DD dynamic load balancing with GPU offload | | 01/29/2020 11:23 AM | |
| 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 |
| 3355 | GROMACS | Feature | Accepted | Normal | New PME parallel (GPU) scheme | Jonathan Vincent | 02/12/2020 11:58 AM | |
| 3353 | GROMACS | Task | New | Normal | Document gmx densmap output | | 01/23/2020 12:52 PM | |
| 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 |
| 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 |

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|------|---------|---------|-------------|----------|---|---------------|---------------------|----------------------------|
| 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 |
| 3337 | GROMACS | Task | New | Normal | GPU update-constraints: Merge Leap-Frog, LINCS and SETTLE kernels. | Artem Zhmurov | 01/23/2020 11:55 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 |
| 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 |
| 3332 | GROMACS | Feature | New | Normal | gmx helixorient doesn't have a -tu option to change time unit | | 01/22/2020 11:57 AM | |
| 3331 | GROMACS | Task | New | Low | Run physical validation tests in Gitlab | Paul Bauer | 02/27/2020 11:09 PM | future |
| 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 |
| 3323 | GROMACS | Task | In Progress | Normal | Rework the StatePropagatorDataGpu | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3322 | GROMACS | Task | Accepted | Normal | Add reallocate(...) function that does not care about the contents of the buffer | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3321 | GROMACS | Task | Accepted | Normal | Add D2D wrapper | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3320 | GROMACS | Task | In Progress | Normal | Remove duplicating D2H/H2D wrappers in NBNXM | Artem Zhmurov | 01/22/2020 09:50 AM | 2021-refactoring |
| 3319 | GROMACS | Task | In Progress | Normal | Use DeviceBuffer instead of native GPU types in NBNXM | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring |
| 3318 | GROMACS | Feature | In Progress | Normal | Use wrappers for the GPU buffer copy/allocations | Artem Zhmurov | 01/23/2020 12:01 PM | 2021-refactoring |
| 3317 | GROMACS | Task | Resolved | Normal | Improve testing of the GPU code | Artem Zhmurov | 10/06/2020 12:15 PM | 2021-refactoring |
| 3316 | GROMACS | Task | Accepted | Normal | Context and Stream manager | Artem Zhmurov | 01/22/2020 09:49 AM | 2021-refactoring |
| 3315 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceContext | Artem Zhmurov | 03/11/2020 04:15 PM | 2021-refactoring |
| 3314 | GROMACS | Task | Resolved | Normal | Platform agnostic DeviceStream | Artem Zhmurov | 03/20/2020 09:55 AM | 2021-refactoring |

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|------|---------|---------|--------------------|----------|---|----------------|---------------------|----------------------------|
| 3313 | GROMACS | Feature | Accepted | Normal | Introduce and use opaque types for the DeviceStream and DeviceContext | Artem Zhmurov | 01/23/2020 12:00 PM | 2021-refactoring |
| 3312 | GROMACS | Task | In Progress | Normal | Data type for coordinates, xyzq data, LJ parameters data to use for GPU buffers | Artem Zhmurov | 03/20/2020 09:54 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 |
| 3306 | GROMACS | Task | New | Normal | Document gmx dos tool more clearly | Christian Blau | 01/20/2020 02:31 PM | future |
| 3305 | GROMACS | Bug | New | Normal | Case gives FPE with Debug build when GPU update is enabled | | 01/21/2020 05:44 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 |
| 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 |
| 3295 | GROMACS | Feature | New | Normal | Expand gmxapi.modify_input use cases. | Eric Irrgang | 01/16/2020 05:13 PM | 2021-refactoring |
| 3294 | GROMACS | Bug | New | Normal | multiple tests fail on fedora 31 | Paul Bauer | 02/28/2020 03:12 PM | 2020.2 |
| 3290 | GROMACS | Task | Resolved | Normal | Require CMake >= 3.12 | | 04/14/2020 02:45 PM | 2021-refactoring |
| 3289 | GROMACS | Task | New | Normal | Distinguish identifying and non-identifying inputs to API operations. | Eric Irrgang | 01/10/2020 11:30 AM | |
| 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 |
| 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 |
| 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 |
| 3275 | GROMACS | Task | New | Normal | Document Gitlab CI instead of Jenkins and releng | Paul Bauer | 03/09/2020 05:55 PM | 2021-infrastructure-stable |
| 3274 | GROMACS | Bug | New | Normal | Remove ARM NEON SIMD | | 12/28/2019 07:53 AM | 2021-infrastructure-stable |

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| 3273 | GROMACS | Bug | New | Normal | gmxapi setup.py complains too much | | 12/27/2019 06:42 PM | 2021-infrastructure-stable |
| 3272 | GROMACS | Task | New | Normal | Port complete CI testing to Gitlab | Paul Bauer | 02/27/2020 11:04 AM | 2021-infrastructure-stable |
| 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 |
| 3266 | GROMACS | Bug | New | High | gmx density show wrong symmetrize density profile using -symm? | Super duper | 02/28/2020 08:24 AM | 2020.2 |
| 3265 | GROMACS | Bug | Blocked, need info | Low | regressiontests/complex fails on ppc64le | Erik Lindahl | 01/09/2020 05:00 PM | |
| 3264 | GROMACS | Task | New | Normal | Break up MdrunMpiTests | Paul Bauer | 12/23/2019 11:44 AM | 2021-infrastructure-stable |
| 3262 | GROMACS | Task | New | High | Trjconv - dimer protein-ligand | | 12/20/2019 09:26 PM | |
| 3260 | GROMACS | Task | New | Low | keep up to with mdspan reference implementation | Christian Blau | 12/20/2019 01:16 PM | 2021-infrastructure-stable |
| 3258 | GROMACS | Task | New | Normal | GPU update-constraints: Enable free energy perturbation | Artem Zhmurov | 01/23/2020 11:54 AM | 2021-infrastructure-stable |
| 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 | |
| 3249 | GROMACS | Bug | In Progress | Low | cmake bad tests for avx512 on AMD | Erik Lindahl | 02/26/2020 05:00 PM | |
| 3246 | GROMACS | Bug | Accepted | Normal | GPU code misses settle error check, simulation crashes with segfault without any further output | Artem Zhmurov | 12/20/2019 09:52 AM | 2021-infrastructure-stable |
| 3244 | GROMACS | Bug | In Progress | Normal | center of mass motion removal with position restraints can lead to artifacts | Berk Hess | 12/27/2019 10:40 AM | 2021 |
| 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 | |
| 3236 | GROMACS | Task | New | Normal | GPU update-constraints: Pulling support | Artem Zhmurov | 01/23/2020 11:53 AM | 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 |
| 3234 | GROMACS | Bug | Accepted | Normal | Signal: Floating point exception Signal code: Floating point divide-by-zero | Erik Lindahl | 12/16/2019 03:40 PM | |
| 3233 | GROMACS | Bug | New | Normal | clang-format incorrectly aligning altered function arguments | | 12/13/2019 12:41 PM | |

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| 3229 | GROMACS | Task | New | Normal | Move checkpointing to the beginning of the MD step | | 01/16/2020 04:31 PM | 2021-infrastructure-stable |
| 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 |
| 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 | |
| 3216 | GROMACS | Task | New | Normal | improve CPU force reductions | Szilárd Páll | 12/04/2019 09:24 PM | |
| 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 | |
| 3203 | GROMACS | Task | Accepted | Normal | Tools should check that input is valid when first using it | Paul Bauer | 12/03/2019 05:26 PM | 2021-infrastructure-stable |
| 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 |
| 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 | |
| 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 |
| 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 | |

| # | 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 |
| 3179 | GROMACS | Feature | New | Normal | Clarify access to parallel data outputs | Eric Irrgang | 10/26/2019 12:23 PM | |
| 3177 | GROMACS | Feature | New | Normal | Spack package management support | | 11/06/2019 06:37 PM | |
| 3174 | GROMACS | Task | Feedback wanted | Low | Proposed gmxapi syntax update: "input" and "output" key word arguments -> "inputs" and "outputs" | Eric Irrgang | 10/23/2019 06:34 PM | |
| 3172 | GROMACS | Feature | New | Normal | QM/MM Interface with CP2K | Dmitry Morozov | 01/17/2020 12:18 PM | future |
| 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 | |
| 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 |
| 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 |
| 3155 | GROMACS | Task | Accepted | Normal | Unify DD and CPU-GPU gather & scatter | Artem Zhmurov | 10/17/2019 03:50 PM | 2021-infrastructure-stable |
| 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 |
| 3150 | GROMACS | Bug | New | Normal | gmxapi data type annotations are confusing and inadequate | Eric Irrgang | 10/22/2019 03:08 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 | |
| 3148 | GROMACS | Feature | New | Normal | Roadmap for gmxapi filesystem interactions. | Eric Irrgang | 10/15/2019 06:23 PM | 2021-infrastructure-stable |
| 3147 | GROMACS | Feature | New | Normal | gmxapi workflow checkpointing | Eric Irrgang | 10/15/2019 06:18 PM | 2021-infrastructure-stable |
| 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 |
| 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 |
| 3141 | GROMACS | Bug | New | Normal | gmxapi File placeholders missing from beta release | Eric Irrgang | 12/10/2019 02:02 PM | 2021-infrastructure-stable |
| 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 |
| 3139 | GROMACS | Task | New | Normal | gmxapi Futures should be subscribable | Eric Irrgang | 10/15/2019 03:56 PM | |
| 3138 | GROMACS | Feature | New | Normal | Improve ensemble support in Context specification. | | 10/15/2019 03:56 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 |
| 3135 | GROMACS | Feature | New | Normal | Make GPU traits into opaque types | | 10/14/2019 10:24 AM | |
| 3134 | GROMACS | Feature | Feedback wanted | Normal | gmxapi Python exception names may need improvement | Eric Irrgang | 10/13/2019 01:50 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|--------------------|----------|---|-----------------|---------------------|----------------------------|
| 3133 | GROMACS | Task | In Progress | Normal | Cookiecutter for sample_restraint | Eric Irrgang | 12/10/2019 01:59 PM | 2021-infrastructure-stable |
| 3132 | GROMACS | Task | New | Normal | gmxapi testing support tools | | 10/31/2019 03:35 PM | |
| 3131 | GROMACS | Task | New | Normal | support ccache with clang-tidy | Mark Abraham | 12/20/2019 08:20 AM | 2021-infrastructure-stable |
| 3130 | GROMACS | Task | New | Normal | Interim handling of gmxapi data references. | Eric Irrgang | 12/11/2019 11:26 AM | 2021-infrastructure-stable |
| 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 |
| 3117 | GROMACS | Feature | New | Normal | Coulomb FEP PME on GPU | Magnus Lundborg | 02/17/2020 03:58 PM | 2021-infrastructure-stable |
| 3116 | GROMACS | Bug | New | Normal | regressiontests/freenenergy core dumps on ppc64le | Paul Bauer | 10/04/2019 10:52 PM | |
| 3115 | GROMACS | Feature | New | Normal | Device stream manager | | 10/04/2019 09:00 AM | |
| 3114 | GROMACS | Feature | New | Normal | Improve GPU update-constraints module | Artem Zhmurov | 02/10/2020 04:30 PM | 2021 |
| 3113 | GROMACS | Bug | New | Low | Use of read_tps_conf is deprecated | Paul Bauer | 10/01/2019 11:36 AM | 2021-infrastructure-stable |
| 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 |
| 3101 | GROMACS | Bug | Blocked, need info | Normal | detect compilation failed | Erik Lindahl | 12/27/2019 10:52 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 |
| 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 | |
| 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 | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 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 |
| 3075 | GROMACS | Bug | New | Normal | Frozen atoms are moving | Erik Lindahl | 12/27/2019 10:51 AM | |
| 3073 | GROMACS | Bug | New | Normal | Total potential energy goes crazy, but I don't know why this happens. | | 09/04/2019 07:25 PM | |
| 3072 | GROMACS | Task | New | Normal | Use gm::index for indexing instead of int | Christian Blau | 09/03/2019 04:23 PM | 2021-infrastructure-stable |
| 3071 | GROMACS | Bug | Accepted | Normal | complex.nbnxn-ljpm-LB-geometric failing with OpenCL timing debug mode assertions | Szilárd Páll | 02/25/2020 03:39 PM | 2020.2 |
| 3069 | GROMACS | Feature | New | Low | Iterator over span and indices into this span (zip-style iterator) | Christian Blau | 08/29/2019 11:11 AM | future |
| 3068 | GROMACS | Bug | New | Normal | Misleading warning on rerun | | 08/26/2019 03:44 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 | |
| 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 | |
| 3057 | GROMACS | Task | New | Normal | re-enable fusion on Power8/9 | Szilárd Páll | 12/27/2019 04:22 PM | 2021 |
| 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 | |
| 3050 | GROMACS | Bug | New | Low | Fix tests on Solaris | Vedran Miletic | 02/27/2020 11:05 AM | 2020.2 |
| 3049 | GROMACS | Bug | New | Low | gmx nmeig should plot a real infrared spectrum | David van der Spoel | 09/24/2019 03:25 PM | future |
| 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 | |
| 3038 | GROMACS | Feature | New | Normal | Improvements to MD plugin development environment | Eric Irrgang | 12/10/2019 01:58 PM | 2021-infrastructure-stable |
| 3035 | GROMACS | Task | New | Normal | Provide central logger in wrapper binary | Paul Bauer | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 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 |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------|---------------------|----------------------------|
| 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 gmxfatal | | 09/06/2019 02:34 PM | 2021-infrastructure-stable |
| 3014 | GROMACS | Task | In Progress | Normal | gmxfapi example Python scripts | | 01/03/2020 11:00 AM | 2021-infrastructure-stable |
| 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 gmxf 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 |
| 2996 | GROMACS | Feature | In Progress | Normal | gmxfapi execution model | Eric Irrgang | 12/10/2019 01:57 PM | 2021-infrastructure-stable |
| 2994 | GROMACS | Feature | New | Normal | Data flow topology in gmxfapi 2020 | | 12/11/2019 11:33 AM | 2021-infrastructure-stable |
| 2993 | GROMACS | Feature | New | Normal | Scalar and structured type expression and definitions for API | Eric Irrgang | 10/17/2019 09:55 AM | |
| 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 |
| 2984 | GROMACS | Feature | New | Normal | More Extensive Selections Examples | Dallas Warren | 06/18/2019 11:50 PM | |
| 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 | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-------------|----------|--|----------------|---------------------|----------------------------|
| 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 | |
| 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 |
| 2944 | GROMACS | Feature | New | Normal | Roadmap for thermostats / barostats in new propagation/integration scheme | Michael Shirts | 12/27/2019 04:00 PM | 2021 |
| 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 | |
| 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 |
| 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 | |
| 2916 | GROMACS | Task | New | Normal | Decide future of symtab | Paul Bauer | 09/06/2019 02:35 PM | 2021-infrastructure-stable |
| 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 | |
| 2908 | GROMACS | Task | New | Normal | Renaming things in nbxnm | Berk Hess | 03/28/2019 10:10 AM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 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 |
| 2889 | GROMACS | Task | New | Normal | update grompp warnings for brevity, usefulness and actionability | Mark Abraham | 12/27/2019 04:38 PM | future |
| 2883 | GROMACS | Bug | New | Normal | essentialdynamics fail with Intel MPI | | 03/08/2019 03:10 AM | |
| 2882 | GROMACS | Task | New | Normal | evaluate different storage layouts for GPU coordinates/changes/forces | Szilárd Páll | 03/07/2019 06:21 PM | |
| 2877 | GROMACS | Task | New | Normal | use gmx::Options more | Mark Abraham | 12/20/2019 01:22 PM | 2021 |
| 2876 | GROMACS | Bug | New | Normal | 2019.1 make check fails on AVX and AVX2 (Intel 2018u3) | Erik Lindahl | 03/08/2019 10:32 AM | |
| 2875 | GROMACS | Task | Accepted | Normal | SIMD version of the free-energy kernel | Berk Hess | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2874 | GROMACS | Task | New | Normal | Refactor Gromacs (cluster) neighborlist into separate module | Erik Lindahl | 02/28/2019 11:36 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 | |
| 2866 | GROMACS | Feature | New | Normal | Alternative non-bonded potentials | David van der Spoel | 03/05/2019 03:50 PM | future |
| 2864 | GROMACS | Task | New | Normal | Building incompatibilities | Benson Muite | 02/19/2019 02:00 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 | |
| 2854 | GROMACS | Bug | New | Normal | OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1 | Paul Bauer | 02/04/2019 11:17 AM | |
| 2853 | GROMACS | Bug | New | Normal | EwaldUnitTests segfault on armv7hl with gcc-9.0.1 | Paul Bauer | 02/04/2019 05:34 PM | |
| 2852 | GROMACS | Bug | New | Low | the in-tree regressiontest download can get out of sync with code | | 01/30/2019 03:58 PM | |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 2850 | GROMACS | Task | In Progress | Normal | assess Raptor Talos for testing | Szilárd Páll | 02/12/2019 01:14 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 | |
| 2834 | GROMACS | Task | In Progress | Normal | C++ matrix classes | Christian Blau | 12/29/2019 10:32 AM | 2021 |
| 2833 | GROMACS | Task | New | Normal | Update topology datastructures | Paul Bauer | 12/02/2019 01:43 PM | 2021-infrastructure-stable |
| 2832 | GROMACS | Bug | New | Low | PaddedVector move operations broken | Mark Abraham | 12/28/2019 10:40 AM | 2021 |
| 2828 | GROMACS | Bug | Feedback wanted | Normal | Installation issue on Power 9 system with SIMD support | | 01/18/2019 11:54 AM | |
| 2822 | GROMACS | Task | Accepted | Normal | Make nbxn a module | Berk Hess | 12/18/2019 10:49 AM | future |
| 2818 | GROMACS | Task | In Progress | Normal | bonded GPU kernel fusion | Magnus Lundborg | 07/03/2019 09:01 PM | |
| 2806 | GROMACS | Feature | New | Normal | SIMD algorithms for ARM SVE // nobonded 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 | |
| 2791 | GROMACS | Feature | In Progress | Normal | Implement a module for lambda-dynamics simulations (lambda_site module) | Thomas Ullmann | 03/01/2019 01:36 AM | future |
| 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 | |
| 2774 | GROMACS | Feature | New | Normal | Refactor shell code into its own integrator | David van der Spoel | 12/27/2019 04:05 PM | 2021 |
| 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 |
| 2766 | GROMACS | Task | In Progress | Normal | Improve hardware option selection | Kevin Boyd | 12/20/2019 02:34 PM | 2021 |
| 2764 | GROMACS | Task | New | Normal | gmxapi version updates for post release-2019 | Eric Irrgang | 11/21/2018 12:53 PM | |
| 2763 | GROMACS | Bug | New | Normal | GMXAPI layout / grouping in development docs "modules" page | | 12/14/2018 12:49 PM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------------|----------|--|----------------|---------------------|----------------------------|
| 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 |
| 2755 | GROMACS | Feature | New | Low | md5 sums and sha256, sha512 hashes | Benson Muite | 02/19/2019 11:00 PM | |
| 2754 | GROMACS | Bug | New | Normal | Simulated Tempering seems to be broken | Michael Shirts | 02/05/2019 03:58 PM | |
| 2740 | GROMACS | Bug | New | Normal | mdrun reports incorrect error with -bonded gpu without gpu | Mark Abraham | 11/07/2018 01:59 PM | |
| 2739 | GROMACS | Feature | New | Normal | Parallel continuous tempering and enhanced sampling feature | | 11/13/2018 11:36 PM | |
| 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 |
| 2734 | GROMACS | Bug | In Progress | Normal | regressiontests/kernel core dumps on ppc64le | Paul Bauer | 06/15/2019 04:12 PM | future |
| 2733 | GROMACS | Bug | Blocked, need info | Normal | MdrunUtilityMpiUnitTests timesout on i686 and armv7hl with OpenMPI 2.1.5 | Paul Bauer | 01/17/2020 08:40 AM | |
| 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 |
| 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 dvdI 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 |
| 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 |
| 2696 | GROMACS | Task | In Progress | Normal | ensure PME queue is flushed | Szilárd Páll | 12/31/2018 11:21 AM | 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 |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|----------|----------|---|---------------------|---------------------|----------------|
| 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 | |
| 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 |
| 2660 | GROMACS | Task | New | Low | rework OpenCL nbnxn kernel constants | Szilárd Páll | 12/28/2019 10:53 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 |
| 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 | |
| 2644 | GROMACS | Task | New | Normal | Replace compute_globals | Mark Abraham | 09/24/2018 05:51 PM | future |
| 2643 | GROMACS | Feature | New | Low | mdp options and/or docs for anisotropic aspects of implementations | | 09/12/2018 02:23 PM | |
| 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 |
| 2621 | GROMACS | Task | New | Normal | Fine-Grained API to Describe Force Calculation and Neighbourhood Search | Prashanth Kanduri | 08/22/2018 11:36 AM | 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 | |
| 2603 | GROMACS | Task | New | Normal | Add ability to properly check coordinate files during testing | Paul Bauer | 10/15/2018 01:16 PM | future |
| 2602 | GROMACS | Bug | New | Low | build information gets outdated if build tree is reused | | 08/13/2018 09:04 PM | |
| 2601 | GROMACS | Feature | New | Normal | Free energy calculations, soft-core potential | Vytautas Gapsys | 02/10/2020 11:29 AM | future |
| 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 |
| 2596 | GROMACS | Feature | New | Normal | Constant potential method | Benson Muite | 05/10/2019 09:54 AM | |
| 2595 | GROMACS | Task | New | Normal | Reusable Utilities for Schedules | Prashanth Kanduri | 02/22/2019 03:48 PM | future |
| 2594 | GROMACS | Feature | New | Normal | Multi-level GMX API | Prashanth Kanduri | 02/22/2019 03:48 PM | future |
| 2590 | GROMACS | Task | New | Normal | Essential Dynamics as module providing forces | Christian Blau | 08/22/2018 05:03 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 | |
| 2582 | GROMACS | Bug | Blocked, need info | Normal | Compilation issues with CUDA V9.1.85 and both gcc5 and gcc6 | Szilárd Páll | 07/23/2018 07:46 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 | |
| 2574 | GROMACS | Feature | New | Normal | iForceSchedule Abstraction | Prashanth Kanduri | 03/29/2019 05:20 PM | future |
| 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 | |
| 2556 | GROMACS | Feature | New | Normal | make default selections suitable for DNA and RNA | Mark Abraham | 06/20/2018 01:48 PM | |
| 2555 | GROMACS | Bug | New | Low | building GROMACS 2018.2 | | 07/03/2018 11:41 PM | |
| 2547 | GROMACS | Feature | New | Low | Add option of averaging and obtaining error bars for AWH PMFs | Viveca Lindahl | 06/06/2018 11:31 AM | future |
| 2546 | GROMACS | Task | New | Normal | Add more assertions to AWH code | Viveca Lindahl | 06/06/2018 11:20 AM | future |
| 2545 | GROMACS | Feature | New | Normal | Should grompp fix periodicity of input files? | David van der Spoel | 10/03/2018 11:32 PM | future |
| 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 |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|-----------------|---------------------|----------------|
| 2538 | GROMACS | Task | New | Normal | organize more of the PME GPU code along task-specific lines | Mark Abraham | 05/31/2018 05:41 PM | |
| 2537 | GROMACS | Task | New | Normal | Simplify PME solve reduction | Aleksei Lupinov | 12/20/2019 12:21 PM | future |
| 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 |
| 2516 | GROMACS | Task | New | Low | Support PME OpenCL execution width < 16 | Aleksei Lupinov | 06/05/2019 05:32 PM | |
| 2514 | GROMACS | Task | New | Normal | PME OpenCL reductions with intrinsics | | 05/31/2018 12:27 AM | future |
| 2513 | GROMACS | Bug | Feedback wanted | Normal | ref_t and temperature incorrect with coulomb-type = user | Yu Du | 05/31/2018 04:05 PM | |
| 2501 | GROMACS | Task | New | Normal | Documentation section on log file contents | Kevin Boyd | 10/03/2018 09:48 PM | 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 | |
| 2495 | GROMACS | Task | Accepted | Normal | replace -noconfout with mdp option | Mark Abraham | 12/28/2019 10:39 AM | 2021 |
| 2492 | GROMACS | Task | New | Normal | implement force calculation via ForceProviders containing collections of IForceProvider | Mark Abraham | 09/19/2018 03:13 PM | future |
| 2491 | GROMACS | Feature | New | Low | Allow constant bias AWH simulations | Viveca Lindahl | 06/05/2018 10:38 PM | future |
| 2490 | GROMACS | Task | New | Normal | evaluate two-step communicators | Szilárd Páll | 10/03/2018 09:47 PM | future |
| 2488 | GROMACS | Task | New | Normal | use MPI non-blocking collectives to overlap pull comm | | 04/25/2018 04:19 PM | |
| 2483 | GROMACS | Bug | New | Low | gmx dump writes mdp files that can not be parsed by grompp | Paul Bauer | 10/08/2018 10:50 AM | future |

| # | Project | Tracker | Status | Priority | Subject | Assignee | Updated | Target version |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 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 |
| 2480 | GROMACS | Bug | New | Normal | pdb2gmx does not protonate correctly for united-atom Gromos | Mark Abraham | 12/20/2019 12:17 PM | 2021 |
| 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 | |
| 2453 | GROMACS | Task | Resolved | High | PME OpenCL porting effort | Aleksei lupinov | 12/20/2019 12:18 PM | 2021 |
| 2452 | GROMACS | Task | In Progress | Normal | Reduce data dependencies in mdrun algorithms | Berk Hess | 03/14/2018 08:47 PM | |
| 2451 | GROMACS | Feature | Resolved | Normal | Linear virtual sites with fixed distance | David van der Spoel | 09/16/2019 01:15 PM | |
| 2448 | GROMACS | Task | Accepted | Normal | should mdrun -multidir permit only one directory? | | 03/21/2018 12:10 PM | |

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