

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	
2902	GROMACS	Bug	New	Normal	2019.1 equilibration issue? (Intel 2018u3)		04/30/2019 08:17 AM	
2876	GROMACS	Bug	New	Normal	2019.1 make check fails on AVX and AVX2 (Intel 2018u3)	Erik Lindahl	03/08/2019 10:32 AM	
2035	GROMACS	Task	New	Normal	A common trajectory analysis data exchange format		03/15/2017 05:46 PM	future
2068	GROMACS	Feature	New	Normal	Access to low level classes		03/02/2019 01:37 AM	future
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2456	GROMACS	Task	New	Normal	Add a pull module external potential tests		03/15/2018 03:02 PM	
2603	GROMACS	Task	New	Normal	Add ability to properly check coordinate files during testing	Paul Bauer	10/15/2018 01:16 PM	future
2928	GROMACS	Feature	New	Normal	Add ability to use expression "count of ATOM_EXPR" in selection statements.		04/16/2019 04:52 PM	
2579	GROMACS	Feature	New	Normal	Add dimensionality option to gmx trjconv -center		07/19/2018 04:53 PM	future
2185	GROMACS	Task	New	Normal	add docs on MPI + CUDA w/wo MPS		05/24/2017 05:17 PM	
3026	GROMACS	Task	New	Normal	add flags for GPU force buffer op / reduction activation		08/01/2019 04:46 PM	2020
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2383	GROMACS	Task	New	Normal	Add JSON interface to write and read files	Paul Bauer	01/16/2018 02:01 PM	future
2128	GROMACS	Feature	New	Normal	add means to verify at build/run-time that source tarball is not tainted		03/06/2018 10:39 PM	
1523	GROMACS	Task	New	Normal	add missing code-paths to CUDA emulation kernel		07/11/2016 08:09 PM	
3037	GROMACS	Task	New	Normal	add missing cycle counters related to buffer ops/reduction launches		09/24/2019 03:27 PM	2020
1373	GROMACS	Task	New	Low	Add missing nbxn tests	Mark Abraham	06/09/2014 08:36 PM	
2546	GROMACS	Task	New	Normal	Add more assertions to AWH code	Viveca Lindahl	06/06/2018 11:20 AM	future
2001	GROMACS	Feature	New	Normal	add MPI info to the mdrun log header		07/06/2016 05:21 PM	
2682	GROMACS	Task	New	Normal	Add MSAN configuration		10/09/2018 06:28 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
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 PM	
2957	GROMACS	Feature	New	Normal	add support for the Hygon Dhyana architecture		05/21/2019 01:00 PM	2020
701	GROMACS	Task	New	Normal	Add symbol visibility macros		03/02/2019 01:46 AM	future
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		08/22/2019 06:34 PM	2020
2730	GROMACS	Task	New	Normal	Add tests for gmx_genion	Joe Jordan	11/02/2018 06:42 PM	2020

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2686	GROMACS	Task	New	Normal	add tests for gpu bonded interactions		11/29/2018 10:44 AM	2020
1641	GROMACS	Feature	New	Normal	Add toolchain file for Cray systems		06/06/2015 11:24 PM	
3062	GROMACS	Task	New	Normal	add twin cut-off mdrun test		08/19/2019 06:21 PM	2020
1948	GROMACS	Feature	New	Low	add warning when non-identical GPUs are used		06/12/2017 08:45 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	
1303	GROMACS	Feature	New	Normal	Adding lambda dependent distance for pull code	Michael Shirts	07/11/2016 08:18 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	
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
2855	GROMACS	Task	New	Normal	Allow compiling GROMACS without C compiler		01/31/2019 08:44 PM	
2491	GROMACS	Feature	New	Low	Allow constant bias AWH simulations	Viveca Lindahl	06/05/2018 10:38 PM	future
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irrgang	10/15/2019 03:56 PM	2020
2735	GROMACS	Task	New	Normal	Allow gmx_genrestr to write correct position restraints for molecules after the first molecule	Joe Jordan	11/09/2018 12:19 PM	2020
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	
3078	GROMACS	Task	New	Normal	Allow MD modules to register energy output fields themselves		09/06/2019 11:36 AM	
2787	GROMACS	Task	New	Normal	allow passing flags to allocateDeviceBuffer		12/03/2018 01:54 PM	
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future
2045	GROMACS	Task	New	Normal	API design and language bindings	Peter Kasson	10/17/2019 09:55 AM	
2990	GROMACS	Bug	New	Normal	ARM neon SIMD4 error		09/24/2019 03:25 PM	2020-beta2
2987	GROMACS	Bug	New	Normal	assess the bonded GPU task assignment default		06/19/2019 06:02 PM	2020
2341	GROMACS	Task	New	Low	assess the state of building and using GROMACS on Windows		07/29/2019 11:09 PM	future
2412	GROMACS	Task	New	Normal	attempt to do better FFTW planning		03/15/2018 05:01 PM	
2015	GROMACS	Feature	New	Normal	Auto recovery from dd communication error		07/28/2016 03:17 PM	
2221	GROMACS	Task	New	Normal	Avoid preprocessor for SIMD functions		02/21/2018 01:43 PM	
2715	GROMACS	Feature	New	Normal	Avoid requesting the user to recompile gromacs for Intel OpenCL support		10/31/2018 12:16 PM	2020
2351	GROMACS	Task	New	Normal	Avoid the SIMD module depending on non-trivial parts of Gromacs		12/14/2017 02:47 AM	future
2478	GROMACS	Task	New	Low	avoid use of getenv in static initialization		04/13/2018 11:57 AM	

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3024	GROMACS	Bug	New	Normal	Bad logic for Sphinx detection CMake output		07/05/2019 05:44 PM	2020
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		08/04/2019 09:44 PM	2020
2925	GROMACS	Bug	New	Normal	BasicVector addition operator yields unexpected result when adding scalar	Christian Blau	04/20/2019 05:39 PM	2020
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		05/02/2019 12:20 PM	
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2695	GROMACS	Task	New	Low	bonded GPU module timing		01/21/2019 01:19 PM	2020
1634	GROMACS	Feature	New	Normal	Boxed Molecular Dynamics		11/04/2014 04:40 PM	
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	
2831	GROMACS	Task	New	Normal	Bump required version numbers of infrastructure for 2020	Mark Abraham	08/23/2019 03:24 PM	2020-infrastructure-update-post-beta1
2834	GROMACS	Task	New	Normal	C++ matrix classes	Christian Blau	01/23/2019 12:19 PM	2020
996	GROMACS	Task	New	Normal	C++ MPI Framework	Roland Schulz	07/14/2014 11:53 AM	future
2919	GROMACS	Task	New	Normal	C++ style guidelines for namespace use		04/15/2019 01:21 PM	
948	GROMACS	Task	New	Normal	C++ thread synchronization primitives	Sander Pronk	07/11/2016 08:24 PM	
1017	GROMACS	Task	New	Normal	C++ Vector/Matrix classes		07/11/2016 08:23 PM	
2048	GROMACS	Task	New	Normal	C++11: CUDA dependency on general headers		09/07/2016 10:30 PM	
1339	GROMACS	Bug	New	Normal	Center of mass drift with Nose-Hoover, MTK and md-vv	Michael Shirts	06/18/2015 08:53 PM	future
3142	GROMACS	Feature	New	High	centralize and clarify GPU force buffer clearing		10/14/2019 04:56 PM	2020-beta2
2770	GROMACS	Task	New	Normal	change branch maintenance policy		11/29/2018 02:51 PM	2020
2672	GROMACS	Task	New	Normal	check & document execution width requirements in OpenCL		12/31/2018 11:20 AM	future
2379	GROMACS	Task	New	Normal	check leftover FIXMEs in r2018	Szilárd Páll	12/31/2018 11:16 AM	future
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelization codepaths		10/04/2019 12:17 PM	2020
3118	GROMACS	Task	New	Normal	clang-tidy segfaulting in CI		10/04/2019 11:34 AM	2020-beta2
2375	GROMACS	Task	New	Normal	Clarify execution phases for MD simulation		04/30/2019 12:59 PM	
2857	GROMACS	Task	New	Normal	Clarify recommended function specifies (constexpr, noexcept, pure)		02/04/2019 04:48 AM	
2796	GROMACS	Task	New	Low	clarify what mdrun -cpt means		01/03/2019 02:09 PM	
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	
3032	GROMACS	Feature	New	Normal	Clean up dev-manual structure		07/11/2019 11:48 AM	2020
1793	GROMACS	Task	New	Normal	cleanup of integration loop	Mark Abraham	10/31/2018 10:49 PM	future

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3000	GROMACS	Bug	New	Normal	CMake "webpage" target does not fail when it should		06/25/2019 02:43 PM	
2949	GROMACS	Bug	New	Normal	cmake fails when building mdrun only		07/08/2019 10:04 AM	
1827	GROMACS	Bug	New	Low	cmake multi-configuration generator support partly broken		12/11/2017 05:20 PM	future
1963	GROMACS	Task	New	Low	collect examples of systems where users tried to do something that performed badly	Mark Abraham	08/09/2016 07:30 AM	
2958	GROMACS	Bug	New	Normal	Compiling master (to become 2020) using CUDA 9.0		10/14/2019 09:15 PM	2020-beta2
3021	GROMACS	Feature	New	Normal	Completion of docs for GPU developments		07/04/2019 10:45 AM	2020
2158	GROMACS	Task	New	Normal	consider adding post-submit test that runs PME with 2xNN kernels		04/19/2017 08:04 PM	
2462	GROMACS	Task	New	Normal	consider adding STL misuse tests		03/23/2018 01:23 AM	
2535	GROMACS	Task	New	Normal	consider compiling opencl fft kernels once		05/31/2018 01:33 PM	
1947	GROMACS	Task	New	Normal	Consider fixing corner case in TinyXML2	Mark Abraham	04/19/2016 01:40 AM	
2909	GROMACS	Task	New	Normal	consider implementing mechanisms to ensure pair lists are not used past their max lifetime		04/03/2019 05:14 PM	
2531	GROMACS	Task	New	Low	Consider optimizing tabulated data access on GPU		07/30/2018 12:31 PM	
3002	GROMACS	Task	New	Normal	consider splitting bonded work into local/nonlocal		06/25/2019 04:06 PM	
2530	GROMACS	Task	New	Normal	consider using CUDA Driver API		09/23/2018 11:47 PM	future
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 PM	
2713	GROMACS	Feature	New	Normal	Constant offset for external electric fields		10/28/2018 12:57 AM	
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
2367	GROMACS	Task	New	Normal	construct pbc_simd less often		09/24/2018 11:02 PM	future
2060	GROMACS	Feature	New	Normal	Convert enum to enum class		10/17/2016 05:27 PM	
1855	GROMACS	Task	New	Normal	Convert preprocessor use so that symbols are always defined		06/28/2016 02:17 PM	
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2231	GROMACS	Bug	New	Normal	convert-tpz aborts when saving subset of the system		01/12/2018 03:52 PM	
3133	GROMACS	Task	New	Normal	Cookiecutter for sample_restraint	Eric Irrgang	10/13/2019 01:07 PM	2020
3042	GROMACS	Bug	New	Normal	core dump error in grompp command		10/09/2019 07:30 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	
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	10/04/2019 09:16 AM	future
3015	GROMACS	Task	New	Normal	Create central log handle for calls to gmxf_fatal		09/06/2019 02:34 PM	2021-infrastructure-stable
1670	GROMACS	Feature	New	Normal	create mdrun option checking mini-tool		06/23/2016 04:06 PM	

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1422	GROMACS	Feature	New	Normal	CSH angle incorrect with GROMOS force field and virtual sites	David van der Spoel	06/12/2014 12:01 AM	
2888	GROMACS	Feature	New	Low	CUDA Update and Constraints module	Artem Zhmurov	10/08/2019 03:09 PM	2020
2887	GROMACS	Feature	New	Normal	CUDA version of Leap Frog algorithm	Artem Zhmurov	10/02/2019 12:00 PM	2020
2885	GROMACS	Feature	New	Normal	CUDA version of LINCS	Artem Zhmurov	03/12/2019 01:33 PM	2020
2886	GROMACS	Feature	New	Normal	CUDA version of SETTLE	Artem Zhmurov	10/02/2019 12:02 PM	2020
2208	GROMACS	Bug	New	Normal	cuFFT linking		06/30/2017 01:58 PM	
2380	GROMACS	Bug	New	Low	cycle counter issues with separate PME rank + GPUs		01/16/2018 10:21 PM	
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxapi 2020		06/24/2019 01:53 PM	2020
3017	GROMACS	Bug	New	Normal	ddBalanceRegionHandler triggers need fixing		09/24/2019 03:25 PM	2020-beta2
2182	GROMACS	Task	New	Low	de-duplicate code in densorder and hydorder		05/16/2017 11:29 AM	
1768	GROMACS	Task	New	Normal	decide future of command-line options vs env vars		11/03/2016 05:51 PM	future
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 PM	2021-infrastructure-stable
1653	GROMACS	Feature	New	Normal	Decide how to represent multiple lambda states in the .top file and how to parse them	Michael Shirts	06/05/2018 03:58 PM	
1652	GROMACS	Feature	New	Normal	Decide how to represent multiple lambda states internally	Michael Shirts	06/05/2018 03:58 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	
2901	GROMACS	Feature	New	Normal	Declare external Resources in mdp / tpr files.	Christian Blau	03/27/2019 04:27 PM	2020
2798	GROMACS	Bug	New	Normal	Default mpi rank number fails when there are 16 cores and 3 gpus	Berk Hess	12/11/2018 10:11 PM	2020
988	GROMACS	Task	New	Normal	Definition of "public API"		08/28/2019 02:50 PM	future
2282	GROMACS	Feature	New	Normal	Density map toolset	Christian Blau	03/21/2019 06:08 PM	future
1102	GROMACS	Feature	New	Normal	Detect incompletely written itp files		06/19/2014 03:23 PM	
1323	GROMACS	Task	New	Normal	determine future of existing tools for	David van der Spoel	12/04/2018 11:53 AM	
2354	GROMACS	Feature	New	Normal	develop configuration file support for control of task layout		09/19/2018 03:01 PM	future
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
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	
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	

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3128	GROMACS	Task	New	High	do not fall back to CPU path on energy-only steps	Alan Gray	10/11/2019 11:55 AM	2020-beta2
2304	GROMACS	Task	New	Normal	Document and propose tracking mdrun heuristics		10/03/2018 09:39 PM	future
2501	GROMACS	Task	New	Normal	Documentation section on log file contents	Kevin Boyd	10/03/2018 09:48 PM	future
1489	GROMACS	Feature	New	Normal	Don't solely rely on filename extension		04/30/2014 05:23 AM	
1885	GROMACS	Feature	New	Normal	DPD Thermostat		01/26/2016 10:17 AM	
1658	GROMACS	Feature	New	Normal	Electrostatics treatment for multiple lambda sites	Berk Hess	07/11/2016 08:05 PM	
3159	GROMACS	Task	New	High	eliminate regression due to moving gmx_pme_send_coordinates()	Alan Gray	10/17/2019 02:57 PM	2020
1518	GROMACS	Feature	New	Low	Enable automatic build checking for newer versions	Mark Abraham	06/04/2014 04:13 PM	future
3087	GROMACS	Feature	New	Normal	enable GPU peer to peer access		09/12/2019 04:24 PM	2020
2532	GROMACS	Task	New	Normal	enable queue priorities in OpenCL		05/29/2018 02:29 PM	
2089	GROMACS	Task	New	Normal	Encourage code review		01/10/2017 12:03 AM	
742	GROMACS	Feature	New	Normal	Enhancing the performance of the free energy code		08/26/2019 04:55 PM	future
2360	GROMACS	Bug	New	Low	error at counter reset with PME-only rank		01/05/2018 12:43 PM	future
2590	GROMACS	Task	New	Normal	Essential Dynamics as module providing forces	Christian Blau	08/22/2018 05:03 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	
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		08/21/2019 06:08 PM	2020
2490	GROMACS	Task	New	Normal	evaluate two-step communicators	Szilárd Páll	10/03/2018 09:47 PM	future
2853	GROMACS	Bug	New	Normal	EwaldUnitTests segfault on armv7hl with gcc-9.0.1	Paul Bauer	02/04/2019 05:34 PM	
1828	GROMACS	Task	New	Normal	Exception handling in mdrun		10/07/2015 11:36 AM	
1849	GROMACS	Feature	New	Normal	expanded ensemble -- Adaptive Integration Method	Christopher Mirabzadeh	07/11/2016 08:01 PM	
1246	GROMACS	Task	New	Normal	expanded ensemble .tpr cannot be rerun	Michael Shirts	06/19/2015 01:56 PM	
3001	GROMACS	Task	New	Normal	explore simplifying virial and shift force reduction		06/25/2019 04:03 PM	2020
1994	GROMACS	Feature	New	Low	explore using JIT for CUDA		07/11/2016 10:20 PM	future
3013	GROMACS	Task	New	Normal	Extend logging levels in MDLogger		09/06/2019 02:34 PM	2021-infrastructure-stable
1972	GROMACS	Feature	New	Normal	external potential modules for refinement against experimental data		08/22/2018 05:03 PM	future
1811	GROMACS	Bug	New	Normal	Extrae build issues		12/13/2017 03:43 AM	
2924	GROMACS	Bug	New	Normal	Failing version check when reading new tpr file with older gromacs version		04/12/2019 10:52 AM	
2496	GROMACS	Task	New	Low	find system xdr properly		05/02/2018 02:19 PM	

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2621	GROMACS	Task	New	Normal	Fine-Grained API to Describe Force Calculation and Neighbourhood Search	Prashanth Kanduri	08/22/2018 11:36 AM	future
1247	GROMACS	Feature	New	Normal	fix hardcoded references to atom names in analysis tools	Mark Abraham	06/12/2014 01:20 AM	future
2728	GROMACS	Bug	New	Normal	Fix NB kernel picking		11/02/2018 03:51 PM	2020
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	07/29/2019 12:38 PM	2020
2283	GROMACS	Feature	New	Normal	Force distribution analysis	Bernd Doser	10/27/2017 11:44 AM	
2606	GROMACS	Bug	New	Normal	Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert		08/10/2018 01:48 AM	
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	03/05/2019 01:44 AM	future
3075	GROMACS	Bug	New	Normal	Frozen atoms are moving		09/04/2019 08:00 PM	
2005	GROMACS	Feature	New	Normal	Full Correlation Analysis (FCA) as Trajectory Analysis Module	Christian Blau	02/07/2018 02:19 PM	future
2229	GROMACS	Feature	New	High	Full Object Oriented Modularization of GROMACS MDRUN Codebase	Mark Abraham	08/22/2018 05:03 PM	future
1862	GROMACS	Task	New	Normal	Fully replace t_topology by gmx_mtop_t		02/13/2019 04:53 PM	
1347	GROMACS	Feature	New	Normal	future of tables	Mark Abraham	03/27/2019 05:24 PM	future
1829	GROMACS	Task	New	Normal	Future of thread level parallelism		11/18/2016 05:29 PM	
1411	GROMACS	Task	New	Normal	Future of thread_mpi	Mark Abraham	02/26/2018 04:56 PM	future
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	
2954	GROMACS	Bug	New	Normal	genion changes residue numbering		05/26/2019 12:08 AM	
2945	GROMACS	Task	New	Normal	Give MdModules access to simulation resources (e.g. atom selection manager or communication infrastructure)	Christian Blau	05/19/2019 01:26 PM	2020
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
1730	GROMACS	Bug	New	Normal	gmx compare does not compare all fields of a .tpr		06/12/2015 09:33 PM	future
1667	GROMACS	Bug	New	Normal	gmx convert-tpr writes wrong number of mol in output tpr	David van der Spoel	06/27/2016 08:29 PM	
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
2568	GROMACS	Bug	New	Low	gmx editconf -rotate does not rotate the box		07/10/2018 10:27 AM	future
1397	GROMACS	Feature	New	Normal	gmx eneconv -offset 1.998 -dt 2 is broken for large times	Mark Abraham	06/12/2014 01:31 AM	future
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	
1583	GROMACS	Bug	New	Normal	gmx msd with mol flag requires excessive memory		12/18/2017 03:34 PM	
3049	GROMACS	Bug	New	Low	gmx nmeig should plot a real infrared spectrum	David van der Spoel	09/24/2019 03:25 PM	future
1602	GROMACS	Feature	New	Low	gmx order S per slice along all 3 axes		09/22/2014 07:25 AM	

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2576	GROMACS	Bug	New	Normal	gmx potential -correct outputs the wrong potential		07/25/2018 02:58 PM	
2544	GROMACS	Bug	New	Normal	gmx rmsf does not fix periodicity in reference structure	David van der Spoel	08/21/2018 10:36 AM	future
2427	GROMACS	Bug	New	Normal	gmx select gives syntax error for selection involving evaluating simple arithmetic expression		02/27/2018 05:15 PM	
2872	GROMACS	Bug	New	Normal	gmx solvate and genion topology update		02/27/2019 10:18 AM	
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	
2133	GROMACS	Task	New	Low	gmx traj needs reform		03/07/2017 02:02 PM	
2211	GROMACS	Bug	New	Low	gmx writes normal output to stderr		03/05/2018 02:00 PM	future
2698	GROMACS	Task	New	Normal	gmxapi documentation integration		03/02/2019 01:31 AM	
3014	GROMACS	Task	New	Normal	gmxapi example Python scripts		06/28/2019 11:07 AM	2020
2996	GROMACS	Feature	New	Normal	gmxapi execution model	Eric Irgang	06/24/2019 02:16 PM	2020
3086	GROMACS	Bug	New	Normal	gmxapi fails with MPI build of GROMACS 2020		09/25/2019 04:18 PM	
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irgang	10/15/2019 03:57 PM	2020
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irgang	10/15/2019 03:56 PM	
2763	GROMACS	Bug	New	Normal	GMXAPI layout / grouping in development docs "modules" page		12/14/2018 12:49 PM	future
2722	GROMACS	Bug	New	Normal	gmxapi may over-manage RPATH	Mark Abraham	10/16/2019 10:28 AM	2020-beta3
3132	GROMACS	Task	New	Low	gmxapi testing support tools		10/13/2019 01:00 PM	
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irgang	11/21/2018 12:53 PM	
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3144	GROMACS	Bug	New	Normal	gmxapi.mdrun does not clearly expose the output trajectory.	Eric Irgang	10/14/2019 06:55 PM	2020-beta2
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irgang	10/14/2019 08:16 PM	2020-beta2
2113	GROMACS	Bug	New	Normal	Google tests and execution order		03/05/2018 02:05 PM	
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 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	
2915	GROMACS	Feature	New	High	GPU direct communications		10/11/2019 05:53 PM	
2217	GROMACS	Bug	New	Low	GPU emulation and separate PME ranks doesn't work properly		12/12/2017 11:50 AM	
2254	GROMACS	Feature	New	Normal	GPU extensions for Google Tests		09/19/2017 05:01 PM	
2890	GROMACS	Feature	New	High	GPU Halo Exchange		10/17/2019 02:00 PM	2020

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2816	GROMACS	Feature	New	High	GPU offload / optimization for update&constraints, buffer ops and multi-gpu communication	Alan Gray	10/14/2019 01:32 PM	2020
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		09/24/2019 06:52 PM	2020-beta2
3052	GROMACS	Feature	New	Normal	GPU virial reduction/calculation		08/01/2019 05:26 PM	
2934	GROMACS	Feature	New	Normal	GPU X Buffer ops		09/24/2019 06:07 PM	2020
2907	GROMACS	Bug	New	Normal	Gromacs autocompletion appears to be broken with ZSH		07/16/2019 04:46 AM	
1625	GROMACS	Feature	New	Normal	Gromacs Python API		03/02/2019 01:44 AM	future
2216	GROMACS	Task	New	Normal	GROMACS SIMD acceleration: generation 3	Erik Lindahl	07/17/2017 06:57 PM	future
2607	GROMACS	Bug	New	Normal	Grompp becomes extremely slow when many pull groups are present		08/11/2018 08:54 AM	
2767	GROMACS	Bug	New	Normal	grompp warns about md + FEP even for fully coupled states		11/19/2018 11:41 AM	2020
1481	GROMACS	Bug	New	Low	g_chi output file chi.log reports atomic definitions for phi and psi that do not correspond to the angles output in the .xvg files	David van der Spoel	06/12/2014 01:37 PM	
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	
1498	GROMACS	Feature	New	Low	g_dipoles does not work properly with ionic systems	David van der Spoel	07/11/2016 08:11 PM	
843	GROMACS	Feature	New	Low	g_helixorient could benefit from more documentation	Erik Lindahl	05/23/2014 02:02 PM	
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 PM	
1166	GROMACS	Bug	New	Low	g_order is incorrect for unsaturated carbons	David van der Spoel	06/18/2017 04:40 PM	future
986	GROMACS	Task	New	Normal	Handling C++ out-of-memory errors		12/24/2014 08:42 PM	future
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2961	GROMACS	Feature	New	Normal	How should Python package find GROMACS resources under various circumstances?		10/02/2019 02:06 PM	
1654	GROMACS	Feature	New	Normal	How to carry out movement between chemical end states in a multiple end state framework?	Michael Shirts	07/11/2016 08:05 PM	
1966	GROMACS	Feature	New	Low	Hydrogen mass repartiniog		05/25/2016 06:04 PM	future
2435	GROMACS	Task	New	Normal	identify and note about/tune task offload in GPU-bound runs		03/02/2018 04:08 PM	
2574	GROMACS	Feature	New	Normal	iForceSchedule Abstraction	Prashanth Kanduri	03/29/2019 05:20 PM	future
2521	GROMACS	Task	New	Normal	Implement alternating PME/NB wait for OpenCL		10/15/2018 12:39 PM	
3092	GROMACS	Task	New	Normal	implement better receiver ready / notify in halo exchange		09/18/2019 02:47 AM	2020
1104	GROMACS	Feature	New	Low	Implement dihedral restraints		02/06/2013 07:04 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3160	GROMACS	Feature	New	Normal	implement direct comm for different src/target memory spaces	Alan Gray	10/17/2019 03:02 PM	2020
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 PM	future
1162	GROMACS	Feature	New	Normal	Implement gb_saltconc	Berk Hess	02/26/2013 05:33 PM	future
3104	GROMACS	Task	New	Normal	implement GPU DD cycle counting		09/24/2019 03:19 PM	2020
3105	GROMACS	Task	New	Normal	implement GPU PME/PP comm cycle counting		09/24/2019 03:19 PM	2020
2469	GROMACS	Task	New	Normal	implement GPU timer reduction for reporting		03/27/2018 05:08 PM	
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	
3106	GROMACS	Task	New	Normal	Implement multiple pulses with GPU communication	Alan Gray	09/25/2019 02:23 PM	
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		01/14/2019 10:09 AM	
1464	GROMACS	Feature	New	Normal	implement PP-PME re-balancing	Szilárd Páll	10/16/2015 08:34 AM	future
760	GROMACS	Feature	New	Low	Implement rigid body groups	Berk Hess	12/30/2012 06:04 AM	future
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	
2175	GROMACS	Task	New	Normal	improve clang static analyzer docs further		01/04/2018 04:13 PM	future
2009	GROMACS	Task	New	Normal	improve command-line reporting of useful things		07/26/2016 12:54 PM	
1715	GROMACS	Feature	New	Low	improve cycle counting GPU sharing and multi-sim		08/03/2016 12:32 PM	future
3138	GROMACS	Feature	New	Normal	Improve ensemble support in Context specification.		10/15/2019 03:56 PM	
2697	GROMACS	Task	New	Normal	improve FFT library flavor/version reporting		12/10/2018 01:49 PM	2020
1665	GROMACS	Feature	New	Normal	improve free energy non-bonded kernel performance		08/26/2019 03:47 PM	future
838	GROMACS	Task	New	Normal	Improve generic error reporting routines		07/11/2016 08:29 PM	
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		11/21/2018 10:28 AM	2020
1515	GROMACS	Task	New	Normal	improve g_bar output	Szilárd Páll	07/11/2016 08:10 PM	
1505	GROMACS	Task	New	Normal	improve handling of logging	Mark Abraham	01/02/2019 06:06 PM	
2353	GROMACS	Task	New	Normal	improve on relative tolerance for constructing tables		10/30/2018 04:17 AM	2020
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		06/24/2019 03:07 PM	2020
1587	GROMACS	Task	New	Normal	improve the configurability of regression tests		01/18/2019 06:17 AM	2020
1182	GROMACS	Feature	New	Normal	improve trajectory writing to support parallel I/O		05/13/2014 10:42 AM	future
1211	GROMACS	Task	New	Low	improve use of preprocessor macros in CUDA kernels	Szilárd Páll	01/12/2015 06:42 PM	future
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		02/15/2019 06:34 PM	
1335	GROMACS	Feature	New	Normal	Improved interaction of free energies with pull code to better support Hamiltonian replica exchange with umbrella sampling	Michael Shirts	05/13/2014 10:38 AM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2792	GROMACS	Task	New	Normal	Improvement of PME gather and spread CUDA kernels		09/12/2019 12:23 PM	
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	07/17/2019 02:15 PM	2020
765	GROMACS	Task	New	Normal	Improving serialization of data structures prior to communication	Mark Abraham	05/13/2014 10:04 AM	future
2785	GROMACS	Bug	New	Normal	Inconsistent and erroneous behaviour of trjconv when writing a partial TNG		11/30/2018 02:36 PM	
1568	GROMACS	Bug	New	Low	inconsistent/incorrect threading checks and reporting in mdrun		05/25/2016 02:01 AM	
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		02/13/2019 08:17 PM	2020
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	
2468	GROMACS	Bug	New	Low	incorrect GPU timing reported with OpenCL and domain decomposition		12/17/2018 01:28 PM	future
3152	GROMACS	Feature	New	Low	Infrastructure and patterns for expressing public interfaces		10/17/2019 10:40 AM	2021-infrastructure-stable
2707	GROMACS	Bug	New	Normal	Installed OpenCL files include clh file from gpu_utils directory		10/30/2018 04:02 AM	
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	10/15/2019 09:07 AM	2020-beta2
2132	GROMACS	Feature	New	Normal	Intermediate code for xvg handling		03/08/2017 05:12 PM	future
3016	GROMACS	Task	New	Normal	intermittent failure of essentialdynamics test		07/18/2019 05:23 PM	
2936	GROMACS	Task	New	Normal	introduce check that CPU-GPU transfers are made between arrays of compatible types		05/13/2019 09:23 AM	2020
1562	GROMACS	Feature	New	Normal	introducing a Monte Carlo framework (first application: MC barostat)	Michael Shirts	07/11/2016 08:08 PM	
1826	GROMACS	Task	New	Normal	investigate non-optimal results with CPU-GPU balancing on AMD		09/16/2015 06:32 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	
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
1214	GROMACS	Task	New	Normal	Keep track of important changes for Changelog	Mark Abraham	06/26/2013 11:24 AM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 AM	
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
2930	GROMACS	Feature	New	Normal	Limited range for reference group detection in cylinder pulling		04/26/2019 05:17 PM	
2761	GROMACS	Feature	New	Low	lincs-order 4 is too conservative for some force fields		11/16/2018 09:55 AM	
3083	GROMACS	Bug	New	Normal	Listed forces tests failing on ICC19 with AVX2_256 nightly build		09/10/2019 11:56 AM	
2975	GROMACS	Feature	New	Normal	LJ PME calculations on GPUs		06/12/2019 01:17 PM	
1120	GROMACS	Feature	New	Low	Make build work with multi-cofiguration generators		06/03/2014 03:04 PM	future

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2567	GROMACS	Bug	New	Normal	make check fails at test 23 SIMD errors		07/10/2018 09:35 AM	
1867	GROMACS	Feature	New	Normal	make coupling implementations reversible		12/02/2015 07:43 AM	
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 PM	
3135	GROMACS	Feature	New	Normal	Make GPU traits ino opaque types		10/14/2019 10:24 AM	
2839	GROMACS	Task	New	Normal	make module and file naming consistent		04/09/2019 04:27 PM	2020
2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		10/30/2018 12:01 PM	2020
2632	GROMACS	Task	New	Low	make sure cmake defines proper hwloc versionc with cross-compilation enabled		12/03/2018 01:35 PM	future
677	GROMACS	Task	New	Normal	Make sure manual uses consistent style throughout		06/19/2014 11:49 AM	
2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2376	GROMACS	Task	New	Normal	max_mpi_ranks has wrong name		02/10/2018 11:03 AM	
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2039	GROMACS	Bug	New	Normal	mdrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 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	
2252	GROMACS	Bug	New	Low	Memory allocation failures with large page sizes during PME tuning		12/14/2017 04:27 AM	
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	
3054	GROMACS	Bug	New	Normal	Missing dihedral define		08/02/2019 05:47 PM	
2910	GROMACS	Feature	New	Normal	Mixed scaling for 1-4 interactions		04/10/2019 10:13 PM	
2616	GROMACS	Task	New	Normal	Model for MD state		09/14/2018 05:12 PM	
2423	GROMACS	Task	New	Normal	modernize constraints code	Mark Abraham	09/19/2018 03:01 PM	future
3020	GROMACS	Feature	New	Low	modernize DeviceBuffer and GPU memory management		08/13/2019 06:01 PM	
2758	GROMACS	Task	New	Low	Modernize genconf		11/15/2018 07:38 AM	future
3022	GROMACS	Feature	New	Normal	modernized naming for new GPU developments		07/04/2019 10:48 AM	2020
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 PM	
2118	GROMACS	Feature	New	Low	More verbose comments requested in header of gmx distance -oxyz		02/08/2017 05:46 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
2178	GROMACS	Task	New	Normal	Move checks for specific warnings to source repo		05/12/2017 03:57 PM	
3156	GROMACS	Task	New	Normal	move ddUsesGpuDirectCommunication and related conditionals into the workload data structures	Alan Gray	10/17/2019 02:00 PM	2020-beta3
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		10/11/2019 05:53 PM	2020
3005	GROMACS	Task	New	Normal	Move logging in gmx preprocess to MDLogger		06/26/2019 10:01 AM	
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
3143	GROMACS	Task	New	Normal	move the non-force accumulation/accounting tasks out of the GPU wait functions	Szilárd Páll	10/14/2019 05:14 PM	2020
3004	GROMACS	Task	New	Normal	Move trajectory analysis logging to MDLogger		06/26/2019 09:59 AM	
1745	GROMACS	Task	New	Normal	Moving to C++11 after Gromacs-5.1		06/01/2016 03:01 PM	
2084	GROMACS	Task	New	Low	MPI and stderr/log output		11/28/2016 06:37 PM	
2371	GROMACS	Task	New	Normal	mtop searching needs reconsideration		01/04/2018 11:54 AM	future
2594	GROMACS	Feature	New	Normal	Multi-level GMX API	Prashanth Kanduri	02/22/2019 03:48 PM	future
1448	GROMACS	Bug	New	Normal	multiple successive crashes during REMD can lead to .log files that do not represent the actual replica exchanges to match the .xtc files (complicating demultiplexing)	Mark Abraham	06/23/2016 03:15 PM	
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
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
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	
3097	GROMACS	Bug	New	Normal	nbnxm grid issue with regressiontest complex/nbnxn_rzero with gpubufferops path		09/24/2019 03:26 PM	2020-beta2
1666	GROMACS	Feature	New	Normal	new approach for Verlet-scheme kernel generation	Erik Lindahl	10/08/2018 07:04 PM	future
1785	GROMACS	Task	New	Low	no pV term written to energy file when pressure coupling is anisotropic		07/26/2015 01:47 PM	future
2255	GROMACS	Bug	New	Normal	nstlist override stopped affecting the input parameter listing		12/17/2017 08:05 AM	
1476	GROMACS	Bug	New	Low	Odd behavior with verlet-buffer-drift		05/25/2016 01:45 AM	future
1530	GROMACS	Task	New	Low	Offer binary downloads		06/29/2014 02:58 PM	
1437	GROMACS	Feature	New	Normal	Online help formatting improvements		06/04/2015 09:20 PM	future
2854	GROMACS	Bug	New	Normal	OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1	Paul Bauer	02/04/2019 11:17 AM	
2522	GROMACS	Task	New	Normal	OpenCL context duplication		10/30/2018 12:07 PM	2020
1973	GROMACS	Task	New	Normal	OpenCL implementation wish list		05/27/2016 03:42 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2498	GROMACS	Task	New	Normal	OpenCL memory pinning/mapping		10/30/2018 12:07 PM	2020
3125	GROMACS	Bug	New	Normal	OpenCL on Volta and Turing broken		10/13/2019 11:46 PM	2020-beta2
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 AM	
3045	GROMACS	Feature	New	Low	Option to remove v-sites in trjconv?		07/19/2019 04:42 PM	
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	02/12/2019 03:22 PM	2020
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
2232	GROMACS	Bug	New	Normal	pdb2gmx can't form special bonds with terminal patched atoms		12/03/2017 01:35 PM	
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/17/2018 01:27 PM	2020
731	GROMACS	Feature	New	Normal	pdb2gmx should warn about missing residues when bonds are too long		06/22/2014 10:55 AM	
1235	GROMACS	Bug	New	Normal	peptide dihedral angle definitions violate IUPAC	David van der Spoel	06/19/2015 12:24 AM	future
2965	GROMACS	Task	New	Normal	Performance of GPU direct communications		05/31/2019 03:12 PM	2020
2463	GROMACS	Task	New	Low	PME GPU decomposition		03/26/2018 10:42 AM	
2528	GROMACS	Task	New	Normal	PME GPU tuning		12/31/2018 11:18 AM	future
2402	GROMACS	Task	New	Normal	PME kernels general performance improvements		03/26/2018 10:41 AM	future
2514	GROMACS	Task	New	Normal	PME OpenCL reductions with intrinsics		05/31/2018 12:27 AM	future
2788	GROMACS	Bug	New	Normal	PME will not run on AMD GPU with NVidia GPU present		01/03/2019 02:24 PM	
3077	GROMACS	Task	New	Normal	PME/PP GPU Comms unique pointer deletion causes seg fault when CUDA calls exist in destructor		09/20/2019 01:04 PM	
2891	GROMACS	Feature	New	High	PME/PP GPU communications		10/17/2019 02:57 PM	
665	GROMACS	Task	New	Normal	Port existing trajectory analysis tools to use the new framework		07/14/2014 11:29 AM	future
2442	GROMACS	Task	New	Normal	Port gmx saxs and gmx sans to c++	Joe Jordan	06/28/2018 10:06 PM	future
2974	GROMACS	Bug	New	Normal	position-restraints regressiontest fails on intel GPU		10/01/2019 11:12 AM	2019.5
3114	GROMACS	Task	New	Low	Possible improvements to update-constraints	Artem Zhmurov	10/07/2019 11:38 AM	
2020	GROMACS	Bug	New	Normal	Possible issue with md-vv integrator	Mark Abraham	03/11/2017 08:30 AM	
1500	GROMACS	Feature	New	Normal	Post-5.0 feature clean-up plan	Mark Abraham	08/26/2019 03:47 PM	
2186	GROMACS	Feature	New	Low	Potential change for logical improvements: move control of constraints purely to the .mdp	Michael Shirts	11/27/2018 11:27 AM	future
2137	GROMACS	Feature	New	Normal	Preliminary refactoring of constraints and update machinery.	Michael Shirts	03/11/2017 08:32 AM	future

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2977	GROMACS	Feature	New	Normal	print DD load balancing improvement		06/13/2019 10:56 AM	
1635	GROMACS	Feature	New	Normal	Proper Unicode support		06/18/2015 08:34 PM	
1137	GROMACS	Feature	New	Normal	Proposal for integrator framework (do_md) in future GROMACS	Michael Shirts	02/21/2017 12:48 AM	future
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	09/19/2018 03:06 PM	2020
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
2018	GROMACS	Feature	New	Normal	Pulling along a line between given points		07/27/2016 09:59 AM	
2985	GROMACS	Feature	New	Normal	Python package documentation		06/19/2019 12:24 PM	2020
1786	GROMACS	Task	New	Normal	Python style standards in developer docs	Peter Kasson	07/30/2015 05:45 PM	
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 PM	
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	08/12/2019 11:41 AM	2020
2003	GROMACS	Task	New	Normal	reconsider various simd flags		07/07/2016 11:23 PM	
2518	GROMACS	Task	New	Normal	redesign task-assignment code for OpenCL		12/28/2018 12:38 PM	2020
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	
2622	GROMACS	Feature	New	Low	Reduce severity of Berendsen warning		08/23/2018 11:16 PM	future
1509	GROMACS	Task	New	Low	Reduce the distance dependence of shifted potentials for free energies if possible	Michael Shirts	07/11/2016 08:10 PM	
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
3040	GROMACS	Task	New	Normal	Refactor Restraint module		07/18/2019 03:59 PM	
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	03/29/2019 05:20 PM	2020
2396	GROMACS	Task	New	Normal	Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation	Paul Bauer	10/08/2018 07:29 PM	2020
2241	GROMACS	Bug	New	Low	refdata can segfault when reading		09/07/2017 11:57 AM	
3088	GROMACS	Bug	New	Normal	Reference to theory needed for cylindrical pull geometry		09/13/2019 11:26 AM	
2053	GROMACS	Task	New	Normal	refine notation in GPU code		09/04/2019 01:47 PM	2020
3116	GROMACS	Bug	New	Normal	regressiontests/freeenergy core dumps on ppc64le	Paul Bauer	10/04/2019 10:52 PM	
909	GROMACS	Task	New	Normal	Reimplement displacement calculation module		07/14/2014 11:30 AM	future
2169	GROMACS	Task	New	Normal	remove 'continuation' mdp option		10/12/2018 10:36 PM	2020
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
2608	GROMACS	Task	New	Normal	Remove code duplication between OpenCL and CUDA		09/24/2018 12:47 PM	
1852	GROMACS	Task	New	Normal	Remove group scheme		09/27/2019 03:13 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2670	GROMACS	Task	New	Low	remove old/backward compatibility OpenCL support from releng		10/04/2018 06:06 PM	
1456	GROMACS	Task	New	Low	remove the use of nbat->alloc/free pointers	Szilárd Páll	06/20/2015 11:53 PM	
3041	GROMACS	Task	New	Normal	Remove workaround for gcc bug 58265		07/23/2019 12:27 PM	
1971	GROMACS	Task	New	Normal	Removing buggy features vs. keeping workflows		01/19/2018 01:36 PM	future
2056	GROMACS	Feature	New	Low	rename "gmx select"		10/03/2016 08:24 PM	
2527	GROMACS	Task	New	Normal	Rename GpuEventSynchronizer to something more fitting (after mergin PME OpenCL)		10/30/2018 04:06 AM	future
2943	GROMACS	Task	New	Normal	Rename Integrator	Pascal Merz	05/23/2019 08:04 PM	2020
2908	GROMACS	Task	New	Normal	Renaming things in nbnxm	Berk Hess	03/28/2019 10:10 AM	
1876	GROMACS	Task	New	Normal	Reorganize vector input passed to core MD routines		06/01/2016 01:59 PM	future
2495	GROMACS	Task	New	Normal	replace -noconfout with mdp option	Mark Abraham	10/12/2018 10:34 PM	2020
2644	GROMACS	Task	New	Normal	Replace compute_globals	Mark Abraham	09/24/2018 05:51 PM	future
2671	GROMACS	Task	New	Normal	replace constants like M_PI		10/05/2018 08:58 AM	2020
1842	GROMACS	Feature	New	Normal	Replace XML with JSON		01/18/2018 05:12 PM	
1974	GROMACS	Feature	New	Normal	Report atom numbers and types in the error message about missed parameters		05/30/2016 09:24 AM	
2220	GROMACS	Feature	New	Normal	report relevant env var behaviour to console		07/31/2017 09:40 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	
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
1729	GROMACS	Task	New	Normal	Resolve whether and how to resolve "state" variables stored in .tpr		05/13/2015 10:48 AM	future
2564	GROMACS	Bug	New	Normal	Result Summary Different For Jobs With Different Numbers of Nodes		07/05/2018 02:39 PM	
2595	GROMACS	Task	New	Normal	Reusable Utilities for Schedules	Prashanth Kanduri	02/22/2019 03:48 PM	future
2650	GROMACS	Task	New	Normal	revise OpenCL stack recommendations		12/31/2018 11:19 AM	future
3093	GROMACS	Task	New	High	rework GPU direct halo-exchange related force reduction complexities		10/11/2019 05:53 PM	2020
2660	GROMACS	Task	New	Low	rework OpenCL nbnxn kernel constants	Szilárd Páll	10/30/2018 12:10 PM	2020
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irrgang	10/15/2019 06:23 PM	2021-infrastructure-stable
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	05/08/2019 05:50 PM	2020
2897	GROMACS	Bug	New	Normal	rotation/flex2 can still fail on cpu-only run on OpenCL build		04/04/2019 06:24 PM	
3030	GROMACS	Feature	New	Normal	RST style guidelines		07/09/2019 03:38 PM	

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2956	GROMACS	Feature	New	Normal	SAXS resolution		05/17/2019 09:58 AM	
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
2658	GROMACS	Task	New	Normal	Secondary structure assignment via DSSP as native gromacs code	Christian Blau	10/09/2018 04:51 PM	future
2645	GROMACS	Bug	New	Normal	Security		09/28/2018 01:16 PM	
2981	GROMACS	Bug	New	Normal	segfault in opencl build		06/18/2019 03:30 AM	
1770	GROMACS	Bug	New	Normal	segmentation fault with free energy changes and multiple GPU's		07/14/2015 03:24 AM	
3076	GROMACS	Task	New	Normal	Selectively activate MdModules during simulation instead of instantiating all of them	Christian Blau	09/05/2019 11:36 AM	2021-infrastructure-stable
2710	GROMACS	Feature	New	Normal	Separate dvdI for each molecule (of couple-moltype) when running FEP		10/26/2018 10:24 AM	2020
3157	GROMACS	Task	New	Normal	separate PME x receive sync	Alan Gray	10/17/2019 02:44 PM	
3047	GROMACS	Task	New	Normal	Set required versions for GROMACS 2021		08/24/2019 05:25 PM	2021-infrastructure-stable
2846	GROMACS	Feature	New	Low	Set rpath in FindLibStdCpp.cmake		02/02/2019 08:09 AM	
2693	GROMACS	Bug	New	Normal	Several memory leaks in mdrun		12/18/2018 04:22 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
3124	GROMACS	Bug	New	Normal	significant performance loss due to DLB auto-off when PP/PME load >1		10/09/2019 04:33 PM	
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobbonded cluster and others		12/12/2018 05:52 PM	2020
2948	GROMACS	Bug	New	Normal	SIMD support detected as none on AMD R5 2500U		05/21/2019 12:58 PM	
2069	GROMACS	Task	New	Low	Simple thread-parallelism inside routines		11/09/2016 06:06 PM	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2382	GROMACS	Task	New	Normal	Simplify Doxygen guidelines		01/13/2018 12:40 AM	
2537	GROMACS	Task	New	Normal	Simplify PME solve reduction	Aleksei Lupinov	10/30/2018 12:08 PM	2020
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/08/2018 08:06 PM	2020
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	
2207	GROMACS	Feature	New	Normal	solvent excluded volume of large molecule with periodic boundary condition		06/16/2017 10:37 AM	
2978	GROMACS	Bug	New	Normal	Some suggestions about the gmx current tool		06/13/2019 12:41 PM	
2992	GROMACS	Task	New	Normal	Split hw_opt in const user options and dynamic settings		09/24/2019 03:23 PM	2020
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	

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3126	GROMACS	Feature	New	Normal	State propagator GPU data manager		10/09/2019 02:42 PM	
1937	GROMACS	Task	New	Low	stop supporting changing CUDA host compiler	Mark Abraham	10/15/2018 05:19 PM	future
2524	GROMACS	Task	New	Normal	struct alignment/packing for OpenCL host & device code		10/30/2018 12:06 PM	2020
2667	GROMACS	Feature	New	Normal	Suggested steps for calculating entropy in solution and binding	David van der Spoel	10/30/2018 02:06 PM	2020
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	10/15/2019 07:23 AM	
2516	GROMACS	Task	New	Low	Support PME OpenCL execution width < 16	Aleksei lupinov	06/05/2019 05:32 PM	
1142	GROMACS	Feature	New	Low	Synchronizing the differences between point estimation and histogram estimation for free energies	Michael Shirts	02/20/2014 08:27 PM	future
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
2980	GROMACS	Bug	New	Normal	taskassignment fails with unit tests when GPUs and custom number of ranks is used		06/17/2019 05:28 PM	
2699	GROMACS	Task	New	Normal	Test POWER9		04/05/2019 04:50 PM	2020
2840	GROMACS	Feature	New	Normal	Test that functionality does not compile that is not supposed to.		01/25/2019 02:35 PM	future
2425	GROMACS	Task	New	Normal	testing multisim with multiple ranks per simulation	Mark Abraham	11/29/2018 11:20 AM	2020
2092	GROMACS	Task	New	Normal	Tests running on GPU, and hardware assignment		12/19/2017 05:27 PM	future
2852	GROMACS	Bug	New	Low	the in-tree regressiontest download can get out of sync with code		01/30/2019 03:58 PM	
2065	GROMACS	Bug	New	Normal	thread-MPI internal errors		11/08/2018 03:43 PM	
1028	GROMACS	Feature	New	Normal	Tool to calculate fraction of native contacts during simulation		11/01/2012 10:27 PM	
2598	GROMACS	Bug	New	Normal	Tools using read_next_x cannot read TNG files with sanitizers		10/15/2018 01:16 PM	future
3073	GROMACS	Bug	New	Normal	Total potential energy goes crazy, but I don't know why this happens.		09/04/2019 07:25 PM	
1936	GROMACS	Task	New	Normal	treat default-able mdp fields as strings		04/02/2016 10:32 PM	future
2520	GROMACS	Task	New	Normal	Treat OpenCL kernel width more diligently		05/24/2018 06:21 PM	
1167	GROMACS	Feature	New	Low	trjconv -center would be more intuitive if it centered the center of mass, not the midpoint between minimum and maximum values	David van der Spoel	06/23/2014 04:13 AM	future
2052	GROMACS	Bug	New	Low	trjconv does not recognize periodic molecules	David van der Spoel	01/12/2018 11:05 AM	
2115	GROMACS	Task	New	Normal	trjconv does too many things, and combinations of them work poorly		10/02/2018 09:04 AM	
2034	GROMACS	Feature	New	Normal	Unit tests for bonded forces	David van der Spoel	06/29/2019 10:22 AM	future
2481	GROMACS	Task	New	Low	Update gmx report-methods to write more method information		09/20/2018 07:43 AM	2020

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2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	03/11/2019 02:15 PM	2020
2723	GROMACS	Task	New	Normal	Update mdrun-performance.rst to clearly express the nature of task	Joe Jordan	09/24/2019 03:21 PM	2020
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	04/02/2019 12:39 PM	2020

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