

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3205	GROMACS	Task	New	High	address Debian experimental issues		11/18/2019 11:17 AM	2020-beta3
3195	GROMACS	Task	New	High	assess nightly master failures		11/01/2019 09:21 PM	2020-beta3
3142	GROMACS	Feature	In Progress	High	centralize and clarify GPU force buffer clearing		11/01/2019 04:28 PM	2020-beta3
2107	GROMACS	Task	Accepted	High	Change to clang-format		08/02/2019 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	
2888	GROMACS	Feature	New	High	CUDA Update and Constraints module	Artem Zhmurov	10/21/2019 03:59 PM	2020
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	
3159	GROMACS	Task	In Progress	High	eliminate regression due to moving gmx_pme_send_coordinates()	Alan Gray	11/01/2019 11:26 AM	2020-beta3
2229	GROMACS	Feature	New	High	Full Object Oriented Modularization of GROMACS MDRUN Codebase	Mark Abraham	08/22/2018 05:03 PM	future
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2915	GROMACS	Feature	New	High	GPU direct communications		10/24/2019 10:59 AM	
3029	GROMACS	Feature	In Progress	High	GPU force buffer ops + reduction		11/01/2019 04:28 PM	2020-beta3
2890	GROMACS	Feature	New	High	GPU Halo Exchange		10/17/2019 02:00 PM	2020
2816	GROMACS	Feature	New	High	GPU offload / optimization for update&constraints, buffer ops and multi-gpu communication	Alan Gray	11/01/2019 06:56 PM	2020
2817	GROMACS	Feature	In Progress	High	GPU X/F buffer ops		11/01/2019 04:28 PM	2020-beta3
3163	GROMACS	Bug	New	High	gpuupdate / task assignment stabilization	Artem Zhmurov	11/14/2019 06:01 PM	2020-beta3
3160	GROMACS	Feature	In Progress	High	implement direct comm for different src/target memory spaces	Alan Gray	11/11/2019 04:43 PM	2020-beta3
3189	GROMACS	Task	New	High	implement heuristics for switching between different spread/gather kernel layouts	Jonathan Vincent	11/16/2019 08:50 PM	2020-beta3
3208	GROMACS	Task	New	High	improve PP-PME tuning		11/18/2019 09:39 PM	2020
2519	GROMACS	Task	New	High	Improve/remove PME OpenCL kernel barriers		02/15/2019 06:34 PM	
2792	GROMACS	Task	New	High	Improvement of PME gather and spread CUDA kernels		10/30/2019 01:29 PM	
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
2188	TNG trajectory library	Feature	Resolved	High	Masses missing from TNG specification	Magnus Lundborg	06/13/2017 05:08 PM	
3164	GROMACS	Bug	In Progress	High	mdrun-mpi-test with separate PME ranks and PP-PME CPU comm crashes	Alan Gray	11/14/2019 12:41 PM	2020-beta3
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		10/11/2019 05:53 PM	2020
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	10/03/2019 09:41 PM	2020

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2453	GROMACS	Task	Resolved	High	PME OpenCL porting effort	Aleksei lupinov	06/05/2019 05:32 PM	2020
2891	GROMACS	Feature	New	High	PME/PP GPU communications		11/01/2019 06:56 PM	
2935	Support Platforms	Bug	New	High	redmine issue updates about gerrit uploads stopped working		06/11/2019 01:42 PM	current
3093	GROMACS	Task	In Progress	High	rework GPU direct halo-exchange related force reduction complexities		11/01/2019 08:58 PM	2020-beta3
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	
2099	Support Platforms	Feature	New	High	sharing accounts/credentials		12/06/2017 08:11 PM	
3120	GROMACS	Bug	Resolved	High	Uninitialized energy and virial contributions with PME on GPU on PME-only rank		10/09/2019 11:15 AM	2019.5
3071	GROMACS	Bug	Accepted	Normal	complex.nbnxn-ljpmc-LB-geometric failing with OpenCL timing debug mode assertions	Szilárd Páll	09/02/2019 10:19 PM	2020
1964	GROMACS	Feature	Accepted	Normal	"pull=no" should not produce warnings about "unknown" pull keywords		05/20/2016 02:37 PM	
3206	GROMACS	Bug	New	Normal	2 not-critical bugs in analyse tool		11/15/2019 03:53 PM	2019.5
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
2218	GROMACS	Feature	Feedback wanted	Normal	A tiny feature: damping for umbrella pull		08/16/2017 07:20 PM	
2068	GROMACS	Feature	New	Normal	Access to low level classes		03/02/2019 01:37 AM	future
3207	GROMACS	Task	New	Normal	Ad cycle counting to StatePropagatorDataGpu		11/18/2019 06:04 PM	
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	
687	Support Platforms	Feature	New	Normal	Add content on the front page		09/02/2019 01:08 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
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

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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	
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 PM	
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmcif) support		10/05/2018 07:14 PM	
2957	GROMACS	Feature	New	Normal	add support for the Hygon Dhyana architecture		05/21/2019 01:00 PM	2020
1192	GROMACS	Feature	Accepted	Normal	Add support for Verlet scheme with Buckingham	Berk Hess	07/11/2016 08:19 PM	
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
920	GROMACS	Task	In Progress	Normal	Add test framework for trajectory analysis modules	Teemu Murtola	07/11/2016 08:27 PM	
2730	GROMACS	Task	New	Normal	Add tests for gmx_genion	Joe Jordan	11/02/2018 06:42 PM	2020
2686	GROMACS	Task	New	Normal	add tests for gpu bonded interactions		11/29/2018 10:44 AM	2020
907	GROMACS	Feature	Accepted	Normal	Add tests for verifying installed headers		03/11/2014 09:15 PM	future
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
3162	GROMACS	Feature	New	Normal	Add virtual site support to GPU version of update-constraints.		10/21/2019 03:59 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	
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irrgang	10/15/2019 03:56 PM	2020
2623	GROMACS	Task	Resolved	Normal	Allow extensible MDModules and forceProviders.		10/15/2018 03:44 PM	
2735	GROMACS	Task	New	Normal	Allow gmx_genrest 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	10/23/2019 09:16 AM	
2990	GROMACS	Bug	New	Normal	ARM neon SIMD4 error		11/01/2019 03:24 PM	2020-beta3

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2850	GROMACS	Task	In Progress	Normal	assess Raptor Talos for testing	Szilárd Páll	02/12/2019 01:14 PM	
2987	GROMACS	Bug	New	Normal	assess the bonded GPU task assignment default		10/21/2019 04:15 PM	2020
1648	GROMACS	Bug	Feedback wanted	Normal	Atoms with zero LJ parameters but partial charges appear to cause crashes in free energy calculations when perturbed in the presence of other charges	Michael Shirts	06/25/2015 06:07 AM	
2482	GROMACS	Bug	Feedback wanted	Normal	Atoms/molecules in freezegrps move and system crashes		05/18/2018 07:13 PM	
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
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	
1010	GROMACS	Task	In Progress	Normal	Better support for multiple AnalysisData datasets	Teemu Murtola	07/11/2016 08:23 PM	
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2675	GROMACS	Task	In Progress	Normal	bonded CUDA offload task		10/29/2019 03:11 PM	2020
2818	GROMACS	Task	In Progress	Normal	bonded GPU kernel fusion	Magnus Lundborg	07/03/2019 09:01 PM	
1634	GROMACS	Feature	New	Normal	Boxed Molecular Dynamics		11/04/2014 04:40 PM	
1367	TNG trajectory library	Feature	In Progress	Normal	Break tng_io.c into smaller files	Magnus Lundborg	10/25/2013 10:49 AM	version 1
2395	GROMACS	Task	In Progress	Normal	break up commrec	Mark Abraham	09/19/2018 03:13 PM	2020
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	
2912	GROMACS	Task	Resolved	Normal	C++ extension module for Python bindings	Eric Irrgang	07/05/2019 09:00 AM	
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	

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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, MTTK and md-vv	Michael Shirts	06/18/2015 08:53 PM	future
2859	GROMACS	Task	Fix uploaded	Normal	Change ArrayRef iterator type from pointer to std::iterator		02/08/2019 11:00 PM	
2770	GROMACS	Task	New	Normal	change branch maintenance policy		11/29/2018 02:51 PM	2020
652	GROMACS	Task	Blocked, need info	Normal	Change selection method implementation to use C++		04/23/2017 08:05 PM	future
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 parallelizaton codepaths		10/04/2019 12:17 PM	2020
3179	GROMACS	Feature	New	Normal	Clarify access to parallel data outputs	Eric Irrgang	10/26/2019 12:23 PM	
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	
1140	GROMACS	Task	New	Normal	Class design for passing options and data		07/11/2016 08:19 PM	
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		08/24/2019 05:23 PM	2021-infrastructure-stable
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
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	
3166	GROMACS	Bug	New	Normal	Compilation failing on Ubuntu 19.04 with Cuda 10.1		10/19/2019 09:13 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	
2958	GROMACS	Bug	New	Normal	Compiling master (to become 2020) using CUDA 9.0		11/01/2019 03:24 PM	2020-beta3
3021	GROMACS	Feature	Feedback wanted	Normal	Completion of docs for GPU developments		11/01/2019 06:29 PM	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	
3194	GROMACS	Task	New	Normal	consider passing GPU dependency list to both dependency producers and consumers		11/01/2019 07:10 PM	

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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
3181	GROMACS	Task	New	Normal	consolidate task assignment and workload data initialization		10/28/2019 02:53 PM	
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	
3201	GROMACS	Task	In Progress	Normal	Convert mdp parameters to key value tree		11/06/2019 06:06 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-tpr 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	
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 gmx_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	
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	
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	
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		11/01/2019 03:23 PM	2020-beta3
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

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921	GROMACS	Feature	Blocked, need info	Normal	Default index groups and selections		07/11/2016 08:27 PM	
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
2168	GROMACS	Task	Feedback wanted	Normal	Design for multiple comparisons against same test reference data		05/08/2017 02:45 PM	future
3101	GROMACS	Bug	Blocked, need info	Normal	detect compilation failed		09/24/2019 05:26 PM	
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	
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	
2862	GROMACS	Bug	In Progress	Normal	Division by zero in restrained dihedrals		04/01/2019 11:53 AM	2020
2304	GROMACS	Task	New	Normal	Document and propose tracking mdrun heuristics		10/03/2018 09:39 PM	future
1731	Support Platforms	Bug	In Progress	Normal	document jenkins configuration and set up means to track changes		05/31/2017 06:13 PM	
1967	Support Platforms	Bug	Resolved	Normal	Documentation pages generated by Jenkins do not render properly		08/27/2016 02:04 AM	
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	
1627	GROMACS	Feature	In Progress	Normal	DPD integrator		07/11/2016 08:08 PM	
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	
3183	GROMACS	Task	Accepted	Normal	enable bonded interactions on GPU		10/31/2019 11:49 AM	2020-beta3
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
2696	GROMACS	Task	In Progress	Normal	ensure PME queue is flushed	Szilárd Páll	12/31/2018 11:21 AM	future
3055	GROMACS	Bug	Feedback wanted	Normal	Error in gmx xpm2ps		08/22/2019 03:27 PM	

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3058	GROMACS	Bug	Feedback wanted	Normal	Error when using a large PME grid on a GPU		09/04/2019 07:26 PM	
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
3196	GROMACS	Bug	New	Normal	ExponentialMovingAverage.DeterminesCorrectlyIfIncreasing failing		11/01/2019 11:28 PM	
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	
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	
3178	GROMACS	Bug	Accepted	Normal	Fatal Error when launching mdrun on host with busy/unavailable GPU(s)	Szilárd Páll	10/28/2019 10:38 PM	2019.5
987	Support Platforms	Feature	New	Normal	Feature wishlist should be moved to Redmine		08/03/2012 12:22 PM	
1200	TNG trajectory library	Feature	New	Normal	Field for the PDB format 'segment identifier'	Magnus Lundborg	04/24/2013 09:32 AM	version 2
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
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
1198	TNG trajectory library	Feature	In Progress	Normal	Full documentation for the high-level API	Magnus Lundborg	06/25/2013 10:05 PM	version 2
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	
2149	Support Platforms	Bug	New	Normal	gerrit server excessive CPU usage		04/05/2017 07:25 PM	
1551	Support Platforms	Bug	Feedback wanted	Normal	git index.lock issue		05/31/2017 05:37 PM	
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
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	
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	
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	
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	
2166	GROMACS	Task	Accepted	Normal	gmx trjconv functionality should check for mismatch between the tpr and the trajectory		05/05/2017 04:32 PM	
3150	GROMACS	Bug	New	Normal	gmxapi data type annotations are confusing and inadequate	Eric Irrgang	10/22/2019 03:08 PM	2021-infrastructure-stable
2698	GROMACS	Task	New	Normal	gmxapi documentation integration		03/02/2019 01:31 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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 Irrgang	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 Irrgang	10/15/2019 03:57 PM	2020
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	10/15/2019 03:56 PM	
2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		10/29/2019 05:38 PM	2020-beta3
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
2895	GROMACS	Task	Resolved	Normal	gmxapi Output proxy establishes execution dependency.	Eric Irrgang	03/29/2019 05:18 PM	2020
3134	GROMACS	Feature	Feedback wanted	Normal	gmxapi Python exception names may need improvement	Eric Irrgang	10/13/2019 01:50 PM	
3132	GROMACS	Task	New	Normal	gmxapi testing support tools		10/31/2019 03:35 PM	
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 PM	
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irrgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irrgang	10/22/2019 03:09 PM	2020-beta3
2628	GROMACS	Bug	Fix uploaded	Normal	GMXRC removes trailing colon from existing MANPATH		08/28/2018 03:13 PM	
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	
2238	GROMACS	Task	In Progress	Normal	GPU emulation mode support for rolling pruning missing	Berk Hess	12/21/2017 03:21 PM	
2254	GROMACS	Feature	New	Normal	GPU extensions for Google Tests		09/19/2017 05:01 PM	
2464	GROMACS	Task	New	Normal	GPU performance goals overview		03/26/2018 10:42 AM	
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		10/31/2019 03:35 PM	2020-beta3
3167	GROMACS	Task	New	Normal	GPU update path user documentation		10/21/2019 04:09 PM	2020-beta3
3168	GROMACS	Feature	New	Normal	GPU update release notes		11/14/2019 06:03 PM	2020-rc1
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	
2390	GROMACS	Bug	Feedback wanted	Normal	GROMACS build system should check for valid nvcc flags before use		01/30/2019 06:16 PM	2020
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

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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
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 PM	
1618	GROMACS	Bug	In Progress	Normal	g_protonate segfaults unconditionally	Erik Lindahl	08/17/2015 02:10 PM	
895	GROMACS	Feature	In Progress	Normal	g_rmsf previous frame as reference		04/29/2013 07:39 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	
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
3173	GROMACS	Bug	Resolved	Normal	Illegal memory access in free-energy calculations	Berk Hess	10/23/2019 01:30 PM	2019.5
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
2521	GROMACS	Task	New	Normal	Implement alternating PME/NB wait for OpenCL		10/15/2018 12:39 PM	
1815	Support Platforms	Task	In Progress	Normal	implement and execute plan for new releng machinery		10/15/2016 05:37 PM	
3092	GROMACS	Task	New	Normal	implement better receiver ready / notify in halo exchange		09/18/2019 02:47 AM	2020
2492	GROMACS	Task	New	Normal	implement force calculation via ForceProviders containing collections of IForceProvider	Mark Abraham	09/19/2018 03:13 PM	future
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 PM	
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	11/01/2019 11:05 AM	future
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		10/29/2019 09:03 PM	
868	GROMACS	Feature	In Progress	Normal	Implement parallelization support to analysis framework	Kevin Boyd	02/07/2019 02:08 AM	2020
1464	GROMACS	Feature	New	Normal	implement PP-PME re-balancing	Szilárd Páll	10/16/2015 08:34 AM	future
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2175	GROMACS	Task	New	Normal	improve clang static analyzer docs further		01/04/2018 04:13 PM	future
1083	GROMACS	Feature	In Progress	Normal	Improve collective error/warning/note handling in mdrun		07/11/2016 08:21 PM	
2009	GROMACS	Task	New	Normal	improve command-line reporting of useful things		07/26/2016 12:54 PM	
2674	GROMACS	Task	Accepted	Normal	Improve domain decomposition for bilayer systems		12/07/2018 04:03 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	
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2018 06:40 PM	2020
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
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
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	
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		02/13/2019 08:17 PM	2020
2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	12/03/2018 01:15 PM	2020
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	
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	
2585	GROMACS	Feature	Resolved	Normal	Infrastructure supporting external API		03/31/2019 04:47 PM	
3028	GROMACS	Bug	Feedback wanted	Normal	install fail on Centos 6		07/15/2019 12:32 PM	
2828	GROMACS	Bug	Feedback wanted	Normal	Installation issue on Power 9 system with SIMD support		01/18/2019 11:54 AM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2707	GROMACS	Bug	New	Normal	Installed OpenCL files include clh file from gpu_utils directory		10/30/2018 04:02 AM	
2893	GROMACS	Task	Resolved	Normal	Integrate gmxapi Python package	Eric Irrgang	10/23/2019 09:16 AM	2020
3209	GROMACS	Bug	New	Normal	Interactive molecular dynamics with VMD becomes stuttering after reconnecting		11/19/2019 11:36 AM	
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	10/22/2019 03:09 PM	2020-beta3
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	
3204	GROMACS	Bug	Resolved	Normal	intermolecular interactions on OpenMPI multiple threads (gromacs 2019.4)	Berk Hess	11/19/2019 12:30 PM	2019.5
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	Szilárd Páll	11/18/2019 09:35 PM	2020
2611	GROMACS	Bug	New	Normal	issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX		08/14/2018 07:03 PM	
1309	Support Platforms	Task	New	Normal	Jenkins verification improvements		06/01/2017 02:34 PM	
1214	GROMACS	Task	New	Normal	Keep track of important changes for Changelog	Mark Abraham	06/26/2013 11:24 AM	
1053	GROMACS	Feature	In Progress	Normal	L-BFGS doesn't use constraints or call do_em_step	Berk Hess	01/18/2013 11:00 AM	future
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 AM	
2930	GROMACS	Feature	New	Normal	Limited range for reference group detection in cylinder pulling		04/26/2019 05:17 PM	
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	
629	Support Platforms	Task	In Progress	Normal	List of users needs cleanup	Rossen Apostolov	02/21/2018 02:07 PM	
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	
2947	GROMACS	Task	Accepted	Normal	make an end to end test for membed		09/24/2019 03:22 PM	future
869	GROMACS	Task	In Progress	Normal	Make analysis data histogramming and multipoint data easier to use in parallel	Teemu Murtola	07/11/2016 08:28 PM	
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 into 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
2822	GROMACS	Task	Accepted	Normal	Make nbnxn a module	Berk Hess	01/03/2019 03:07 PM	2020

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2475	GROMACS	Task	New	Normal	make OpenCL 1st class-citizen in the build system		10/30/2018 12:01 PM	2020
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	
2620	GROMACS	Feature	In Progress	Normal	MD signaling API		03/02/2019 01:24 AM	
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future
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	
3161	GROMACS	Bug	New	Normal	mdrun-test hangs with -ntmpi2		10/17/2019 05:34 PM	2020
2733	GROMACS	Bug	Blocked, need info	Normal	MdrunUtilityMpiUnitTests timeout on i686 and armv7hl with OpenMPI 2.1.5	Paul Bauer	11/08/2018 04:27 PM	
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
3022	GROMACS	Feature	Resolved	Normal	modernized naming for new GPU developments		11/11/2019 01:03 PM	2020
2017	GROMACS	Task	In Progress	Normal	Modularize simulation option storage and reading from mdp files	Christian Blau	04/06/2018 06:07 PM	future
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
1221	GROMACS	Feature	Accepted	Normal	More generic position mapping for selections		06/10/2014 02:58 PM	future
2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 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
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
3005	GROMACS	Task	New	Normal	Move logging in gmx preprocess to MDLogger		06/26/2019 10:01 AM	
3027	GROMACS	Task	In Progress	Normal	Move sample_restraint development from GitHub to Gerrit	Eric Irrgang	11/01/2019 03:23 PM	2020-beta3
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
1328	GROMACS	Feature	Accepted	Normal	Names for selection positions		07/11/2016 08:15 PM	
3097	GROMACS	Bug	New	Normal	nbnxm grid issue with regressiontest complex/nbnxn_rzero with gpubufferops path		11/01/2019 03:22 PM	2020-beta3
1666	GROMACS	Feature	New	Normal	new approach for Verlet-scheme kernel generation	Erik Lindahl	10/08/2018 07:04 PM	future
1442	GROMACS	Bug	Feedback wanted	Normal	Not consistent solvation free energies differencies	Michael Shirts	07/11/2016 08:13 PM	
2255	GROMACS	Bug	New	Normal	nstlist override stopped affecting the input parameter listing		12/17/2017 08:05 AM	
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	
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 borken		11/04/2019 11:37 AM	2020-beta3
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 AM	
2538	GROMACS	Task	New	Normal	organize more of the PME GPU code along task-specific lines	Mark Abraham	05/31/2018 05:41 PM	
1202	TNG trajectory library	Feature	New	Normal	Other hash types		06/25/2013 10:02 PM	version 2
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2147	GROMACS	Bug	Feedback wanted	Normal	Parrinello-Rahman barostat not properly working		06/06/2017 07:53 AM	
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
1843	GROMACS	Bug	In Progress	Normal	pbc=xy with 2 walls floating point exception with the verlet scheme	Berk Hess	10/31/2016 11:35 AM	
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	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
2070	GROMACS	Feature	In Progress	Normal	Physical validation testing	Michael Shirts	10/12/2018 10:36 PM	2020
2702	GROMACS	Bug	Accepted	Normal	PME gather reduction race in OpenCL (and CUDA)		03/28/2019 03:14 PM	
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	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	
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
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	
1880	GROMACS	Bug	Feedback wanted	Normal	PP-PME load balancing issue	Berk Hess	10/03/2018 09:45 PM	future
2137	GROMACS	Feature	New	Normal	Preliminary refactoring of constraints and update machinery.	Michael Shirts	03/11/2017 08:32 AM	future
3182	GROMACS	Bug	New	Normal	pressure coupling buggy with GPU update		10/28/2019 11:34 PM	
2977	GROMACS	Feature	New	Normal	print DD load balancing improvement		06/13/2019 10:56 AM	
1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
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
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	
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	
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		11/08/2019 08:55 PM	2020
2896	GROMACS	Feature	In Progress	Normal	Python packaging		10/09/2019 04:08 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	

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3172	GROMACS	Feature	New	Normal	QM/MM Interface with CP2K	Dmitry Morozov	10/22/2019 12:35 PM	future
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
1781	GROMACS	Task	Accepted	Normal	re-design benchmarking functionality	Mark Abraham	10/08/2018 07:04 PM	2020
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	08/12/2019 11:41 AM	2020
2391	GROMACS	Task	Accepted	Normal	re-enable TPI test	Berk Hess	01/09/2019 05:17 PM	2020
3188	GROMACS	Task	New	Normal	re-enable parallel spline calculation for #threads/atoms > 4		11/03/2019 09:18 PM	2020
2979	GROMACS	Task	Accepted	Normal	Reconsider default 1 OpenMP thread per thread-MPI rank	Berk Hess	11/01/2019 03:24 PM	2020-rc1
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	
2096	Support Platforms	Bug	New	Normal	Redmine internal error with special characters		05/31/2017 08:48 PM	
2452	GROMACS	Task	In Progress	Normal	Reduce data dependencies in mdrun algorithms	Berk Hess	03/14/2018 08:47 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
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
2513	GROMACS	Bug	Feedback wanted	Normal	ref_t and temperature incorrect with coulomb-type = user	Yu Du	05/31/2018 04:05 PM	
3116	GROMACS	Bug	New	Normal	regressiontests/freenenergy core dumps on ppc64le	Paul Bauer	10/04/2019 10:52 PM	
2734	GROMACS	Bug	In Progress	Normal	regressiontests/kernel core dumps on ppc64le	Paul Bauer	06/15/2019 04:12 PM	future
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	
1925	GROMACS	Task	In Progress	Normal	remove concept of unilateral global communication		07/15/2019 06:42 PM	2020
3180	GROMACS	Task	New	Normal	Remove extra D2H and H2D copies of coordinates when the COM motion is compensated.	Artem Zhmurov	11/14/2019 05:48 PM	
1852	GROMACS	Task	New	Normal	Remove group scheme		09/27/2019 03:13 PM	future
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

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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 nbxnm	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	
2233	GROMACS	Bug	Accepted	Normal	replica exchange and -append bugged?		03/05/2018 01:38 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	
2281	GROMACS	Task	In Progress	Normal	Represent data on regularly spaced N-dimensional grids.	Christian Blau	08/06/2019 08:48 AM	2020
2294	GROMACS	Task	New	Normal	Require identical hardware on nodes on parallel runs		11/19/2017 08:54 PM	
1252	TNG trajectory library	Bug	Feedback wanted	Normal	residual ids and atomIDs	Magnus Lundborg	06/12/2013 10:35 AM	version 1
1199	TNG trajectory library	Feature	New	Normal	residue numbering	Magnus Lundborg	04/24/2013 09:33 AM	version 2
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
1732	Support Platforms	Bug	New	Normal	review and extend jenkins tests setups, coverage		05/03/2016 05:30 AM	
2650	GROMACS	Task	New	Normal	revise OpenCL stack recommendations		12/31/2018 11:19 AM	future
2706	GROMACS	Task	Accepted	Normal	Rework classic QM/MM interface		11/05/2018 10:06 AM	2020
1197	TNG trajectory library	Feature	New	Normal	Rework the molecule descriptions		03/18/2013 04:16 PM	version 2

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