

Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3151	GROMACS	Bug	In Progress	Normal	integrator md-vv does not print at nstlog	Pascal Merz	10/17/2019 02:23 AM	2020-beta2
3144	GROMACS	Bug	New	Normal	gmxapi.mdrun does not clearly expose the output trajectory.	Eric Irrgang	10/14/2019 06:55 PM	2020-beta2
3141	GROMACS	Bug	New	Normal	gmxapi File placeholders missing from beta release	Eric Irrgang	10/15/2019 03:57 PM	2020
3136	GROMACS	Bug	New	Normal	gmxapi.operation data flow topology unclear or incomplete	Eric Irrgang	10/14/2019 08:16 PM	2020-beta2
3127	GROMACS	Bug	New	Normal	mdrun-mpi-test -ntmpi 2 runs out of memory with OpenCL on Nvidia		10/09/2019 05:33 PM	
3125	GROMACS	Bug	New	Normal	OpenCL on Volta and Turing broken		10/13/2019 11:46 PM	2020-beta2
3124	GROMACS	Bug	New	Normal	significant performance loss due to DLB auto-off when PP/PME load >1		10/09/2019 04:33 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
3116	GROMACS	Bug	New	Normal	regressiontests/freeenergy core dumps on ppc64le	Paul Bauer	10/04/2019 10:52 PM	
3113	GROMACS	Bug	New	Low	Use of read_tps_conf is deprecated	Paul Bauer	10/01/2019 11:36 AM	2021-infrastructure-stable
3111	GROMACS	Bug	Fix uploaded	Low	sample_restraint testing should not download files	Eric Irrgang	10/16/2019 06:00 PM	2020-beta2
3101	GROMACS	Bug	Blocked, need info	Normal	detect compilation failed		09/24/2019 05:26 PM	
3100	GROMACS	Bug	In Progress	Normal	crash with GPU comm DD		09/27/2019 01:28 PM	2020-beta2
3097	GROMACS	Bug	New	Normal	nbnxm grid issue with regressiontest complex/nbnxn_rzero with gpubufferops path		09/24/2019 03:26 PM	2020-beta2
3088	GROMACS	Bug	New	Normal	Reference to theory needed for cylindrical pull geometry		09/13/2019 11:26 AM	
3086	GROMACS	Bug	New	Normal	gmxapi fails with MPI build of GROMACS 2020		09/25/2019 04:18 PM	
3085	GROMACS	Bug	Fix uploaded	High	gromacs-toolchain.cmake file does not work on OS X		10/06/2019 04:59 PM	2020-beta2
3083	GROMACS	Bug	New	Normal	Listed forces tests failing on ICC19 with AVX2_256 nightly build		09/10/2019 11:56 AM	
3075	GROMACS	Bug	New	Normal	Frozen atoms are moving		09/04/2019 08:00 PM	
3074	GROMACS	Bug	Feedback wanted	Normal	box volume is affected by decoupled molecule when using couple-moltype mdp option	Berk Hess	10/17/2019 10:55 AM	
3073	GROMACS	Bug	New	Normal	Total potential energy goes crazy, but I don't know why this happens.		09/04/2019 07:25 PM	
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
3068	GROMACS	Bug	New	Normal	Misleading warning on rerun		08/26/2019 03:44 PM	
3066	GROMACS	Bug	New	Normal	Gauss transform and density fit classes should operate on real values instead of float	Christian Blau	08/26/2019 11:53 AM	

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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	
3055	GROMACS	Bug	Feedback wanted	Normal	Error in gmx xpm2ps		08/22/2019 03:27 PM	
3054	GROMACS	Bug	New	Normal	Missing dihedral define		08/02/2019 05:47 PM	
3050	GROMACS	Bug	New	Low	Fix tests on Solaris	Vedran Miletic	07/29/2019 12:38 PM	2020
3049	GROMACS	Bug	New	Low	gmx nmeig should plot a real infrared spectrum	David van der Spoel	09/24/2019 03:25 PM	future
3048	GROMACS	Bug	New	Normal	Dihedral parameters for N-terminal in gromos53a6 force field in the aminoacids.n.tdb file with different values in versions 4.6.7 and gromacs 2019/2016/5.1.5		07/29/2019 10:41 AM	
3042	GROMACS	Bug	New	Normal	core dump error in grompp command		10/09/2019 07:30 PM	
3028	GROMACS	Bug	Feedback wanted	Normal	install fail on Centos 6		07/15/2019 12:32 PM	
3024	GROMACS	Bug	New	Normal	Bad logic for Sphinx detection CMake output		07/05/2019 05:44 PM	2020
3017	GROMACS	Bug	New	Normal	ddBalanceRegionHandler triggers need fixing		09/24/2019 03:25 PM	2020-beta2
3000	GROMACS	Bug	New	Normal	CMake "webpage" target does not fail when it should		06/25/2019 02:43 PM	
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
2981	GROMACS	Bug	New	Normal	segfault in opencl build		06/18/2019 03:30 AM	
2980	GROMACS	Bug	New	Normal	taskassignment fails with unit tests when GPUs and custom number of ranks is used		06/17/2019 05:28 PM	
2978	GROMACS	Bug	New	Normal	Some suggestions about the gmx current tool		06/13/2019 12:41 PM	
2974	GROMACS	Bug	New	Normal	position-restraints regressiontest fails on intel GPU		10/01/2019 11:12 AM	2019.5
2958	GROMACS	Bug	New	Normal	Compiling master (to become 2020) using CUDA 9.0		10/14/2019 09:15 PM	2020-beta2
2954	GROMACS	Bug	New	Normal	genion changes residue numbering		05/26/2019 12:08 AM	
2949	GROMACS	Bug	New	Normal	cmake fails when building mdrun only		07/08/2019 10:04 AM	
2948	GROMACS	Bug	New	Normal	SIMD support detected as none on AMD R5 2500U		05/21/2019 12:58 PM	
2927	GROMACS	Bug	Feedback wanted	Low	CMake 3.14.1 fails to properly run gmxDetectCpu.make		10/01/2019 11:13 AM	2019.5
2925	GROMACS	Bug	New	Normal	BasicVector addition operator yields unexpected result when adding scalar	Christian Blau	04/20/2019 05:39 PM	2020
2924	GROMACS	Bug	New	Normal	Failing version check when reading new tpr file with older gromacs version		04/12/2019 10:52 AM	
2907	GROMACS	Bug	New	Normal	Gromacs autocompletion appears to be broken with ZSH		07/16/2019 04:46 AM	
2902	GROMACS	Bug	New	Normal	2019.1 equilibration issue? (Intel 2018u3)		04/30/2019 08:17 AM	

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2897	GROMACS	Bug	New	Normal	rotation/flex2 can still fail on cpu-only run on OpenCL build		04/04/2019 06:24 PM	
2883	GROMACS	Bug	New	Normal	essentialdynamics fail with Intel MPI		03/08/2019 03:10 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	
2873	GROMACS	Bug	New	Normal	Simple way to get last frame from trajectory		02/28/2019 11:14 PM	
2872	GROMACS	Bug	New	Normal	gmx solvate and genion topology update		02/27/2019 10:18 AM	
2870	GROMACS	Bug	New	Normal	GPU detection error message missing from the output		03/05/2019 03:55 PM	
2869	GROMACS	Bug	New	Normal	GPU detection error only issued as a note to the log		03/05/2019 04:09 PM	
2862	GROMACS	Bug	In Progress	Normal	Division by zero in restrained dihedrals		04/01/2019 11:53 AM	2020
2854	GROMACS	Bug	New	Normal	OnlineHelpUnitTests segfaults on s390x with gcc-9.0.1	Paul Bauer	02/04/2019 11:17 AM	
2853	GROMACS	Bug	New	Normal	EwaldUnitTests segfault on armv7hl with gcc-9.0.1	Paul Bauer	02/04/2019 05:34 PM	
2852	GROMACS	Bug	New	Low	the in-tree regressiontest download can get out of sync with code		01/30/2019 03:58 PM	
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	
2832	GROMACS	Bug	New	Low	PaddedVector move operations broken	Mark Abraham	02/12/2019 03:22 PM	2020
2828	GROMACS	Bug	Feedback wanted	Normal	Installation issue on Power 9 system with SIMD support		01/18/2019 11:54 AM	
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
2788	GROMACS	Bug	New	Normal	PME will not run on AMD GPU with NVidia GPU present		01/03/2019 02:24 PM	
2785	GROMACS	Bug	New	Normal	Inconsistent and erroneous behaviour of trjconv when writing a partial TNG		11/30/2018 02:36 PM	
2767	GROMACS	Bug	New	Normal	grompp warns about md + FEP even for fully coupled states		11/19/2018 11:41 AM	2020
2763	GROMACS	Bug	New	Normal	GMXAPI layout / grouping in development docs "modules" page		12/14/2018 12:49 PM	future
2762	GROMACS	Bug	Blocked, need info	Normal	incorrect results with Ubuntu 18.04 / glibc 2.27 (?) and >20 threads		07/01/2019 11:26 PM	
2754	GROMACS	Bug	New	Normal	Simulated Tempering seems to be broken	Michael Shirts	02/05/2019 03:58 PM	
2740	GROMACS	Bug	New	Normal	mdrun reports incorrect error with -bonded gpu without gpu	Mark Abraham	11/07/2018 01:59 PM	
2737	GROMACS	Bug	Accepted	Low	AMD OpenCl failes release build in complex tests	Szilárd Páll	10/14/2019 09:16 PM	2020-beta2
2734	GROMACS	Bug	In Progress	Normal	regressiontests/kernel core dumps on ppc64le	Paul Bauer	06/15/2019 04:12 PM	future
2733	GROMACS	Bug	Blocked, need info	Normal	MdrunUtilityMpiUnitTests timesout on i686 and armv7hl with OpenMPI 2.1.5	Paul Bauer	11/08/2018 04:27 PM	
2728	GROMACS	Bug	New	Normal	Fix NB kernel picking		11/02/2018 03:51 PM	2020
2722	GROMACS	Bug	New	Normal	gmxapi may over-manage RPATH	Mark Abraham	10/16/2019 10:28 AM	2020-beta3

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2707	GROMACS	Bug	New	Normal	Installed OpenCL files include clh file from gpu_utils directory		10/30/2018 04:02 AM	
2702	GROMACS	Bug	Accepted	Normal	PME gather reduction race in OpenCL (and CUDA)		03/28/2019 03:14 PM	
2693	GROMACS	Bug	New	Normal	Several memory leaks in mdrun		12/18/2018 04:22 AM	future
2657	GROMACS	Bug	New	Normal	Biphasic tutorial		09/28/2018 10:02 AM	
2649	GROMACS	Bug	New	Normal	Virial calculation necessary for correct energy calculation on GPU		12/17/2018 02:32 PM	future
2645	GROMACS	Bug	New	Normal	Security		09/28/2018 01:16 PM	
2637	GROMACS	Bug	New	High	gmx solvate tears apart molecules		09/11/2018 07:43 PM	
2628	GROMACS	Bug	Fix uploaded	Normal	GMXRC removes trailing colon from existing MANPATH		08/28/2018 03:13 PM	
2624	GROMACS	Bug	New	Normal	GPU build system not robust enough		09/05/2018 02:00 AM	
2611	GROMACS	Bug	New	Normal	issues with gpu_utils-test with GMX_BUILD_UNITTESTS=OFF and on OSX		08/14/2018 07:03 PM	
2607	GROMACS	Bug	New	Normal	Grompp becomes extremely slow when many pull groups are present		08/11/2018 08:54 AM	
2606	GROMACS	Bug	New	Normal	Free Energy Calculation -- Function type Fourier Dih. Not implemented in ip_pert		08/10/2018 01:48 AM	
2602	GROMACS	Bug	New	Low	build information gets outdated if build tree is reused		08/13/2018 09:04 PM	
2600	GROMACS	Bug	New	High	coul-lambdas turns off all coulombic interactions in system instead of the molecule specified in the couple-moltype		08/07/2018 06:50 PM	
2598	GROMACS	Bug	New	Normal	Tools using read_next_x cannot read TNG files with sanitizers		10/15/2018 01:16 PM	future
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	
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	
2576	GROMACS	Bug	New	Normal	gmx potential -correct outputs the wrong potential		07/25/2018 02:58 PM	
2573	GROMACS	Bug	New	High	Different mdp files describing the same change yield different free energy on the same trajectory		07/19/2018 06:52 PM	
2568	GROMACS	Bug	New	Low	gmx editconf -rotate does not rotate the box		07/10/2018 10:27 AM	future
2567	GROMACS	Bug	New	Normal	make check fails at test 23 SIMD errors		07/10/2018 09:35 AM	
2564	GROMACS	Bug	New	Normal	Result Summary Different For Jobs With Different Numbers of Nodes		07/05/2018 02:39 PM	
2563	GROMACS	Bug	New	Normal	Windows 7 Compilation with GPU support		07/02/2018 09:58 AM	
2555	GROMACS	Bug	New	Low	building GROMACS 2018.2		07/03/2018 11:41 PM	
2553	GROMACS	Bug	Accepted	Normal	Incorrect COM velocity correction with frozen atoms	Berk Hess	12/03/2018 01:15 PM	2020

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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
2526	GROMACS	Bug	New	Normal	Bug of gmx hbond		05/30/2018 03:12 PM	
2513	GROMACS	Bug	Feedback wanted	Normal	ref_t and temperature incorrect with coulomb-type = user	Yu Du	05/31/2018 04:05 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
2482	GROMACS	Bug	Feedback wanted	Normal	Atoms/molecules in freezegrps move and system crashes		05/18/2018 07:13 PM	
2480	GROMACS	Bug	New	Normal	pdb2gmx does not protonate correctly for united-atom Gromos	Mark Abraham	12/17/2018 01:27 PM	2020
2473	GROMACS	Bug	New	Normal	mdrun sometimes stalls due to large coordinates with no constraints		04/04/2018 10:15 PM	
2468	GROMACS	Bug	New	Low	incorrect GPU timing reported with OpenCL and domain decomposition		12/17/2018 01:28 PM	future
2460	GROMACS	Bug	New	Normal	Allow inclusion of user libraries through CMake cache variables		03/28/2018 08:47 PM	
2427	GROMACS	Bug	New	Normal	gmx select gives syntax error for selection involving evaluating simple arithmetic expression		02/27/2018 05:15 PM	
2393	GROMACS	Bug	New	Normal	incorrect error message with omitted command line flag before its argument		01/24/2018 11:24 PM	
2390	GROMACS	Bug	Feedback wanted	Normal	GROMACS build system should check for valid nvcc flags before use		01/30/2019 06:16 PM	2020
2380	GROMACS	Bug	New	Low	cycle counter issues with separate PME rank + GPUs		01/16/2018 10:21 PM	
2373	GROMACS	Bug	New	Low	gmx -nice can't work		01/04/2018 11:17 AM	
2360	GROMACS	Bug	New	Low	error at counter reset with PME-only rank		01/05/2018 12:43 PM	future
2255	GROMACS	Bug	New	Normal	nstlist override stopped affecting the input parameter listing		12/17/2017 08:05 AM	
2252	GROMACS	Bug	New	Low	Memory allocation failures with large page sizes during PME tuning		12/14/2017 04:27 AM	
2241	GROMACS	Bug	New	Low	refdata can segfault when reading		09/07/2017 11:57 AM	
2233	GROMACS	Bug	Accepted	Normal	replica exchange and -append bugged?		03/05/2018 01:38 PM	
2232	GROMACS	Bug	New	Normal	pdb2gmx can't form special bonds with terminal patched atoms		12/03/2017 01:35 PM	
2231	GROMACS	Bug	New	Normal	convert-tpr aborts when saving subset of the system		01/12/2018 03:52 PM	
2217	GROMACS	Bug	New	Low	GPU emulation and separate PME ranks doesn't work properly		12/12/2017 11:50 AM	
2211	GROMACS	Bug	New	Low	gmx writes normal output to stderr		03/05/2018 02:00 PM	future
2208	GROMACS	Bug	New	Normal	cuFFT linking		06/30/2017 01:58 PM	

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2192	GROMACS	Bug	Accepted	Low	grompp should read floats (e.g charge) from data files to double, to avoid accumulating round-off error	Berk Hess	12/03/2018 01:25 PM	2020
2147	GROMACS	Bug	Feedback wanted	Normal	Parrinello-Rahman barostat not properly working		06/06/2017 07:53 AM	
2113	GROMACS	Bug	New	Normal	Google tests and execution order		03/05/2018 02:05 PM	
2094	GROMACS	Bug	New	Normal	Solvation Consistency with MARTINI forcefield water across GROMACS versions with user-specified VDW size		01/20/2017 04:56 PM	
2065	GROMACS	Bug	New	Normal	thread-MPI internal errors		11/08/2018 03:43 PM	
2052	GROMACS	Bug	New	Low	trjconv does not recognize periodic molecules	David van der Spoel	01/12/2018 11:05 AM	
2039	GROMACS	Bug	New	Normal	mdrun -pinstride defaults are too confusing		12/13/2017 04:14 AM	
2020	GROMACS	Bug	New	Normal	Possible issue with md-vv integrator	Mark Abraham	03/11/2017 08:30 AM	
1985	GROMACS	Bug	Fix uploaded	Low	CUDA build system refactoring awaiting review		10/15/2018 05:21 PM	2020
1977	GROMACS	Bug	Feedback wanted	Low	warning: __WORDSIZE not defined		09/21/2018 06:19 PM	2020
1934	GROMACS	Bug	New	Normal	QMMM with ORCA: memory leaks, buffer overflows and much more		07/10/2016 09:26 AM	
1919	GROMACS	Bug	Accepted	Normal	static linking issues cause by hwloc support		10/12/2018 10:49 PM	future
1880	GROMACS	Bug	Feedback wanted	Normal	PP-PME load balancing issue	Berk Hess	10/03/2018 09:45 PM	future
1843	GROMACS	Bug	In Progress	Normal	pbcs=xy with 2 walls floating point exception with the verlet scheme	Berk Hess	10/31/2016 11:35 AM	
1839	GROMACS	Bug	Accepted	Low	pdb2gmx: Failure to rename non-standard hydrogen atom names after generating missing hydrogens in pdb2gmx		07/09/2016 07:27 PM	future
1827	GROMACS	Bug	New	Low	cmake multi-configuration generator support partly broken		12/11/2017 05:20 PM	future
1811	GROMACS	Bug	New	Normal	Extrac build issues		12/13/2017 03:43 AM	
1770	GROMACS	Bug	New	Normal	segmentation fault with free energy changes and multiple GPU's		07/14/2015 03:24 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	
1655	GROMACS	Bug	New	Normal	g_membed and box type		12/09/2014 01:33 PM	
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	
1618	GROMACS	Bug	In Progress	Normal	g_protonate segfaults unconditionally	Erik Lindahl	08/17/2015 02:10 PM	
1583	GROMACS	Bug	New	Normal	gmx msd with mol flag requires excessive memory		12/18/2017 03:34 PM	

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1568	GROMACS	Bug	New	Low	inconsistent/incorrect threading checks and reporting in mdrun		05/25/2016 02:01 AM	
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	
1476	GROMACS	Bug	New	Low	Odd behavior with verlet-buffer-drift		05/25/2016 01:45 AM	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	
1442	GROMACS	Bug	Feedback wanted	Normal	Not consistent solvation free energies differences	Michael Shirts	07/11/2016 08:13 PM	
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 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
1235	GROMACS	Bug	New	Normal	peptide dihedral angle definitions violate IUPAC	David van der Spoel	06/19/2015 12:24 AM	future
1190	GROMACS	Bug	New	Normal	Use of FORCE in setting cached variables	Mark Abraham	06/17/2014 06:09 AM	
1166	GROMACS	Bug	New	Low	g_order is incorrect for unsaturated carbons	David van der Spoel	06/18/2017 04:40 PM	future
2935	Support Platforms	Bug	New	High	redmine issue updates about gerrit uploads stopped working		06/11/2019 01:42 PM	current
2149	Support Platforms	Bug	New	Normal	gerrit server excessive CPU usage		04/05/2017 07:25 PM	
2096	Support Platforms	Bug	New	Normal	Redmine internal error with special characters		05/31/2017 08:48 PM	
1967	Support Platforms	Bug	Resolved	Normal	Documentation pages generated by Jenkins do not render properly		08/27/2016 02:04 AM	
1836	Support Platforms	Bug	New	Normal	Support a way to retrigger part of matrix job		07/22/2017 12:30 AM	
1732	Support Platforms	Bug	New	Normal	review and extend jenkins tests setups, coverage		05/03/2016 05:30 AM	
1731	Support Platforms	Bug	In Progress	Normal	document jenkins configuration and set up means to track changes		05/31/2017 06:13 PM	
1551	Support Platforms	Bug	Feedback wanted	Normal	git index.lock issue		05/31/2017 05:37 PM	
2937	TNG trajectory library	Bug	New	Normal	tng_num_frames_get reports incorrect num frames		04/29/2019 11:30 AM	
2362	TNG trajectory library	Bug	New	Normal	tng_*_of_particle_nr_get() functions return wrong result for structures with multiple molecule types		12/21/2017 11:51 AM	
1536	TNG trajectory library	Bug	New	Normal	TNG uses incorrect format for size_t on 32bit		06/28/2014 03:56 AM	
1252	TNG trajectory library	Bug	Feedback wanted	Normal	residual ids and atomIDs	Magnus Lundborg	06/12/2013 10:35 AM	version 1
1106	Benchmark suite	Feature	New	Normal	publish benchmark numbers		06/19/2014 12:08 PM	

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1105	Benchmark suite	Feature	New	Normal	produce a benchmark suite		09/13/2016 10:31 PM	
3160	GROMACS	Feature	New	Normal	implement direct comm for different src/target memory spaces	Alan Gray	10/17/2019 03:02 PM	2020
3152	GROMACS	Feature	New	Low	Infrastructure and patterns for expressing public interfaces		10/17/2019 10:40 AM	2021-infrastructure-stable
3149	GROMACS	Feature	New	Normal	Python user interface for obtaining simulation artifacts as files.	Eric Irrgang	10/15/2019 06:21 PM	
3148	GROMACS	Feature	New	Normal	Roadmap for gmxapi filesystem interactions.	Eric Irrgang	10/15/2019 06:23 PM	2021-infrastructure-stable
3147	GROMACS	Feature	New	Normal	gmxapi workflow checkpointing	Eric Irrgang	10/15/2019 06:18 PM	2021-infrastructure-stable
3142	GROMACS	Feature	New	High	centralize and clarify GPU force buffer clearing		10/14/2019 04:56 PM	2020-beta2
3140	GROMACS	Feature	New	Normal	Allow explicit input definition for gmxapi.operation function wrapper	Eric Irrgang	10/15/2019 03:56 PM	2020
3138	GROMACS	Feature	New	Normal	Improve ensemble support in Context specification.		10/15/2019 03:56 PM	
3135	GROMACS	Feature	New	Normal	Make GPU traits into opaque types		10/14/2019 10:24 AM	
3134	GROMACS	Feature	Feedback wanted	Normal	gmxapi Python exception names may need improvement	Eric Irrgang	10/13/2019 01:50 PM	
3126	GROMACS	Feature	New	Normal	State propagator GPU data manager		10/09/2019 02:42 PM	
3117	GROMACS	Feature	New	Normal	Coulomb FEP PME on GPU	Magnus Lundborg	10/04/2019 09:16 AM	future
3115	GROMACS	Feature	New	Normal	Device stream manager		10/04/2019 09:00 AM	
3087	GROMACS	Feature	New	Normal	enable GPU peer to peer access		09/12/2019 04:24 PM	2020
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
3052	GROMACS	Feature	New	Normal	GPU virial reduction/calculation		08/01/2019 05:26 PM	
3045	GROMACS	Feature	New	Low	Option to remove v-sites in trjconv?		07/19/2019 04:42 PM	
3038	GROMACS	Feature	New	Normal	Improvements to MD plugin development environment	Eric Irrgang	07/17/2019 02:15 PM	2020
3032	GROMACS	Feature	New	Normal	Clean up dev-manual structure		07/11/2019 11:48 AM	2020
3030	GROMACS	Feature	New	Normal	RST style guidelines		07/09/2019 03:38 PM	
3029	GROMACS	Feature	In Progress	High	GPU force buffer ops + reduction		10/11/2019 11:55 AM	2020-beta2
3022	GROMACS	Feature	New	Normal	modernized naming for new GPU developments		07/04/2019 10:48 AM	2020
3021	GROMACS	Feature	New	Normal	Completion of docs for GPU developments		07/04/2019 10:45 AM	2020
3020	GROMACS	Feature	New	Low	modernize DeviceBuffer and GPU memory management		08/13/2019 06:01 PM	
2996	GROMACS	Feature	New	Normal	gmxapi execution model	Eric Irrgang	06/24/2019 02:16 PM	2020
2994	GROMACS	Feature	New	Normal	Data flow topology in gmxapi 2020		06/24/2019 01:53 PM	2020
2993	GROMACS	Feature	New	Normal	Scalar and structured type expression and definitions for API	Eric Irrgang	10/17/2019 09:55 AM	
2985	GROMACS	Feature	New	Normal	Python package documentation		06/19/2019 12:24 PM	2020

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2984	GROMACS	Feature	New	Normal	More Extensive Selections Examples	Dallas Warren	06/18/2019 11:50 PM	
2977	GROMACS	Feature	New	Normal	print DD load balancing improvement		06/13/2019 10:56 AM	
2975	GROMACS	Feature	New	Normal	LJ PME calculations on GPUs		06/12/2019 01:17 PM	
2967	GROMACS	Feature	New	Normal	GPU reallocateDeviceBuffer improvements		09/24/2019 06:52 PM	2020-beta2
2961	GROMACS	Feature	New	Normal	How should Python package find GROMACS resources under various circumstances?		10/02/2019 02:06 PM	
2957	GROMACS	Feature	New	Normal	add support for the Hygon Dhyana architecture		05/21/2019 01:00 PM	2020
2956	GROMACS	Feature	New	Normal	SAXS resolution		05/17/2019 09:58 AM	
2944	GROMACS	Feature	New	Normal	Roadmap for thermostats / barostats in new propagation/integration scheme	Michael Shirts	05/08/2019 05:50 PM	2020
2934	GROMACS	Feature	New	Normal	GPU X Buffer ops		09/24/2019 06:07 PM	2020
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
2930	GROMACS	Feature	New	Normal	Limited range for reference group detection in cylinder pulling		04/26/2019 05:17 PM	
2928	GROMACS	Feature	New	Normal	Add ability to use expression "count of ATOM_EXPR" in selection statements.		04/16/2019 04:52 PM	
2915	GROMACS	Feature	New	High	GPU direct communications		10/11/2019 05:53 PM	
2910	GROMACS	Feature	New	Normal	Mixed scaling for 1-4 interactions		04/10/2019 10:13 PM	
2901	GROMACS	Feature	New	Normal	Declare external Resources in mdp / tpr files.	Christian Blau	03/27/2019 04:27 PM	2020
2896	GROMACS	Feature	In Progress	Normal	Python packaging		10/09/2019 04:08 PM	2020
2891	GROMACS	Feature	New	High	PME/PP GPU communications		10/17/2019 02:57 PM	
2890	GROMACS	Feature	New	High	GPU Halo Exchange		10/17/2019 02:00 PM	2020
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
2886	GROMACS	Feature	New	Normal	CUDA version of SETTLE	Artem Zhmurov	10/02/2019 12:02 PM	2020
2885	GROMACS	Feature	New	Normal	CUDA version of LINGS	Artem Zhmurov	03/12/2019 01:33 PM	2020
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future
2860	GROMACS	Feature	New	Normal	Option for outputting min/max coordinates in gmx traj		02/08/2019 12:35 AM	
2846	GROMACS	Feature	New	Low	Set rpath in FindLibStdC.cpp.cmake		02/02/2019 08:09 AM	
2840	GROMACS	Feature	New	Normal	Test that functionality does not compile that is not supposed to.		01/25/2019 02:35 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2817	GROMACS	Feature	In Progress	High	GPU X/F buffer ops		10/11/2019 11:55 AM	2020-beta2
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
2806	GROMACS	Feature	New	Normal	SIMD algorithms for ARM SVE // nobonded cluster and others		12/12/2018 05:52 PM	2020
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
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	03/29/2019 05:20 PM	2020
2761	GROMACS	Feature	New	Low	lincs-order 4 is too conservative for some force fields		11/16/2018 09:55 AM	
2755	GROMACS	Feature	New	Low	md5 sums and sha256, sha512 hashes	Benson Muite	02/19/2019 11:00 PM	
2739	GROMACS	Feature	New	Normal	Parallel continuous tempering and enhanced sampling feature		11/13/2018 11:36 PM	
2715	GROMACS	Feature	New	Normal	Avoid requesting the user to recompile gromacs for Intel OpenCL support		10/31/2018 12:16 PM	2020
2713	GROMACS	Feature	New	Normal	Constant offset for external electric fields		10/28/2018 12:57 AM	
2710	GROMACS	Feature	New	Normal	Separate dvdI for each molecule (of couple-moltype) when running FEP		10/26/2018 10:24 AM	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
2643	GROMACS	Feature	New	Low	mdp options and/or docs for anisotropic aspects of implementations		09/12/2018 02:23 PM	
2622	GROMACS	Feature	New	Low	Reduce severity of Berendsen warning		08/23/2018 11:16 PM	future
2620	GROMACS	Feature	In Progress	Normal	MD signaling API		03/02/2019 01:24 AM	
2615	GROMACS	Feature	Accepted	Normal	Switch to Python3		07/05/2019 02:57 PM	2020
2601	GROMACS	Feature	New	Normal	Free energy calculations, soft-core potential	Vytautas Gapsys	03/05/2019 01:44 AM	future
2596	GROMACS	Feature	New	Normal	Constant potential method	Benson Muite	05/10/2019 09:54 AM	
2594	GROMACS	Feature	New	Normal	Multi-level GMX API	Prashanth Kanduri	02/22/2019 03:48 PM	future
2587	GROMACS	Feature	In Progress	Normal	Provide Context (e.g. to runner code) to manage client and runtime environment		10/15/2018 03:34 PM	
2586	GROMACS	Feature	Resolved	Normal	Versioned libgmxapi target for build, install, headers, docs		03/02/2019 01:32 AM	
2585	GROMACS	Feature	Resolved	Normal	Infrastructure supporting external API		03/31/2019 04:47 PM	
2581	GROMACS	Feature	Accepted	Normal	User interface for hybrid Monte Carlo		10/15/2018 05:21 PM	2020
2579	GROMACS	Feature	New	Normal	Add dimensionality option to gmx trjconv -center		07/19/2018 04:53 PM	future
2574	GROMACS	Feature	New	Normal	iForceSchedule Abstraction	Prashanth Kanduri	03/29/2019 05:20 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2570	GROMACS	Feature	New	Normal	Better string formatting and printing		05/02/2019 12:20 PM	
2556	GROMACS	Feature	New	Normal	make default selections suitable for DNA and RNA	Mark Abraham	06/20/2018 01:48 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
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	10/03/2018 11:32 PM	future
2491	GROMACS	Feature	New	Low	Allow constant bias AWH simulations	Viveca Lindahl	06/05/2018 10:38 PM	future
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	
2429	GROMACS	Feature	New	Normal	Add option of periodic chain topology to pdb2gmx		03/10/2018 01:01 PM	
2428	GROMACS	Feature	New	Normal	Add way of selecting interactive arguments of pdb2gmx by string rather than an index		02/27/2018 06:28 PM	
2426	GROMACS	Feature	In Progress	Normal	Trajectory analysis tool for functional mode analysis by partial least squares fitting (PLS-FMA)		10/03/2018 11:31 PM	future
2354	GROMACS	Feature	New	Normal	develop configuration file support for control of task layout		09/19/2018 03:01 PM	future
2310	GROMACS	Feature	Accepted	Low	Let mdrun dump coordinates with non-finite energy		10/03/2018 09:47 PM	future
2289	GROMACS	Feature	New	Normal	gmx spatial add ability to perform over multiple reference structures		11/08/2017 12:31 AM	
2288	GROMACS	Feature	Accepted	Low	gmx msd doesn't optimally handle missing input trajectory frames		11/10/2017 11:03 AM	
2283	GROMACS	Feature	New	Normal	Force distribution analysis	Bernd Doser	10/27/2017 11:44 AM	
2282	GROMACS	Feature	New	Normal	Density map toolset	Christian Blau	03/21/2019 06:08 PM	future
2254	GROMACS	Feature	New	Normal	GPU extensions for Google Tests		09/19/2017 05:01 PM	
2248	GROMACS	Feature	New	Normal	Label all SIMD functions as pure/nodiscard		02/04/2019 04:49 AM	
2239	GROMACS	Feature	New	Normal	split libgromacs into base and full		01/07/2019 01:47 AM	
2229	GROMACS	Feature	New	High	Full Object Oriented Modularization of GROMACS MDRUN Codebase	Mark Abraham	08/22/2018 05:03 PM	future
2226	GROMACS	Feature	New	Normal	Harmonise commands for exit in make_ndx and distance		08/04/2017 12:24 PM	
2224	GROMACS	Feature	New	Normal	Proposed feature: conditional stop	Vedran Miletic	09/19/2018 03:06 PM	2020
2220	GROMACS	Feature	New	Normal	report relevant env var behaviour to console		07/31/2017 09:40 PM	
2218	GROMACS	Feature	Feedback wanted	Normal	A tiny feature: damping for umbrella pull		08/16/2017 07:20 PM	
2207	GROMACS	Feature	New	Normal	solvent excluded volume of large molecule with periodic boundary condition		06/16/2017 10:37 AM	
2194	GROMACS	Feature	Accepted	Low	xvg output requested as an output option in place of xpm files		05/31/2017 04:26 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
2139	GROMACS	Feature	New	Normal	More precise/explicit documentation conventions		01/07/2018 11:54 PM	
2137	GROMACS	Feature	New	Normal	Preliminary refactoring of constraints and update machinery.	Michael Shirts	03/11/2017 08:32 AM	future
2132	GROMACS	Feature	New	Normal	Intermediate code for xvg handling		03/08/2017 05:12 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	
2126	GROMACS	Feature	New	Normal	implement native CUDA support in CMake		01/14/2019 10:09 AM	
2118	GROMACS	Feature	New	Low	More verbose comments requested in header of gmx distance -oxyz		02/08/2017 05:46 AM	
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 PM	
2101	GROMACS	Feature	New	Low	warninp could print the offending line, as well as its number		01/20/2017 03:06 PM	
2097	GROMACS	Feature	New	Low	Move output of dhdl file entirely to edr, rather than having a separate text dhdl file		01/05/2017 05:21 PM	future
2090	GROMACS	Feature	New	Normal	redirecting stdout or stderr for testing	Mark Abraham	12/15/2016 03:15 AM	
2080	GROMACS	Feature	New	Normal	add grompp warning for suitability for domain decomposition		11/23/2016 03:03 PM	
2070	GROMACS	Feature	In Progress	Normal	Physical validation testing	Michael Shirts	10/12/2018 10:36 PM	2020
2068	GROMACS	Feature	New	Normal	Access to low level classes		03/02/2019 01:37 AM	future
2060	GROMACS	Feature	New	Normal	Convert enum to enum class		10/17/2016 05:27 PM	
2056	GROMACS	Feature	New	Low	rename "gmx select"		10/03/2016 08:24 PM	
2054	GROMACS	Feature	Accepted	High	PME on GPU	Aleksei lupinov	10/03/2019 09:41 PM	2020
2034	GROMACS	Feature	New	Normal	Unit tests for bonded forces	David van der Spoel	06/29/2019 10:22 AM	future
2018	GROMACS	Feature	New	Normal	Pulling along a line between given points		07/27/2016 09:59 AM	
2015	GROMACS	Feature	New	Normal	Auto recovery from dd communication error		07/28/2016 03:17 PM	
2005	GROMACS	Feature	New	Normal	Full Correlation Analysis (FCA) as Trajectory Analysis Module	Christian Blau	02/07/2018 02:19 PM	future
2001	GROMACS	Feature	New	Normal	add MPI info to the mdrun log header		07/06/2016 05:21 PM	
1994	GROMACS	Feature	New	Low	explore using JIT for CUDA		07/11/2016 10:20 PM	future
1974	GROMACS	Feature	New	Normal	Report atom numbers and types in the error message about missed parameters		05/30/2016 09:24 AM	
1972	GROMACS	Feature	New	Normal	external potential modules for refinement against experimental data		08/22/2018 05:03 PM	future
1966	GROMACS	Feature	New	Low	Hydrogen mass repartitioning		05/25/2016 06:04 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1964	GROMACS	Feature	Accepted	Normal	"pull=no" should not produce warnings about "unknown" pull keywords		05/20/2016 02:37 PM	
1953	GROMACS	Feature	New	Low	use more regular polymorphism for GPU code		05/06/2016 10:06 PM	future
1948	GROMACS	Feature	New	Low	add warning when non-identical GPUs are used		06/12/2017 08:45 PM	
1902	GROMACS	Feature	Accepted	Low	Add grompp check that non-excluded atoms are not too close to each other in the starting structure		02/15/2016 01:34 PM	
1900	GROMACS	Feature	New	Normal	Implement some new errors in grompp		06/22/2016 05:20 PM	
1885	GROMACS	Feature	New	Normal	DPD Thermostat		01/26/2016 10:17 AM	
1867	GROMACS	Feature	New	Normal	make coupling implementations reversible		12/02/2015 07:43 AM	
1864	GROMACS	Feature	New	Normal	write tng files with energies	Magnus Lundborg	07/11/2016 08:00 PM	
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
1849	GROMACS	Feature	New	Normal	expanded ensemble -- Adaptive Integration Method	Christopher Mirabzadeh	07/11/2016 08:01 PM	
1842	GROMACS	Feature	New	Normal	Replace XML with JSON		01/18/2018 05:12 PM	
1715	GROMACS	Feature	New	Low	improve cycle counting GPU sharing and multi-sim		08/03/2016 12:32 PM	future
1688	GROMACS	Feature	New	Low	g_cluster "middle" is not exactly the same as the definition in the cited paper		04/01/2015 05:53 AM	
1670	GROMACS	Feature	New	Normal	create mdrun option checking mini-tool		06/23/2016 04:06 PM	
1666	GROMACS	Feature	New	Normal	new approach for Verlet-scheme kernel generation	Erik Lindahl	10/08/2018 07:04 PM	future
1665	GROMACS	Feature	New	Normal	improve free energy non-bonded kernel performance		08/26/2019 03:47 PM	future
1658	GROMACS	Feature	New	Normal	Electrostatics treatment for multiple lambda sites	Berk Hess	07/11/2016 08:05 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	
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	
1641	GROMACS	Feature	New	Normal	Add toolchain file for Cray systems		06/06/2015 11:24 PM	
1635	GROMACS	Feature	New	Normal	Proper Unicode support		06/18/2015 08:34 PM	
1634	GROMACS	Feature	New	Normal	Boxed Molecular Dynamics		11/04/2014 04:40 PM	
1627	GROMACS	Feature	In Progress	Normal	DPD integrator		07/11/2016 08:08 PM	
1625	GROMACS	Feature	New	Normal	Gromacs Python API		03/02/2019 01:44 AM	future
1602	GROMACS	Feature	New	Low	gmx order S per slice along all 3 axes		09/22/2014 07:25 AM	
1562	GROMACS	Feature	New	Normal	introducing a Monte Carlo framework (first application: MC barostat)	Michael Shirts	07/11/2016 08:08 PM	
1518	GROMACS	Feature	New	Low	Enable automatic build checking for newer versions	Mark Abraham	06/04/2014 04:13 PM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1511	GROMACS	Feature	Accepted	Normal	add PDBx (ie mmcif) support		10/05/2018 07:14 PM	
1500	GROMACS	Feature	New	Normal	Post-5.0 feature clean-up plan	Mark Abraham	08/26/2019 03:47 PM	
1498	GROMACS	Feature	New	Low	g_dipoles does not work properly with ionic systems	David van der Spoel	07/11/2016 08:11 PM	
1489	GROMACS	Feature	New	Normal	Don't solely rely on filename extension		04/30/2014 05:23 AM	
1464	GROMACS	Feature	New	Normal	implement PP-PME re-balancing	Szilárd Páll	10/16/2015 08:34 AM	future
1437	GROMACS	Feature	New	Normal	Online help formatting improvements		06/04/2015 09:20 PM	future
1422	GROMACS	Feature	New	Normal	CSH angle incorrect with GROMOS force field and virtual sites	David van der Spoel	06/12/2014 12:01 AM	
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
1377	GROMACS	Feature	Feedback wanted	Low	Replica exchange if replicas not in ascendent T	David van der Spoel	06/23/2016 03:48 PM	
1347	GROMACS	Feature	New	Normal	future of tables	Mark Abraham	03/27/2019 05:24 PM	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
1332	GROMACS	Feature	In Progress	Normal	Supporting multiple end states instead of just A and B	Michael Shirts	06/05/2018 03:58 PM	
1328	GROMACS	Feature	Accepted	Normal	Names for selection positions		07/11/2016 08:15 PM	
1303	GROMACS	Feature	New	Normal	Adding lambda dependent distance for pull code	Michael Shirts	07/11/2016 08:18 PM	
1247	GROMACS	Feature	New	Normal	fix hardcoded references to atom names in analysis tools	Mark Abraham	06/12/2014 01:20 AM	future
1221	GROMACS	Feature	Accepted	Normal	More generic position mapping for selections		06/10/2014 02:58 PM	future
1192	GROMACS	Feature	Accepted	Normal	Add support for Verlet scheme with Buckingham	Berk Hess	07/11/2016 08:19 PM	
1182	GROMACS	Feature	New	Normal	improve trajectory writing to support parallel I/O		05/13/2014 10:42 AM	future
1168	GROMACS	Feature	In Progress	Low	g_density does not do what users think it does, given PBC over z and constant pressure simulation	Erik Lindahl	10/20/2018 12:49 AM	future
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
1165	GROMACS	Feature	Accepted	Low	Multi-SIMD binaries		01/23/2019 02:08 PM	2020
1162	GROMACS	Feature	New	Normal	Implement gb_saltconc	Berk Hess	02/26/2013 05:33 PM	future
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
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	
1137	GROMACS	Feature	New	Normal	Proposal for integrator framework (do_md) in future GROMACS	Michael Shirts	02/21/2017 12:48 AM	future

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
1120	GROMACS	Feature	New	Low	Make build work with multi-configuration generators		06/03/2014 03:04 PM	future
1104	GROMACS	Feature	New	Low	Implement dihedral restraints		02/06/2013 07:04 PM	future
1102	GROMACS	Feature	New	Normal	Detect incompletely written itp files		06/19/2014 03:23 PM	
1083	GROMACS	Feature	In Progress	Normal	Improve collective error/warning/note handling in mdrun		07/11/2016 08:21 PM	
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
1030	GROMACS	Feature	Fix uploaded	Low	adding -tu option to some analysis tools	Rossen Apostolov	07/11/2016 08:22 PM	
1028	GROMACS	Feature	New	Normal	Tool to calculate fraction of native contacts during simulation		11/01/2012 10:27 PM	
1026	GROMACS	Feature	New	Low	request for gen_vel to work with multiple temperature coupling groups at different temperatures		11/17/2016 04:39 PM	
951	GROMACS	Feature	New	Normal	Multiple versions of Gromacs (e.g., single and double) in the same library/binary		01/07/2019 02:10 AM	future
950	GROMACS	Feature	New	Normal	Path/directory/filename handling in Gromacs		07/11/2016 08:24 PM	
921	GROMACS	Feature	Blocked, need info	Normal	Default index groups and selections		07/11/2016 08:27 PM	
907	GROMACS	Feature	Accepted	Normal	Add tests for verifying installed headers		03/11/2014 09:15 PM	future
895	GROMACS	Feature	In Progress	Normal	g_rmsf previous frame as reference		04/29/2013 07:39 PM	future
868	GROMACS	Feature	In Progress	Normal	Implement parallelization support to analysis framework	Kevin Boyd	02/07/2019 02:08 AM	2020
843	GROMACS	Feature	New	Low	g_helixorient could benefit from more documentation	Erik Lindahl	05/23/2014 02:02 PM	
760	GROMACS	Feature	New	Low	Implement rigid body groups	Berk Hess	12/30/2012 06:04 AM	future
742	GROMACS	Feature	New	Normal	Enhancing the performance of the free energy code		08/26/2019 04:55 PM	future
731	GROMACS	Feature	New	Normal	pdb2gmx should warn about missing residues when bonds are too long		06/22/2014 10:55 AM	
720	GROMACS	Feature	Accepted	Low	permit pdb2gmx to choose a kind of HIS based on proton position		11/17/2016 03:51 PM	future
438	GROMACS	Feature	In Progress	Low	New tool: g_correl	Alexey Shvetsov	06/20/2014 10:38 AM	future
2180	Support Platforms	Feature	Fix uploaded	Low	relog matrices would work better with a hint for execution		05/19/2017 01:02 AM	
2099	Support Platforms	Feature	New	High	sharing accounts/credentials		12/06/2017 08:11 PM	
1601	Support Platforms	Feature	New	Normal	use Git for Jenkins Config		05/24/2015 10:59 AM	
987	Support Platforms	Feature	New	Normal	Feature wishlist should be moved to Redmine		08/03/2012 12:22 PM	
694	Support Platforms	Feature	Feedback wanted	Normal	Write instructions/policy for issue handling	Rossen Apostolov	05/31/2017 05:41 PM	
687	Support Platforms	Feature	New	Normal	Add content on the front page		09/02/2019 01:08 PM	
2188	TNG trajectory library	Feature	Resolved	High	Masses missing from TNG specification	Magnus Lundborg	06/13/2017 05:08 PM	

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
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
1229	TNG trajectory library	Feature	Resolved	Normal	Selection groups	Magnus Lundborg	11/29/2013 04:38 PM	version 1
1206	TNG trajectory library	Feature	New	Low	XTC Compression		10/25/2013 03:43 PM	version 2
1202	TNG trajectory library	Feature	New	Normal	Other hash types		06/25/2013 10:02 PM	version 2
1200	TNG trajectory library	Feature	New	Normal	Field for the PDB format 'segment identifier'	Magnus Lundborg	04/24/2013 09:32 AM	version 2
1199	TNG trajectory library	Feature	New	Normal	residue numbering	Magnus Lundborg	04/24/2013 09:33 AM	version 2
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
1197	TNG trajectory library	Feature	New	Normal	Rework the molecule descriptions		03/18/2013 04:16 PM	version 2
3159	GROMACS	Task	New	High	eliminate regression due to moving gmx_pme_send_coordinates()	Alan Gray	10/17/2019 02:57 PM	2020
3158	GROMACS	Task	New	Normal	use MPI_Isend() in sendFTToPpCudaDirect and receiveCoordinatesFromPpCudaDirect	Alan Gray	10/17/2019 02:48 PM	
3157	GROMACS	Task	New	Normal	separate PME x receive sync	Alan Gray	10/17/2019 02:44 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
3155	GROMACS	Task	Accepted	Normal	Unify DD and CPU-GPU gather & scatter	Artem Zhmurov	10/17/2019 03:50 PM	2021-infrastructure-stable
3154	GROMACS	Task	New	Low	Update use of Python subprocess for >=3.5		10/17/2019 01:46 PM	
3153	GROMACS	Task	New	Low	Let CMake process module directories earlier to support more modern CMake idioms.		10/17/2019 10:40 AM	2021-infrastructure-stable
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
3139	GROMACS	Task	New	Normal	gmxapi Futures should be subscribable	Eric Irrgang	10/15/2019 03:56 PM	
3133	GROMACS	Task	New	Normal	Cookiecutter for sample_restraint	Eric Irrgang	10/13/2019 01:07 PM	2020
3132	GROMACS	Task	New	Low	gmxapi testing support tools		10/13/2019 01:00 PM	
3131	GROMACS	Task	New	Normal	support ccache with clang-tidy	Mark Abraham	10/15/2019 07:23 AM	
3130	GROMACS	Task	New	Normal	Interim handling of gmxapi data references.	Eric Irrgang	10/15/2019 09:07 AM	2020-beta2
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
3123	GROMACS	Task	New	Normal	address sanitizer coverage of parallelization code-paths		10/05/2019 12:32 AM	
3119	GROMACS	Task	New	Normal	clang-tidy coverage of parallelization codepaths		10/04/2019 12:17 PM	2020

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3118	GROMACS	Task	New	Normal	clang-tidy segfaulting in CI		10/04/2019 11:34 AM	2020-beta2
3114	GROMACS	Task	New	Low	Possible improvements to update-constraints	Artem Zhmurov	10/07/2019 11:38 AM	
3106	GROMACS	Task	New	Normal	Implement multiple pulses with GPU communication	Alan Gray	09/25/2019 02:23 PM	
3105	GROMACS	Task	New	Normal	implement GPU PME/PP comm cycle counting		09/24/2019 03:19 PM	2020
3104	GROMACS	Task	New	Normal	implement GPU DD cycle counting		09/24/2019 03:19 PM	2020
3096	GROMACS	Task	New	Normal	Multiple time-stepping: correct coupling algorithms, virial calculation and energy output	Christian Blau	09/18/2019 02:18 PM	2021-infrastructure-stable
3093	GROMACS	Task	New	High	rework GPU direct halo-exchange related force reduction complexities		10/11/2019 05:53 PM	2020
3092	GROMACS	Task	New	Normal	implement better receiver ready / notify in halo exchange		09/18/2019 02:47 AM	2020
3082	GROMACS	Task	New	High	move launch/synchronization points to clarify task dependencies		10/11/2019 05:53 PM	2020
3078	GROMACS	Task	New	Normal	Allow MD modules to register energy output fields themselves		09/06/2019 11:36 AM	
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	
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
3072	GROMACS	Task	New	Normal	Use gm::index for indexing instead of int	Christian Blau	09/03/2019 04:23 PM	2021-infrastructure-stable
3064	GROMACS	Task	New	Normal	add test for perturbed bonded forces		08/22/2019 06:34 PM	2020
3062	GROMACS	Task	New	Normal	add twin cut-off mdrun test		08/19/2019 06:21 PM	2020
3061	GROMACS	Task	Resolved	Normal	support for Zen2		10/17/2019 03:32 PM	2020-beta2
3057	GROMACS	Task	New	Normal	re-enable fusion on Power8/9	Szilárd Páll	08/12/2019 11:41 AM	2020
3047	GROMACS	Task	New	Normal	Set required versions for GROMACS 2021		08/24/2019 05:25 PM	2021-infrastructure-stable
3041	GROMACS	Task	New	Normal	Remove workaround for gcc bug 58265		07/23/2019 12:27 PM	
3040	GROMACS	Task	New	Normal	Refactor Restraint module		07/18/2019 03:59 PM	
3037	GROMACS	Task	New	Normal	add missing cycle counters related to buffer ops/reduction launches		09/24/2019 03:27 PM	2020
3035	GROMACS	Task	New	Normal	Provide central logger in wrapper binary	Paul Bauer	09/06/2019 02:34 PM	2021-infrastructure-stable
3033	GROMACS	Task	In Progress	Normal	Clean up and modernize googletest bundling and usage		08/24/2019 05:23 PM	2021-infrastructure-stable
3031	GROMACS	Task	New	Normal	evaluate the impact of particle order on PME		08/21/2019 06:08 PM	2020
3027	GROMACS	Task	In Progress	Normal	Move sample_restraint development from GitHub to Gerrit	Eric Irrgang	09/24/2019 03:23 PM	2020-beta2
3026	GROMACS	Task	New	Normal	add flags for GPU force buffer op / reduction activation		08/01/2019 04:46 PM	2020
3016	GROMACS	Task	New	Normal	intermittent failure of essentialdynamics test		07/18/2019 05:23 PM	
3015	GROMACS	Task	New	Normal	Create central log handle for calls to gm_fatal		09/06/2019 02:34 PM	2021-infrastructure-stable

#	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
3013	GROMACS	Task	New	Normal	Extend logging levels in MDLogger		09/06/2019 02:34 PM	2021-infrastructure-stable
3010	GROMACS	Task	In Progress	Normal	upgrade OpenCL stack on bs-gpu01		08/23/2019 03:23 PM	2020-infrastructure-update-post-beta1
3008	GROMACS	Task	New	Normal	verify block size choice of CUDA bonded kernel		06/26/2019 08:38 PM	2020
3005	GROMACS	Task	New	Normal	Move logging in gmx preprocess to MDLogger		06/26/2019 10:01 AM	
3004	GROMACS	Task	New	Normal	Move trajectory analysis logging to MDLogger		06/26/2019 09:59 AM	
3003	GROMACS	Task	New	Normal	implement heuristic fallback to CPU when there is too little work for GPU offload		06/25/2019 04:10 PM	
3002	GROMACS	Task	New	Normal	consider splitting bonded work into local/nonlocal		06/25/2019 04:06 PM	
3001	GROMACS	Task	New	Normal	explore simplifying virial and shift force reduction		06/25/2019 04:03 PM	2020
2999	GROMACS	Task	New	Normal	Move all logging in core library and tools to use MDLogger		09/06/2019 02:36 PM	2021-infrastructure-stable
2998	GROMACS	Task	In Progress	Normal	Update Python detection		08/16/2019 09:57 AM	2020-infrastructure-update-post-beta1
2997	GROMACS	Task	New	Normal	improve performance of alchemical free energy calculations		06/24/2019 03:07 PM	2020
2992	GROMACS	Task	New	Normal	Split hw_opt in const user options and dynamic settings		09/24/2019 03:23 PM	2020
2988	GROMACS	Task	In Progress	Low	clean up and refactor code to modern standards		06/20/2019 02:14 PM	2020
2983	GROMACS	Task	New	Normal	better suited data-types for bonded GPU kernels		07/11/2019 04:32 PM	
2979	GROMACS	Task	Accepted	Normal	Reconsider default 1 OpenMP thread per thread-MPI rank	Berk Hess	09/24/2019 03:22 PM	2020-beta2
2976	GROMACS	Task	New	Normal	Basic math for Multidimensional arrays		08/04/2019 09:44 PM	2020
2965	GROMACS	Task	New	Normal	Performance of GPU direct communications		05/31/2019 03:12 PM	2020
2947	GROMACS	Task	Accepted	Normal	make an end to end test for membed		09/24/2019 03:22 PM	future
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
2943	GROMACS	Task	New	Normal	Rename Integrator	Pascal Merz	05/23/2019 08:04 PM	2020
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
2933	GROMACS	Task	New	Normal	Convert walls to a ForceProvider		04/25/2019 02:43 PM	
2919	GROMACS	Task	New	Normal	C++ style guidelines for namespace use		04/15/2019 01:21 PM	
2916	GROMACS	Task	New	Normal	Decide future of symtab	Paul Bauer	09/06/2019 02:35 PM	2021-infrastructure-stable
2912	GROMACS	Task	Resolved	Normal	C++ extension module for Python bindings	Eric Irrgang	07/05/2019 09:00 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	
2908	GROMACS	Task	New	Normal	Renaming things in nbxnm	Berk Hess	03/28/2019 10:10 AM	
2905	GROMACS	Task	New	Normal	Add a Jenkins configuration with std library assert		08/24/2019 05:22 PM	
2899	GROMACS	Task	In Progress	Normal	Update testing matrix versions for GROMACS 2020 release	Mark Abraham	10/12/2019 09:44 PM	2020-infrastructure-update-post-beta1

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2898	GROMACS	Task	New	Low	Naming common variables		03/26/2019 11:46 PM	
2895	GROMACS	Task	Resolved	Normal	gmxapi Output proxy establishes execution dependency.	Eric Irrgang	03/29/2019 05:18 PM	2020
2894	GROMACS	Task	Resolved	Normal	Wrap importable Python code.	Eric Irrgang	05/09/2019 11:30 AM	2020
2893	GROMACS	Task	Resolved	Normal	Integrate gmxapi Python package	Eric Irrgang	04/09/2019 12:20 PM	2020
2889	GROMACS	Task	New	Normal	update grompp warnings for brevity, usefulness and actionability	Mark Abraham	03/11/2019 02:15 PM	2020
2882	GROMACS	Task	New	Normal	evaluate different storage layouts for GPU coordinates/changes/forces	Szilárd Páll	03/07/2019 06:21 PM	
2877	GROMACS	Task	New	Normal	use gmx::Options more	Mark Abraham	04/02/2019 06:14 PM	2020
2875	GROMACS	Task	Accepted	Normal	SIMD version of the free-energy kernel	Berk Hess	08/26/2019 03:47 PM	2020
2874	GROMACS	Task	New	Normal	Refactor Gromacs (cluster) neighborlist into separate module	Erik Lindahl	02/28/2019 11:36 AM	
2864	GROMACS	Task	New	Normal	Building incompatibilities	Benson Muite	02/19/2019 02:00 PM	
2863	GROMACS	Task	New	Normal	improve PBC handling		03/11/2019 04:28 PM	
2859	GROMACS	Task	Fix uploaded	Normal	Change ArrayRef iterator type from pointer to std::iterator		02/08/2019 11:00 PM	
2857	GROMACS	Task	New	Normal	Clarify recommended function specifies (constexpr, noexcept, pure)		02/04/2019 04:48 AM	
2855	GROMACS	Task	New	Normal	Allow compiling GROMACS without C compiler		01/31/2019 08:44 PM	
2850	GROMACS	Task	In Progress	Normal	assess Raptor Talos for testing	Szilárd Páll	02/12/2019 01:14 PM	
2839	GROMACS	Task	New	Normal	make module and file naming consistent		04/09/2019 04:27 PM	2020
2835	GROMACS	Task	New	Normal	Matrix class constraint to upper or lower triangle		02/07/2019 02:44 PM	
2834	GROMACS	Task	New	Normal	C++ matrix classes	Christian Blau	01/23/2019 12:19 PM	2020
2833	GROMACS	Task	New	Normal	Update topology datastructures	Paul Bauer	04/02/2019 12:39 PM	2020
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
2822	GROMACS	Task	Accepted	Normal	Make nbxn a module	Berk Hess	01/03/2019 03:07 PM	2020
2818	GROMACS	Task	In Progress	Normal	bonded GPU kernel fusion	Magnus Lundborg	07/03/2019 09:01 PM	
2796	GROMACS	Task	New	Low	clarify what mdrun -cpt means		01/03/2019 02:09 PM	
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		02/13/2019 08:17 PM	2020
2792	GROMACS	Task	New	Normal	Improvement of PME gather and spread CUDA kernels		09/12/2019 12:23 PM	
2787	GROMACS	Task	New	Normal	allow passing flags to allocateDeviceBuffer		12/03/2018 01:54 PM	
2773	GROMACS	Task	New	Normal	improve GPU error handling and make such handling uniform across modules		11/21/2018 10:28 AM	2020
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/08/2018 08:06 PM	2020
2770	GROMACS	Task	New	Normal	change branch maintenance policy		11/29/2018 02:51 PM	2020

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
2766	GROMACS	Task	In Progress	Normal	Improve hardware option selection	Kevin Boyd	12/20/2018 06:40 PM	2020
2764	GROMACS	Task	New	Normal	gmxapi version updates for post release-2019	Eric Irrgang	11/21/2018 12:53 PM	
2758	GROMACS	Task	New	Low	Modernize genconf		11/15/2018 07:38 AM	future
2756	GROMACS	Task	In Progress	Normal	gmxapi integration testing		08/16/2019 09:56 AM	2020-infrastructure-update-post-beta1
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

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