Issues

#	Project	Tracker	Status	Priority	Subject	Assignee	Updated	Target version
3386	GROMACS	Bug	Closed	Normal	gmx disre crashed when number of pairs larger than number of restraints	David van der Spoel	02/18/2020 10:17 PM	2019.6
3384	GROMACS	Bug	Closed	Normal	Inconsisten labels in distance restraints can crash gmx disre	David van der Spoel	02/24/2020 03:36 PM	2019.6
3375	GROMACS	Bug	Closed	Normal	Orires consistency check too strict	David van der Spoel	02/21/2020 08:14 AM	2019.6
3049	GROMACS	Bug	New	Low	gmx nmeig should plot a real infrared spectrum	David van der Spoel	09/24/2019 03:25 PM	future
2862	GROMACS	Bug	Closed	Normal	Division by zero in restrained dihedrals		02/28/2020 09:13 AM	2020.1
2844	GROMACS	Bug	Closed	High	Test SEGV with -DGMX_DOUBLE due to LAPACK	David van der Spoel	02/05/2019 07:01 PM	2020
2843	GROMACS	Bug	Closed	Normal	Building with GMX_BUILD_OWN_FFTW		01/28/2019 04:38 PM	2020
2815	GROMACS	Bug	Closed	Normal	gmx msd -mol broken	David van der Spoel	12/26/2018 11:39 AM	2020
2720	GROMACS	Bug	Closed	Normal	Normal-mode analysis with vsites or shells works for first molecule of each type only		11/28/2018 03:33 PM	
2641	GROMACS	Bug	Closed	Normal	Possible l-bfgs improvements	David van der Spoel	04/05/2019 04:27 PM	2019.2
2568	GROMACS	Bug	New	Low	gmx editconf -rotate does not rotate the box		07/10/2018 10:27 AM	future
2544	GROMACS	Bug	New	Normal	gmx rmsf does not fix periodicity in reference structure	David van der Spoel	08/21/2018 10:36 AM	future
2444	GROMACS	Bug	Rejected	Normal	Eneergy minimization crashes due to vsites	David van der Spoel	03/13/2018 02:03 PM	2018.1
2119	GROMACS	Bug	Closed	Normal	gmx solvate -shell does not add anything	David van der Spoel	12/11/2017 12:17 PM	
2052	GROMACS	Bug	New	Low	trjconv does not recognize periodic molecules	David van der Spoel	01/12/2018 11:05 AM	
2019	GROMACS	Bug	Closed	Low	gmx velacc lacking documentation	David van der Spoel	12/14/2017 10:27 PM	
2011	GROMACS	Bug	Closed	Low	gmx clustsize -mol ignores index file	David van der Spoel	12/31/2017 05:00 PM	
1996	GROMACS	Bug	Closed	Normal	gmx dos does not work at all	David van der Spoel	06/27/2016 07:27 PM	5.1.3
1884	GROMACS	Bug	Closed	Normal	gmx_output_env_t not visible from trajectoryanalysis modules	David van der Spoel	12/28/2015 06:16 PM	5.1.2
1860	GROMACS	Bug	Closed	Normal	convert-tpr messes up gmx_mtop_t structure	David van der Spoel	11/24/2015 06:22 PM	5.1.2
1859	GROMACS	Bug	Closed	Normal	make_ndx does not work	David van der Spoel	01/12/2016 04:23 PM	5.1.2
1791	GROMACS	Bug	Closed	Normal	Spurious interactions that should not be there / Table routines work with 1/r leading to NaN.	David van der Spoel	07/11/2016 08:34 PM	
1645	GROMACS	Bug	Closed	Normal	Difference in energy with Verlet scheme due to PME dipole correction	David van der Spoel	06/22/2015 06:03 PM	4.6.8
1630	GROMACS	Bug	Closed	Normal	grompp allows to specify vdwtype = PME and dispcorr != no	David van der Spoel	10/24/2014 02:32 PM	5.0.3
1592	GROMACS	Bug	Rejected	Low	Manual of trjconv is unclear about precision.	David van der Spoel	06/22/2015 06:13 AM	
1510	GROMACS	Bug	Closed	Normal	gmx check and gmx dump do not work for tng files	Magnus Lundborg	07/15/2014 06:45 AM	5.0
1502	GROMACS	Bug	Closed	Normal	trjconv incorrect tng defaults	Magnus Lundborg	06/05/2014 04:48 PM	5.0
1473	GROMACS	Bug	Closed	Normal	gmx energy -driftcorr broken.	David van der Spoel	07/11/2016 07:48 PM	

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1469	GROMACS	Bug	Closed	Normal	sizeof call generates compilation error in src/gromacs/simd/impl_x86_sse2/impl_x86_sse2.h	Erik Lindahl	04/03/2014 07:36 PM	5.0
1395	GROMACS	Bug	Closed	Normal	rtp errors gromos and opls	David van der Spoel	06/24/2014 08:29 PM	4.6.6
1354	GROMACS	Bug	New	Normal	Constant acceleration NEMD is broken.	David van der Spoel	01/09/2019 04:42 PM	
1343	GROMACS	Bug	Closed	Normal	vsiten particles are not integrated	Berk Hess	09/29/2013 03:53 PM	5.0
1272	GROMACS	Bug	Closed	Normal	Energy minimization with domain decomposition crashes	Berk Hess	06/16/2015 11:50 PM	
1249	GROMACS	Bug	Closed	Normal	no-PBC no-cutoff is broken with SIMD group kernels in 4.6.1	Erik Lindahl	03/04/2015 10:47 PM	4.6.x
1183	GROMACS	Bug	Closed	Normal	g_mindist -pi bug with triclinic boxes	David van der Spoel	12/16/2013 05:40 PM	4.5.7
1156	GROMACS	Bug	Closed	Normal	mdrun -nt > 1 crashes with old tpr	Michael Shirts	12/16/2013 05:39 PM	4.6.1
972	GROMACS	Bug	Closed	Normal	g_hbond crashes with openmp and -ac	David van der Spoel	11/11/2012 02:01 PM	4.5.6
901	GROMACS	Bug	Closed	Normal	Dispersion correction incorrect with energy minimization	Berk Hess	04/26/2012 08:27 PM	4.5.6
900	GROMACS	Bug	Closed	High	crash in OpenMP code.	Berk Hess	06/23/2012 06:46 PM	4.6
847	GROMACS	Bug	Rejected	Normal	tpbconv with index file can produce incorrect tpr files		12/29/2012 12:18 AM	4.6
743	GROMACS	Bug	Closed	Normal	Angular momentum removal incorrect	David van der Spoel	03/05/2012 11:27 AM	4.5.6
741	GROMACS	Bug	Closed	Normal	tpbconv can not read cpt file	Berk Hess	06/29/2011 06:27 AM	
713	GROMACS	Bug	Closed	Normal	MD with polarization does not work in parallel	David van der Spoel	01/04/2012 01:21 PM	
620	GROMACS	Bug	Closed	Normal	Total dipole in energy files is incorrect		12/28/2012 08:15 PM	4.6
608	GROMACS	Bug	Closed	Normal	Molecules with large charge groups give wrong neighborlist	David van der Spoel	11/02/2010 06:18 PM	4.0.7
579	GROMACS	Bug	Closed	Normal	nstcalcenergy = -1 leads to wrong pressure	Erik Lindahl	10/05/2010 12:43 PM	4.5.1
564	GROMACS	Bug	Closed	Normal	g_dipoles has a memory hole	David van der Spoel	09/20/2010 01:51 PM	4.5.1
523	GROMACS	Bug	Closed	Normal	g_rms gives nonsense values when the number of atoms differs between tpr and xtc	David van der Spoel	08/31/2010 12:06 PM	CVS
520	GROMACS	Bug	Closed	Normal	Editconf with index can not do other things	David van der Spoel	08/31/2010 10:42 AM	CVS
440	GROMACS	Bug	Closed	Normal	Double precision man pages are installed as program_d.1	David van der Spoel	09/01/2010 10:22 PM	CVS
434	GROMACS	Bug	Closed	Normal	pdb2gmx opens all rtp files	Erik Lindahl	06/14/2010 03:42 PM	CVS
274	GROMACS	Bug	Closed	Normal	Crashes in mdrun with DD code, not sequential	Berk Hess	01/06/2009 03:35 PM	4.0_rc1
224	GROMACS	Bug	Closed	Normal	grompp does not process encads topologies correctly	Erik Lindahl	10/08/2008 05:40 PM	4.0_rc1
214	GROMACS	Bug	Closed	Normal	Configure fails in 64 bit	Erik Lindahl	10/08/2008 07:11 AM	4.0_rc1
206	GROMACS	Bug	Closed	Normal	Protein atom naming in pdb files incorrect	David van der Spoel	10/08/2008 02:38 AM	CVS
181	GROMACS	Bug	Closed	Normal	Pressure scaling distorts dodecahedron boxes	Erik Lindahl	02/18/2016 11:59 PM	3.3.1
103	GROMACS	Bug	Closed	High	Possible problems in g_sas	David van der Spoel	09/21/2007 02:02 PM	3.3.1
85	GROMACS	Bug	Closed	High	mdrun with PME gives different results with MPI	David van der Spoel	09/11/2007 12:07 PM	3.3.1
80	GROMACS	Bug	Closed	High	bug in avcsix calculation for dispersion correction	David van der Spoel	05/11/2006 08:43 AM	3.3.1
71	GROMACS	Bug	Closed	High	grompp takes excessive time for large systems	David van der Spoel	07/21/2007 03:11 PM	3.3.1

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69	GROMACS	Bug	Closed	High	x2top improvements	David van der Spoel	08/20/2006 02:43 PM	3.3.1
67	GROMACS	Bug	Closed	High	g_rdf has GROMOS atom names hardocoded	David van der Spoel	08/21/2006 01:28 PM	3.3.1
66	GROMACS	Bug	Closed	High	graph problem with distance restraints	David van der Spoel	04/14/2007 03:24 PM	3.3.1
63	GROMACS	Bug	Closed	High	eneconv produces NaN	David van der Spoel	08/21/2006 01:09 PM	3.3
60	GROMACS	Bug	Closed	High	genion mixes up ions	David van der Spoel	03/30/2006 10:28 AM	CVS
53	GROMACS	Bug	Closed	High	Angle definitions maybe wrong in g_chi	David van der Spoel	04/02/2006 05:11 PM	3.3
50	GROMACS	Bug	Closed	High	grompp -check14 SEGVs	David van der Spoel	02/28/2006 09:51 AM	3.3
45	GROMACS	Bug	Closed	High	pdb2gmx crashes when force field files in workdir	David van der Spoel	02/28/2006 01:58 PM	3.3
7	GROMACS	Bug	Closed	High	Environment variable IAMCOOL crashes program luck	David van der Spoel	09/05/2005 05:39 PM	3.3_rc1
2931	GROMACS	Feature	New	Normal	Tables in Verlet kernels		04/29/2019 12:01 PM	
2866	GROMACS	Feature	New	Normal	Alternative non-bonded potentials	David van der Spoel	03/05/2019 03:50 PM	future
2774	GROMACS	Feature	New	Normal	Refactor shell code into its own integrator	David van der Spoel	12/27/2019 04:05 PM	2021
2545	GROMACS	Feature	New	Normal	Should grompp fix periodicity of input files?	David van der Spoel	10/03/2018 11:32 PM	future
2451	GROMACS	Feature	Resolved	Normal	Linear virtual sites with fixed distance	David van der Spoel	09/16/2019 01:15 PM	
2272	GROMACS	Feature	Closed	Low	pdb2gmx does not accept tips3p as a water model	David van der Spoel	11/28/2017 05:59 PM	2018
2132	GROMACS	Feature	New	Normal	Intermediate code for xvg handling		03/08/2017 05:12 PM	future
2111	GROMACS	Feature	In Progress	Normal	Implement Gaussian screening of electrostatics		02/23/2019 12:33 PM	
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	
2036	GROMACS	Feature	Closed	Normal	gmx solvate should work with molecules		08/23/2016 03:25 PM	2018
2034	GROMACS	Feature	New	Normal	Unit tests for bonded forces	David van der Spoel	06/29/2019 10:22 AM	future
1864	GROMACS	Feature	New	Normal	write tng files with energies	Magnus Lundborg	07/11/2016 08:00 PM	
1863	GROMACS	Feature	Closed	Normal	write tng files with velocities from mdrun	Magnus Lundborg	07/11/2016 08:01 PM	2016
1854	GROMACS	Feature	New	Normal	Remove all cyclic dependencies		05/25/2017 08:34 AM	
1837	GROMACS	Feature	Closed	High	Design of new table classes	David van der Spoel	03/17/2018 12:31 AM	
1564	GROMACS	Feature	Closed	Low	g_gyrate help text and manual is confusing	David van der Spoel	07/11/2016 07:47 PM	5.0.7
1524	GROMACS	Feature	Closed	Low	More uniform options to programs.	David van der Spoel	08/17/2016 02:25 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	
1377	GROMACS	Feature	Feedback wanted	Low	Replica exchange if replicas not in ascendent T	David van der Spoel	06/23/2016 03:48 PM	
879	GROMACS	Feature	Closed	Low	Normal modes with vsites and/or shells does not work	David van der Spoel	07/11/2016 08:28 PM	2016
846	GROMACS	Feature	Closed	Low	Warning messages should be added to programs reducing the precision of coordinates/velocities etc.	David van der Spoel	07/11/2016 08:44 PM	

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720	GROMACS	Feature	Accepted	Low	permit pdb2gmx to choose a kind of HIS based on proton position		11/17/2016 03:51 PM	future
2795	GROMACS	Task	New	Normal	Incorporate regressiontests into core gromacs		12/02/2019 01:44 PM	2021-infrastructure-stable
2771	GROMACS	Task	New	Normal	Size independent Hessian for normal mode analysis		12/28/2019 10:50 AM	future
2071	GROMACS	Task	In Progress	High	Low accuracy default settings yield incorrect liquid densities	Berk Hess	01/05/2018 03:32 PM	
1345	GROMACS	Task	Closed	Low	Charmm - CMAP weirdness in grompp	Erik Lindahl	07/15/2014 06:42 AM	5.0
1170	GROMACS	Task	New	Normal	mdlib reorganization		11/17/2016 03:47 PM	future