

## Issues

| #    | Project | Tracker | Status          | Priority | Subject   | Assignee            | Updated             | Target version             |
|------|---------|---------|-----------------|----------|---|---------------------|---------------------|----------------------------|
| 2068 | GROMACS | Feature | New             | Normal   | Access to low level classes                                     |                     | 03/02/2019 01:37 AM | future                     |
| 2866 | GROMACS | Feature | New             | Normal   | Alternative non-bonded potentials                               | David van der Spoel | 03/05/2019 03:50 PM | future                     |
| 1354 | GROMACS | Bug     | New             | Normal   | Constant acceleration NEMD is broken.                           | David van der Spoel | 01/09/2019 04:42 PM |                            |
| 2060 | GROMACS | Feature | New             | Normal   | Convert enum to enum class                                      |                     | 10/17/2016 05:27 PM |                            |
| 2568 | GROMACS | Bug     | New             | Low      | gmx editconf -rotate does not rotate the box                    |                     | 07/10/2018 10:27 AM | future                     |
| 3049 | GROMACS | Bug     | New             | Low      | gmx nmeig should plot a real infrared spectrum                  | David van der Spoel | 09/24/2019 03:25 PM | future                     |
| 2544 | GROMACS | Bug     | New             | Normal   | gmx rmsf does not fix periodicity in reference structure        | David van der Spoel | 08/21/2018 10:36 AM | future                     |
| 1498 | GROMACS | Feature | New             | Low      | g_dipoles does not work properly with ionic systems             | David van der Spoel | 07/11/2016 08:11 PM |                            |
| 2795 | GROMACS | Task    | New             | Normal   | Incorporate regressiontests into core gromacs                   |                     | 12/02/2019 01:44 PM | 2021-infrastructure-stable |
| 2132 | GROMACS | Feature | New             | Normal   | Intermediate code for xvg handling                              |                     | 03/08/2017 05:12 PM | future                     |
| 1170 | GROMACS | Task    | New             | Normal   | mdlib reorganization  |                     | 11/17/2016 03:47 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                       |
| 1854 | GROMACS | Feature | New             | Normal   | Remove all cyclic dependencies                                  |                     | 05/25/2017 08:34 AM |                            |
| 2545 | GROMACS | Feature | New             | Normal   | Should grompp fix periodicity of input files?                   | David van der Spoel | 10/03/2018 11:32 PM | future                     |
| 2771 | GROMACS | Task    | New             | Normal   | Size independent Hessian for normal mode analysis               |                     | 12/28/2019 10:50 AM | future                     |
| 2931 | GROMACS | Feature | New             | Normal   | Tables in Verlet kernels  |                     | 04/29/2019 12:01 PM |                            |
| 2052 | GROMACS | Bug     | New             | Low      | trjconv does not recognize periodic molecules                   | David van der Spoel | 01/12/2018 11:05 AM |                            |
| 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 |                            |
| 720  | GROMACS | Feature | Accepted        | Low      | permit pdb2gmx to choose a kind of HIS based on proton position |                     | 11/17/2016 03:51 PM | future                     |
| 2111 | GROMACS | Feature | In Progress     | Normal   | Implement Gaussian screening of electrostatics                  |                     | 02/23/2019 12:33 PM |                            |
| 2071 | GROMACS | Task    | In Progress     | High     | Low accuracy default settings yield incorrect liquid densities  | Berk Hess           | 01/05/2018 03:32 PM |                            |
| 2451 | GROMACS | Feature | Resolved        | Normal   | Linear virtual sites with fixed distance                        | David van der Spoel | 09/16/2019 01:15 PM |                            |
| 2444 | GROMACS | Bug     | Rejected        | Normal   | Eneergy minimization crashes due to vsites                      | David van der Spoel | 03/13/2018 02:03 PM | 2018.1                     |
| 1592 | GROMACS | Bug     | Rejected        | Low      | Manual of trjconv is unclear about precision.                   | David van der Spoel | 06/22/2015 06:13 AM |                            |
| 847  | GROMACS | Bug     | Rejected        | Normal   | tpbconv with index file can produce incorrect tpr files         |                     | 12/29/2012 12:18 AM | 4.6                        |
| 1377 | GROMACS | Feature | Feedback wanted | Low      | Replica exchange if replicas not in ascendent T                 | David van der Spoel | 06/23/2016 03:48 PM |                            |
| 53   | GROMACS | Bug     | Closed          | High     | Angle definitions maybe wrong in g_chi                          | David van der Spoel | 04/02/2006 05:11 PM | 3.3                        |
| 743  | GROMACS | Bug     | Closed          | Normal   | Angular momentum removal incorrect                              | David van der Spoel | 03/05/2012 11:27 AM | 4.5.6                      |
| 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                      |

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|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 2843 | GROMACS | Bug     | Closed | Normal   | Building with GMX_BUILD_OWN_FFTW  |                     | 01/28/2019 04:38 PM | 2020           |
| 1345 | GROMACS | Task    | Closed | Low      | Charmm - CMAP weirdness in grompp                                       | Erik Lindahl        | 07/15/2014 06:42 AM | 5.0            |
| 214  | GROMACS | Bug     | Closed | Normal   | Configure fails in 64 bit   | Erik Lindahl        | 10/08/2008 07:11 AM | 4.0_rc1        |
| 1860 | GROMACS | Bug     | Closed | Normal   | convert-tpz messes up gmx_mtop_t structure                              | David van der Spoel | 11/24/2015 06:22 PM | 5.1.2          |
| 900  | GROMACS | Bug     | Closed | High     | crash in OpenMP code.   | Berk Hess           | 06/23/2012 06:46 PM | 4.6            |
| 274  | GROMACS | Bug     | Closed | Normal   | Crashes in mdrun with DD code, not sequential                           | Berk Hess           | 01/06/2009 03:35 PM | 4.0_rc1        |
| 1837 | GROMACS | Feature | Closed | High     | Design of new table classes   | David van der Spoel | 03/17/2018 12:31 AM |                |
| 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          |
| 901  | GROMACS | Bug     | Closed | Normal   | Dispersion correction incorrect with energy minimization                | Berk Hess           | 04/26/2012 08:27 PM | 4.5.6          |
| 2862 | GROMACS | Bug     | Closed | Normal   | Division by zero in restrained dihedrals                                |                     | 02/28/2020 09:13 AM | 2020.1         |
| 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            |
| 520  | GROMACS | Bug     | Closed | Normal   | Editconf with index can not do other things                             | David van der Spoel | 08/31/2010 10:42 AM | CVS            |
| 63   | GROMACS | Bug     | Closed | High     | eneconv produces NaN  | David van der Spoel | 08/21/2006 01:09 PM | 3.3            |
| 1272 | GROMACS | Bug     | Closed | Normal   | Energy minimization with domain decomposition crashes                   | Berk Hess           | 06/16/2015 11:50 PM |                |
| 7    | GROMACS | Bug     | Closed | High     | Environment variable IAMCOOL crashes program luck                       | David van der Spoel | 09/05/2005 05:39 PM | 3.3_rc1        |
| 60   | GROMACS | Bug     | Closed | High     | genion mixes up ions  | David van der Spoel | 03/30/2006 10:28 AM | CVS            |
| 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            |
| 2011 | GROMACS | Bug     | Closed | Low      | gmx clustsize -mol ignores index file                                   | David van der Spoel | 12/31/2017 05:00 PM |                |
| 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         |
| 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          |
| 1473 | GROMACS | Bug     | Closed | Normal   | gmx energy -driftcorr broken.   | David van der Spoel | 07/11/2016 07:48 PM |                |
| 2815 | GROMACS | Bug     | Closed | Normal   | gmx msd -mol broken   | David van der Spoel | 12/26/2018 11:39 AM | 2020           |
| 2119 | GROMACS | Bug     | Closed | Normal   | gmx solvate -shell does not add anything                                | David van der Spoel | 12/11/2017 12:17 PM |                |
| 2036 | GROMACS | Feature | Closed | Normal   | gmx solvate should work with molecules                                  |                     | 08/23/2016 03:25 PM | 2018           |
| 2019 | GROMACS | Bug     | Closed | Low      | gmx velacc lacking documentation  | David van der Spoel | 12/14/2017 10:27 PM |                |
| 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          |
| 66   | GROMACS | Bug     | Closed | High     | graph problem with distance restraints                                  | David van der Spoel | 04/14/2007 03:24 PM | 3.3.1          |
| 50   | GROMACS | Bug     | Closed | High     | grompp -check14 SEGVs   | David van der Spoel | 02/28/2006 09:51 AM | 3.3            |
| 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          |
| 224  | GROMACS | Bug     | Closed | Normal   | grompp does not process encads topologies correctly                     | Erik Lindahl        | 10/08/2008 05:40 PM | 4.0_rc1        |
| 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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|------|---------|---------|--------|----------|---|---------------------|---------------------|----------------|
| 564  | GROMACS | Bug     | Closed | Normal   | g_dipoles has a memory hole   | David van der Spoel | 09/20/2010 01:51 PM | 4.5.1          |
| 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          |
| 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          |
| 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          |
| 67   | GROMACS | Bug     | Closed | High     | g_rdf has GROMOS atom names hardcoded   | David van der Spoel | 08/21/2006 01:28 PM | 3.3.1          |
| 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            |
| 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         |
| 1859 | GROMACS | Bug     | Closed | Normal   | make_ndx does not work  | David van der Spoel | 01/12/2016 04:23 PM | 5.1.2          |
| 713  | GROMACS | Bug     | Closed | Normal   | MD with polarization does not work in parallel  | David van der Spoel | 01/04/2012 01:21 PM |                |
| 1156 | GROMACS | Bug     | Closed | Normal   | mdrun -nt > 1 crashes with old tpr  | Michael Shirts      | 12/16/2013 05:39 PM | 4.6.1          |
| 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          |
| 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          |
| 1524 | GROMACS | Feature | Closed | Low      | More uniform options to programs.   | David van der Spoel | 08/17/2016 02:25 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          |
| 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           |
| 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 |                |
| 579  | GROMACS | Bug     | Closed | Normal   | nstcalcenergy = -1 leads to wrong pressure  | Erik Lindahl        | 10/05/2010 12:43 PM | 4.5.1          |
| 3375 | GROMACS | Bug     | Closed | Normal   | Orires consistency check too strict   | David van der Spoel | 02/21/2020 08:14 AM | 2019.6         |
| 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            |
| 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           |
| 434  | GROMACS | Bug     | Closed | Normal   | pdb2gmx opens all rtp files   | Erik Lindahl        | 06/14/2010 03:42 PM | CVS            |
| 2641 | GROMACS | Bug     | Closed | Normal   | Possible l-bfgs improvements  | David van der Spoel | 04/05/2019 04:27 PM | 2019.2         |
| 103  | GROMACS | Bug     | Closed | High     | Possible problems in g_sas  | David van der Spoel | 09/21/2007 02:02 PM | 3.3.1          |
| 181  | GROMACS | Bug     | Closed | Normal   | Pressure scaling distorts dodecahedron boxes  | Erik Lindahl        | 02/18/2016 11:59 PM | 3.3.1          |
| 206  | GROMACS | Bug     | Closed | Normal   | Protein atom naming in pdb files incorrect  | David van der Spoel | 10/08/2008 02:38 AM | CVS            |
| 1395 | GROMACS | Bug     | Closed | Normal   | rtp errors gromos and opls  | David van der Spoel | 06/24/2014 08:29 PM | 4.6.6          |
| 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            |
| 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 |                |
| 2844 | GROMACS | Bug     | Closed | High     | Test SEGV with -DGMX_DOUBLE due to LAPACK   | David van der Spoel | 02/05/2019 07:01 PM | 2020           |
| 620  | GROMACS | Bug     | Closed | Normal   | Total dipole in energy files is incorrect   |                     | 12/28/2012 08:15 PM | 4.6            |

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|------|---------|---------|--------|----------|--|---------------------|---------------------|----------------|
| 741  | GROMACS | Bug     | Closed | Normal   | tpbconv can not read cpt file  | Berk Hess           | 06/29/2011 06:27 AM |                |
| 1502 | GROMACS | Bug     | Closed | Normal   | trjconv incorrect tng defaults   | Magnus Lundborg     | 06/05/2014 04:48 PM | 5.0            |
| 1343 | GROMACS | Bug     | Closed | Normal   | vsiten particles are not integrated  | Berk Hess           | 09/29/2013 03:53 PM | 5.0            |
| 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 |                |
| 1863 | GROMACS | Feature | Closed | Normal   | write tng files with velocities from mdrun   | Magnus Lundborg     | 07/11/2016 08:01 PM | 2016           |
| 69   | GROMACS | Bug     | Closed | High     | x2top improvements   | David van der Spoel | 08/20/2006 02:43 PM | 3.3.1          |