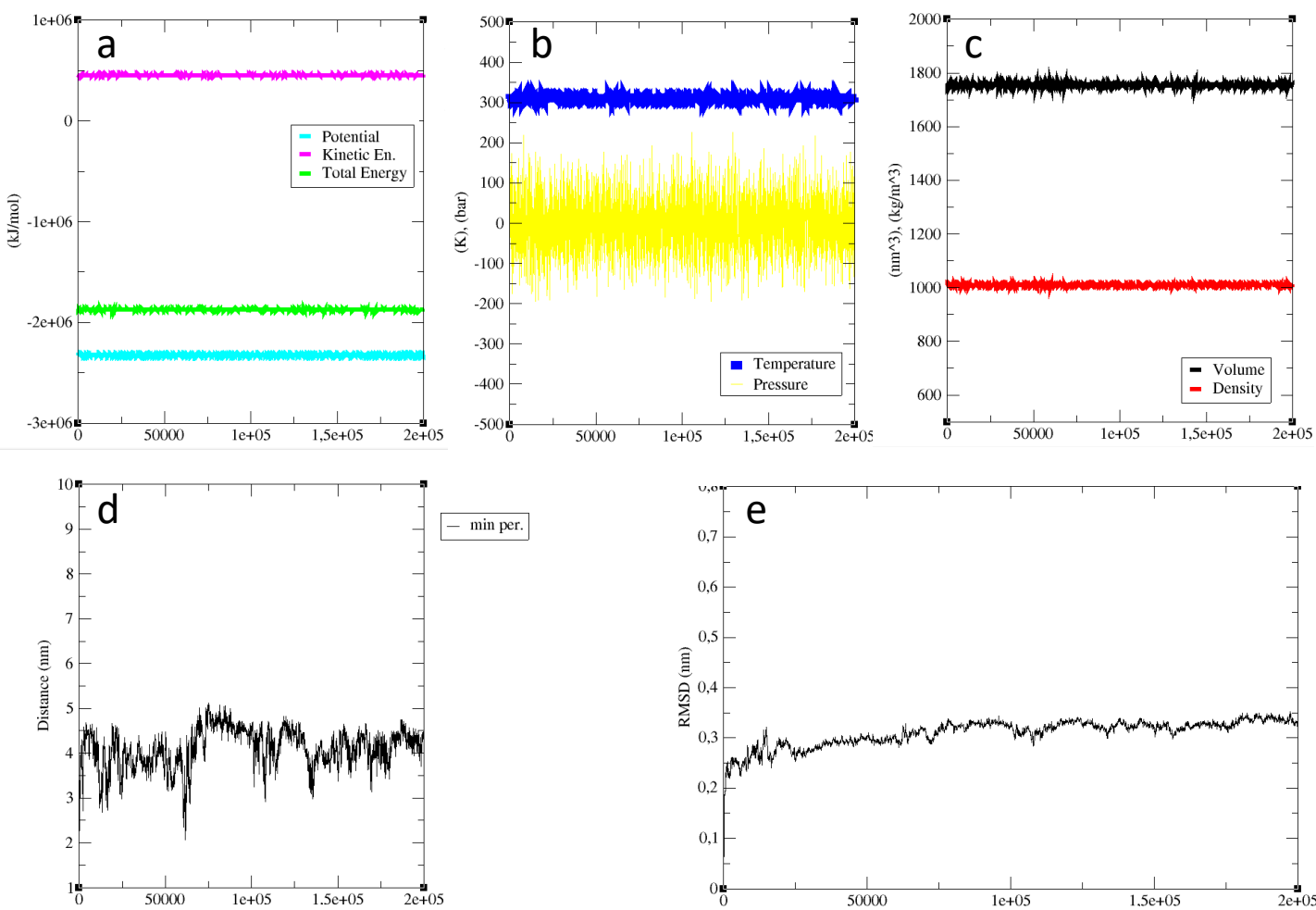


Supplementary File 1

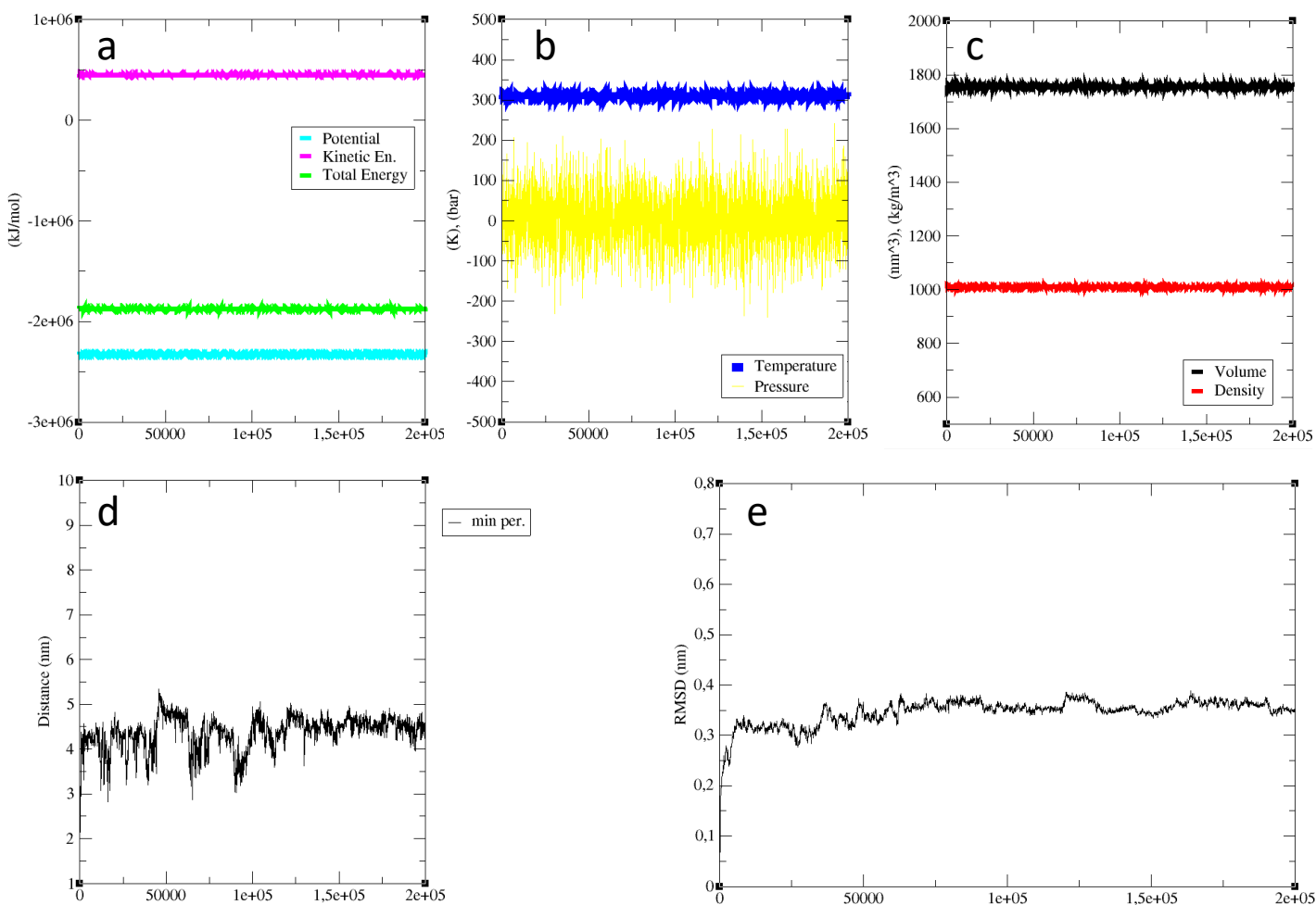
Quality check for wtGALT at 310K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances..

Supplementary File 2

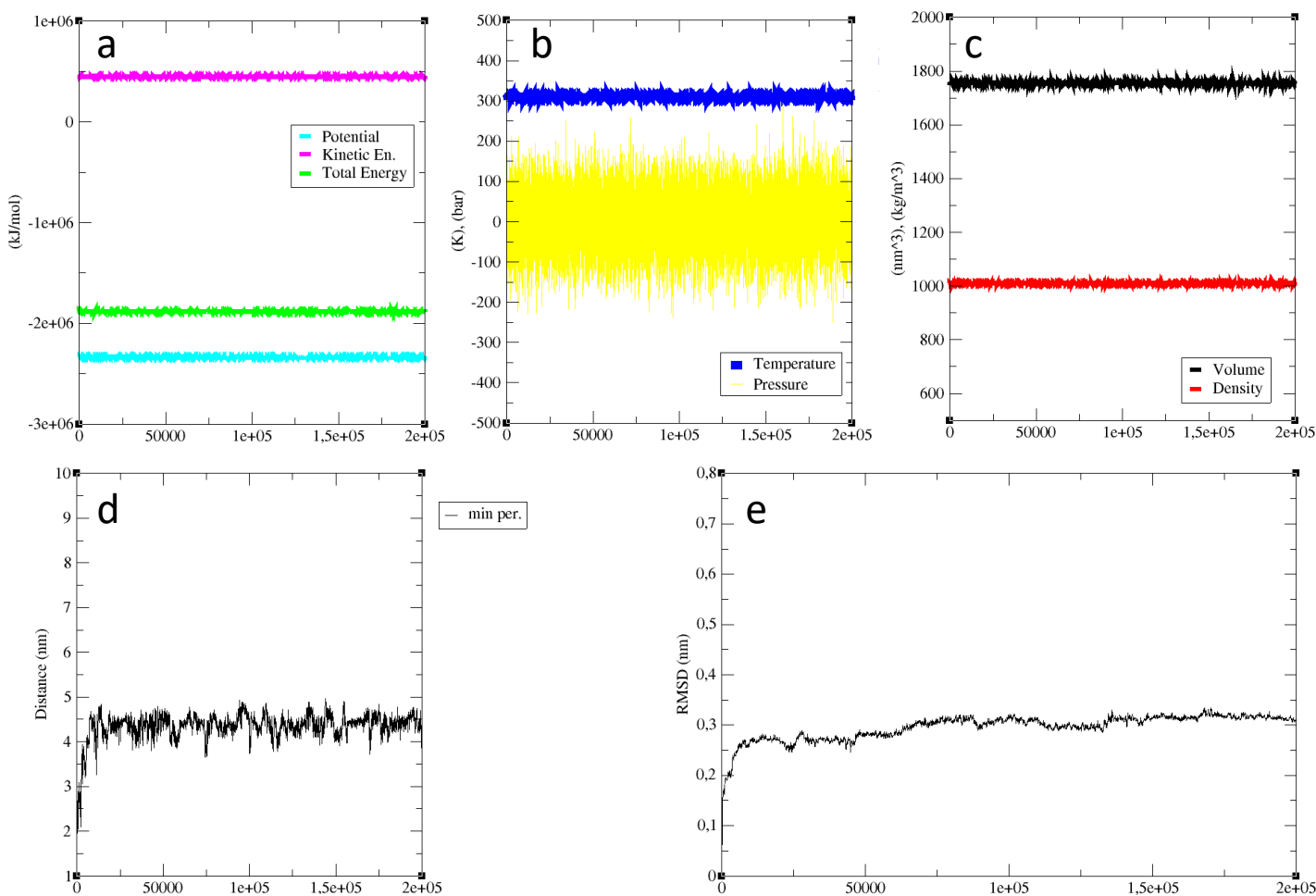
Quality check for p.Gln188Arg at 310K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances.

Supplementary File 3

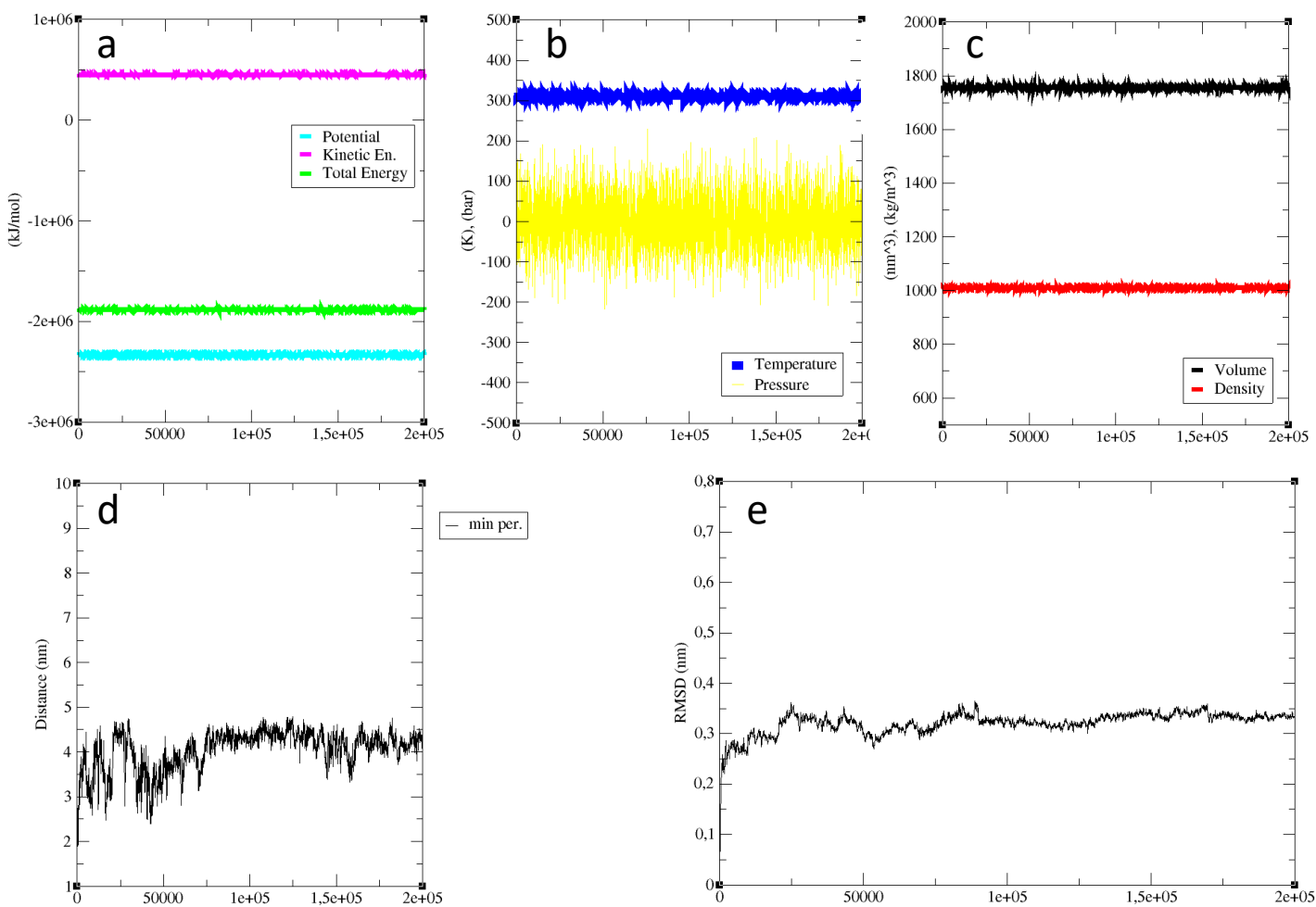
Quality check for wtGALT + ligands at 310K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances.

Supplementary File 4

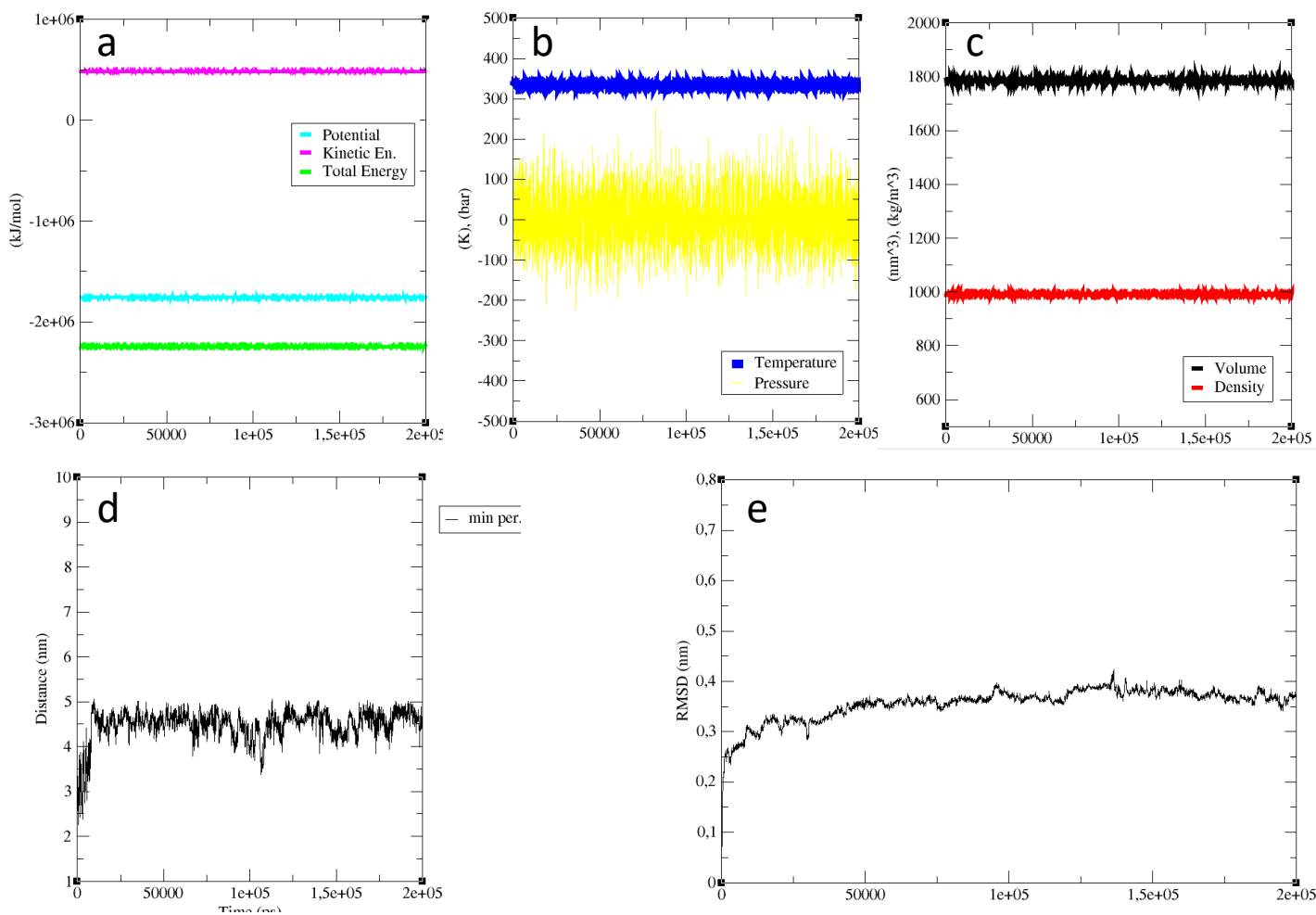
Quality check for p.Gln188Arg + ligands at 310K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances.

Supplementary File 5

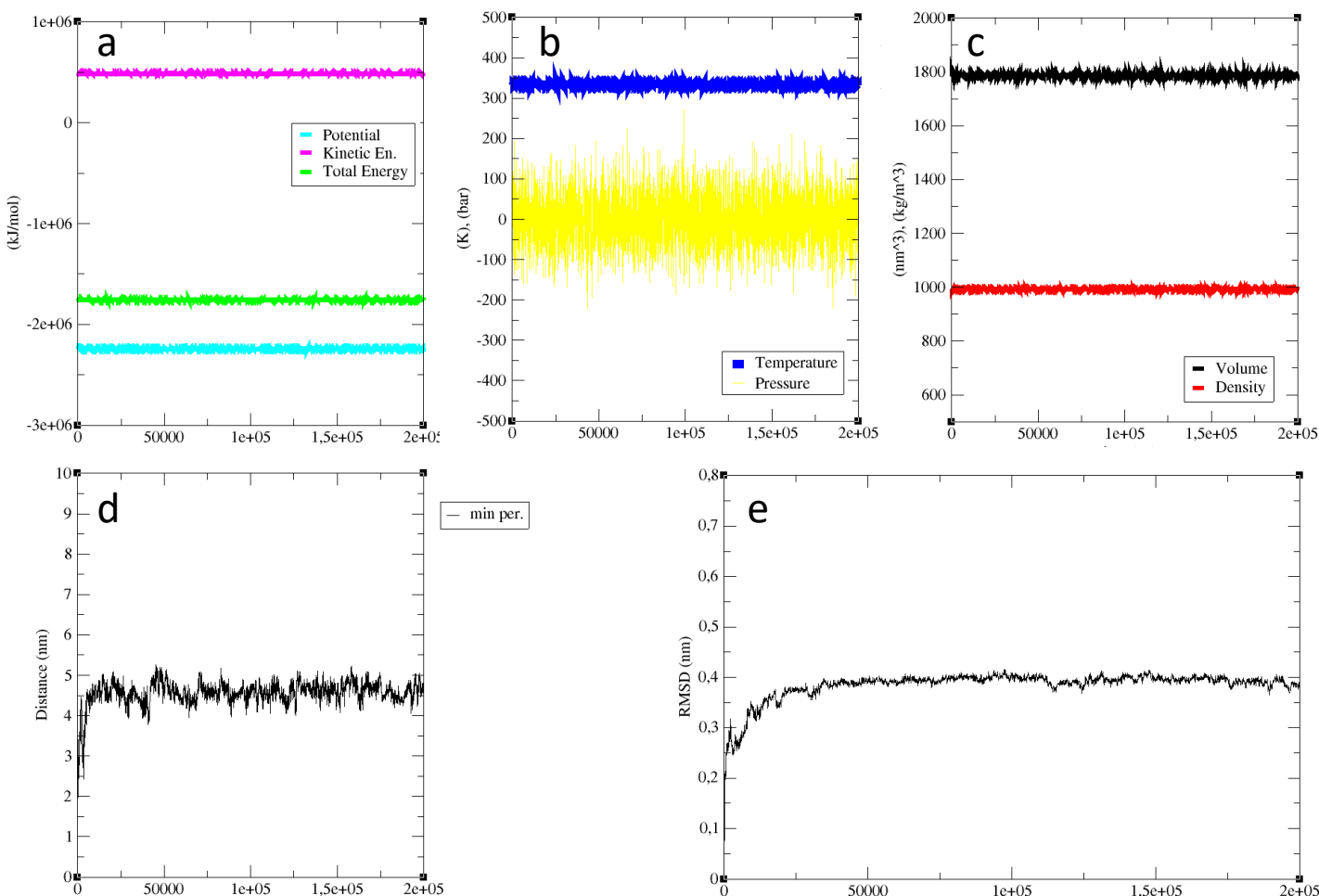
Quality check for wtGALT at 334K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances.

Supplementary File 6

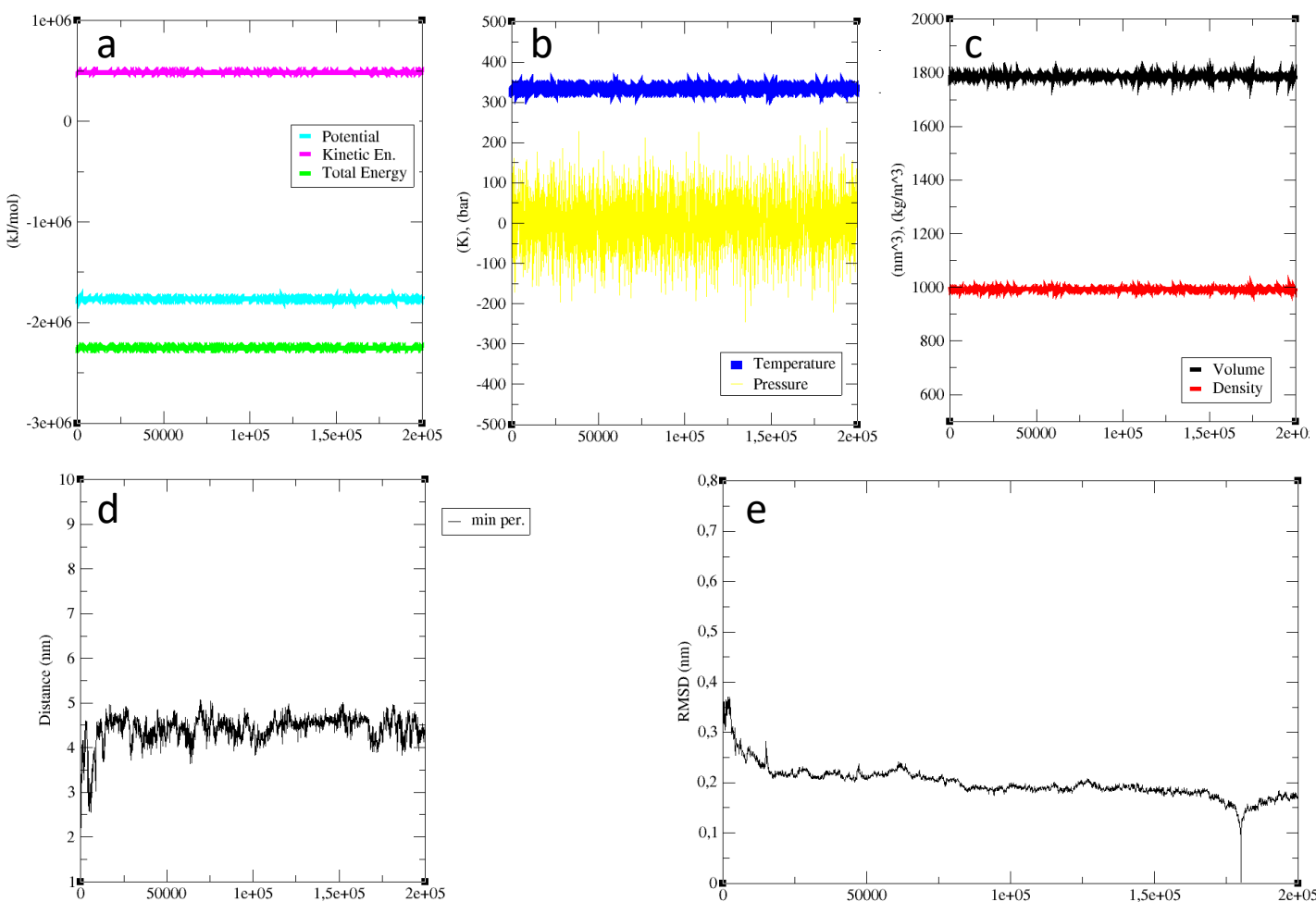
Quality check for p.Gln188Arg at 334K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances.

Supplementary File 7

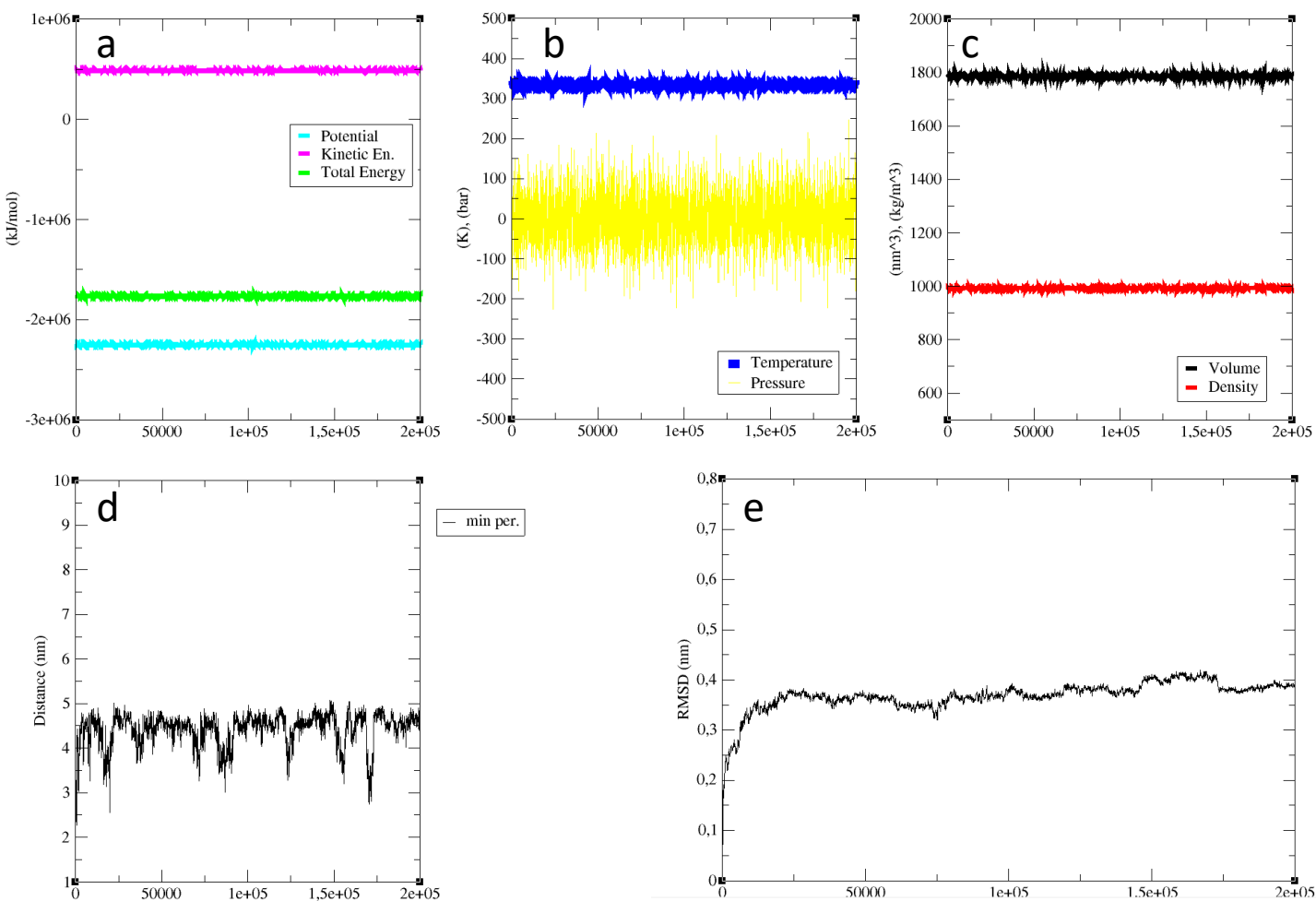
Quality check for wtGALT + ligands at 334K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances.

Supplementary File 8

Quality check for p.Gln188Arg + ligands at 334K



Legend: a: evolution of potential, kinetic and total energy; b: evolution of temperature and pressure; c: evolution of volume and density; d: variation of minimum distance between periodic images; e: root mean square deviation (RMSD) of atom distances.