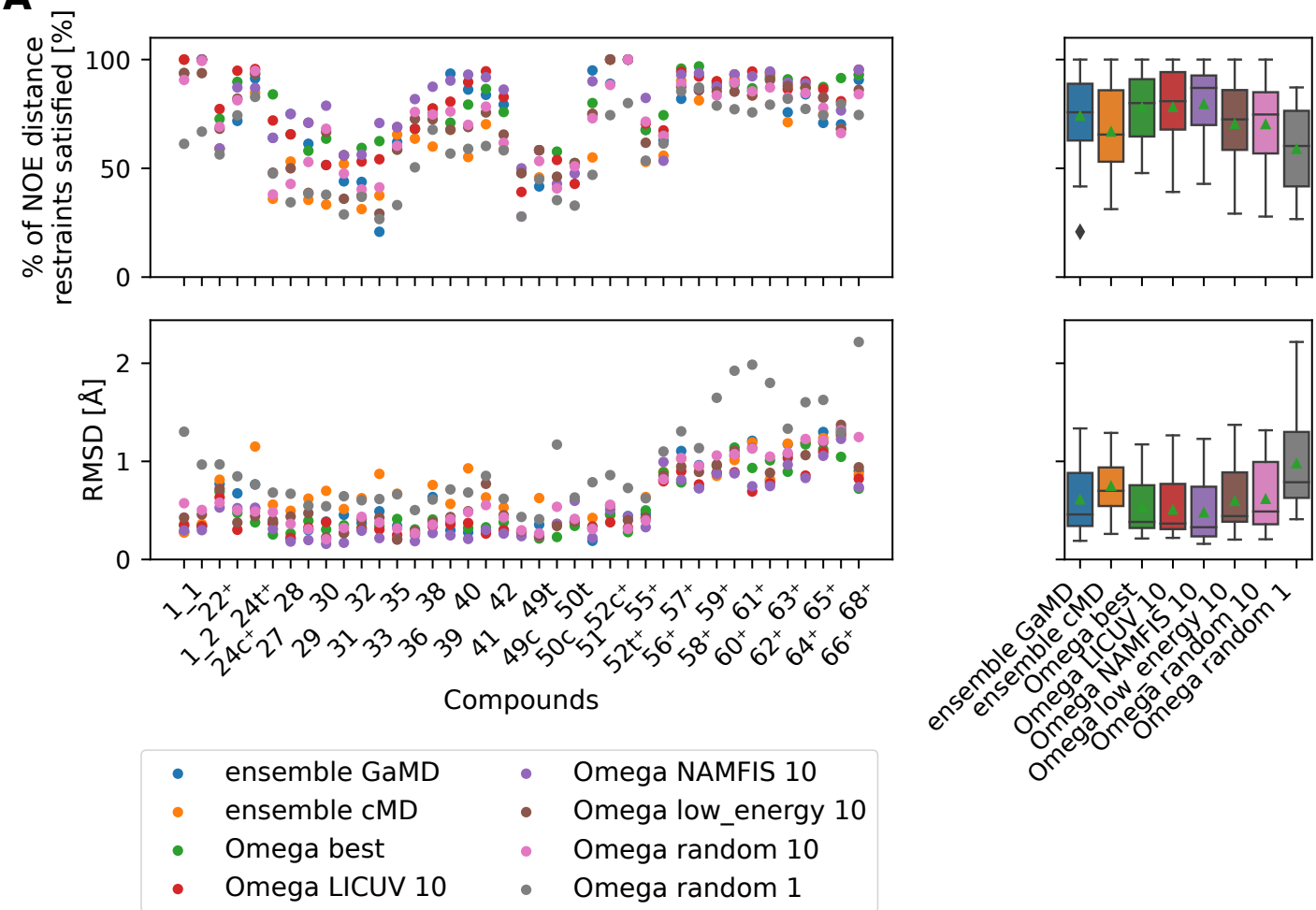
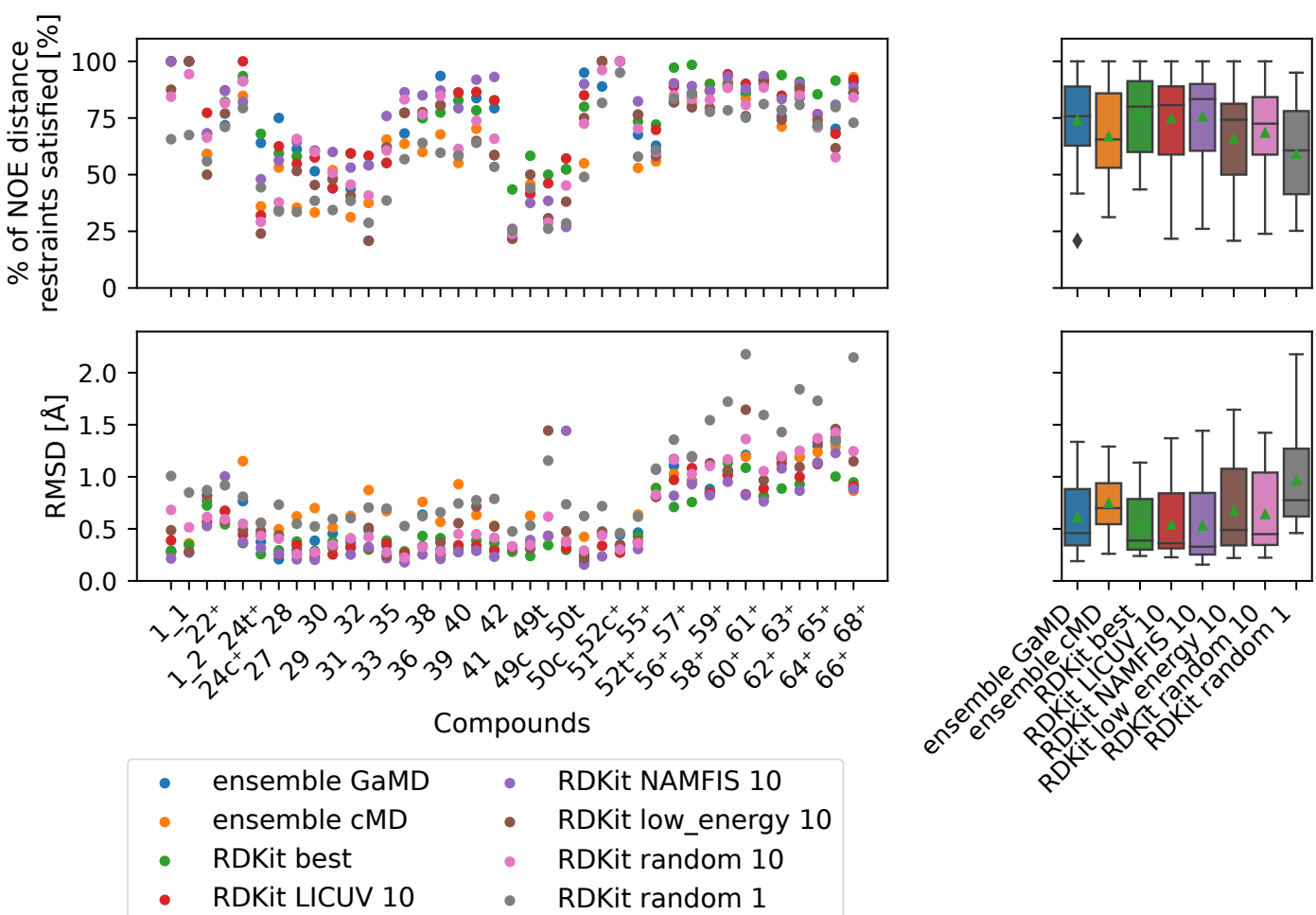
A


% of NOE distance restraints satisfied [%]
RMSD [Å]
Compounds
ensemble GaMD
ensemble cMD
Omega best
Omega LICUV 10
Omega NAMFIS 10
Omega low_energy 10
Omega random 10
Omega random 1


% of NOE distance restraints satisfied [%]
RMSD [Å]
Compounds
ensemble GaMD
ensemble cMD
RDKit best
RDKit LICUV 10
RDKit NAMFIS 10
RDKit low_energy 10
RDKit random 10
RDKit random 1