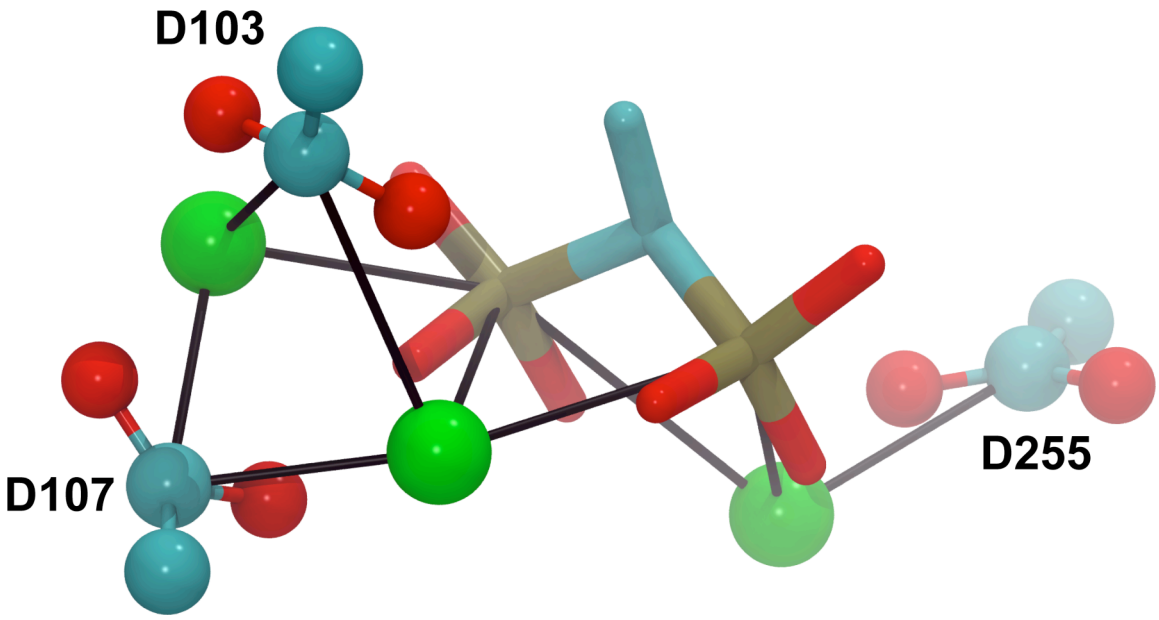

Figure S1. The restraints used in the molecular dynamics simulation. The side chains of Mg^{2+}-coordinating aspartate residues are shown in CPK. A portion of the minodronate ligand is shown in licorice. The three Mg^{2+} cations of the active site are shown as green spheres. Restraints, represented by black lines, were used to prevent the relevant atomic distances from deviating from the crystal-structure values by applying a harmonic potential with a force constant of 50 kcal/Å^2.