To carry out the refinements, the process was initially executed on Olex2 and aborted after a few seconds. The ORCA input generated during this process was modified and run on another machine with the modified DFs. After each calculation was finished, the WFN files were copied to the main folder to be read by NoSpherA2. Because of this, all CIF files indicate that the refinement was done with the Olex2 defaults (B3LYP/def2-SVP), since these were generated with Olex2. The name of each CIF file indicates how the refinement was carried out (functional, HF exchange percentage, etc.).