This .sdf files contains NMReDATA based on DFT (for structure) and GIAO (for chemical shifts and couplings)

The NMReDATA can be viewer opening the file with any text editor. The structure can be viewer using chemdraw, pymol, etc.

This files is very rich of data (including couplings in 2D spectra and comments). In principle one can simulate all 2D and 2D spectra based on the data.

It is meant to be used to verify .sdf file readers