Layered double hydroxides (LDH) are a promising material for use as a drug carrier thanks to their capacity for the intercalation of various anionic species, as well as their very low toxicity for the human body. Atorvastatin (ATS) is a drug used for blood cholesterol level lowering and cardiovascular disease prevention. Current methods of ATS delivery are quite ineffective, leading to the need for prescribing high ATS doses, which may cause discomfort to patients due to the drug's adverse side effects, most commonly including nausea, indigestion, joint pain or muscle pain. The intercalation of ATS into LDH could facilitate a controlled, targeted release of the drug into the patient's body, making a lower dose of drug more effective and thus alleviating the side effects of ATS. Molecular simulations utilising the COMPASS force field were used to assess three different models of ATS intercalated into Mg_2Al LDH with ATS concentrations of 61.99 %, 73.64 % and 70.64 %, corresponding to basal spacing of LDH layers of 3.751 nm, 3.808 nm and 3.823 nm, taken from X-ray diffraction experiments. Different starting orientations of ATS anions in the LDH interlayers were explored. The highest concentration of ATS appeared the most promising and lead to the most stable structure. Geometry optimisations and subsequent molecular dynamics simulations showed that the ATS anions interact with the LDH layers through hydrogen bonding between carboxyl groups of ATS and hydroxyl groups of LDH. This interaction was observed in nuclear magnetic resonance experiments as well, confirming the validity of the molecular simulations' results.