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Synthesis, Crystal Structure, and Non-Covalent Interactions in Ethyl 4-Hydrazinobenzoate Hydrochloride.

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ABSTRACT

The compound ethyl 4-hydrazinobenzoate hydrochloride (E-4HB), $C_9H_{13}N_2O_2Cl$, has been synthesized and characterized by FT-IR, 1H and ^{13}C NMR and X-ray diffraction. The compound crystallizes as colourless plates in the triclinic space group $P-1$, with $Z' = 2$ and cell parameters $a = 5.9566$ (4) Å, $b = 7.4498$ (6) Å, $c = 23.5349$ (17) Å, $\alpha = 84.323$ (3), $\beta = 84.521$ (3), $\gamma = 80.257$ (3), $V = 1020.95$ (13) Å³. The component ions are linked by two N-H...N hydrogen bonds and eight N-H...Cl hydrogen bonds to form complex sheets in which each of the chloride ions accepts hydrogen bonds from four different cations. Calculations on the Non-Covalent Interactions (NCI) amplify the crystallographic conclusions concerning the intermolecular hydrogen bonds.

Keywords: synthesis, crystal structure, molecular structure, hydrogen bonding, modelling of non-covalent interactions.

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