The Crystal Structure of N,N'-Bis-(1,3-dihydroxy-2-methylprop-2-yl)-pyrazine-2,3-dicarboxamide Semihydrate

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Crystal Structure, N,N'-Bis-(1,3-dihydroxy-2-methylprop-2-yl)-pyrazine-2,3-dicarboxamide Semihydrate, Hematoregulatory Active Compounds

Crystals of the title compound were obtained by recrystallization of N,N'-bis-(1,3-dihydroxy-2-methylprop-2-yl)-pyrazine-2,3-dicarboxamide in aqueous methanol. $C_{14}H_{22}N_4O_6 \cdot 1/2H_2O$ crystallizes in the triclinic system, s. g. P$\bar{1}$ (No. 2) with a = 9.339(4) Å, b = 13.218(9) Å, c = 14.5137(9) Å, α = 70.95(4)°, β = 87.66(4)°, γ = 87.13(4)°, Z = 4. Its crystal structure has been determined from diffractometer data and refined to a conventional R of 0.050 (4008 observations, 464 variable parameters). The structure contains two crystallographically independent molecules which are alternatingly stacked above each other along the [001]-direction. Extensive intermolecular hydrogen bonding between these stacks leads to the formation of slabs parallel to (010). The hydrate water is only loosely attached to one of the molecules and has no apparent influence on the stacking.