Crystal structure of methyl-4-(4-ethylenzamido)-
2-sulfamoylbenzoate, C₁₇H₁₈N₂O₅S

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Abstract
C₁₇H₁₈N₂O₅S, triclinic, P₁̅ (no. 2), a = 8.650(3) Å, b = 8.832(3) Å, c = 11.619(4) Å, α = 76.445(5)°, β = 79.684(5)°, γ = 78.770(5)°, V = 838.1 Å³, Z = 2, Rₑ(F) = 0.052, wRₑ(F) = 0.052, S(l) = 1.2 t/eq(C)]. The H atoms bonded to C and Ν atoms were positioned geometrically and refined using a riding model [aliphatic (H) = 1.5 t/eq(O)], the H atoms bonded to O atoms were located in difference Fourier maps and refined with Ω(O) = 0.85(2) Å and d(N—H) = 0.86 Å, t/eq(C)]. The H atoms bonded to C and Ν atoms were positioned geometrically and refined using a riding model. The H atoms bonded to O atoms were located in difference Fourier maps and refined with Ω(O) = 0.85(2) Å and d(N—H) = 0.86 Å, t/eq(C)].

The benzene ring in the title crystal structure is planar. The carboxamide moiety is coplanar with the benzene ring [dihedral angle 176.2(3)°]. The interatomic distance for C9—O1 is 1.218(4) Å, revealing a normal C=O double bond. In addition, the X-ray data also indicate intermolecular and intramolecular H-bonding interactions.

Table 1. Data collection and handling.

| Crystal | colorless cubbed, size 0.14 × 0.24 × 0.26 mm |
| Wavelength | Mo Kα radiation (0.71073 Å) |
| μ | 2.24 cm⁻¹ |
| Diffractometer, scan mode | Broker SMART CCD, φ/ω |
| 2Θmax | 50.04° |
| N(hkl)measured, N(hkl)unique | 4276, 2943 |
| Criterion for lobs, N(lobs) | lobs > 2σ(lobs), 2106 |
| N(param)refined | 240 |
| Programs | SHELXS-97 [5], SHELXL-97 [6], SHELXTL [7] |

Table 2. Atomic coordinates and displacement parameters (in Å²).

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Discussion
Amides are very useful starting materials for the synthesis of various bioactive molecules [2]. These compounds are also widely applied in medicine [3] and agriculture [4]. In view of these facts and in continuation of our interest in the agriculture, we attempted to synthesize a series of amide derivatives, some of which have comparatively high fungicidal activity.

* e-mail: xinghai.liu@yahoo.com.cn
Table 3. Continued.

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