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# *N*-(4-Ethoxyphenyl)-2-[(4-ethoxyphenylcarbamoyl)methoxy]acetamide monohydrate, a supramolecular chain structure formed by hydrogen bonds

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**Key indicators**

Single-crystal X-ray study
$T$ = 294 K
Mean $\sigma$(C–C) = 0.004 Å
H-atom completeness 93%
$R$ factor = 0.049
$wR$ factor = 0.124
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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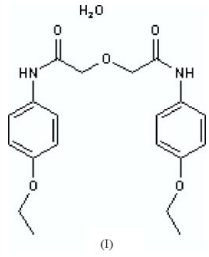
In the title compound, $C_{20}H_{24}N_2O_5\cdot H_2O$, the molecules are linked to each other by hydrogen bonds, and form a supramolecular chain structure. The organic and water molecules lie on crystallographic twofold rotation axes.

## Comment

Hydrogen-bonding interactions are regarded as among the most important driving forces in crystal engineering (Ranganaham *et al.*, 1999). Whitesides *et al.* (1995) have designed a family of self-assembled aggregates by hydrogen bonding between cyanuric acid and melamine. Recently, this method was also introduced for the construction of supramolecular nanostructures (Kosonen *et al.*, 2000). In our work, hydrogen bonds between water and the O atoms of $C_{20}H_{24}N_2O_5$ were used to form a novel supramolecular cavity.




(I)

In the title compound, (I), the water molecule (O4) forms two hydrogen bonds with O2 and a symmetry-equivalent O2′, the O4···O2 distance being 2.813 (3) Å, and the angle O2···O4···O2′ being 103.7 (2) Å. N—H forms a hydrogen bond with an O atom of another molecule (Table 2).

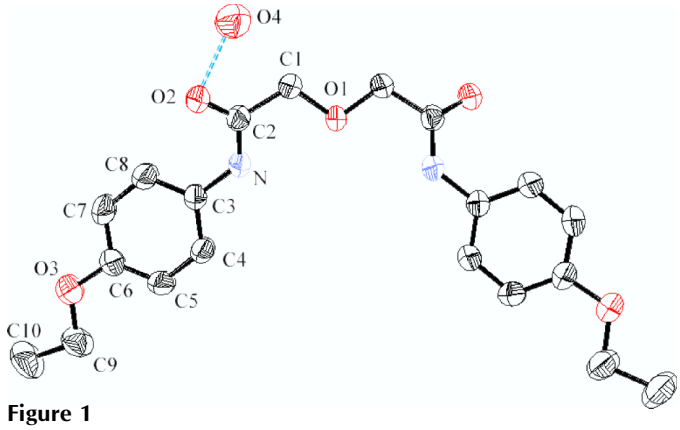



**Figure 1**
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. Dashed lines indicate a hydrogen-bonding interaction.

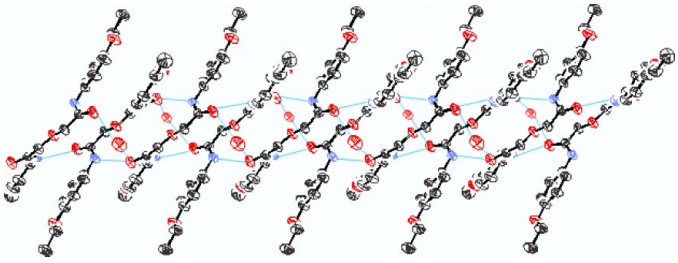


**Figure 2**
The chain-like supramolecular structure of (I). H atoms have been omitted for clarity. Dashed lines indicate hydrogen-bonding interactions.

The molecules are linked by O···O and N···O hydrogen bonds to form a one-dimensional supramolecular chain structure (Fig. 2). Adjacent molecules adopt opposite orientations due to the bulk of the benzene rings. A cavity formed by hydrogen bonds is observed (Fig. 3).

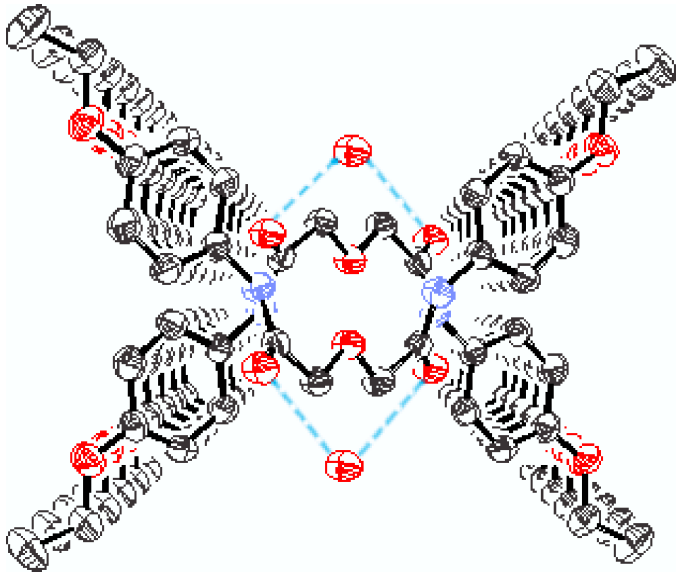


**Figure 3**
Supramolecular cavity formed by hydrogen bonds. H atoms are omitted for clarity. Dashed lines indicate hydrogen-bonding interactions.

## Experimental

The title compound was prepared by the direct reaction of chlorocarbonylmethoxyacetyl chloride with 4-ethoxyphenylamine in pyridine. The resulting mixture was separated by flash chromatography (ethyl acetate/benzene, 1:4). Suitable crystals were obtained by evaporation of an ethanol solution. Spectroscopic analysis, IR (KBr, $\nu$, cm$^{-1}$): 1666, 1117, 1235; $^1$H NMR ($CDCl_3$, $\delta$): 4.24 (*s*, 2H), 8.23 (*s*, 1H), 6.81–7.53 (*d*, 1H), 3.87–4.13 (*d*, 2H), 1.25–1.42 (*d*, 3H); analysis, calculated for $C_{20}H_{26}N_2O_6$: C 61.53, H 6.71, N 7.17%; found: C 61.94, H 6.44, N 7.06%.

### *Crystal data*

$C_{20}H_{24}N_2O_5\cdot H_2O$
$M_r$ = 390.43
Monoclinic, $C2/c$
$a$ = 30.575 (5) Å
$b$ = 7.929 (1) Å
$c$ = 8.356 (2) Å
$\beta$ = 95.09 (2)°
$V$ = 2017.7 (6) Å$^3$
$Z$ = 4
$D_x$ = 1.285 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 2.7–12.1°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 294 (2) K
Rhomboidal plate, colourless
0.70 × 0.52 × 0.06 mm

### *Data collection*

Siemens *P*4 diffractometer
$\omega$ scans
Absorption correction: none
2017 measured reflections
1771 independent reflections
880 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 25.0°
$h = 0 \rightarrow 36$
$k = 0 \rightarrow 9$
$l = -9 \rightarrow 9$
3 standard reflections
every 97 reflections
intensity decay: 4.4%

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.124
$S$ = 0.84
1771 reflections
130 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0027 (6)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C1$^{i}$ | 1.414 (3) | O3—C9 | 1.424 (3) |
| O1—C1 | 1.414 (3) | N—C2 | 1.338 (3) |
| O2—C2 | 1.232 (3) | N—C3 | 1.425 (3) |
| O2—O4 | 2.813 (3) | C1—C2 | 1.506 (3) |
| O3—C6 | 1.370 (3) | C9—C10 | 1.503 (4) |
| | | | |
| C1$^{i}$—O1—C1 | 110.3 (3) | N—C2—C1 | 117.1 (2) |
| C2—O2—O4 | 118.28 (16) | C4—C3—C8 | 118.9 (3) |
| C6—O3—C9 | 117.8 (2) | C4—C3—N | 119.5 (2) |
| C2—N—C3 | 126.2 (2) | C8—C3—N | 121.6 (2) |
| O1—C1—C2 | 112.9 (2) | O3—C6—C5 | 125.6 (3) |
| O2—C2—N | 124.8 (2) | O3—C6—C7 | 115.2 (3) |
| O2—C2—C1 | 118.1 (2) | O3—C9—C10 | 106.8 (3) |

Symmetry code: (i) $-x, y, \frac{5}{2} - z$.

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N—H0N···O2$^{ii}$ | 0.86 | 2.14 | 2.930 (3) | 153 |
| C4—H4···O4$^{iii}$ | 0.93 | 2.56 | 3.469 (3) | 167 |

Symmetry codes: (ii) $x, -y, \frac{1}{2} + z$; (iii) $-x, -y, 2 - z$.

All H atoms were positioned geometrically and refined with riding model constraints, except for those on the water molecule, which were not included.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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