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N-{2-[4-(Aminosulfonyl)phenyl]ethyl}-2-(4-hydroxyphenyl)acetamide

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Key indicators

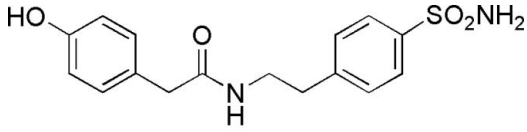
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.111
Data-to-parameter ratio = 13.4

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

The crystal structure of the title sulfonamide, $C_{16}H_{18}N_2O_4S$, is stabilized by strong N—H···O and O—H···O intermolecular hydrogen bonds.

Comment

The title compound, (I) (Fig. 1), was synthesized during structure–activity investigations aimed at optimizing the natural product template for bovine carbonic anhydrase II inhibition (Poulsen *et al.*, 2006). The amide group is almost planar [C9—N1—C8—O8 = −3.6 (3)°], with the carbonyl and NH bonds adopting a *trans* configuration. The *p*-hydroxyphenyl group folds back over the aminosulfonylphenyl group with a dihedral angle of 76.2 (1)° between the mean planes of the two benzene rings.



(I)

The crystal structure is characterized by a network of strong intermolecular N—H···O hydrogen bonds between the

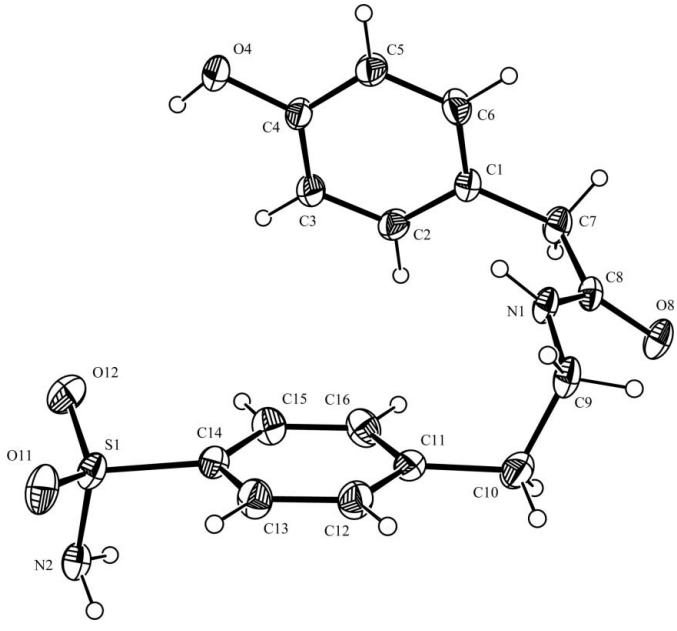


Figure 1
A view of the molecular structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms).

sulfonamido and amide H atoms and the sulfonamide, ketone and hydroxy O atoms, and O—H···O hydrogen bonds between the hydroxyl group and the ketone O-atom acceptor (Table 1).

Experimental

The title compound was prepared as previously reported (Poulsen *et al.*, 2006). Crystals of (I) suitable for X-ray diffraction studies were obtained by slow evaporation of a methanol solution of the compound (m.p. 476–478 K).

Crystal data

$C_{16}H_{18}N_2O_4S$
M_r = 334.39
Monoclinic, $P2_1/n$
a = 15.715 (3) Å
b = 10.250 (2) Å
c = 9.819 (3) Å
β = 91.862 (18)°
V = 1580.8 (6) Å^3
Z = 4
D_x = 1.405 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 295 K
Prism, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku AFC-7R diffractometer
ω–2θ scans
Absorption correction: none
3219 measured reflections
2779 independent reflections
2100 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°
3 standard reflections
every 150 reflections
intensity decay: 0.8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.03
2779 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.3548P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O11^{i}	0.86	2.22	2.909 (2)	138
N2—H2A···O8^{ii}	0.87	2.09	2.951 (2)	174
N2—H2B···O4^{iii}	0.87	2.19	3.001 (3)	155
O4—H4···O8^{iv}	0.86	1.86	2.698 (2)	165

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

The H atoms were positioned geometrically (C—H = 0.94–0.96 Å, N—H = 0.86–0.87 Å and O—H = 0.86 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier).

Data collection: *MSC/AFC7 Diffractometer Control for Windows* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC7 Diffractometer Control for Windows*; data reduction: *TEXSAN* for Windows (Molecular Structure Corporation, 2001); program(s) used to solve structure: *TEXSAN* for Windows; program(s) used to refine structure: *TEXSAN* for Windows and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN* for Windows and *PLATON* (Spek, 2003).

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References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Molecular Structure Corporation (1999). *MSC/AFC7 Diffractometer Control for Windows*. Version 1.02. MSC, The Woodlands, Texas, USA.
Molecular Structure Corporation (2001). *TEXSAN for Windows*. Version 1.06. MSC, The Woodlands, Texas, USA.
Poulsen, S.-A., Davis, R. A. & Keys, T. G. (2006). *Bioorg. Med. Chem.* **14**, 510–515.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.