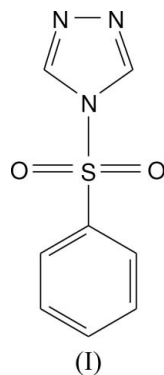
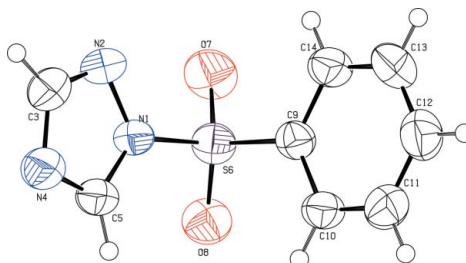


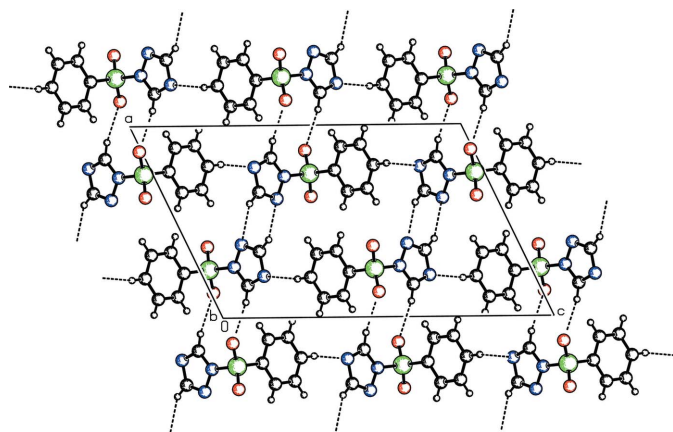
1-Phenylsulfonyl-1*H*-1,2,4-triazoleS. Naveen,<sup>a</sup> S. B. Benaka Prasad,<sup>b</sup>  
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## Key indicators

Single-crystal X-ray study  
*T* = 295 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
*R* factor = 0.045  
*wR* factor = 0.125  
Data-to-parameter ratio = 12.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.In the title compound,  $\text{C}_8\text{H}_7\text{N}_3\text{O}_2\text{S}$ , the dihedral angle  
between the 1,2,4-triazole ring and the phenyl ring is  
 $82.17(14)^\circ$ . The geometry around the S atom is distorted  
tetrahedral. The molecules are linked by intermolecular C—  
H $\cdots$ N and C—H $\cdots$ O hydrogen bonds.Received 13 November 2006  
Accepted 20 November 2006

## Comment

1,2,4-Triazoles have attracted considerable attention in the  
fields of medicine and agrochemical research and also in  
materials science due to their unique structures and proper-  
ties. Fluconazole, which contains two 1,2,4-triazole residues, is  
a powerful antifungal agent (Al-Soud *et al.*, 2004). Substituted  
1,2,4-triazoles have been found to exhibit anti-inflammatory,  
insecticidal, antifungal and antimicrobial activities (Boschelli  
*et al.*, 1993). Sulfonamides are among the most widely used  
antibacterial agents in the world, chiefly because of their low  
cost, low toxicity and excellent activity against common  
bacterial diseases. In the light of the above information, the  
title compound, (I), was synthesized and we report here its  
crystal structure.The molecular structure and the atom-numbering scheme of  
(I) are shown in Fig. 1. In (I), the dihedral angle between the**Figure 1**  
The molecular structure of (I), shown with 50% probability displacement  
ellipsoids.



**Figure 2**  
The packing of (I), viewed down the *b* axis. Dashed lines indicate intermolecular hydrogen bonds.

1,2,4-triazole ring and the phenyl ring is  $82.17(14)^\circ$ . The geometry around the S atom is distorted tetrahedral, with the largest deviations being observed for the O–S–O and O–S–N angles (Table 1). The O–S–O widening may be due to the repulsive interaction between the two short S=O bonds. The S–N bond distances lie within the expected range of 1.63–1.69 Å. The reduction of the N1–S6–C9 angle to  $103.86(10)^\circ$  from the ideal tetrahedral value is attributed to the Thorpe–Ingold effect (Bassindale *et al.*, 1984).

The crystal packing is stabilized by C–H...N and C–H...O hydrogen bonds (Table 2). These hydrogen bonds link the molecules into chains (Fig. 2).

## Experimental

1-Benzenesulfonyl-1*H*-1,2,4-triazole was obtained by the condensation of 1,2,4-triazole with benzenesulfonyl chloride in the presence of triethylamine as the base. First, 1,2,4-triazole (1 g, 14.4 mmol) was dissolved in dichloromethane (10 ml) and cooled to 273–278 K in an ice bath. Triethylamine (4.37 g, 43.2 mmol) was then added to the cold reaction mixture and the resulting solution was stirred for 10 min. Benzenesulfonyl chloride (2.44 g, 14.4 mmol) was added to the reaction mixture which was then allowed to cool to room temperature and stirred for 5 h. The reaction mass was monitored by thin-layer chromatography. On completion of the reaction, the solvent was removed under reduced pressure and the residue was taken up in water and extracted with ethyl acetate. Finally, the organic layer was washed with water and dried over anhydrous sodium sulfate. The product was a white crystalline solid (yield 2.25 g, 89%), which was dissolved in ethyl acetate–methanol (3:1) and kept for 4 d. Upon slow evaporation of the solvent, white crystals of (I) developed (m.p. 442.15 K).

### Crystal data

$C_8H_7N_3O_2S$	$Z = 4$
$M_r = 209.23$	$D_x = 1.513 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 11.395(14) \text{ \AA}$	$\mu = 0.33 \text{ mm}^{-1}$
$b = 5.045(3) \text{ \AA}$	$T = 295(2) \text{ K}$
$c = 17.698(19) \text{ \AA}$	Block, white
$\beta = 115.445(3)^\circ$	$0.25 \times 0.20 \times 0.20 \text{ mm}$
$V = 918.7(16) \text{ \AA}^3$	

### Data collection

MacScience DIPLabo 32001  
diffractometer  
 $\omega$  scans  
Absorption correction: none  
2728 measured reflections

1535 independent reflections  
1284 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$   
 $\theta_{\text{max}} = 25.0^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.125$   
 $S = 1.06$   
1535 reflections  
128 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.33P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$   
Extinction correction: *SHELXL97*  
Extinction coefficient: 0.038 (5)

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

S6–O7	1.413 (3)	N1–C5	1.346 (4)
S6–O8	1.422 (3)	N2–C3	1.307 (4)
S6–N1	1.699 (3)	N4–C3	1.347 (5)
S6–C9	1.741 (3)	N4–C5	1.299 (4)
N1–N2	1.361 (3)		
O7–S6–O8	121.63 (11)	N2–N1–C5	109.50 (19)
O7–S6–N1	105.74 (11)	N1–N2–C3	101.2 (2)
O7–S6–C9	110.69 (12)	C3–N4–C5	102.6 (2)
O8–S6–N1	103.42 (11)	N2–C3–N4	116.3 (3)
O8–S6–C9	109.69 (11)	N1–C5–N4	110.4 (2)
N1–S6–C9	103.85 (10)	S6–C9–C10	119.12 (19)
S6–N1–N2	122.01 (17)	S6–C9–C14	119.47 (18)
S6–N1–C5	128.08 (17)		

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3–H3...N2 <sup>i</sup>	0.93	2.55	3.425 (6)	157
C5–H5...O8 <sup>ii</sup>	0.93	2.38	3.296 (5)	169
C12–H12...N4 <sup>iii</sup>	0.93	2.57	3.490 (6)	169

Symmetry codes: (i)  $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $-x, -y + 1, -z + 1$ ; (iii)  $x, -y - \frac{1}{2}, z - \frac{1}{2}$ .

H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C–H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$ .

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *PLATON*.

The authors are grateful to DST–CSIR, New Delhi for financial support under the projects SP/I2/FOO/93 and 01(1904)/03/EMR-II 2004. Analytical and IR spectroscopic data were obtained from instruments funded by DST–FIST and UGC–SAP (phase I).

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