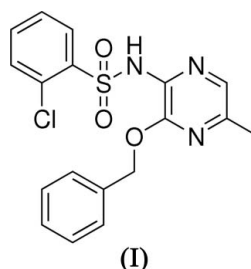
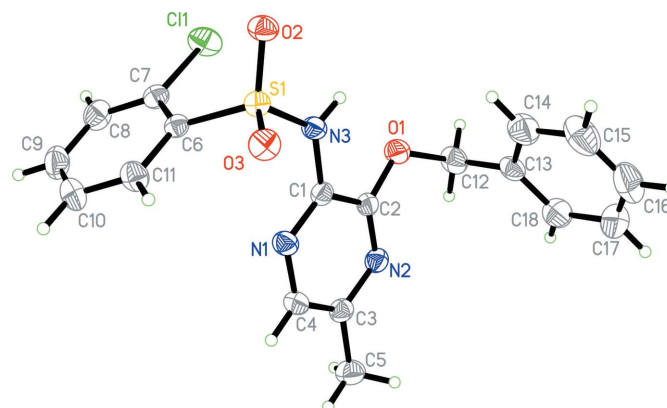


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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.045
 wR factor = 0.106
Data-to-parameter ratio = 15.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***N*-(3-Benzyloxy-5-methylpyrazin-2-yl)-
2-chlorobenzenesulfonamide**Molecules of the title compound, $\text{C}_{18}\text{H}_{16}\text{ClN}_3\text{O}_3\text{S}$, crystallize as centrosymmetric dimers, connected by intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds. The dimers are interlinked *via* $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds.Received 29 March 2006
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Comment

The vasoconstrictive peptide endothelin has been implicated as a causative factor in a number of diseases, and as such it has become a popular target in drug discovery (Wu *et al.*, 2001; Murugesan *et al.*, 2000; Arai *et al.*, 1990). Sulfonamides have been identified as important non-peptide and selective endothelin antagonists (Stein *et al.*, 1995). We have synthesized a series of *N*-pyrazin-2-ylphenylsulfonamides and we report here the crystal structure of the title compound, (I).The structure of the molecule of (I) is shown in Fig. 1. The bond lengths and angles (Table 1) are normal. The C6–C11 and C13–C18 benzene rings are oriented at angles of 88.83 (7) and 84.33 (9)°, respectively, with respect to the pyrazine plane. Intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds result in the formation of a dimer in the crystal structure; adjacent dimers are linked *via* $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Table 2).**Figure 1**
View of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

Compound (I) was prepared according to the literature procedure of Bradbury *et al.* (1997). Colourless prismatic single crystals of (I) were grown from a saturated solution in dichloromethane.

Crystal data

$C_{18}H_{16}ClN_3O_3S$ $Z = 4$
 $M_r = 389.85$ $D_x = 1.414 \text{ Mg m}^{-3}$
 Monoclinic, $P2_1/n$ Mo $K\alpha$ radiation
 $a = 11.764 (3) \text{ \AA}$ $\mu = 0.35 \text{ mm}^{-1}$
 $b = 13.519 (4) \text{ \AA}$ $T = 293 (2) \text{ K}$
 $c = 12.068 (4) \text{ \AA}$ Prism, colourless
 $\beta = 107.466 (5)^\circ$ $0.26 \times 0.22 \times 0.20 \text{ mm}$
 $V = 1830.7 (9) \text{ \AA}^3$

Data collection

Bruker SMART 1000 CCD area-detector diffractometer 10398 measured reflections
 φ and ω scans 3745 independent reflections
 Absorption correction: multi-scan 2227 reflections with $I > 2\sigma(I)$
 (SADABS; Sheldrick, 1996) $R_{int} = 0.050$
 $T_{min} = 0.915, T_{max} = 0.934$ $\theta_{max} = 26.4^\circ$

Refinement

Refinement on F^2 H-atom parameters constrained
 $R[F^2 > 2\sigma(F^2)] = 0.045$ $w = 1/[\sigma^2(F_o^2) + (0.0461P)^2]$
 $wR(F^2) = 0.106$ where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.01$ $(\Delta/\sigma)_{max} = 0.002$
 3745 reflections $\Delta\rho_{max} = 0.24 \text{ e \AA}^{-3}$
 236 parameters $\Delta\rho_{min} = -0.32 \text{ e \AA}^{-3}$

Table 1 Selected geometric parameters ($\text{\AA}, ^\circ$).

S1—O3	1.4246 (18)	N2—C2	1.308 (3)
S1—O2	1.4310 (17)	N2—C3	1.356 (3)
S1—N3	1.629 (2)	N3—C1	1.401 (3)
S1—C6	1.775 (2)	O1—C2	1.350 (3)
N1—C1	1.309 (3)	O1—C12	1.447 (3)
N1—C4	1.349 (3)		
O3—S1—O2	118.26 (11)	N3—S1—C6	105.64 (11)
O3—S1—N3	110.20 (11)	C2—N2—C3	116.9 (2)
O2—S1—N3	105.34 (11)	C1—N3—S1	124.52 (18)
O3—S1—C6	107.38 (11)	N2—C2—O1	122.7 (2)
O2—S1—C6	109.35 (11)	O1—C2—C1	115.1 (2)

Table 2 Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N3—H3...O2 ⁱ	0.86	2.26	3.061 (3)	156
C11—H11...Cl1 ⁱⁱ	0.93	2.66	3.488 (3)	149

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

H atoms were placed in calculated positions ($N-H = 0.86 \text{ \AA}$ and $C-H = 0.93-0.97 \text{ \AA}$) and included in the final cycles of refinement in

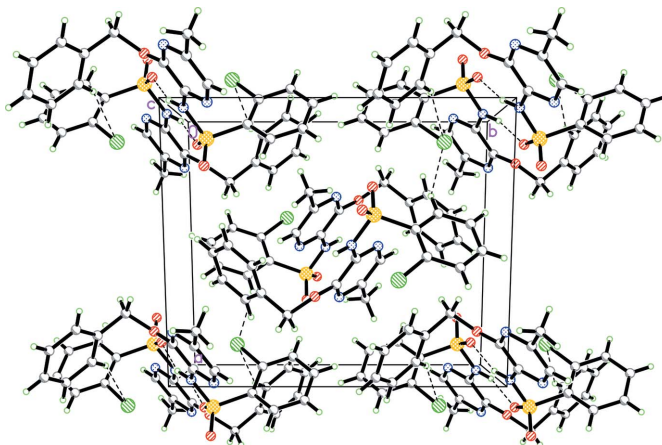


Figure 2 The crystal packing of (I), viewed down the c axis. Hydrogen bonds are shown as dashed lines.

the riding-model approximation, with $U_{iso}(H) = 1.2$ or 1.5 (methyl) times $U_{eq}(C,N)$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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