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An additional methylene group driving the conformation and assembly of two arylsulfonamide *para*-alkoxychalcone hybrids

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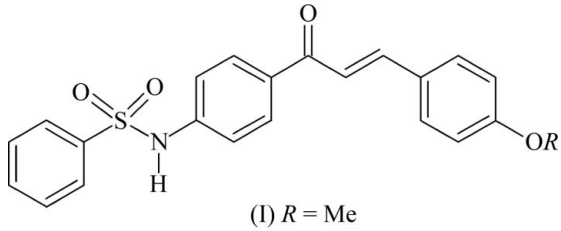
The structures of two arylsulfonamide *para*-alkoxychalcones, namely, *N*-{4-[(*E*)-3-(4-methoxyphenyl)prop-2-enoyl]phenyl}-benzenesulfonamide, $C_{22}H_{19}NO_4S$, (I), and *N*-{4-[(*E*)-3-(4-ethoxyphenyl)prop-2-enoyl]phenyl}benzenesulfonamide, $C_{23}H_{21}NO_4S$, (II), reveal the effect of the inclusion of one $-CH_2-$ group between the CH_3 branch and the alkoxy O atom on the conformation and crystal structure. Although the molecular conformations and one-dimensional chain motifs are the same in both structures, their crystallographic symmetry, number of independent molecules and crystal packing are different. The crystal packing of (I) is stabilized by weak C—H$\cdots\pi$ and π–π interactions, while only C—H$\cdots\pi$ contacts occur in the structure of (II). The role of the additional methylene group in the crystal packing can also be seen in the fact that the alkoxy O atom is an acceptor in nonclassical hydrogen bonds only in the *para*-ethoxy analogue, (II). The remarkable similarity between the crystal packing features of (I) and (II) lies in the formation of N—H$\cdots$O hydrogen-bonded ribbons, a synthon commonly found in related compounds.

Comment

Compounds containing a sulfonamide group are well known to possess strong antibacterial effects, and they are widely used against common bacterial diseases due to their low cost, low toxicity and excellent pharmacological profiles (Ozbek *et al.*, 2007). The sulfonamide group is also present in many biologically active compounds, such as antimicrobial, antithyroid, antitumour and antimalarial drugs (Ozdemir *et al.*, 2009; Seo *et al.*, 2010; Domínguez *et al.*, 2005; Connor, 1998; Hanson *et al.*, 1999). In addition, many substituted aromatic and heterocyclic sulfonamides have been synthesized and their activity against glaucoma has been evaluated (Remko *et al.*, 2010). Chalcones containing an arylsulfonamide group are emerging compounds for which antimalarial properties have already been demonstrated (Domínguez *et al.*, 2005).

As part of our ongoing studies of sulfonamides in terms of their structural features (Martins *et al.*, 2009; Fernandes *et al.*, 2011), in this study the arylsulfonamide *para*-alkoxychalcones, *N*-{4-[(*E*)-3-(4-methoxyphenyl)prop-2-enoyl]phenyl}benzenesulfonamide, (I), and *N*-{4-[(*E*)-3-(4-ethoxyphenyl)prop-2-enoyl]phenyl}benzenesulfonamide, (II), differing only in one methylene group in the *para*-alkoxy fragment on the chalcone skeleton, were synthesized and their crystal structures determined using single-crystal X-ray diffraction. This molecular difference of only one $-CH_2-$ group is enough to change the crystal assembly and symmetry. Likewise, the absence of methylene in the *para*-alkoxy group of (I) is also related to the conformational variability observed in this compound.



(I) *R* = Me
(II) *R* = Et

Because of the slight molecular structure differences between (I) and (II), they crystallize in different crystal systems and space groups. While the crystal structure of (I) was solved in the centrosymmetric triclinic space group $P\overline{1}$, with two independent molecules in the asymmetric unit, (II) crystallizes in the monoclinic space group $P2_1/c$ with only one molecule in the asymmetric unit (Fig. 1).

Compound (I) has two conformers in its crystal structure, labelled *A* and *B*. The chalcone molecular backbones of both conformers are almost completely planar [r.m.s. deviations = 0.0537 and 0.0440 Å, respectively, for conformers *A* and *B*, with the greatest deviations being −0.2053 Å for atom C18*A* and 0.2076 Å for atom C8*B*, where the chalcone plane is defined by atoms C13–C15/O3 and the C atoms of rings *B* (central) and *C* (alkoxy-substituted) in Fig. 1] and therefore similar, even though there are slight rotations about the sulfamyl S1—N1 and sulfonyl S1—C1 bridging bond axes (Fig. 2). More specifically, the chalcone group of conformer *A* is more planar than that of conformer *B*. In the latter, there are three slight rotations on the bond axes of: (i) C10*B*—C13*B*, which displaces central ring *B* from the neighbouring carbonyl group [*e.g.* the C9*B*—C10*B*—C13*B*—O3*B* torsion angle is 8.3 (4)°, *cf.* 5.6 (5)° for the corresponding torsion angle in conformer *A*]; (ii) C15*B*—C16*B*, twisting the *para*-alkoxy-substituted ring *C* from the C14=C15 group [*e.g.* the C14*B*—C15*B*—C16*B*—C21*B* torsion angle is −7.8 (4)°, *cf.* −0.6 (6)° for the corresponding torsion angle in conformer *A*]; (iii) C19*B*—O4*B*, setting the methyl group of the methoxy in the *para* position out of the ring *C* plane [*e.g.* the C18*B*—C19*B*—O4*B*—C22*B* torsion angle is 7.8 (4)°, *cf.* 6.9 (5)° for the corresponding torsion angle in conformer *A*]. The rotation on this last bond axis is also appreciable in conformer *A* of (I)

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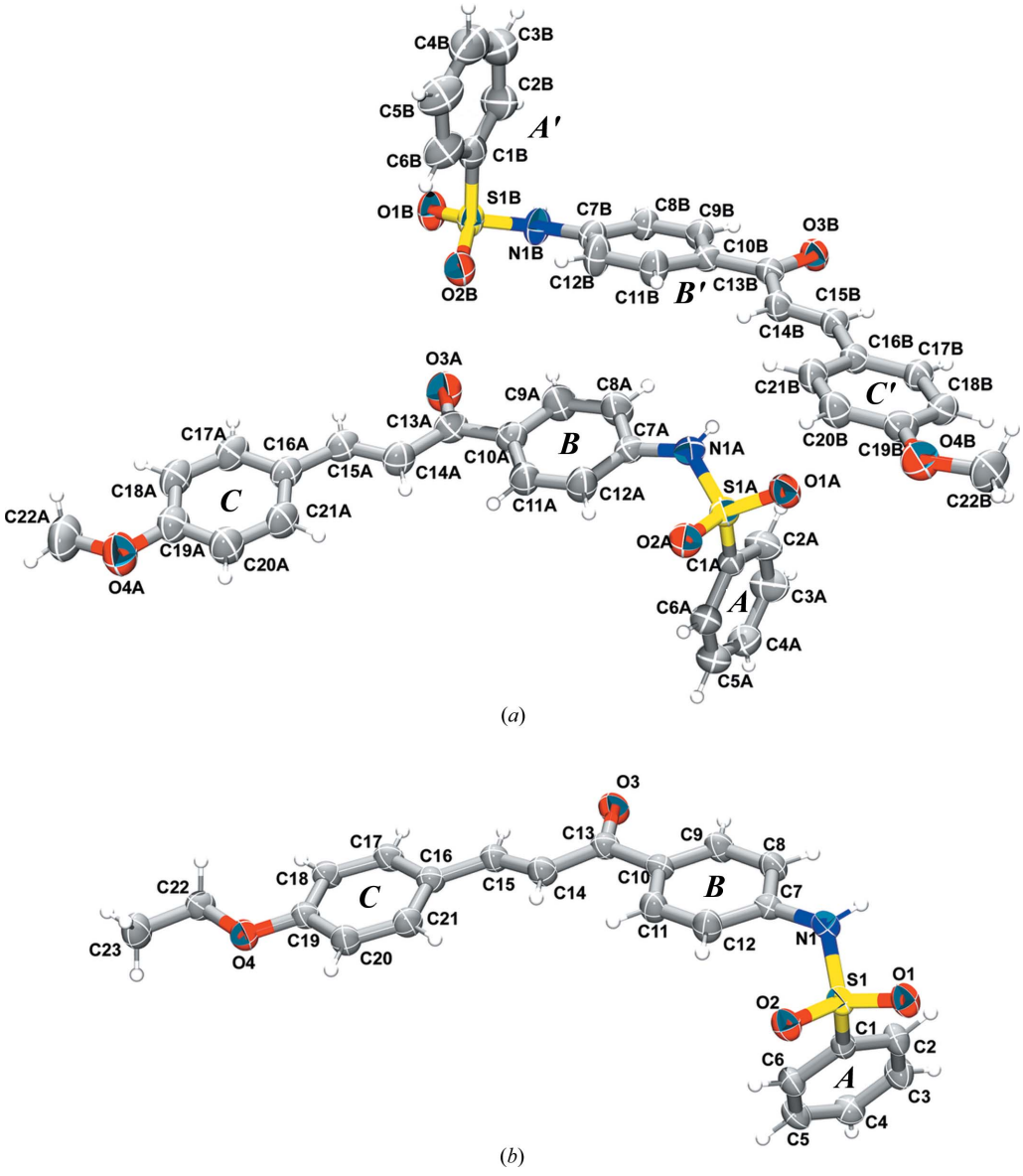

Figure 1
A view of the molecular structures of (*a*) (I) and (*b*) (II), showing the atom- and ring-labelling schemes. Displacement ellipsoids are drawn at the 30% probability level.

and in (II), which also shows a remarkable planarity of its chalcone skeleton (r.m.s. deviation = 0.0371 Å, with the greatest deviation being 0.1563 Å for atom C8), except that the ethyl group is slightly out of the ring *C* plane, as mentioned above.

It is interesting to note that in the crystal structure of the only other example of an arylsulfonamide chalcone hybrid found in the Cambridge Structural Database (CSD, Version 5.33, August 2012 update; Allen, 2002), namely, 4′-(*p*-toluenesulfonylamino)-4-hydroxychalcone (TSAHC; CSD refcode NARZIR; Seo *et al.*, 2010), the chalcone skeleton is strongly twisted, wherein the least-squares planes through the corresponding rings *B* and *C* form an angle of 33.9 (8)°. We observe values of 10.8 (1), 10.02 (8) and 5.2 (8)° in molecules *A* and *B* of (I) and in (II), respectively. In the structure of TSAHC, the observed twist may be related to the presence of a further intermolecular classical O—H···O hydrogen bond involving the *para*-hydroxy and sulfamyl groups of TSAHC, which is not present in (I) and (II). However, the N—H···O hydrogen bonding between the amino and carbonyl groups is

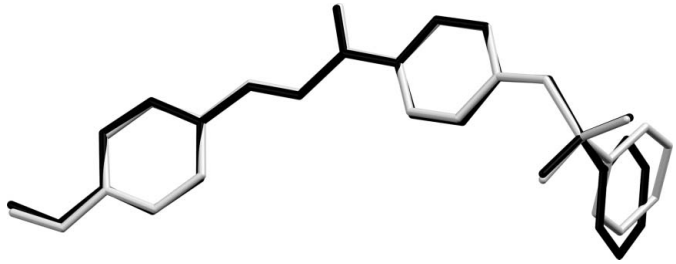

Figure 2
A superposition of the conformers *A* (grey) and *B* (black) of (I). H atoms have been omitted for clarity.

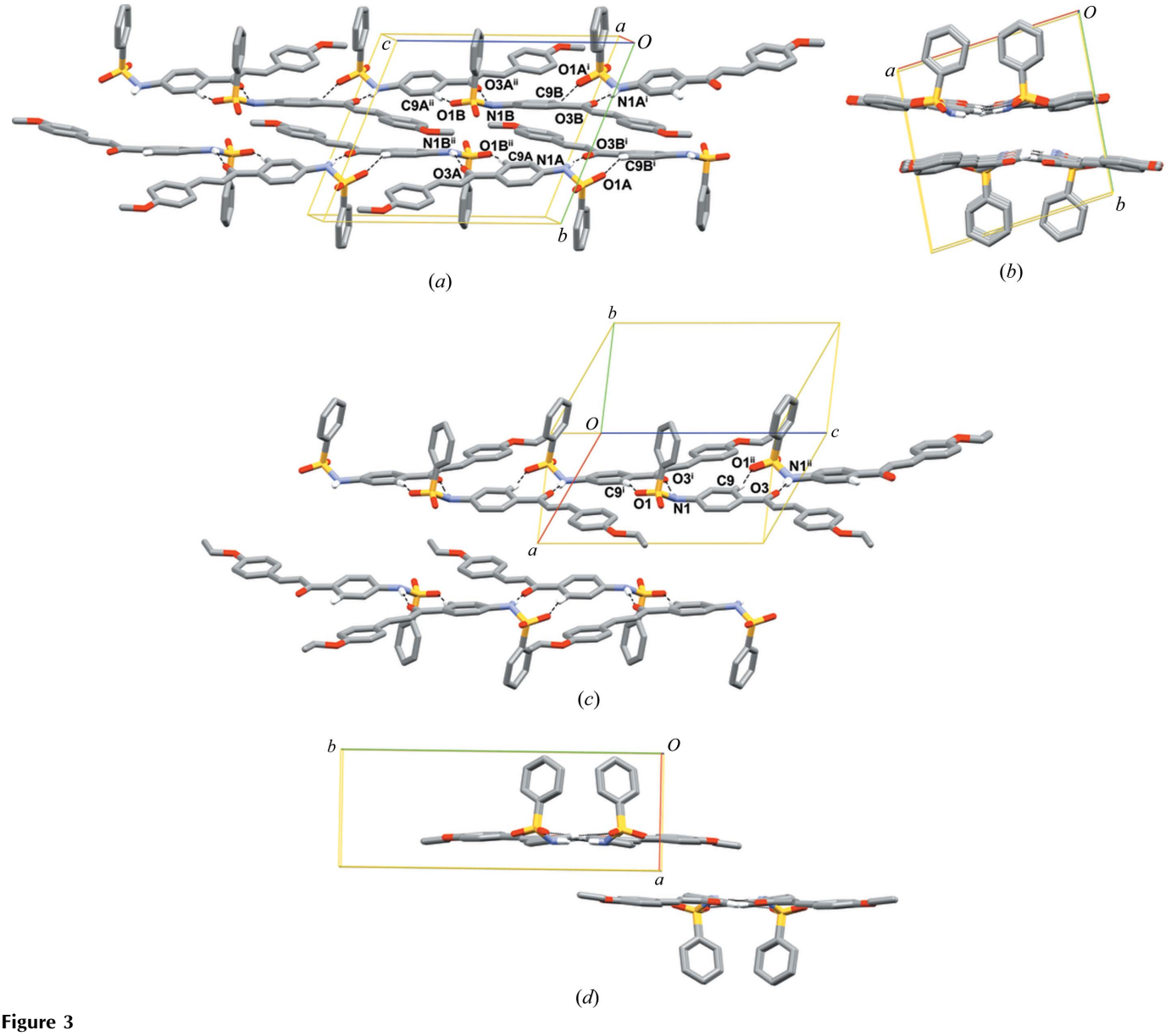

Figure 3
(*a*) The infinite one-dimensional chains of (I), propagating along the [001] direction, (*b*) the stacking of the chains of (I), (*c*) the infinite one-dimensional chains of (II), propagating along the [001] direction, and (*d*) the stacking of the chains of (II). Classical N—H···O and nonclassical C—H···O hydrogen-bond interactions are shown as dashed lines. [Symmetry codes, (*a*): (i) $-x+1, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$; (*c*): (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.]

conserved in the structures of TSAHC, (I) and (II). In all three sulfonamide chalcone derivatives, these N—H···O interactions give rise to infinite one-dimensional ribbons running along the [001] (or [010] in TSAHC) direction (Fig. 3). In the structures of both (I) and (II), each chain has all phenyl rings *A* oriented towards the same side of the sulfonamide–chalcone plane (Fig. 3). These ribbons are made up of alternating molecules *A* and *B* in (I), while *c*-glide-related units assemble these supramolecular motifs in (II). The linear ribbons are stacked face-to-face, along the [120] direction in (I) and along the *a* axis in (II). In contrast, a zigzag chain is formed with 2_1-screw axis symmetry-related molecules in TSAHC.

In addition to the classical hydrogen bonds, the ribbons in (I) and (II) are supported by C9—H9···O1 hydrogen bonds (Tables 1 and 2). The pairwise interactions co-exist with a degree of coplanarity between sulfonamide–chalcone fragments of the hydrogen-bonded molecules. Between successive molecules along the chain, these fragments, defined as the chalcone plane plus atoms N1 and S1, form dihedral angles of 15.0 and 6.4° in (I) and (II).

The supramolecular assemblies of (I) and (II) are thus similar in the formation of linear ribbons, but the structural similarities between them end there. While the crystal packing of (I) is stabilized by weak C—H···π and π–π interactions, only the former interactions occur in (II). In (I), inversion-related molecules *A* interact through their CH_3 groups and phenyl *A* rings in very weak but co-operative C—H···π interactions involving two methyl H atoms ($CgA\cdots H22D^{iv}$ =

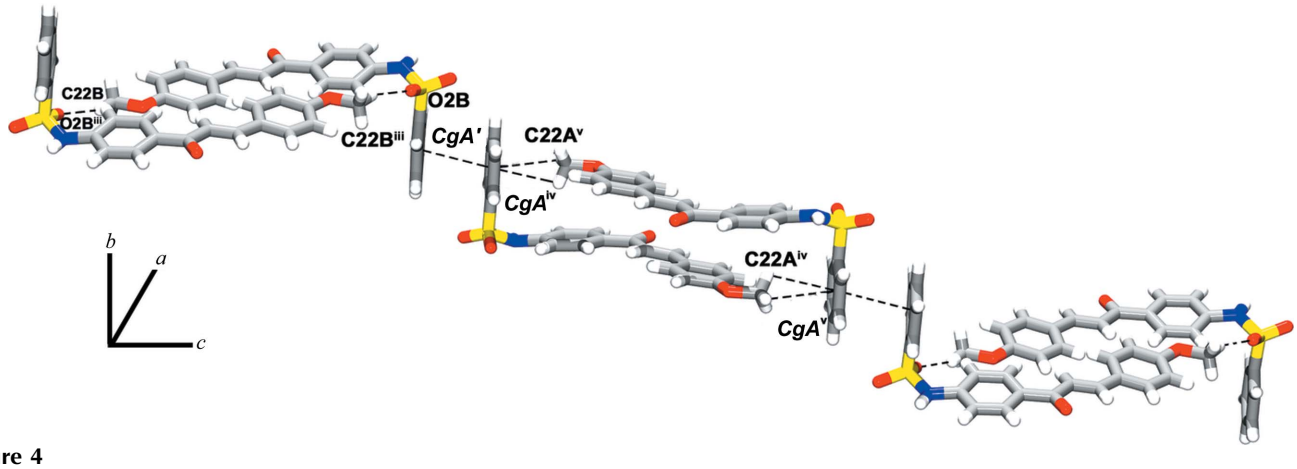

Figure 4
The C—H···O, C—H···π and π–π interactions (dashed lines) in the structure of (I). [Symmetry codes: (iii) $-x, -y+1, -z$; (iv) $x, y-1, z+1$; (v) $-x, -y+1, -z+2$.]

3.28 Å and $CgA\cdots H22E^{iv}$ = 3.33 Å, where *CgA* is the centroid calculated through the ring *A* C atoms of molecule *A*; see Table 1 for symmetry code) (Fig. 4). The rings of both molecules *A* and *B* are further connected by weak π–π interactions in (I), with a $CgA\cdots CgA'$ distance between translation symmetry-related molecules at $(x, y+1, z-1)$ of 3.72 (5) Å (Fig. 4). However, the ethoxy CH_3 group in (II) is involved in C—H···π contacts in this structure and π–π interactions do not occur. The intercalation between the CH_3 group and the O4 atom by a CH_2 moiety of the ethoxy group in (II) leads to the formation of a C23—H23*A*···*CgA* interaction ($CgA\cdots H23A^{iii}$ = 3.04 Å; see Table 2 for symmetry code), assembling dimers made up of inversion-related molecules (Fig. 5*a*). In this figure, it is possible to see the occurrence of a π–π interaction between the π-electrons of the double bond between atoms C14 and C15 and the C atoms of ring *B* [$CgD\cdots CgB^{v}$ = 3.56 Å, where *CgD* is the centroid calculated through atoms C14 and C15, and *CgB* is the centroid calcu-

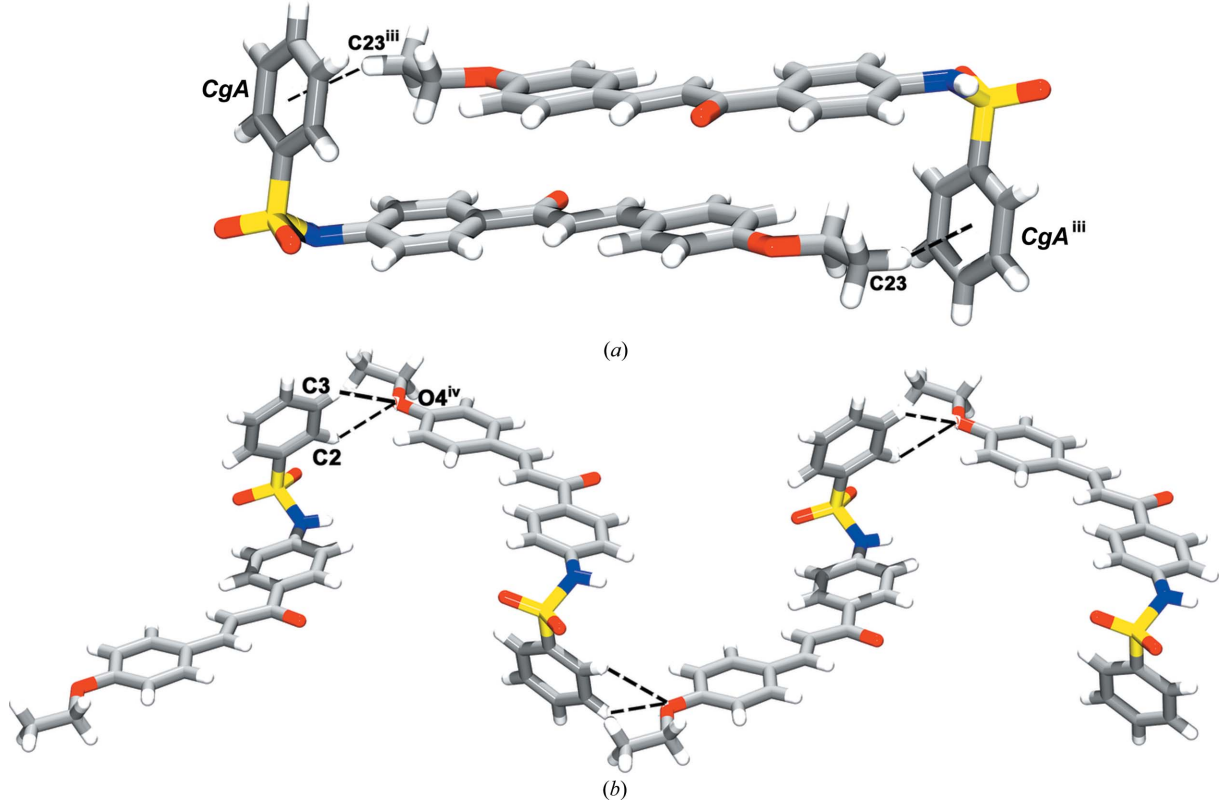

Figure 5
(*a*) The C—H···π interaction and (*b*) the bifurcated C—H···O hydrogen-bond contacts in the structure of (II). These interactions are shown as dashed lines. [Symmetry codes: (iii) $-x+1, -y, -z+2$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.]

lated through the C atoms of ring *B*; symmetry code: (v) $-x+1$, $-y$, $-z+2$]. In this structure, the role of the additional methylene group in the crystal packing and symmetry can also be seen in the fact that alkoxy atom O4 is involved as an acceptor in weak acceptor-bifurcated nonclassical hydrogen bonds, having as donors the neighbouring C2—H2 and C3—H3 groups of phenyl ring *A*. Both C2—H2···O4^{iv} and C3—H3···O4^{iv} contacts occur between 2_1-screw axis symmetry-related molecules assembled into zigzag chains along the [010] direction (see Fig. 5*b* for symmetry code). These contacts and chains are not observed in (I). In the structure of (I), the methoxy group is involved in nonclassical C—H···O hydrogen bonding, *viz.* C22*B*—H22*A*···O2*B*^{iii}, as a donor to an O atom of SO_2 in an inversion-related molecule *B* (Fig. 4) (see Table 1 for symmetry code).

In conclusion, this study presents an interesting example in which a molecular difference of only one CH_2 group in the terminal alkoxy group has altered the crystal packing and symmetry in two otherwise identical compounds. While classical hydrogen-bonding patterns are conserved in both structures investigated here, the combination of weak C—H···O, C—H···π and π–π contacts involving the phenyl heads and alkoxy tails differs, and this is responsible for the differences observed in the conformations and intermolecular architectures of these two chalcone–sulfonamide analogues. From a crystallographic point of view, not only are the crystal systems and space groups different for (I) and (II), but the Z' values also differ. This reveals that their crystal structures must depend on the intermolecular contact patterns involving the methylene group of the alkoxy substituent.

Experimental

Compounds (I) and (II) were synthesized by Claisen–Schmidt condensation from *N*-(4-acetylphenyl)benzenesulfonamide with either *p*-methoxybenzene [for (I)] or *p*-ethoxybenzaldehyde [for (II)], using sodium hydroxide in ethanol (50% *w*/*w*) as catalyst. The reactions were performed at 343 K for about either 22 h [for (I)] or 24 h [for (II)]. In each case, the precipitate was recrystallized from dichloromethane to obtain single crystals. The reaction yields were 57 and 65% for (I) and (II), respectively, and the melting-point ranges were 446–448 K and 425–427 K, respectively.

Compound (I)

Crystal data

$C_{22}H_{19}NO_4S$
M_r = 393.44
Triclinic, $P\overline{1}$
a = 11.8650 (3) Å
b = 12.2420 (3) Å
c = 14.7287 (3) Å
α = 68.075 (1)°
β = 81.665 (1)°
γ = 80.437 (1)°
V = 1948.99 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 298 K
0.28 × 0.15 × 0.08 mm

Data collection

Nonius KappaCCD area-detector diffractometer
22723 measured reflections
8378 independent reflections
5268 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

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

CgA is the centroid calculated through the C atoms of benzenesulfonamide ring *A* of molecule *A*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O3*B*^{i}	0.81 (5)	2.16 (5)	2.950 (3)	166 (5)
N1*B*—H1*B*···O3*A*^{ii}	0.81 (5)	2.11 (5)	2.892 (3)	163 (5)
C9*A*—H9*A*···O1*B*^{ii}	0.93	2.43	3.320 (4)	160
C9*B*—H9*B*···O1*A*^{i}	0.93	2.49	3.366 (3)	157
C22*B*—H22*A*···O2*B*^{iii}	0.96	2.40	3.317 (4)	160
C22*A*—H22*D*···*CgA*^{iv}	0.96	3.28	3.580 (4)	101
C22*A*—H22*E*···*CgA*^{iv}	0.96	3.33	3.580 (4)	97

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

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.152
S = 1.02
8378 reflections
512 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Compound (II)

Crystal data

$C_{23}H_{21}NO_4S$
M_r = 407.47
Monoclinic, $P2_1/c$
a = 8.4506 (2) Å
b = 20.1587 (6) Å
c = 14.2120 (3) Å
β = 119.098 (2)°
V = 2115.49 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 K
0.25 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
7397 measured reflections
4185 independent reflections
3072 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.143
S = 1.05
4185 reflections
265 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

All C-bound H atoms were placed geometrically and refined using a riding model, with C—H = 0.97 (CH_2), 0.96 (CH_3) or 0.93 Å (aromatic groups), and with U_{iso}(H) = 1.2U_{eq}(C). The N-bound H atoms were found in difference Fourier maps and their positional parameters were refined freely; U_{iso}(H) values were set at 1.2U_{eq}(N).

Table 2
Hydrogen-bond geometry (Å, °) for (II).

CgA is the centroid calculated through the C atoms of benzenesulfonamide ring *A*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.91 (3)	2.08 (3)	2.987 (2)	175 (3)
C9—H9···O1^{ii}	0.93	2.34	3.228 (2)	160
C23—H23*A*···*CgA*^{iii}	0.96	3.04	3.816 (3)	138
C2—H2···O4^{iv}	0.93	2.65	3.269 (2)	125
C3—H3···O4^{iv}	0.93	2.68	3.285 (2)	124

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

For both compounds, data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: UK3058). Services for accessing these data are described at the back of the journal.

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supplementary materials

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An additional methylene group driving the conformation and assembly of two arylsulfonamide *para*-alkoxychalcone hybrids

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(I) *N*-{4-[(*E*)-3-(4-Methoxyphenyl)prop-2-enoyl]phenyl}benzenesulfonamide

Crystal data

$C_{22}H_{19}NO_4S$
$M_r = 393.44$
Triclinic, $P\overline{1}$
Hall symbol: -P1
$a = 11.8650\ (3)$ Å
$b = 12.2420\ (3)$ Å
$c = 14.7287\ (3)$ Å
$\alpha = 68.075\ (1)°$
$\beta = 81.665\ (1)°$
$\gamma = 80.437\ (1)°$
$V = 1948.99\ (8)$ Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.341$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6621 reflections
$\theta = 2.4–22.8°$
$\mu = 0.19$ mm^{-1}
$T = 298$ K
Prism, yellow
0.28 × 0.15 × 0.08 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
CCD scans
22723 measured reflections
8378 independent reflections
5268 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 26.9°$, $\theta_{min} = 1.5°$
$h = -15\rightarrow14$
$k = -14\rightarrow15$
$l = -18\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.152$
$S = 1.01$
8378 reflections
512 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.7349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.17904 (5)	0.79421 (6)	−0.03767 (5)	0.0646 (2)
S1B	0.36203 (6)	0.34197 (7)	0.55077 (5)	0.0694 (2)
O3B	0.52135 (14)	0.35404 (17)	0.02461 (12)	0.0722 (5)
O2B	0.25459 (15)	0.40900 (18)	0.52211 (13)	0.0816 (6)
O1B	0.41481 (16)	0.3584 (2)	0.62501 (13)	0.0854 (6)
N1A	0.24599 (18)	0.70776 (19)	0.05831 (16)	0.0661 (6)
O1A	0.21279 (16)	0.73965 (17)	−0.10896 (14)	0.0795 (5)
O2A	0.05999 (14)	0.81540 (18)	−0.00745 (14)	0.0799 (5)
O4B	−0.05735 (17)	0.4984 (2)	−0.28263 (16)	0.0947 (6)
O3A	0.31611 (18)	0.7139 (2)	0.47768 (16)	0.1072 (8)
C7B	0.4446 (2)	0.3629 (2)	0.36402 (17)	0.0602 (6)
C16B	0.2188 (2)	0.4344 (2)	−0.11850 (18)	0.0582 (6)
C17B	0.2373 (2)	0.4527 (2)	−0.21827 (18)	0.0635 (6)
H17B	0.3123	0.4498	−0.2471	0.076*
N1B	0.45667 (19)	0.3690 (2)	0.45617 (16)	0.0751 (7)
C11B	0.3353 (2)	0.3661 (3)	0.23888 (19)	0.0766 (8)
H11B	0.2642	0.3687	0.218	0.092*
C7A	0.2392 (2)	0.7274 (2)	0.14772 (18)	0.0602 (6)
C21B	0.1051 (2)	0.4378 (2)	−0.0777 (2)	0.0706 (7)
H21B	0.0897	0.425	−0.011	0.085*
C12B	0.3402 (2)	0.3639 (3)	0.3323 (2)	0.0850 (9)
H12B	0.2734	0.3631	0.3741	0.102*
C15B	0.3171 (2)	0.4082 (2)	−0.06264 (18)	0.0601 (6)
H15B	0.3879	0.3988	−0.0971	0.072*
C18B	0.1485 (2)	0.4750 (2)	−0.27569 (19)	0.0689 (7)
H18B	0.1635	0.4873	−0.3423	0.083*
C8B	0.5424 (2)	0.3574 (2)	0.30272 (18)	0.0647 (6)
H8B	0.6135	0.3533	0.3242	0.078*
C13B	0.4309 (2)	0.3695 (2)	0.07319 (17)	0.0565 (6)
C9B	0.5370 (2)	0.3578 (2)	0.21029 (18)	0.0630 (6)
H9B	0.6046	0.3535	0.1703	0.076*
C1A	0.2357 (2)	0.9295 (2)	−0.07958 (17)	0.0630 (6)
C10B	0.43259 (19)	0.3645 (2)	0.17527 (17)	0.0546 (5)
O4A	−0.2762 (2)	0.9286 (3)	0.78912 (19)	0.1242 (9)
C14B	0.3211 (2)	0.3955 (2)	0.03014 (18)	0.0618 (6)
H14B	0.253	0.4032	0.0687	0.074*
C13A	0.2292 (3)	0.7493 (3)	0.4336 (2)	0.0765 (8)

C10A	0.2314 (2)	0.7464 (2)	0.3332 (2)	0.0689 (7)
C16A	0.0107 (3)	0.8190 (2)	0.62976 (19)	0.0719 (7)
C6A	0.1643 (3)	1.0319 (3)	−0.0857 (2)	0.0810 (8)
H6A	0.0865	1.0294	−0.0652	0.097*
C11A	0.1398 (2)	0.7892 (3)	0.2768 (2)	0.0840 (9)
H11A	0.0735	0.826	0.3007	0.101*
C21A	−0.0923 (3)	0.8748 (3)	0.5895 (2)	0.0926 (9)
H21A	−0.0983	0.889	0.5237	0.111*
C15A	0.1104 (3)	0.7821 (3)	0.5737 (2)	0.0760 (8)
H15A	0.1746	0.7466	0.6083	0.091*
C1B	0.3442 (3)	0.1908 (3)	0.58692 (18)	0.0731 (7)
C5A	0.2092 (3)	1.1388 (3)	−0.1228 (3)	0.0997 (10)
H5A	0.1613	1.2089	−0.1283	0.12*
C19B	0.0369 (2)	0.4788 (2)	−0.2336 (2)	0.0690 (7)
C12A	0.1428 (2)	0.7795 (3)	0.1863 (2)	0.0888 (9)
H12A	0.0786	0.8086	0.1509	0.107*
C8A	0.3326 (2)	0.6855 (3)	0.2022 (2)	0.0859 (9)
H8A	0.3995	0.6507	0.1773	0.103*
C17A	0.0138 (3)	0.8004 (3)	0.7279 (2)	0.0867 (9)
H17A	0.0808	0.7627	0.7575	0.104*
C18A	−0.0784 (3)	0.8354 (3)	0.7838 (2)	0.0889 (9)
H18A	−0.0728	0.8222	0.8495	0.107*
C19A	−0.1785 (3)	0.8901 (3)	0.7413 (2)	0.0907 (9)
C2A	0.3500 (3)	0.9334 (3)	−0.1101 (3)	0.0908 (9)
H2A	0.398	0.864	−0.1067	0.109*
C14A	0.1232 (3)	0.7920 (3)	0.4799 (2)	0.0790 (8)
H14A	0.0615	0.8277	0.4421	0.095*
C22B	−0.0381 (3)	0.5009 (3)	−0.3814 (3)	0.1051 (11)
H22A	−0.1104	0.5143	−0.408	0.158*
H22B	0.0024	0.4265	−0.382	0.158*
H22C	0.0067	0.5638	−0.4203	0.158*
C20B	0.0157 (2)	0.4595 (3)	−0.1338 (2)	0.0755 (8)
H20B	−0.0594	0.4612	−0.1051	0.091*
C4A	0.3235 (4)	1.1419 (3)	−0.1512 (2)	0.0980 (10)
H4A	0.3538	1.2138	−0.1744	0.118*
C4B	0.3128 (6)	−0.0426 (4)	0.6518 (3)	0.1318 (15)
H4B	0.302	−0.1222	0.6734	0.158*
C3A	0.3934 (3)	1.0399 (3)	−0.1455 (3)	0.1055 (11)
H3A	0.4712	1.0425	−0.1659	0.127*
C9A	0.3279 (3)	0.6945 (3)	0.2930 (2)	0.0925 (10)
H9A	0.3919	0.6646	0.3286	0.111*
C20A	−0.1851 (3)	0.9093 (3)	0.6440 (3)	0.1008 (10)
H20A	−0.2528	0.9459	0.6151	0.121*
C6B	0.2361 (3)	0.1570 (4)	0.6157 (2)	0.0991 (10)
H6B	0.1729	0.2142	0.6121	0.119*
C5B	0.2204 (4)	0.0392 (5)	0.6498 (3)	0.1245 (15)
H5B	0.1474	0.0161	0.6711	0.149*
C3B	0.4211 (5)	−0.0121 (4)	0.6233 (4)	0.1494 (19)
H3B	0.4834	−0.0698	0.6251	0.179*

C2B	0.4373 (4)	0.1087 (4)	0.5910 (3)	0.1212 (13)
H2B	0.5106	0.1316	0.5727	0.145*
C22A	−0.2706 (4)	0.9231 (4)	0.8865 (3)	0.1404 (16)
H22D	−0.344	0.953	0.9108	0.211*
H22E	−0.2136	0.9704	0.8865	0.211*
H22F	−0.2505	0.8423	0.928	0.211*
H1B	0.521 (4)	0.361 (4)	0.471 (3)	0.169*
H1A	0.308 (4)	0.679 (4)	0.040 (3)	0.169*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0553 (4)	0.0775 (4)	0.0618 (4)	0.0065 (3)	−0.0138 (3)	−0.0289 (3)
S1B	0.0604 (4)	0.1005 (5)	0.0534 (4)	−0.0051 (4)	−0.0090 (3)	−0.0352 (4)
O3B	0.0583 (10)	0.0951 (13)	0.0643 (11)	0.0153 (9)	−0.0088 (8)	−0.0392 (10)
O2B	0.0657 (11)	0.1114 (15)	0.0710 (12)	0.0104 (10)	−0.0165 (9)	−0.0414 (11)
O1B	0.0745 (12)	0.1324 (17)	0.0662 (11)	−0.0121 (11)	−0.0132 (9)	−0.0524 (12)
N1A	0.0606 (13)	0.0687 (13)	0.0635 (13)	0.0062 (11)	−0.0115 (10)	−0.0211 (11)
O1A	0.0751 (12)	0.0964 (14)	0.0790 (12)	0.0091 (10)	−0.0203 (10)	−0.0484 (11)
O2A	0.0517 (10)	0.1042 (15)	0.0810 (12)	0.0051 (10)	−0.0121 (9)	−0.0340 (11)
O4B	0.0730 (13)	0.1227 (17)	0.1015 (16)	0.0099 (12)	−0.0369 (11)	−0.0536 (14)
O3A	0.0757 (14)	0.164 (2)	0.0926 (15)	0.0032 (14)	−0.0336 (12)	−0.0555 (15)
C7B	0.0583 (14)	0.0712 (16)	0.0510 (13)	−0.0083 (12)	−0.0085 (11)	−0.0204 (12)
C16B	0.0558 (14)	0.0639 (15)	0.0597 (14)	0.0014 (11)	−0.0119 (11)	−0.0290 (12)
C17B	0.0593 (15)	0.0751 (17)	0.0599 (15)	−0.0029 (12)	−0.0062 (12)	−0.0305 (13)
N1B	0.0599 (13)	0.1186 (19)	0.0549 (12)	−0.0170 (13)	−0.0065 (10)	−0.0374 (13)
C11B	0.0513 (14)	0.122 (2)	0.0639 (16)	−0.0070 (15)	−0.0116 (12)	−0.0412 (16)
C7A	0.0553 (14)	0.0580 (14)	0.0621 (15)	−0.0011 (11)	−0.0114 (12)	−0.0159 (12)
C21B	0.0653 (16)	0.0911 (19)	0.0630 (16)	0.0027 (14)	−0.0069 (13)	−0.0411 (15)
C12B	0.0521 (15)	0.150 (3)	0.0620 (16)	−0.0130 (16)	−0.0034 (12)	−0.0483 (18)
C15B	0.0570 (14)	0.0673 (15)	0.0591 (14)	0.0024 (12)	−0.0082 (11)	−0.0294 (12)
C18B	0.0739 (17)	0.0772 (17)	0.0601 (15)	−0.0018 (14)	−0.0158 (13)	−0.0292 (13)
C8B	0.0514 (14)	0.0833 (18)	0.0603 (15)	−0.0081 (12)	−0.0112 (11)	−0.0246 (13)
C13B	0.0575 (14)	0.0554 (13)	0.0564 (14)	0.0043 (11)	−0.0095 (11)	−0.0230 (11)
C9B	0.0479 (13)	0.0803 (17)	0.0600 (15)	−0.0009 (12)	−0.0055 (11)	−0.0268 (13)
C1A	0.0626 (15)	0.0704 (16)	0.0516 (13)	0.0099 (13)	−0.0095 (11)	−0.0226 (12)
C10B	0.0537 (13)	0.0562 (13)	0.0531 (13)	0.0010 (11)	−0.0097 (10)	−0.0201 (11)
O4A	0.126 (2)	0.159 (2)	0.1018 (18)	−0.0054 (18)	−0.0049 (16)	−0.0699 (17)
C14B	0.0543 (14)	0.0764 (16)	0.0590 (15)	0.0043 (12)	−0.0090 (11)	−0.0327 (13)
C13A	0.0696 (18)	0.089 (2)	0.0734 (18)	−0.0095 (15)	−0.0217 (15)	−0.0258 (15)
C10A	0.0612 (16)	0.0761 (17)	0.0700 (17)	−0.0040 (13)	−0.0155 (13)	−0.0251 (14)
C16A	0.0840 (19)	0.0770 (18)	0.0593 (15)	−0.0168 (15)	−0.0189 (14)	−0.0223 (14)
C6A	0.0802 (19)	0.079 (2)	0.0747 (19)	0.0129 (16)	−0.0063 (15)	−0.0275 (16)
C11A	0.0661 (17)	0.114 (2)	0.0673 (17)	0.0186 (16)	−0.0137 (14)	−0.0364 (17)
C21A	0.100 (2)	0.120 (3)	0.0650 (18)	−0.002 (2)	−0.0263 (17)	−0.0391 (18)
C15A	0.0801 (19)	0.0826 (19)	0.0682 (17)	−0.0127 (15)	−0.0256 (15)	−0.0221 (15)
C1B	0.0768 (18)	0.093 (2)	0.0503 (14)	−0.0054 (16)	−0.0095 (13)	−0.0269 (14)
C5A	0.118 (3)	0.074 (2)	0.092 (2)	0.012 (2)	−0.004 (2)	−0.0243 (18)
C19B	0.0652 (16)	0.0740 (17)	0.0773 (18)	0.0078 (13)	−0.0270 (14)	−0.0371 (14)
C12A	0.0637 (17)	0.127 (3)	0.0692 (18)	0.0210 (17)	−0.0213 (14)	−0.0364 (18)

C8A	0.0595 (16)	0.114 (2)	0.092 (2)	0.0184 (16)	−0.0214 (15)	−0.0536 (19)
C17A	0.097 (2)	0.102 (2)	0.0659 (18)	−0.0175 (18)	−0.0259 (17)	−0.0260 (17)
C18A	0.108 (3)	0.108 (2)	0.0611 (17)	−0.028 (2)	−0.0124 (18)	−0.0346 (17)
C19A	0.103 (3)	0.102 (2)	0.078 (2)	−0.021 (2)	−0.0070 (19)	−0.0424 (19)
C2A	0.0691 (19)	0.074 (2)	0.116 (3)	0.0040 (16)	−0.0033 (17)	−0.0263 (18)
C14A	0.0752 (19)	0.098 (2)	0.0655 (17)	−0.0035 (16)	−0.0215 (14)	−0.0293 (16)
C22B	0.099 (2)	0.136 (3)	0.099 (2)	0.002 (2)	−0.050 (2)	−0.055 (2)
C20B	0.0546 (15)	0.101 (2)	0.0814 (19)	0.0029 (14)	−0.0103 (13)	−0.0483 (17)
C4A	0.121 (3)	0.078 (2)	0.085 (2)	−0.014 (2)	−0.002 (2)	−0.0197 (17)
C4B	0.179 (5)	0.113 (3)	0.105 (3)	−0.033 (4)	−0.019 (3)	−0.032 (3)
C3A	0.084 (2)	0.092 (2)	0.124 (3)	−0.010 (2)	0.003 (2)	−0.025 (2)
C9A	0.0646 (18)	0.129 (3)	0.094 (2)	0.0162 (18)	−0.0349 (16)	−0.053 (2)
C20A	0.089 (2)	0.133 (3)	0.087 (2)	0.006 (2)	−0.0235 (18)	−0.050 (2)
C6B	0.089 (2)	0.116 (3)	0.090 (2)	−0.019 (2)	−0.0312 (18)	−0.024 (2)
C5B	0.132 (4)	0.127 (4)	0.109 (3)	−0.046 (3)	−0.045 (3)	−0.011 (3)
C3B	0.167 (5)	0.107 (4)	0.137 (4)	0.012 (3)	0.030 (3)	−0.029 (3)
C2B	0.111 (3)	0.110 (3)	0.117 (3)	0.000 (2)	0.026 (2)	−0.030 (2)
C22A	0.186 (5)	0.159 (4)	0.090 (3)	−0.029 (3)	0.015 (3)	−0.067 (3)

Geometric parameters (Å, º)

S1A—O1A	1.4220 (18)	C10A—C9A	1.381 (4)
S1A—O2A	1.4293 (17)	C16A—C17A	1.381 (4)
S1A—N1A	1.637 (2)	C16A—C21A	1.393 (4)
S1A—C1A	1.749 (3)	C16A—C15A	1.451 (4)
S1B—O2B	1.4235 (19)	C6A—C5A	1.382 (4)
S1B—O1B	1.4258 (18)	C6A—H6A	0.93
S1B—N1B	1.624 (2)	C11A—C12A	1.377 (4)
S1B—C1B	1.764 (3)	C11A—H11A	0.93
O3B—C13B	1.229 (3)	C21A—C20A	1.371 (4)
N1A—C7A	1.414 (3)	C21A—H21A	0.93
N1A—H1A	0.82 (4)	C15A—C14A	1.330 (4)
O4B—C19B	1.359 (3)	C15A—H15A	0.93
O4B—C22B	1.428 (4)	C1B—C2B	1.356 (4)
O3A—C13A	1.228 (3)	C1B—C6B	1.373 (4)
C7B—C8B	1.372 (3)	C5A—C4A	1.362 (5)
C7B—C12B	1.382 (3)	C5A—H5A	0.93
C7B—N1B	1.416 (3)	C19B—C20B	1.389 (4)
C16B—C17B	1.391 (3)	C12A—H12A	0.93
C16B—C21B	1.396 (3)	C8A—C9A	1.375 (4)
C16B—C15B	1.447 (3)	C8A—H8A	0.93
C17B—C18B	1.375 (3)	C17A—C18A	1.381 (4)
C17B—H17B	0.93	C17A—H17A	0.93
N1B—H1B	0.80 (4)	C18A—C19A	1.374 (4)
C11B—C12B	1.376 (4)	C18A—H18A	0.93
C11B—C10B	1.380 (3)	C19A—C20A	1.374 (4)
C11B—H11B	0.93	C2A—C3A	1.369 (4)
C7A—C12A	1.371 (4)	C2A—H2A	0.93
C7A—C8A	1.377 (3)	C14A—H14A	0.93
C21B—C20B	1.370 (4)	C22B—H22A	0.96

C21B—H21B	0.93	C22B—H22B	0.96
C12B—H12B	0.93	C22B—H22C	0.96
C15B—C14B	1.323 (3)	C20B—H20B	0.93
C15B—H15B	0.93	C4A—C3A	1.361 (5)
C18B—C19B	1.379 (4)	C4A—H4A	0.93
C18B—H18B	0.93	C4B—C5B	1.351 (6)
C8B—C9B	1.370 (3)	C4B—C3B	1.362 (6)
C8B—H8B	0.93	C4B—H4B	0.93
C13B—C14B	1.467 (3)	C3A—H3A	0.93
C13B—C10B	1.485 (3)	C9A—H9A	0.93
C9B—C10B	1.389 (3)	C20A—H20A	0.93
C9B—H9B	0.93	C6B—C5B	1.374 (5)
C1A—C2A	1.368 (4)	C6B—H6B	0.93
C1A—C6A	1.372 (4)	C5B—H5B	0.93
O4A—C19A	1.375 (4)	C3B—C2B	1.411 (6)
O4A—C22A	1.421 (4)	C3B—H3B	0.93
C14B—H14B	0.93	C2B—H2B	0.93
C13A—C14A	1.456 (4)	C22A—H22D	0.96
C13A—C10A	1.489 (4)	C22A—H22E	0.96
C10A—C11A	1.376 (4)	C22A—H22F	0.96

O1A—S1A—O2A	119.61 (12)	C12A—C11A—H11A	118.8
O1A—S1A—N1A	104.80 (11)	C20A—C21A—C16A	121.9 (3)
O2A—S1A—N1A	109.01 (11)	C20A—C21A—H21A	119
O1A—S1A—C1A	108.43 (12)	C16A—C21A—H21A	119
O2A—S1A—C1A	107.90 (12)	C14A—C15A—C16A	129.1 (3)
N1A—S1A—C1A	106.36 (12)	C14A—C15A—H15A	115.4
O2B—S1B—O1B	119.17 (12)	C16A—C15A—H15A	115.4
O2B—S1B—N1B	109.69 (12)	C2B—C1B—C6B	120.6 (3)
O1B—S1B—N1B	105.01 (12)	C2B—C1B—S1B	120.0 (3)
O2B—S1B—C1B	107.17 (13)	C6B—C1B—S1B	119.3 (3)
O1B—S1B—C1B	109.08 (13)	C4A—C5A—C6A	120.2 (3)
N1B—S1B—C1B	106.03 (13)	C4A—C5A—H5A	119.9
C7A—N1A—S1A	125.13 (17)	C6A—C5A—H5A	119.9
C7A—N1A—H1A	116 (3)	O4B—C19B—C18B	124.5 (3)
S1A—N1A—H1A	110 (3)	O4B—C19B—C20B	115.7 (3)
C19B—O4B—C22B	116.9 (2)	C18B—C19B—C20B	119.7 (2)
C8B—C7B—C12B	118.7 (2)	C7A—C12A—C11A	120.8 (3)
C8B—C7B—N1B	117.6 (2)	C7A—C12A—H12A	119.6
C12B—C7B—N1B	123.7 (2)	C11A—C12A—H12A	119.6
C17B—C16B—C21B	117.1 (2)	C9A—C8A—C7A	120.6 (3)
C17B—C16B—C15B	118.8 (2)	C9A—C8A—H8A	119.7
C21B—C16B—C15B	124.0 (2)	C7A—C8A—H8A	119.7
C18B—C17B—C16B	122.3 (2)	C18A—C17A—C16A	122.8 (3)
C18B—C17B—H17B	118.9	C18A—C17A—H17A	118.6
C16B—C17B—H17B	118.9	C16A—C17A—H17A	118.6
C7B—N1B—S1B	126.34 (18)	C19A—C18A—C17A	119.2 (3)
C7B—N1B—H1B	117 (3)	C19A—C18A—H18A	120.4
S1B—N1B—H1B	112 (3)	C17A—C18A—H18A	120.4

C12B—C11B—C10B	121.9 (2)	C20A—C19A—C18A	119.6 (3)
C12B—C11B—H11B	119	C20A—C19A—O4A	115.6 (3)
C10B—C11B—H11B	119	C18A—C19A—O4A	124.8 (3)
C12A—C7A—C8A	117.9 (3)	C1A—C2A—C3A	119.7 (3)
C12A—C7A—N1A	123.8 (2)	C1A—C2A—H2A	120.1
C8A—C7A—N1A	118.1 (2)	C3A—C2A—H2A	120.1
C20B—C21B—C16B	121.3 (2)	C15A—C14A—C13A	122.9 (3)
C20B—C21B—H21B	119.3	C15A—C14A—H14A	118.5
C16B—C21B—H21B	119.3	C13A—C14A—H14A	118.5
C11B—C12B—C7B	120.0 (2)	O4B—C22B—H22A	109.5
C11B—C12B—H12B	120	O4B—C22B—H22B	109.5
C7B—C12B—H12B	120	H22A—C22B—H22B	109.5
C14B—C15B—C16B	129.6 (2)	O4B—C22B—H22C	109.5
C14B—C15B—H15B	115.2	H22A—C22B—H22C	109.5
C16B—C15B—H15B	115.2	H22B—C22B—H22C	109.5
C17B—C18B—C19B	119.4 (2)	C21B—C20B—C19B	120.2 (2)
C17B—C18B—H18B	120.3	C21B—C20B—H20B	119.9
C19B—C18B—H18B	120.3	C19B—C20B—H20B	119.9
C9B—C8B—C7B	121.0 (2)	C3A—C4A—C5A	120.1 (3)
C9B—C8B—H8B	119.5	C3A—C4A—H4A	120
C7B—C8B—H8B	119.5	C5A—C4A—H4A	120
O3B—C13B—C14B	120.4 (2)	C5B—C4B—C3B	122.0 (5)
O3B—C13B—C10B	120.0 (2)	C5B—C4B—H4B	119
C14B—C13B—C10B	119.7 (2)	C3B—C4B—H4B	119
C8B—C9B—C10B	121.2 (2)	C4A—C3A—C2A	120.4 (3)
C8B—C9B—H9B	119.4	C4A—C3A—H3A	119.8
C10B—C9B—H9B	119.4	C2A—C3A—H3A	119.8
C2A—C1A—C6A	120.3 (3)	C8A—C9A—C10A	122.3 (3)
C2A—C1A—S1A	119.9 (2)	C8A—C9A—H9A	118.9
C6A—C1A—S1A	119.8 (2)	C10A—C9A—H9A	118.9
C11B—C10B—C9B	117.1 (2)	C21A—C20A—C19A	120.3 (3)
C11B—C10B—C13B	123.7 (2)	C21A—C20A—H20A	119.9
C9B—C10B—C13B	119.2 (2)	C19A—C20A—H20A	119.9
C19A—O4A—C22A	118.1 (3)	C1B—C6B—C5B	120.5 (4)
C15B—C14B—C13B	121.2 (2)	C1B—C6B—H6B	119.7
C15B—C14B—H14B	119.4	C5B—C6B—H6B	119.7
C13B—C14B—H14B	119.4	C4B—C5B—C6B	119.0 (4)
O3A—C13A—C14A	120.3 (3)	C4B—C5B—H5B	120.5
O3A—C13A—C10A	119.9 (3)	C6B—C5B—H5B	120.5
C14A—C13A—C10A	119.7 (2)	C4B—C3B—C2B	118.9 (4)
C11A—C10A—C9A	116.1 (3)	C4B—C3B—H3B	120.6
C11A—C10A—C13A	123.9 (3)	C2B—C3B—H3B	120.6
C9A—C10A—C13A	120.0 (3)	C1B—C2B—C3B	119.0 (4)
C17A—C16A—C21A	116.1 (3)	C1B—C2B—H2B	120.5
C17A—C16A—C15A	120.7 (3)	C3B—C2B—H2B	120.5
C21A—C16A—C15A	123.2 (3)	O4A—C22A—H22D	109.5
C1A—C6A—C5A	119.2 (3)	O4A—C22A—H22E	109.5
C1A—C6A—H6A	120.4	H22D—C22A—H22E	109.5
C5A—C6A—H6A	120.4	O4A—C22A—H22F	109.5

C10A—C11A—C12A	122.3 (3)	H22D—C22A—H22F	109.5
C10A—C11A—H11A	118.8	H22E—C22A—H22F	109.5
O1A—S1A—N1A—C7A	179.4 (2)	C17A—C16A—C15A—C14A	179.6 (3)
O2A—S1A—N1A—C7A	−51.5 (2)	C21A—C16A—C15A—C14A	−0.7 (5)
C1A—S1A—N1A—C7A	64.6 (2)	O2B—S1B—C1B—C2B	161.1 (3)
C21B—C16B—C17B—C18B	0.9 (4)	O1B—S1B—C1B—C2B	−68.6 (3)
C15B—C16B—C17B—C18B	178.3 (2)	N1B—S1B—C1B—C2B	44.0 (3)
C8B—C7B—N1B—S1B	−162.9 (2)	O2B—S1B—C1B—C6B	−22.3 (3)
C12B—C7B—N1B—S1B	18.1 (4)	O1B—S1B—C1B—C6B	108.0 (2)
O2B—S1B—N1B—C7B	−51.6 (3)	N1B—S1B—C1B—C6B	−139.4 (2)
O1B—S1B—N1B—C7B	179.2 (2)	C1A—C6A—C5A—C4A	−1.1 (5)
C1B—S1B—N1B—C7B	63.8 (3)	C22B—O4B—C19B—C18B	7.7 (4)
S1A—N1A—C7A—C12A	33.5 (4)	C22B—O4B—C19B—C20B	−170.9 (3)
S1A—N1A—C7A—C8A	−150.6 (2)	C17B—C18B—C19B—O4B	−179.0 (3)
C17B—C16B—C21B—C20B	−0.7 (4)	C17B—C18B—C19B—C20B	−0.4 (4)
C15B—C16B—C21B—C20B	−177.9 (3)	C8A—C7A—C12A—C11A	−0.1 (5)
C10B—C11B—C12B—C7B	1.5 (5)	N1A—C7A—C12A—C11A	175.9 (3)
C8B—C7B—C12B—C11B	−3.6 (5)	C10A—C11A—C12A—C7A	−0.9 (5)
N1B—C7B—C12B—C11B	175.4 (3)	C12A—C7A—C8A—C9A	0.8 (5)
C17B—C16B—C15B—C14B	175.0 (3)	N1A—C7A—C8A—C9A	−175.3 (3)
C21B—C16B—C15B—C14B	−7.9 (4)	C21A—C16A—C17A—C18A	−0.7 (5)
C16B—C17B—C18B—C19B	−0.4 (4)	C15A—C16A—C17A—C18A	179.1 (3)
C12B—C7B—C8B—C9B	2.7 (4)	C16A—C17A—C18A—C19A	0.7 (5)
N1B—C7B—C8B—C9B	−176.4 (2)	C17A—C18A—C19A—C20A	−0.2 (5)
C7B—C8B—C9B—C10B	0.4 (4)	C17A—C18A—C19A—O4A	179.7 (3)
O1A—S1A—C1A—C2A	−51.2 (3)	C22A—O4A—C19A—C20A	−173.2 (3)
O2A—S1A—C1A—C2A	177.8 (2)	C22A—O4A—C19A—C18A	6.9 (5)
N1A—S1A—C1A—C2A	61.0 (3)	C6A—C1A—C2A—C3A	0.9 (5)
O1A—S1A—C1A—C6A	125.9 (2)	S1A—C1A—C2A—C3A	178.1 (3)
O2A—S1A—C1A—C6A	−5.0 (2)	C16A—C15A—C14A—C13A	−179.4 (3)
N1A—S1A—C1A—C6A	−121.8 (2)	O3A—C13A—C14A—C15A	−8.1 (5)
C12B—C11B—C10B—C9B	1.5 (4)	C10A—C13A—C14A—C15A	170.6 (3)
C12B—C11B—C10B—C13B	−178.6 (3)	C16B—C21B—C20B—C19B	−0.1 (4)
C8B—C9B—C10B—C11B	−2.5 (4)	O4B—C19B—C20B—C21B	179.4 (3)
C8B—C9B—C10B—C13B	177.6 (2)	C18B—C19B—C20B—C21B	0.7 (4)
O3B—C13B—C10B—C11B	−171.6 (2)	C6A—C5A—C4A—C3A	1.7 (5)
C14B—C13B—C10B—C11B	9.8 (4)	C5A—C4A—C3A—C2A	−0.9 (6)
O3B—C13B—C10B—C9B	8.3 (3)	C1A—C2A—C3A—C4A	−0.4 (6)
C14B—C13B—C10B—C9B	−170.3 (2)	C7A—C8A—C9A—C10A	−0.7 (5)
C16B—C15B—C14B—C13B	−179.5 (2)	C11A—C10A—C9A—C8A	−0.2 (5)
O3B—C13B—C14B—C15B	−3.1 (4)	C13A—C10A—C9A—C8A	177.4 (3)
C10B—C13B—C14B—C15B	175.5 (2)	C16A—C21A—C20A—C19A	0.4 (6)
O3A—C13A—C10A—C11A	−177.0 (3)	C18A—C19A—C20A—C21A	−0.3 (5)
C14A—C13A—C10A—C11A	4.3 (4)	O4A—C19A—C20A—C21A	179.7 (3)
O3A—C13A—C10A—C9A	5.6 (5)	C2B—C1B—C6B—C5B	0.5 (5)
C14A—C13A—C10A—C9A	−173.1 (3)	S1B—C1B—C6B—C5B	−176.1 (3)
C2A—C1A—C6A—C5A	−0.2 (4)	C3B—C4B—C5B—C6B	1.6 (7)
S1A—C1A—C6A—C5A	−177.4 (2)	C1B—C6B—C5B—C4B	−1.9 (6)

C9A—C10A—C11A—C12A	1.0 (5)	C5B—C4B—C3B—C2B	0.2 (8)
C13A—C10A—C11A—C12A	−176.5 (3)	C6B—C1B—C2B—C3B	1.3 (6)
C17A—C16A—C21A—C20A	0.1 (5)	S1B—C1B—C2B—C3B	177.9 (3)
C15A—C16A—C21A—C20A	−179.6 (3)	C4B—C3B—C2B—C1B	−1.6 (7)

Hydrogen-bond geometry (Å, º)

*Cg*A is the centroid calculated through the ring A C atoms of molecule A.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O3*B*^{i}	0.81 (5)	2.16 (5)	2.950 (3)	166 (5)
N1*B*—H1*B*···O3*A*^{ii}	0.81 (5)	2.11 (5)	2.892 (3)	163 (5)
C9*A*—H9*A*···O1*B*^{ii}	0.93	2.43	3.320 (4)	160
C9*B*—H9*B*···O1*A*^{i}	0.93	2.49	3.366 (3)	157
C22*B*—H22*A*···O2*B*^{iii}	0.96	2.40	3.317 (4)	160
C22*A*—H22*D*···Cg*A*^{iv}	0.96	3.28	3.580 (4)	101
C22*A*—H22*E*···Cg*A*^{iv}	0.96	3.33	3.580 (4)	97

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*; (iv) −*x*, −*y*+2, −*z*+1.

(II) *N*-{4-[(*E*)-3-(4-Ethoxyphenyl)prop-2-enoyl]phenyl}benzenesulfonamide

Crystal data

$C_{23}H_{21}NO_4S$
M_r = 407.47
Monoclinic, $P2_1/c$
Hall symbol: -P2ybc
a = 8.4506 (2) Å
b = 20.1587 (6) Å
c = 14.2120 (3) Å
β = 119.098 (2)°
V = 2115.49 (9) Å^3
Z = 4
$F(000)$ = 856
D_x = 1.279 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4266 reflections
θ = 2.9–26.4°
μ = 0.18 mm^{-1}
T = 298 K
Prism, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
CCD scans
7397 measured reflections
4185 independent reflections
3072 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 26.4°, θ_{min} = 3.2°
h = −10→10
k = −23→25
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.143
S = 1.05
4185 reflections
265 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0875P)^2 + 0.0704P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.65679 (6)	0.11848 (2)	0.42888 (3)	0.05750 (19)
N1	0.76455 (19)	0.16732 (8)	0.53375 (12)	0.0606 (4)
O1	0.69037 (17)	0.14641 (6)	0.34799 (10)	0.0709 (4)
O2	0.70805 (17)	0.05154 (6)	0.46160 (10)	0.0678 (3)
O4	0.74263 (19)	−0.16891 (7)	1.27909 (10)	0.0753 (4)
C1	0.4242 (2)	0.12732 (8)	0.38628 (13)	0.0546 (4)
C7	0.7578 (2)	0.15805 (8)	0.63097 (14)	0.0565 (4)
C6	0.3341 (2)	0.07890 (9)	0.41042 (16)	0.0677 (5)
H6	0.395	0.0414	0.4491	0.081*
C13	0.7446 (3)	0.13877 (10)	0.92840 (15)	0.0660 (5)
C21	0.7434 (3)	−0.05952 (10)	1.07881 (15)	0.0723 (5)
H21	0.7525	−0.0638	1.0165	0.087*
C10	0.7513 (2)	0.14366 (9)	0.82493 (14)	0.0601 (4)
C19	0.7346 (2)	−0.11021 (9)	1.22857 (14)	0.0640 (5)
O3	0.7338 (2)	0.18963 (7)	0.97259 (11)	0.0833 (4)
C22	0.7544 (3)	−0.16605 (10)	1.38310 (15)	0.0747 (5)
H22A	0.6452	−0.1466	1.3774	0.09*
H22B	0.8569	−0.139	1.4315	0.09*
C15	0.7296 (3)	0.06480 (10)	1.06029 (15)	0.0700 (5)
H15	0.7149	0.1035	1.0908	0.084*
C9	0.7312 (3)	0.20515 (9)	0.77736 (16)	0.0722 (5)
H9	0.7166	0.2424	0.8109	0.087*
C18	0.7174 (3)	−0.04923 (9)	1.26476 (15)	0.0693 (5)
H18	0.7081	−0.0455	1.3271	0.083*
C17	0.7140 (3)	0.00713 (10)	1.20731 (15)	0.0716 (5)
H17	0.7017	0.0484	1.2322	0.086*
C8	0.7323 (3)	0.21237 (9)	0.68120 (15)	0.0684 (5)
H8	0.7157	0.2541	0.65	0.082*
C20	0.7449 (3)	−0.11520 (10)	1.13412 (15)	0.0722 (5)
H20	0.753	−0.1568	1.1084	0.087*
C16	0.7284 (2)	0.00392 (9)	1.11405 (14)	0.0652 (5)
C2	0.3369 (3)	0.18415 (9)	0.33206 (16)	0.0700 (5)
H2	0.4002	0.2173	0.3189	0.084*
C12	0.7835 (3)	0.09649 (10)	0.67957 (16)	0.0743 (5)
H12	0.8052	0.0596	0.6482	0.089*
C5	0.1508 (3)	0.08715 (10)	0.37601 (17)	0.0754 (5)
H5	0.0882	0.055	0.3918	0.09*

C14	0.7485 (3)	0.07314 (10)	0.97391 (16)	0.0720 (5)
H14	0.7649	0.036	0.9408	0.086*
C4	0.0624 (3)	0.14239 (10)	0.31898 (16)	0.0741 (5)
H4	−0.061	0.1471	0.2944	0.089*
C11	0.7769 (3)	0.08960 (10)	0.77449 (15)	0.0728 (5)
H11	0.7901	0.0477	0.8048	0.087*
C3	0.1549 (3)	0.19133 (10)	0.29755 (17)	0.0783 (5)
H3	0.0941	0.2291	0.2598	0.094*
C23	0.7774 (4)	−0.23565 (12)	1.42532 (19)	0.0988 (7)
H23A	0.7856	−0.2351	1.4951	0.148*
H23B	0.8861	−0.2544	1.4309	0.148*
H23C	0.6752	−0.2619	1.377	0.148*
H1	0.763 (3)	0.2108 (14)	0.516 (2)	0.119*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0687 (3)	0.0501 (3)	0.0675 (3)	−0.00035 (18)	0.0439 (2)	−0.00150 (18)
N1	0.0657 (8)	0.0533 (8)	0.0708 (9)	−0.0046 (6)	0.0394 (7)	−0.0013 (7)
O1	0.0923 (9)	0.0643 (8)	0.0829 (8)	−0.0019 (6)	0.0637 (8)	0.0005 (6)
O2	0.0830 (8)	0.0490 (7)	0.0819 (8)	0.0063 (5)	0.0485 (7)	−0.0001 (6)
O4	0.1070 (10)	0.0633 (8)	0.0669 (7)	−0.0010 (7)	0.0510 (7)	−0.0033 (6)
C1	0.0645 (9)	0.0506 (9)	0.0551 (9)	−0.0017 (7)	0.0340 (8)	0.0008 (7)
C7	0.0548 (8)	0.0524 (10)	0.0644 (10)	−0.0059 (7)	0.0306 (8)	−0.0057 (8)
C6	0.0702 (11)	0.0548 (10)	0.0800 (12)	−0.0034 (8)	0.0382 (9)	0.0082 (9)
C13	0.0730 (11)	0.0624 (11)	0.0661 (10)	−0.0069 (8)	0.0367 (9)	−0.0077 (9)
C21	0.0931 (13)	0.0719 (13)	0.0617 (10)	−0.0031 (10)	0.0453 (10)	−0.0083 (9)
C10	0.0624 (9)	0.0547 (10)	0.0650 (10)	−0.0055 (8)	0.0324 (8)	−0.0062 (8)
C19	0.0735 (11)	0.0605 (11)	0.0616 (10)	−0.0038 (8)	0.0356 (9)	−0.0066 (8)
O3	0.1218 (12)	0.0609 (8)	0.0834 (9)	−0.0081 (7)	0.0624 (9)	−0.0125 (7)
C22	0.0906 (13)	0.0795 (13)	0.0630 (11)	−0.0084 (10)	0.0443 (10)	−0.0071 (10)
C15	0.0829 (12)	0.0629 (11)	0.0660 (11)	−0.0072 (9)	0.0378 (10)	−0.0082 (9)
C9	0.0961 (14)	0.0548 (11)	0.0798 (12)	−0.0048 (9)	0.0539 (11)	−0.0092 (9)
C18	0.0853 (12)	0.0675 (12)	0.0656 (11)	−0.0111 (9)	0.0449 (10)	−0.0133 (9)
C17	0.0899 (13)	0.0631 (12)	0.0714 (11)	−0.0095 (9)	0.0466 (10)	−0.0148 (9)
C8	0.0866 (12)	0.0506 (10)	0.0780 (12)	−0.0048 (8)	0.0480 (10)	−0.0030 (9)
C20	0.0974 (14)	0.0605 (11)	0.0687 (11)	0.0015 (9)	0.0483 (11)	−0.0093 (9)
C16	0.0715 (11)	0.0628 (11)	0.0634 (10)	−0.0081 (8)	0.0345 (9)	−0.0081 (9)
C2	0.0730 (11)	0.0614 (11)	0.0834 (12)	0.0005 (9)	0.0442 (10)	0.0143 (9)
C12	0.1028 (14)	0.0555 (11)	0.0735 (12)	0.0111 (10)	0.0498 (11)	0.0002 (9)
C5	0.0743 (12)	0.0674 (13)	0.0917 (14)	−0.0129 (9)	0.0462 (11)	0.0025 (10)
C14	0.0874 (13)	0.0615 (11)	0.0742 (12)	−0.0045 (9)	0.0448 (11)	−0.0070 (9)
C4	0.0628 (10)	0.0768 (13)	0.0832 (12)	−0.0003 (9)	0.0360 (10)	−0.0007 (11)
C11	0.0958 (14)	0.0563 (11)	0.0715 (11)	0.0035 (9)	0.0447 (11)	0.0015 (9)
C3	0.0718 (12)	0.0738 (13)	0.0887 (13)	0.0083 (9)	0.0385 (10)	0.0169 (11)
C23	0.133 (2)	0.0928 (17)	0.0818 (14)	−0.0041 (14)	0.0610 (15)	0.0078 (12)

Geometric parameters (Å, º)

S1—O2	1.4245 (13)	C22—H22B	0.97
S1—O1	1.4269 (12)	C15—C14	1.324 (3)
S1—N1	1.6432 (15)	C15—C16	1.448 (2)
S1—C1	1.7621 (17)	C15—H15	0.93
N1—C7	1.423 (2)	C9—C8	1.379 (3)
N1—H1	0.91 (3)	C9—H9	0.93
O4—C19	1.369 (2)	C18—C17	1.391 (3)
O4—C22	1.434 (2)	C18—H18	0.93
C1—C2	1.378 (2)	C17—C16	1.390 (2)
C1—C6	1.380 (2)	C17—H17	0.93
C7—C8	1.380 (2)	C8—H8	0.93
C7—C12	1.385 (2)	C20—H20	0.93
C6—C5	1.388 (2)	C2—C3	1.376 (3)
C6—H6	0.93	C2—H2	0.93
C13—O3	1.228 (2)	C12—C11	1.384 (3)
C13—C14	1.466 (3)	C12—H12	0.93
C13—C10	1.502 (2)	C5—C4	1.366 (3)
C21—C20	1.367 (3)	C5—H5	0.93
C21—C16	1.402 (2)	C14—H14	0.93
C21—H21	0.93	C4—C3	1.381 (3)
C10—C11	1.378 (2)	C4—H4	0.93
C10—C9	1.382 (3)	C11—H11	0.93
C19—C18	1.367 (3)	C3—H3	0.93
C19—C20	1.390 (2)	C23—H23A	0.96
C22—C23	1.501 (3)	C23—H23B	0.96
C22—H22A	0.97	C23—H23C	0.96
O2—S1—O1	119.26 (7)	C19—C18—C17	119.28 (16)
O2—S1—N1	108.97 (8)	C19—C18—H18	120.4
O1—S1—N1	104.76 (8)	C17—C18—H18	120.4
O2—S1—C1	108.62 (7)	C16—C17—C18	122.35 (17)
O1—S1—C1	108.00 (8)	C16—C17—H17	118.8
N1—S1—C1	106.53 (7)	C18—C17—H17	118.8
C7—N1—S1	122.41 (11)	C9—C8—C7	120.45 (17)
C7—N1—H1	113.0 (16)	C9—C8—H8	119.8
S1—N1—H1	113.6 (17)	C7—C8—H8	119.8
C19—O4—C22	117.85 (14)	C21—C20—C19	120.54 (17)
C2—C1—C6	121.14 (16)	C21—C20—H20	119.7
C2—C1—S1	118.74 (12)	C19—C20—H20	119.7
C6—C1—S1	120.09 (13)	C17—C16—C21	116.63 (17)
C8—C7—C12	118.61 (16)	C17—C16—C15	119.34 (17)
C8—C7—N1	119.22 (15)	C21—C16—C15	124.02 (17)
C12—C7—N1	122.11 (15)	C3—C2—C1	119.25 (17)
C1—C6—C5	118.90 (17)	C3—C2—H2	120.4
C1—C6—H6	120.5	C1—C2—H2	120.4
C5—C6—H6	120.5	C11—C12—C7	120.35 (17)
O3—C13—C14	121.27 (17)	C11—C12—H12	119.8
O3—C13—C10	119.55 (17)	C7—C12—H12	119.8

C14—C13—C10	119.18 (16)	C4—C5—C6	120.08 (17)
C20—C21—C16	121.40 (17)	C4—C5—H5	120
C20—C21—H21	119.3	C6—C5—H5	120
C16—C21—H21	119.3	C15—C14—C13	122.46 (18)
C11—C10—C9	117.89 (16)	C15—C14—H14	118.8
C11—C10—C13	123.20 (17)	C13—C14—H14	118.8
C9—C10—C13	118.90 (16)	C5—C4—C3	120.54 (18)
C18—C19—O4	124.55 (16)	C5—C4—H4	119.7
C18—C19—C20	119.76 (18)	C3—C4—H4	119.7
O4—C19—C20	115.69 (16)	C10—C11—C12	121.23 (18)
O4—C22—C23	107.77 (16)	C10—C11—H11	119.4
O4—C22—H22A	110.2	C12—C11—H11	119.4
C23—C22—H22A	110.2	C2—C3—C4	120.03 (18)
O4—C22—H22B	110.2	C2—C3—H3	120
C23—C22—H22B	110.2	C4—C3—H3	120
H22A—C22—H22B	108.5	C22—C23—H23A	109.5
C14—C15—C16	129.19 (18)	C22—C23—H23B	109.5
C14—C15—H15	115.4	H23A—C23—H23B	109.5
C16—C15—H15	115.4	C22—C23—H23C	109.5
C8—C9—C10	121.40 (17)	H23A—C23—H23C	109.5
C8—C9—H9	119.3	H23B—C23—H23C	109.5
C10—C9—H9	119.3		

O2—S1—N1—C7	−54.26 (15)	C12—C7—C8—C9	−0.5 (3)
O1—S1—N1—C7	177.05 (13)	N1—C7—C8—C9	−177.83 (16)
C1—S1—N1—C7	62.76 (15)	C16—C21—C20—C19	−1.1 (3)
O2—S1—C1—C2	−167.78 (14)	C18—C19—C20—C21	1.9 (3)
O1—S1—C1—C2	−37.10 (16)	O4—C19—C20—C21	−178.15 (18)
N1—S1—C1—C2	74.98 (15)	C18—C17—C16—C21	1.1 (3)
O2—S1—C1—C6	14.36 (17)	C18—C17—C16—C15	−178.05 (18)
O1—S1—C1—C6	145.04 (14)	C20—C21—C16—C17	−0.4 (3)
N1—S1—C1—C6	−102.89 (15)	C20—C21—C16—C15	178.72 (19)
S1—N1—C7—C8	−135.53 (15)	C14—C15—C16—C17	177.28 (19)
S1—N1—C7—C12	47.2 (2)	C14—C15—C16—C21	−1.8 (3)
C2—C1—C6—C5	2.1 (3)	C6—C1—C2—C3	−2.7 (3)
S1—C1—C6—C5	179.91 (14)	S1—C1—C2—C3	179.41 (15)
O3—C13—C10—C11	175.02 (19)	C8—C7—C12—C11	2.3 (3)
C14—C13—C10—C11	−5.8 (3)	N1—C7—C12—C11	179.61 (17)
O3—C13—C10—C9	−4.9 (3)	C1—C6—C5—C4	0.2 (3)
C14—C13—C10—C9	174.23 (18)	C16—C15—C14—C13	179.29 (18)
C22—O4—C19—C18	−7.4 (3)	O3—C13—C14—C15	4.3 (3)
C22—O4—C19—C20	172.68 (17)	C10—C13—C14—C15	−174.90 (17)
C19—O4—C22—C23	−175.26 (17)	C6—C5—C4—C3	−1.8 (3)
C11—C10—C9—C8	1.5 (3)	C9—C10—C11—C12	0.4 (3)
C13—C10—C9—C8	−178.55 (16)	C13—C10—C11—C12	−179.56 (17)
O4—C19—C18—C17	178.87 (18)	C7—C12—C11—C10	−2.3 (3)
C20—C19—C18—C17	−1.2 (3)	C1—C2—C3—C4	1.1 (3)
C19—C18—C17—C16	−0.3 (3)	C5—C4—C3—C2	1.2 (3)
C10—C9—C8—C7	−1.5 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*A is the centroid calculated through the ring A C atoms.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.91 (3)	2.08 (3)	2.987 (2)	175 (3)
C9—H9···O1^{ii}	0.93	2.34	3.228 (2)	160
C23—H23*A*···Cg*A*^{iii}	0.96	3.04	3.816 (3)	138
C2—H2···O4^{iv}	0.93	2.65	3.269 (2)	125
C3—H3···O4^{iv}	0.93	2.68	3.285 (2)	124

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+1, −*y*, −*z*+2; (iv) −*x*+1, *y*+1/2, −*z*+3/2.