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Crystal structures of (*E*)-3-(furan-2-yl)-2-phenyl-*N*-tosylacrylamide and (*E*)-3-phenyl-2-(*m*-tolyl)-*N*-tosylacrylamide

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Keywords: crystal structure; Cu-catalysed azide-alkyne cycloaddition reaction; CuAAC; N—H···O hydrogen bonding; inversion dimers; C—H···π interactions.

CCDC references: 1478730; 1478729

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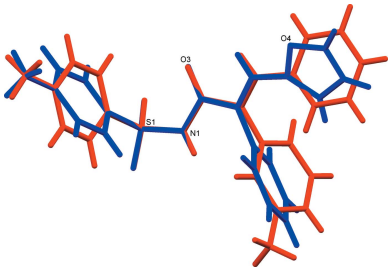
In the title *N*-tosylacrylamide compounds, $C_{20}H_{17}NO_4S$, (I), and $C_{23}H_{21}NO_3S$, (II), the conformation about the C=C bond is *E*. The acrylamide groups, [–NH—C(=O)—C=C–], are almost planar, with the N—C—C=C torsion angle being −170.18 (14)° in (I) and −168.01 (17)° in (II). In (I), the furan, phenyl and 4-methylbenzene rings are inclined to the acrylamide mean plane by 26.47 (11), 69.01 (8) and 82.49 (9)°, respectively. In (II), the phenyl, 3-methylbenzene and 4-methylbenzene rings are inclined to the acrylamide mean plane by 11.61 (10), 78.44 (10) and 78.24 (10)°, respectively. There is an intramolecular C—H···π interaction present in compound (II). In the crystals of both compounds, molecules are linked by pairs of N—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif. In (I), the dimers are reinforced by C—H···O hydrogen bonds and linked by C—H···π interactions, forming chains along [011]. In the crystal of (II), the dimers are linked *via* C—H···O hydrogen bonds, forming chains along [100]. The chains are further linked by C—H···π interactions, forming layers parallel to (010).

1. Chemical context

The Cu-catalysed azide-alkyne cycloaddition (CuAAC) reaction constitutes one of the most interesting examples of the click reaction (Bae *et al.*, 2005; Cheng *et al.*, 2012; Mondal & Pan, 2015). Trisubstituted alkenes are commonly found in the molecular skeleton of natural products and bioactive substances, and they are important building blocks in organic chemistry (Zhu *et al.*, 2012; Manikandan & Jeganmohan, 2015). Therefore, it is highly desirable to develop new efficient and general methods for the stereoselective synthesis of trisubstituted alkenes (Ram & Tittal, 2014; Bae *et al.*, 2005). As part of our work on the application of the CuAAC reaction (Cheng *et al.*, 2012), we report herein on the synthesis and crystal structures of the title compounds, (I) and (II).



2. Structural commentary

The molecular structures of the title compounds, (I) and (II), are illustrated in Figs. 1 and 2, respectively. Both molecules adopt an *E* conformation about the C=C bonds; C9=C16 in (I) and C9=C10 in (II). The acrylamide groups, [–NH—C(=O)—C=C–], are almost planar with the N1—C8—C9=C16 torsion angle being −170.18 (14) ° in (I), and the N1—C8—C9=C10 torsion angle being −168.01 (17)° in (II). The molecular conformation of the two molecules differ somewhat, as shown by the structure overlap illustrated in Fig. 3.

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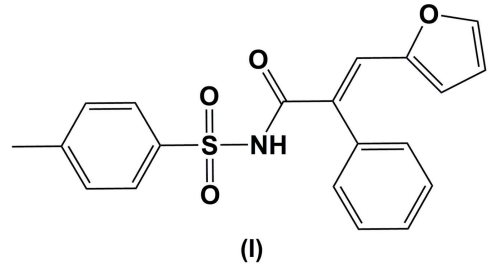
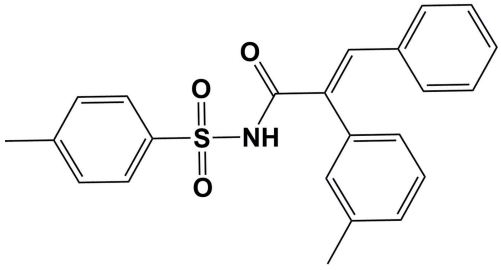


(I)



(II)

In (I) the furan, phenyl and 4-methylbenzene rings are inclined to the acrylamide mean plane [N1/O3/C8/C9/C16; maximum deviation of 0.0779 (15) Å for atom C9] by 26.47 (11), 69.01 (8) and 82.49 (9)°, respectively. The 4-methylbenzene ring is inclined to the furan and phenyl rings by 72.25 (11) and 19.00 (9)°, respectively, the latter two rings being inclined to one another by 66.28 (11)°. In (II), the phenyl, 3-methylbenzene and 4-methylbenzene rings are inclined to the acrylamide mean plane [N1/O3/C8/C9/C10; maximum deviation of 0.0998 (18) Å for atom C9] by 11.61 (10), 78.44 (10) and 78.24 (10)°, respectively. The 4-methylbenzene ring is inclined to the phenyl and 3-methylbenzene rings by dihedral angles of 78.33 (11) and 13.10 (11)°, respectively, the latter two rings being inclined to one another by 75.86 (11)°. There is an intramolecular C—H···π interaction present in compound (II) involving the adjacent phenyl and 3-methylbenzene rings (Table 2 and Fig. 2).

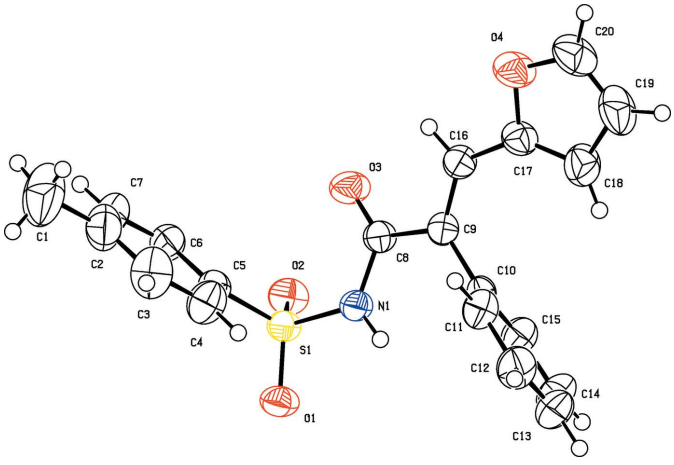


Figure 1
The molecular structure of compound (I), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

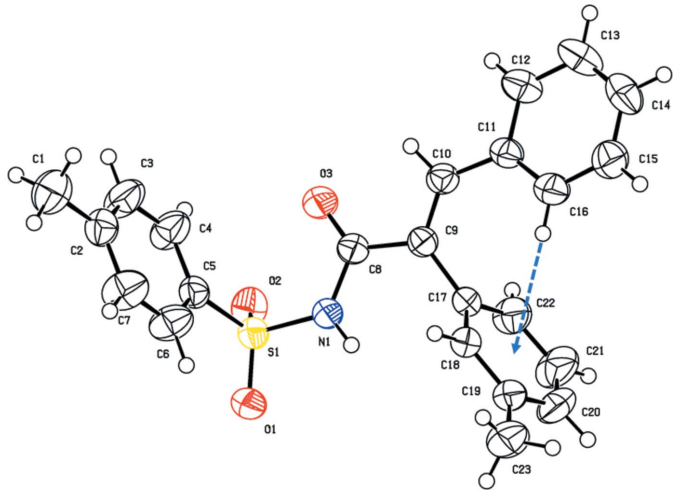


Figure 2
The molecular structure of compound (II), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. The intramolecular C—H···π interaction is shown by the blue dashed arrow (see Table 2).

3. Supramolecular features

In the crystal of both compounds, molecules are linked by pairs of N—H···O hydrogen bonds (Tables 1 and 2), forming inversion dimers with $R_2^2(8)$ ring motifs, as shown in Fig. 4 for (I) and Fig. 5 for (II). In (I), the dimers are reinforced by C—H···O hydrogen bonds and linked by C—H···π interactions (Table 1), forming chains propagating along [011]. In the crystal of (II), the dimers are linked *via* C—H···O hydrogen bonds, forming chains propagating along [100]. There is also a C—H···π interaction present, linking the chains to form layers lying parallel to (010).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, update February 2016; Groom *et al.*, 2016) for the substructure

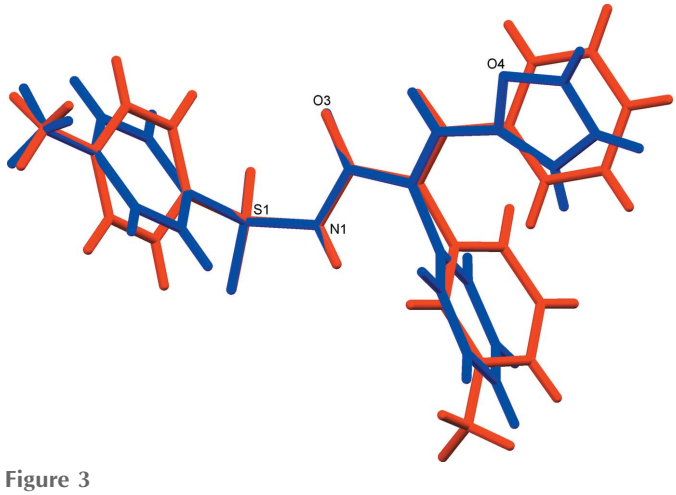


Figure 3
A view of the overlap of molecules (I) (blue) and (II) (red).

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

*Cg*1 is the centroid of the furan ring, O4/C17–C20

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.30	2.904 (2)	127
C4—H4···O1^{i}	0.93	2.55	3.427 (3)	158
C12—H12···*Cg*1^{ii}	0.93	2.81	3.664 (2)	158

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

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

*Cg*2 and *Cg*3 are the centroids of rings C11–C16 and C17–C22, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.31	3.038 (2)	143
C21—H21···O2^{ii}	0.93	2.57	3.468 (4)	163
C16—H16···*Cg*3	0.93	2.88	3.617 (2)	137
C18—H18···*Cg*2^{iii}	0.93	2.83	3.646 (2)	168

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

N-(phenylsulfonyl)acrylamide yielded five hits. Four of these compounds involve the 4-methylbenzenesulfonyl group and one compound involves a phenylsulfonyl group. This later compound, 2-(4-chlorophenyl)-3-(2-furyl)-*N*-(phenylsulfonyl)acrylamide (BIZGOI; Yu & Cao, 2014), is very similar to compound (I). The principal difference in the conformation of this molecule with respect to that of compound (I) is the dihedral angle involving the pyran ring and the adjacent aromatic ring, a phenyl ring in (I) and a chlorobenzene ring in BIZGOI; this angle is 66.18 (11)° in (I) but 88.84 (13)° in BIZGOI. In the crystal of BIZGOI, molecules are linked by pairs of N—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif, similar to the arrangement in the crystals of compounds (I) and (II).

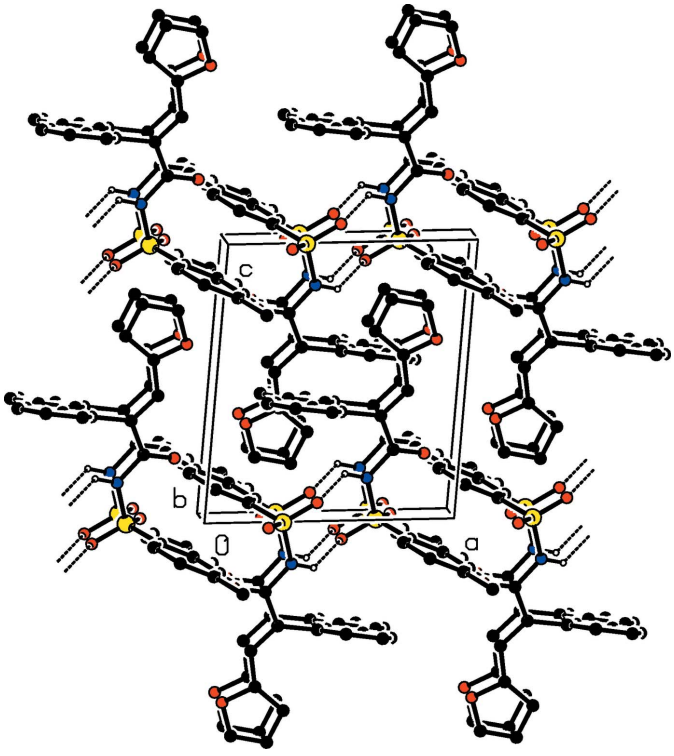


Figure 4
The crystal packing of compound (I), viewed along the *b*-axis direction. The hydrogen bonds are shown as dashed lines (see Table 1), and for clarity only the H atoms involved in the various interactions have been included.

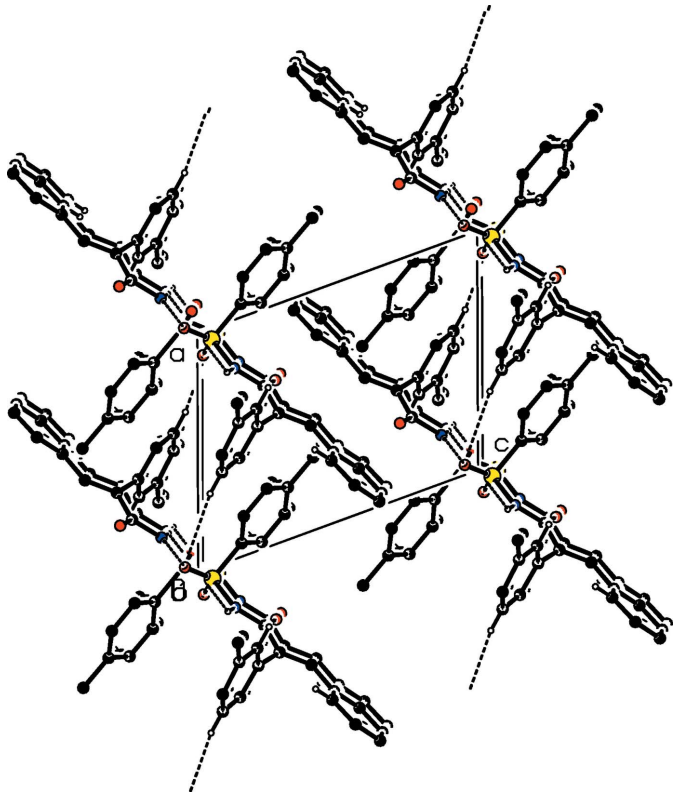


Figure 5
The crystal packing of compound (II), viewed along the *b*-axis direction. The hydrogen bonds are shown as dashed lines (see Table 2), and for clarity only the H atoms involved in the various interactions have been included.

5. Synthesis and crystallization

Compound (I): 4-methylbenzenesulfonyl azide (4.5 mmol), CuI (5.7 mg, 0.03 mmol), Et_4NI (7.7 mg, 0.03 mmol), ethynylbenzene (4.5 mmol), and furan-2-carbaldehyde (3 mmol) were suspended in CH_2Cl_2 (5 ml) in a 10 mL Schlenk tube under nitrogen at rt. LiOH (8.64 mg, 3.6mmol) was then added, and the resulting solution was stirred at this temperature. Upon full consumption of furan-2-carbaldehyde, the reaction was quenched by saturated aqueous NH_4Cl (5 ml) and extracted with CH_2Cl_2 (10 ml × 3). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude residue was purified by column chromatography on silica gel (*n*-hexane/EtOAc 5:1 *v*/*v*) to afford compound (I) as a white solid (yield: 0.79 g, 72%). Part of the purified product was redissolved in *n*-hexane/EtOAc and after

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{20}H_{17}NO_4S$	$C_{23}H_{21}NO_3S$
M_r	367.41	391.47
Crystal system, space group	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	293	293
a, b, c (Å)	10.309 (2), 10.391 (2), 10.566 (2)	9.2595 (10), 10.1158 (11), 11.9271 (12)
α, β, γ (°)	69.598 (2), 75.790 (2), 61.445 (2)	72.396 (1), 67.518 (1), 79.346 (1)
V (Å^3)	927.5 (3)	980.89 (18)
Z	2	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.20	0.19
Crystal size (mm)	0.21 × 0.20 × 0.19	0.23 × 0.22 × 0.19
Data collection		
Diffractometer	Bruker APEXII CCD area-detector	Bruker *SMART* CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.959, 0.963	0.958, 0.965
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8964, 3258, 3012	7136, 3422, 3082
R_{int}	0.024	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595	0.595
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.102, 1.04	0.040, 0.103, 1.00
No. of reflections	3258	3422
No. of parameters	237	255
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.31	0.24, −0.35

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

slow evaporation over several days, colourless crystals suitable for analysis by X-ray diffraction were formed.

Compound (II): 4-methylbenzenesulfonyl azide (4.5 mmol), CuI (5.7 mg, 0.03 mmol), Et_4NI (7.7 mg, 0.03 mmol), 1-ethynyl-3-methylbenzene (4.5 mmol), and benzaldehyde (3 mmol) were suspended in CH_2Cl_2 (5 ml) in a 10 mL Schlenk tube under nitrogen at rt. LiOH (8.64 mg, 3.6mmol) was then added, and the resulting solution was stirred at this temperature. Upon full consumption of benzaldehyde, the reaction was quenched by saturated aqueous NH_4Cl (5 ml) and extracted with CH_2Cl_2 (3 × 10 ml). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated *in vacuo*. The crude residue was purified by column chromatography on silica gel (*n*-hexane/EtOAc 5:1 *v*/*v*) to afford compound (II) as a white solid (0.82, 70%). Part of the purified product was redissolved in *n*-hexane/EtOAc and after slow evaporation over several days, colourless block-like crystals were obtained.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms: C—H = 0.93–0.96 Å and N—H = 0.86 Å, with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C,N) for other H atoms.

Acknowledgements

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supporting information

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Crystal structures of (*E*)-3-(furan-2-yl)-2-phenyl-*N*-tosylacrylamide and (*E*)-3-phenyl-2-(*m*-tolyl)-*N*-tosylacrylamide

Dong Cheng, Xiangzhen Meng, Zeyuan Sheng, Shuangming Wang, Yuanyuan Duan and Ziqian Li

Computing details

For both compounds, data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

(I) (*E*)-3-(Furan-2-yl)-*N*-(4-methylphenylsulfonyl)-2-phenylacrylamide

Crystal data

$C_{20}H_{17}NO_4S$
$M_r = 367.41$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.309$ (2) Å
$b = 10.391$ (2) Å
$c = 10.566$ (2) Å
$\alpha = 69.598$ (2)°
$\beta = 75.790$ (2)°
$\gamma = 61.445$ (2)°
$V = 927.5$ (3) Å^3
$Z = 2$
$F(000) = 384$
$D_x = 1.316$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8167 reflections
$\theta = 2.3$–27.5°
$\mu = 0.20$ mm^{-1}
$T = 293$ K
Block, colorless
0.21 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.959$, $T_{max} = 0.963$
8964 measured reflections
3258 independent reflections
3012 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.102$
$S = 1.04$
3258 reflections
237 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.266P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.029$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), FC*=KFC[1+0.001XFC^{2}Λ^3/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.043 (4)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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	0.31262 (4)	−0.04942 (4)	0.99847 (4)	0.0398 (1)
O1	0.44114 (12)	−0.12030 (13)	1.07038 (11)	0.0504 (4)
O2	0.25505 (13)	−0.14223 (13)	0.98347 (12)	0.0505 (4)
O3	0.14722 (12)	0.13779 (14)	0.75876 (12)	0.0566 (4)
O4	0.14941 (14)	0.51936 (14)	0.33592 (12)	0.0600 (4)
N1	0.36504 (13)	0.03957 (14)	0.84691 (12)	0.0412 (4)
C1	−0.1644 (3)	0.4486 (3)	1.2413 (3)	0.1107 (11)
C2	−0.0458 (2)	0.3231 (2)	1.1810 (2)	0.0702 (7)
C3	0.0932 (3)	0.3215 (3)	1.1313 (2)	0.0737 (8)
C4	0.2016 (2)	0.2091 (2)	1.0754 (2)	0.0599 (6)
C5	0.17206 (17)	0.09570 (18)	1.06750 (15)	0.0433 (5)
C6	0.03613 (18)	0.0933 (2)	1.11682 (17)	0.0529 (6)
C7	−0.0712 (2)	0.2073 (3)	1.1735 (2)	0.0659 (7)
C8	0.27179 (16)	0.12761 (16)	0.74414 (15)	0.0397 (5)
C9	0.33631 (16)	0.20731 (16)	0.61840 (14)	0.0374 (4)
C10	0.49564 (16)	0.17520 (16)	0.60270 (14)	0.0379 (4)
C11	0.53485 (19)	0.28623 (19)	0.60036 (17)	0.0496 (5)
C12	0.6822 (2)	0.2583 (2)	0.58483 (19)	0.0595 (7)
C13	0.7919 (2)	0.1204 (2)	0.5697 (2)	0.0634 (7)
C14	0.7551 (2)	0.0091 (2)	0.5724 (2)	0.0636 (6)
C15	0.60774 (18)	0.03538 (19)	0.59019 (17)	0.0489 (5)
C16	0.24031 (17)	0.31073 (16)	0.52654 (15)	0.0418 (5)
C17	0.27222 (18)	0.39778 (17)	0.39410 (16)	0.0459 (5)
C18	0.3932 (2)	0.3905 (2)	0.30719 (18)	0.0635 (6)
C19	0.3424 (3)	0.5141 (2)	0.18957 (19)	0.0735 (8)
C20	0.1978 (3)	0.5878 (2)	0.2122 (2)	0.0683 (7)
H1	0.45440	0.03080	0.83110	0.0490*
H1A	−0.13250	0.44460	1.32120	0.1660*
H1B	−0.25440	0.43580	1.26480	0.1660*

H1C	−0.18190	0.54530	1.17620	0.1660*
H3	0.11260	0.39830	1.13610	0.0880*
H4	0.29410	0.20900	1.04310	0.0720*
H6	0.01720	0.01620	1.11200	0.0630*
H7	−0.16290	0.20600	1.20750	0.0790*
H11	0.46120	0.38060	0.60930	0.0600*
H12	0.70710	0.33340	0.58460	0.0710*
H13	0.89090	0.10250	0.55770	0.0760*
H14	0.82930	−0.08450	0.56220	0.0760*
H15	0.58380	−0.04160	0.59380	0.0590*
H16	0.14160	0.32800	0.55170	0.0500*
H18	0.49070	0.31910	0.32090	0.0760*
H19	0.40080	0.53830	0.11130	0.0880*
H20	0.13730	0.67450	0.15190	0.0820*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0370 (2)	0.0433 (2)	0.0375 (2)	−0.0226 (2)	−0.0060 (2)	0.0002 (2)
O1	0.0430 (6)	0.0558 (7)	0.0455 (6)	−0.0249 (5)	−0.0132 (5)	0.0052 (5)
O2	0.0530 (7)	0.0483 (6)	0.0544 (7)	−0.0305 (5)	−0.0088 (5)	−0.0036 (5)
O3	0.0423 (6)	0.0675 (8)	0.0527 (7)	−0.0300 (6)	−0.0106 (5)	0.0053 (6)
O4	0.0613 (8)	0.0502 (7)	0.0535 (7)	−0.0213 (6)	−0.0173 (6)	0.0067 (5)
N1	0.0351 (6)	0.0488 (7)	0.0370 (7)	−0.0225 (6)	−0.0040 (5)	−0.0017 (5)
C1	0.113 (2)	0.0914 (19)	0.101 (2)	−0.0286 (17)	0.0316 (17)	−0.0472 (16)
C2	0.0717 (13)	0.0694 (13)	0.0546 (11)	−0.0226 (11)	0.0076 (10)	−0.0209 (9)
C3	0.0871 (15)	0.0661 (12)	0.0762 (14)	−0.0420 (12)	0.0087 (12)	−0.0271 (11)
C4	0.0568 (10)	0.0622 (11)	0.0676 (12)	−0.0359 (9)	0.0055 (9)	−0.0184 (9)
C5	0.0421 (8)	0.0516 (9)	0.0358 (7)	−0.0249 (7)	−0.0034 (6)	−0.0047 (6)
C6	0.0457 (9)	0.0704 (11)	0.0483 (9)	−0.0318 (8)	−0.0001 (7)	−0.0157 (8)
C7	0.0484 (10)	0.0895 (14)	0.0567 (11)	−0.0302 (10)	0.0091 (8)	−0.0254 (10)
C8	0.0380 (8)	0.0397 (8)	0.0393 (8)	−0.0181 (6)	−0.0044 (6)	−0.0061 (6)
C9	0.0389 (8)	0.0341 (7)	0.0370 (7)	−0.0154 (6)	−0.0015 (6)	−0.0093 (6)
C10	0.0402 (8)	0.0404 (8)	0.0303 (7)	−0.0185 (6)	−0.0004 (6)	−0.0068 (6)
C11	0.0504 (9)	0.0458 (9)	0.0537 (10)	−0.0237 (8)	0.0026 (7)	−0.0156 (7)
C12	0.0609 (11)	0.0707 (12)	0.0611 (11)	−0.0436 (10)	0.0024 (9)	−0.0173 (9)
C13	0.0422 (9)	0.0825 (14)	0.0635 (11)	−0.0311 (10)	0.0037 (8)	−0.0175 (10)
C14	0.0418 (9)	0.0593 (11)	0.0755 (13)	−0.0117 (8)	0.0034 (8)	−0.0231 (9)
C15	0.0451 (9)	0.0437 (8)	0.0551 (10)	−0.0175 (7)	−0.0012 (7)	−0.0152 (7)
C16	0.0415 (8)	0.0380 (8)	0.0413 (8)	−0.0160 (6)	−0.0030 (6)	−0.0078 (6)
C17	0.0503 (9)	0.0379 (8)	0.0431 (8)	−0.0169 (7)	−0.0090 (7)	−0.0037 (6)
C18	0.0633 (11)	0.0609 (11)	0.0488 (10)	−0.0233 (9)	0.0028 (9)	−0.0057 (8)
C19	0.0955 (17)	0.0690 (13)	0.0431 (10)	−0.0414 (12)	0.0043 (10)	0.0004 (9)
C20	0.0847 (15)	0.0572 (11)	0.0510 (10)	−0.0331 (11)	−0.0186 (10)	0.0107 (9)

Geometric parameters (Å, º)

S1—O1	1.4305 (14)	C13—C14	1.369 (3)
S1—O2	1.4168 (15)	C14—C15	1.384 (3)
S1—N1	1.6529 (13)	C16—C17	1.436 (2)
S1—C5	1.7506 (18)	C17—C18	1.342 (3)
O3—C8	1.212 (2)	C18—C19	1.426 (3)
O4—C17	1.374 (2)	C19—C20	1.314 (4)
O4—C20	1.354 (3)	C1—H1A	0.9600
N1—C8	1.385 (2)	C1—H1B	0.9600
C1—C2	1.508 (4)	C1—H1C	0.9600
N1—H1	0.8600	C3—H3	0.9300
C2—C3	1.394 (4)	C4—H4	0.9300
C2—C7	1.379 (3)	C6—H6	0.9300
C3—C4	1.368 (3)	C7—H7	0.9300
C4—C5	1.383 (3)	C11—H11	0.9300
C5—C6	1.379 (3)	C12—H12	0.9300
C6—C7	1.379 (3)	C13—H13	0.9300
C8—C9	1.490 (2)	C14—H14	0.9300
C9—C10	1.489 (3)	C15—H15	0.9300
C9—C16	1.343 (2)	C16—H16	0.9300
C10—C15	1.385 (2)	C18—H18	0.9300
C10—C11	1.384 (3)	C19—H19	0.9300
C11—C12	1.381 (3)	C20—H20	0.9300
C12—C13	1.371 (3)		
O1—S1—O2	118.76 (8)	O4—C17—C16	114.34 (16)
O1—S1—N1	103.46 (8)	C17—C18—C19	106.2 (2)
O1—S1—C5	109.41 (8)	C18—C19—C20	107.4 (2)
O2—S1—N1	109.21 (7)	O4—C20—C19	110.31 (19)
O2—S1—C5	110.00 (9)	C2—C1—H1A	110.00
N1—S1—C5	104.98 (7)	C2—C1—H1B	109.00
C17—O4—C20	107.00 (17)	C2—C1—H1C	109.00
S1—N1—C8	123.08 (13)	H1A—C1—H1B	109.00
S1—N1—H1	118.00	H1A—C1—H1C	109.00
C8—N1—H1	118.00	H1B—C1—H1C	109.00
C3—C2—C7	118.2 (2)	C2—C3—H3	119.00
C1—C2—C7	121.3 (2)	C4—C3—H3	119.00
C1—C2—C3	120.5 (2)	C3—C4—H4	120.00
C2—C3—C4	121.2 (3)	C5—C4—H4	120.00
C3—C4—C5	119.2 (2)	C5—C6—H6	121.00
S1—C5—C4	118.85 (15)	C7—C6—H6	121.00
S1—C5—C6	120.12 (14)	C2—C7—H7	119.00
C4—C5—C6	120.99 (17)	C6—C7—H7	119.00
C5—C6—C7	118.76 (19)	C10—C11—H11	120.00
C2—C7—C6	121.6 (2)	C12—C11—H11	120.00
O3—C8—C9	123.90 (15)	C11—C12—H12	120.00
N1—C8—C9	114.94 (15)	C13—C12—H12	120.00

O3—C8—N1	121.15 (15)	C12—C13—H13	120.00
C10—C9—C16	124.12 (14)	C14—C13—H13	120.00
C8—C9—C10	120.46 (13)	C13—C14—H14	120.00
C8—C9—C16	115.38 (16)	C15—C14—H14	120.00
C11—C10—C15	118.34 (18)	C10—C15—H15	120.00
C9—C10—C15	121.55 (16)	C14—C15—H15	120.00
C9—C10—C11	120.11 (15)	C9—C16—H16	116.00
C10—C11—C12	120.69 (17)	C17—C16—H16	116.00
C11—C12—C13	120.3 (2)	C17—C18—H18	127.00
C12—C13—C14	119.8 (2)	C19—C18—H18	127.00
C13—C14—C15	120.26 (18)	C18—C19—H19	126.00
C10—C15—C14	120.62 (18)	C20—C19—H19	126.00
C9—C16—C17	127.63 (18)	O4—C20—H20	125.00
O4—C17—C18	109.06 (15)	C19—C20—H20	125.00
C16—C17—C18	136.58 (17)		

O1—S1—N1—C8	−178.32 (12)	O3—C8—C9—C10	−173.10 (15)
O2—S1—N1—C8	54.28 (14)	O3—C8—C9—C16	9.3 (2)
C5—S1—N1—C8	−63.63 (14)	N1—C8—C9—C10	7.5 (2)
O1—S1—C5—C4	55.32 (16)	N1—C8—C9—C16	−170.18 (14)
O2—S1—C5—C4	−172.53 (14)	C16—C9—C10—C15	−114.84 (18)
N1—S1—C5—C4	−55.15 (16)	C8—C9—C16—C17	−176.14 (15)
O1—S1—C5—C6	−122.64 (14)	C10—C9—C16—C17	6.3 (3)
O2—S1—C5—C6	9.51 (16)	C8—C9—C10—C15	67.7 (2)
N1—S1—C5—C6	126.88 (14)	C8—C9—C10—C11	−112.25 (17)
C17—O4—C20—C19	1.2 (3)	C16—C9—C10—C11	65.2 (2)
C20—O4—C17—C18	−0.8 (2)	C9—C10—C15—C14	178.43 (15)
C20—O4—C17—C16	−179.35 (17)	C9—C10—C11—C12	−179.51 (15)
S1—N1—C8—O3	−3.6 (2)	C15—C10—C11—C12	0.5 (2)
S1—N1—C8—C9	175.84 (11)	C11—C10—C15—C14	−1.6 (2)
C3—C2—C7—C6	−1.0 (3)	C10—C11—C12—C13	0.9 (3)
C1—C2—C7—C6	179.1 (2)	C11—C12—C13—C14	−1.1 (3)
C1—C2—C3—C4	−179.5 (2)	C12—C13—C14—C15	0.1 (3)
C7—C2—C3—C4	0.6 (3)	C13—C14—C15—C10	1.3 (3)
C2—C3—C4—C5	0.4 (3)	C9—C16—C17—O4	−165.28 (16)
C3—C4—C5—S1	−178.90 (16)	C9—C16—C17—C18	16.7 (3)
C3—C4—C5—C6	−1.0 (3)	O4—C17—C18—C19	0.1 (2)
S1—C5—C6—C7	178.49 (14)	C16—C17—C18—C19	178.2 (2)
C4—C5—C6—C7	0.6 (3)	C17—C18—C19—C20	0.6 (3)
C5—C6—C7—C2	0.4 (3)	C18—C19—C20—O4	−1.2 (3)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the furan ring, O4/C17–C20

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.30	2.904 (2)	127

C4—H4···O1^{i}	0.93	2.55	3.427 (3)	158
C12—H12···*Cg*1^{ii}	0.93	2.81	3.664 (2)	158

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

(II) (*E*)-2-(3-Methylphenyl)-*N*-(4-methylphenylsulfonyl)-3-phenylacrylamide

Crystal data

$C_{23}H_{21}NO_3S$
M_r = 391.47
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.2595 (10) Å
b = 10.1158 (11) Å
c = 11.9271 (12) Å
α = 72.396 (1)°
β = 67.518 (1)°
γ = 79.346 (1)°
V = 980.89 (18) Å^3
Z = 2
$F(000)$ = 412
D_x = 1.325 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5782 reflections
θ = 2.4–27.5°
μ = 0.19 mm^{-1}
T = 293 K
Block, colorless
0.23 × 0.22 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.958, T_{max} = 0.965
7136 measured reflections
3422 independent reflections
3082 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.0°, θ_{min} = 1.9°
h = −11→11
k = −11→12
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.103
S = 1.00
3422 reflections
255 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.4517P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.020
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of F^2 > 2sigma(F^2) is used only for calculating -R-factor-obs 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	0.95790 (5)	0.26449 (4)	0.05551 (4)	0.0436 (1)
O1	1.04900 (15)	0.37065 (13)	−0.04088 (12)	0.0547 (4)
O2	0.90276 (16)	0.16492 (14)	0.02290 (13)	0.0569 (5)
O3	0.68817 (16)	0.16464 (13)	0.28061 (14)	0.0597 (5)
N1	0.80466 (16)	0.35319 (15)	0.13653 (14)	0.0451 (5)
C1	1.3053 (3)	−0.0307 (3)	0.4111 (2)	0.0727 (9)
C2	1.2199 (2)	0.0429 (2)	0.32171 (19)	0.0528 (6)
C3	1.1116 (3)	−0.0221 (2)	0.3086 (3)	0.0722 (8)
C4	1.0318 (3)	0.0434 (2)	0.2278 (2)	0.0675 (8)
C5	1.05970 (19)	0.17789 (17)	0.15828 (17)	0.0428 (5)
C6	1.1700 (3)	0.2442 (2)	0.1675 (2)	0.0633 (8)
C7	1.2484 (3)	0.1761 (2)	0.2490 (2)	0.0693 (8)
C8	0.68331 (19)	0.28973 (18)	0.24058 (16)	0.0428 (5)
C9	0.55006 (18)	0.38643 (17)	0.29569 (16)	0.0386 (5)
C10	0.44805 (19)	0.32908 (18)	0.40848 (16)	0.0426 (5)
C11	0.3048 (2)	0.39036 (19)	0.48921 (16)	0.0429 (5)
C12	0.1949 (2)	0.2998 (2)	0.57903 (18)	0.0562 (7)
C13	0.0586 (3)	0.3480 (3)	0.6607 (2)	0.0681 (8)
C14	0.0297 (2)	0.4866 (3)	0.6551 (2)	0.0658 (8)
C15	0.1372 (3)	0.5781 (2)	0.5689 (2)	0.0640 (7)
C16	0.2740 (2)	0.5309 (2)	0.48597 (18)	0.0543 (6)
C17	0.52982 (18)	0.53233 (17)	0.22211 (15)	0.0394 (5)
C18	0.60582 (19)	0.63895 (17)	0.22063 (16)	0.0419 (5)
C19	0.5787 (2)	0.77626 (19)	0.15814 (18)	0.0526 (6)
C20	0.4696 (3)	0.8034 (2)	0.0996 (2)	0.0756 (8)
C21	0.3957 (3)	0.6992 (3)	0.0975 (3)	0.0837 (10)
C22	0.4264 (2)	0.5634 (2)	0.1573 (2)	0.0606 (7)
C23	0.6632 (3)	0.8906 (2)	0.1559 (2)	0.0737 (8)
H1	0.80020	0.44260	0.11300	0.0540*
H1A	1.23480	−0.03780	0.49580	0.1090*
H1B	1.39150	0.02090	0.39490	0.1090*
H1C	1.34430	−0.12220	0.39960	0.1090*
H3	1.09170	−0.11290	0.35580	0.0870*
H4	0.95940	−0.00300	0.22020	0.0810*
H6	1.19150	0.33430	0.11900	0.0760*
H7	1.32280	0.22150	0.25500	0.0830*
H10	0.47200	0.23520	0.44070	0.0510*
H12	0.21380	0.20500	0.58400	0.0670*
H13	−0.01370	0.28600	0.71960	0.0820*
H14	−0.06280	0.51920	0.70970	0.0790*
H15	0.11800	0.67230	0.56630	0.0770*
H16	0.34570	0.59370	0.42760	0.0650*
H18	0.67690	0.61820	0.26250	0.0500*
H20	0.44570	0.89480	0.06040	0.0910*
H21	0.32450	0.72020	0.05570	0.1000*

H22	0.37780	0.49260	0.15420	0.0730*
H23A	0.74480	0.91580	0.07570	0.1100*
H23B	0.70830	0.85900	0.22060	0.1100*
H23C	0.59060	0.97000	0.16980	0.1100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0405 (2)	0.0405 (2)	0.0452 (3)	−0.0018 (2)	−0.0106 (2)	−0.0112 (2)
O1	0.0506 (7)	0.0506 (7)	0.0466 (7)	−0.0047 (6)	−0.0035 (6)	−0.0068 (6)
O2	0.0592 (8)	0.0539 (8)	0.0666 (9)	−0.0005 (6)	−0.0276 (7)	−0.0231 (7)
O3	0.0540 (8)	0.0372 (7)	0.0687 (9)	−0.0055 (6)	−0.0057 (7)	−0.0057 (6)
N1	0.0395 (8)	0.0350 (7)	0.0501 (9)	−0.0023 (6)	−0.0074 (6)	−0.0071 (6)
C1	0.0784 (15)	0.0720 (15)	0.0750 (15)	0.0034 (12)	−0.0401 (13)	−0.0171 (12)
C2	0.0521 (11)	0.0516 (11)	0.0550 (11)	0.0029 (8)	−0.0188 (9)	−0.0178 (9)
C3	0.0748 (14)	0.0441 (11)	0.0995 (18)	−0.0114 (10)	−0.0474 (14)	0.0052 (11)
C4	0.0659 (13)	0.0444 (11)	0.0996 (17)	−0.0145 (9)	−0.0470 (13)	0.0009 (11)
C5	0.0381 (9)	0.0391 (9)	0.0479 (10)	−0.0021 (7)	−0.0104 (7)	−0.0132 (7)
C6	0.0806 (15)	0.0465 (11)	0.0705 (14)	−0.0199 (10)	−0.0357 (12)	−0.0049 (10)
C7	0.0858 (16)	0.0602 (13)	0.0792 (15)	−0.0231 (11)	−0.0462 (13)	−0.0091 (11)
C8	0.0392 (9)	0.0405 (9)	0.0462 (10)	−0.0066 (7)	−0.0135 (7)	−0.0072 (8)
C9	0.0353 (8)	0.0389 (9)	0.0424 (9)	−0.0058 (7)	−0.0150 (7)	−0.0080 (7)
C10	0.0421 (9)	0.0403 (9)	0.0451 (10)	−0.0073 (7)	−0.0159 (8)	−0.0072 (7)
C11	0.0410 (9)	0.0501 (10)	0.0359 (9)	−0.0088 (7)	−0.0120 (7)	−0.0075 (7)
C12	0.0557 (11)	0.0594 (12)	0.0504 (11)	−0.0194 (9)	−0.0073 (9)	−0.0154 (9)
C13	0.0538 (12)	0.0868 (16)	0.0556 (12)	−0.0284 (11)	0.0036 (10)	−0.0227 (11)
C14	0.0470 (11)	0.0891 (17)	0.0547 (12)	−0.0032 (11)	−0.0042 (9)	−0.0280 (12)
C15	0.0663 (13)	0.0598 (12)	0.0554 (12)	0.0057 (10)	−0.0132 (10)	−0.0167 (10)
C16	0.0537 (11)	0.0515 (11)	0.0453 (10)	−0.0060 (9)	−0.0068 (9)	−0.0074 (8)
C17	0.0324 (8)	0.0425 (9)	0.0369 (8)	−0.0024 (7)	−0.0082 (7)	−0.0067 (7)
C18	0.0389 (9)	0.0418 (9)	0.0403 (9)	−0.0023 (7)	−0.0119 (7)	−0.0067 (7)
C19	0.0506 (10)	0.0417 (10)	0.0511 (11)	−0.0034 (8)	−0.0076 (9)	−0.0048 (8)
C20	0.0734 (15)	0.0528 (13)	0.0834 (16)	−0.0018 (11)	−0.0364 (13)	0.0165 (11)
C21	0.0796 (16)	0.0807 (17)	0.0924 (18)	−0.0071 (13)	−0.0594 (15)	0.0143 (14)
C22	0.0561 (12)	0.0641 (13)	0.0659 (13)	−0.0120 (10)	−0.0339 (10)	−0.0019 (10)
C23	0.0822 (16)	0.0438 (11)	0.0838 (16)	−0.0112 (10)	−0.0195 (13)	−0.0091 (11)

Geometric parameters (Å, º)

S1—O2	1.4161 (16)	C18—C19	1.391 (3)
S1—O1	1.4258 (14)	C19—C20	1.380 (3)
S1—N1	1.6605 (16)	C19—C23	1.500 (3)
S1—C5	1.7571 (19)	C20—C21	1.370 (4)
O3—C8	1.209 (2)	C21—C22	1.377 (4)
N1—C8	1.390 (2)	C1—H1A	0.9600
C1—C2	1.504 (3)	C1—H1B	0.9600
N1—H1	0.8600	C1—H1C	0.9600
C2—C3	1.374 (4)	C3—H3	0.9300

C2—C7	1.374 (3)	C4—H4	0.9300
C3—C4	1.375 (4)	C6—H6	0.9300
C4—C5	1.374 (3)	C7—H7	0.9300
C5—C6	1.374 (3)	C10—H10	0.9300
C6—C7	1.377 (4)	C12—H12	0.9300
C8—C9	1.495 (3)	C13—H13	0.9300
C9—C10	1.341 (2)	C14—H14	0.9300
C9—C17	1.491 (2)	C15—H15	0.9300
C10—C11	1.467 (3)	C16—H16	0.9300
C11—C16	1.389 (3)	C18—H18	0.9300
C11—C12	1.393 (3)	C20—H20	0.9300
C12—C13	1.378 (3)	C21—H21	0.9300
C13—C14	1.364 (4)	C22—H22	0.9300
C14—C15	1.374 (3)	C23—H23A	0.9600
C15—C16	1.384 (3)	C23—H23B	0.9600
C17—C22	1.386 (3)	C23—H23C	0.9600
C17—C18	1.385 (3)		

O2—S1—O1	119.71 (8)	C20—C21—C22	120.2 (3)
O2—S1—N1	108.68 (9)	C17—C22—C21	119.9 (2)
O2—S1—C5	109.20 (9)	C2—C1—H1A	110.00
O1—S1—N1	103.40 (8)	C2—C1—H1B	109.00
O1—S1—C5	109.12 (9)	C2—C1—H1C	109.00
N1—S1—C5	105.77 (8)	H1A—C1—H1B	109.00
S1—N1—C8	123.08 (13)	H1A—C1—H1C	109.00
S1—N1—H1	118.00	H1B—C1—H1C	109.00
C8—N1—H1	118.00	C2—C3—H3	119.00
C1—C2—C3	120.9 (2)	C4—C3—H3	119.00
C1—C2—C7	121.6 (2)	C3—C4—H4	120.00
C3—C2—C7	117.5 (2)	C5—C4—H4	120.00
C2—C3—C4	121.8 (2)	C5—C6—H6	120.00
C3—C4—C5	119.5 (2)	C7—C6—H6	120.00
C4—C5—C6	119.8 (2)	C2—C7—H7	119.00
S1—C5—C4	120.43 (17)	C6—C7—H7	119.00
S1—C5—C6	119.78 (15)	C9—C10—H10	115.00
C5—C6—C7	119.5 (2)	C11—C10—H10	115.00
C2—C7—C6	121.9 (2)	C11—C12—H12	119.00
N1—C8—C9	115.33 (15)	C13—C12—H12	119.00
O3—C8—N1	120.79 (17)	C12—C13—H13	120.00
O3—C8—C9	123.88 (17)	C14—C13—H13	120.00
C10—C9—C17	124.16 (16)	C13—C14—H14	120.00
C8—C9—C10	115.24 (16)	C15—C14—H14	120.00
C8—C9—C17	120.42 (15)	C14—C15—H15	120.00
C9—C10—C11	130.45 (17)	C16—C15—H15	120.00
C12—C11—C16	117.83 (18)	C11—C16—H16	120.00
C10—C11—C12	117.32 (17)	C15—C16—H16	120.00
C10—C11—C16	124.79 (17)	C17—C18—H18	119.00
C11—C12—C13	121.2 (2)	C19—C18—H18	119.00

C12—C13—C14	120.0 (2)	C19—C20—H20	119.00
C13—C14—C15	120.0 (2)	C21—C20—H20	119.00
C14—C15—C16	120.4 (2)	C20—C21—H21	120.00
C11—C16—C15	120.46 (19)	C22—C21—H21	120.00
C18—C17—C22	118.86 (17)	C17—C22—H22	120.00
C9—C17—C18	122.21 (16)	C21—C22—H22	120.00
C9—C17—C22	118.87 (17)	C19—C23—H23A	109.00
C17—C18—C19	121.81 (17)	C19—C23—H23B	109.00
C18—C19—C23	121.31 (19)	C19—C23—H23C	109.00
C20—C19—C23	121.30 (19)	H23A—C23—H23B	109.00
C18—C19—C20	117.38 (18)	H23A—C23—H23C	109.00
C19—C20—C21	121.7 (2)	H23B—C23—H23C	110.00

O2—S1—N1—C8	51.45 (17)	C17—C9—C10—C11	−4.3 (3)
O1—S1—N1—C8	179.65 (15)	C8—C9—C17—C18	−85.9 (2)
C5—S1—N1—C8	−65.69 (17)	C8—C9—C17—C22	96.9 (2)
O2—S1—C5—C4	−22.48 (19)	C10—C9—C17—C18	99.4 (2)
O1—S1—C5—C4	−155.02 (16)	C10—C9—C17—C22	−77.8 (2)
N1—S1—C5—C4	94.32 (17)	C9—C10—C11—C12	158.7 (2)
O2—S1—C5—C6	156.34 (16)	C9—C10—C11—C16	−24.1 (3)
O1—S1—C5—C6	23.79 (19)	C10—C11—C12—C13	178.6 (2)
N1—S1—C5—C6	−86.87 (18)	C16—C11—C12—C13	1.1 (3)
S1—N1—C8—C9	−175.81 (13)	C10—C11—C16—C15	−177.9 (2)
S1—N1—C8—O3	3.5 (3)	C12—C11—C16—C15	−0.8 (3)
C1—C2—C3—C4	179.8 (2)	C11—C12—C13—C14	−0.4 (4)
C3—C2—C7—C6	1.3 (3)	C12—C13—C14—C15	−0.7 (4)
C1—C2—C7—C6	−179.7 (2)	C13—C14—C15—C16	1.1 (4)
C7—C2—C3—C4	−1.2 (4)	C14—C15—C16—C11	−0.3 (3)
C2—C3—C4—C5	−0.4 (4)	C9—C17—C18—C19	−175.89 (17)
C3—C4—C5—C6	1.8 (3)	C22—C17—C18—C19	1.3 (3)
C3—C4—C5—S1	−179.38 (19)	C9—C17—C22—C21	174.5 (2)
S1—C5—C6—C7	179.47 (17)	C18—C17—C22—C21	−2.8 (3)
C4—C5—C6—C7	−1.7 (3)	C17—C18—C19—C20	1.5 (3)
C5—C6—C7—C2	0.2 (3)	C17—C18—C19—C23	−179.25 (18)
O3—C8—C9—C10	12.7 (3)	C18—C19—C20—C21	−3.0 (3)
O3—C8—C9—C17	−162.47 (18)	C23—C19—C20—C21	177.8 (2)
N1—C8—C9—C10	−168.01 (17)	C19—C20—C21—C22	1.6 (4)
N1—C8—C9—C17	16.8 (2)	C20—C21—C22—C17	1.4 (4)
C8—C9—C10—C11	−179.30 (19)		

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of rings C11–C16 and C17–C22, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.31	3.038 (2)	143
C21—H21···O2^{ii}	0.93	2.57	3.468 (4)	163

C16—H16···*Cg*3	0.93	2.88	3.617 (2)	137
C18—H18···*Cg*2^{iii}	0.93	2.83	3.646 (2)	168

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