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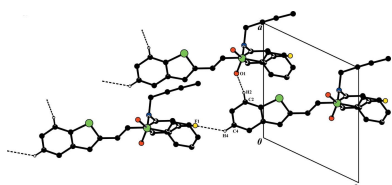
Crystal-structure determination and Hirshfeld surface analysis of two new thiophene derivatives: (*E*)-*N*-{2-[2-(benzo[*b*]thiophen-2-yl)ethenyl]-5-fluorophenyl}benzenesulfonamide and (*E*)-*N*-{2-[2-(benzo[*b*]thiophen-2-yl)ethenyl]-5-fluorophenyl}-*N*-(but-2-yn-1-yl)benzenesulfonamide

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In the title compounds, C₂₂H₁₆FNO₂S₂ (**I**) and C₂₆H₂₀FNO₂S₂ (**II**), the benzothiophene rings are essentially planar with maximum deviations of 0.009 (1) and 0.001 (1) Å for the carbon and sulfur atom in compounds **I** and **II**, respectively. In **I**, the thiophene ring system is almost orthogonal to the phenyl ring attached to the sulfonyl group, with a dihedral angle of 77.7 (1)°. In compound **I**, the molecular structure is stabilized by weak C—H···O intramolecular interactions formed by the sulfone oxygen atoms, which generate two *S*(5) ring motifs. In the crystal of **I**, N—H···O hydrogen bonds link the molecules into *R*₂²(8) rings, which are connected into a *C*(10) chain *via* C—H···F hydrogen bonds. Intermolecular C—H···π interactions are also observed. In compound **II**, the molecules are linked *via* C—H···O and C—H···F hydrogen bonding, generating infinite *C*(11) and *C*(13) chains running parallel to [010].

1. Chemical context

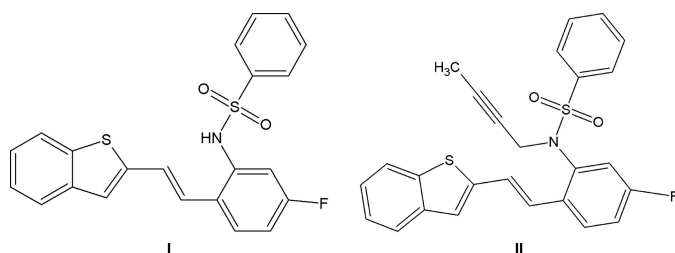
Thiophene, C₄H₄S, belongs to a class of aromatic five-membered heterocycles comprising one S heteroatom. Thiophene derivatives possess pharmacological and biological activities including antibacterial (Mishra *et al.*, 2012), anti-allergic (Gillespie *et al.*, 1985), anti-cancer and anti-toxic (Gewald *et al.*, 1966), analgesic (Laddi *et al.*, 1998; Chen *et al.*, 2008), anti-inflammatory (Ferreira *et al.*, 2006), antioxidant (Jarak *et al.*, 2005), antitumor (Gadad *et al.*, 1994), antimicrobial (Abdel-Rahman *et al.*, 2003), antihypertensive (Monge Vega *et al.*, 1980), anti-diabetes mellitus (Abdelhamid *et al.*, 2009), gonadotropin releasing hormone antagonist (Sabins *et al.*, 1944) and they are building blocks in many agrochemicals (Ansary & Omar, 2001). Thiophene possesses promising pharmacological activities, such as anti-HIV PR inhibitor (Bonini *et al.*, 2005) and anti-breast cancer (Brault *et al.*, 2005). Benzothiophenes are biologically energetic molecules. One of the most significant drugs based on the benzothiophene structure is Raloxifene, used to treat osteoporosis in postmenopausal women (Jordan, 2003). Benzothiophenes are also present in luminescent components used in organic materials (Russell & Press, 1996). Thiophene derivatives have a wide variety of applications in optical and



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electronic systems (Gather *et al.*, 2008; He *et al.*, 2009) and are used extensively in solar cells (Justin Thomas *et al.*, 2008), organic light-emitting diodes (OLEDs) (Mazzeo *et al.*, 2003), organic field-effect transistors (OFETs) (Zhan *et al.*, 2007) and as NLO devices (Bedworth *et al.*, 1996; Raposo *et al.*, 2011). Thieno-pyridine products are used in medicine as allosteric adenosine receptors and in the treatment of adenosine-sensitive cardiac arrhythmias (Tumey *et al.*, 2008; Grunewald *et al.*, 2008). Recognizing the importance of such compounds in drug discovery and our ongoing research into the construction of novel thiophene has prompted us to investigate the title thiophene derivatives and we report herein their synthesis, crystal structures and Hirshfeld surface analysis.



2. Structural commentary

The molecular structure of compound **I**, $C_{22}H_{16}FNO_2S_2$ (Fig. 1), comprises a benzothiophene ring system (S1/C1–C8) attached to an *N*-(5-fluoro-2-vinylphenyl)benzenesulfonamide (C7–C22/N1/S2/O1/O2/F1) while compound **II**, $C_{26}H_{20}FNO_2S_2$ (Fig. 2), comprises a benzothiophene ring system (S1/C1–C8) attached to an *N*-but-2-yn-1-yl-*N*-(5-fluoro-2-vinylphenyl)benzenesulfonamide (C9–C15/N1/S2/O1/O2). In both compounds, the benzothiophene ring systems (S1/C1–C8) are essentially planar with maximum deviations of 0.009 (1) and 0.001 (1) Å for atom C8 and S1 in compounds **I** and **II**, respectively. The mean planes of the thiophene ring system in **I** make dihedral angles of 1.2 (2), 2.3 (2), 77.7 (2)° with the C1–C6, C11–C16 and C17–C22 phenyl rings. The mean planes of the thiophene ring system in **II** make dihedral angles of 0.3 (2), 33.3 (2), 25.2 (2)°, respectively, with the C1–

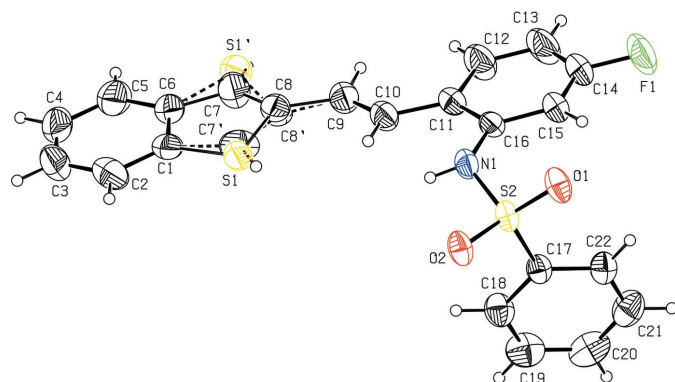


Figure 1
The molecular structure of compound **I**, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C15–H15···O1	0.93	2.30	2.980 (3)	130
C10–H10···O2 ⁱ	0.93	2.51	3.383 (3)	157
N1–H1N···O2 ⁱ	0.83 (2)	2.21 (2)	3.001 (2)	161 (2)
C22–H22···F1 ⁱⁱ	0.93	2.44	3.116 (3)	130

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

C6, C11–C16 and C17–C22 phenyl rings, The benzothiophene ring system in **I** is almost orthogonal to the C17–C22 ring attached to sulfonyl group with dihedral angle of 77.7 (1)° in **I**. For both compounds, the bond lengths and angles are close to those observed for similar structures (Madhan *et al.*, 2022, 2023).

In both compounds, the tetrahedral configuration is distorted around atom S1. The increase in the O2–S2–O1 angle [118.64 (9) in **I** and 120.6 (2)° in **II**], with a simultaneous decrease in the N1–S2–C17 angle [106.35 (9) in **I** and 108.3 (2)° in **II**] from the ideal tetrahedral value (109.5°) are attributed to the Thorpe–Ingold effect (Bassindale, 1984). The widening of the angles may be due to the repulsive interaction between the two short S=O bonds. In compound **II**, the N1–C23 = 1.483 (6) and N1–C16 = 1.450 (5) Å bond lengths in the molecule are longer than the mean Nsp^2 – Csp^2 bond-length value of 1.355 (14) Å [Allen *et al.*, 1987; Cambridge Structural Database (CSD), Version 5.37; Groom *et al.*, 2016]. The elongation observed may be due to the electron-withdrawing character of the phenylsulfonyl group. In compound **II**, the sum of the bond angles around N1 (354.1°) indicates sp^2 hybridization.

In compound (**I**), the molecular structure is stabilized by weak C15–H15···O1 intramolecular interactions formed by the sulfone oxygen atoms, which generate two *S*(5) ring motifs (Fig. 1).

3. Supramolecular features

In the crystal of **I**, the C10–H10···O2ⁱ hydrogen bond generates an inversion dimer with an $R_2^2(14)$ ring motif; within

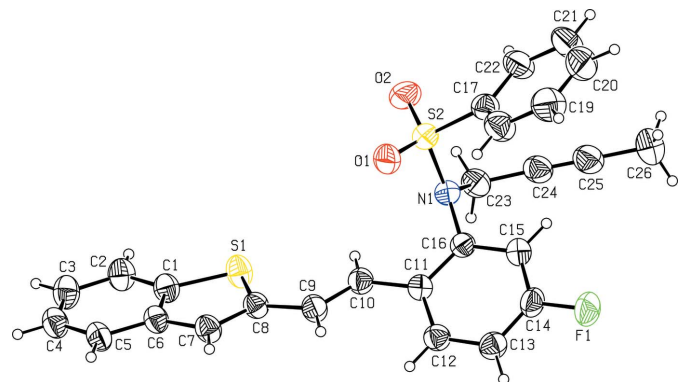


Figure 2
The molecular structure of compound **II**, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

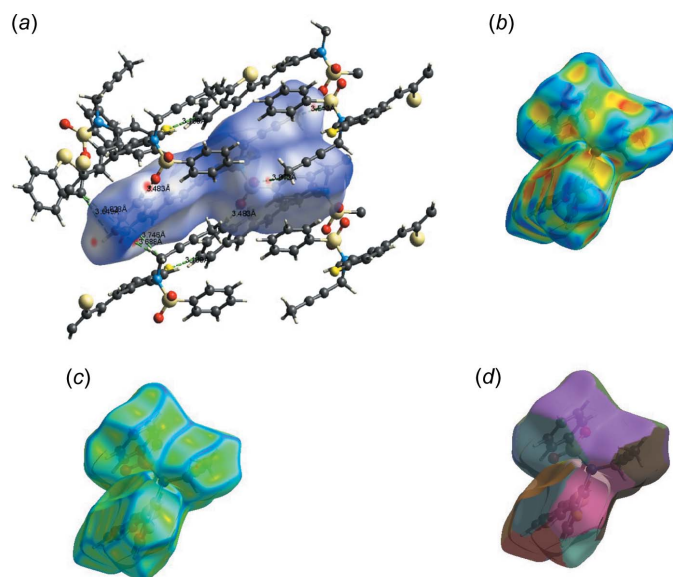


Figure 7
The Hirshfeld surfaces for visualizing the intermolecular contacts of compound **II**: (a) d_{norm} of compound **II**, showing the various intermolecular contacts in the crystal, (b) shape index, (d) curvedness and (e) fragment patches.

through white to blue (distances longer than the sum of the van der Waals radii). The d_{norm} surface was mapped over a fixed colour scale of -0.434 (red) to 1.449 (blue) for compound **I** and -0.119 (red) to 1.765 (blue) for compound **II**, where the red spots indicate the intermolecular contacts involved in the hydrogen bonding. The electrostatic potential was also mapped on the Hirshfeld surface using a STO-3G basis set and the Hartee–Fock level of theory (Spackman *et al.*, 2008; Jayatilaka *et al.*, 2005). The presence of interactions is indicated by a red and blue colour on the shape-index surface (Fig. 6*b* for **I** and 7*b* for **II**). Areas on the Hirshfeld surface

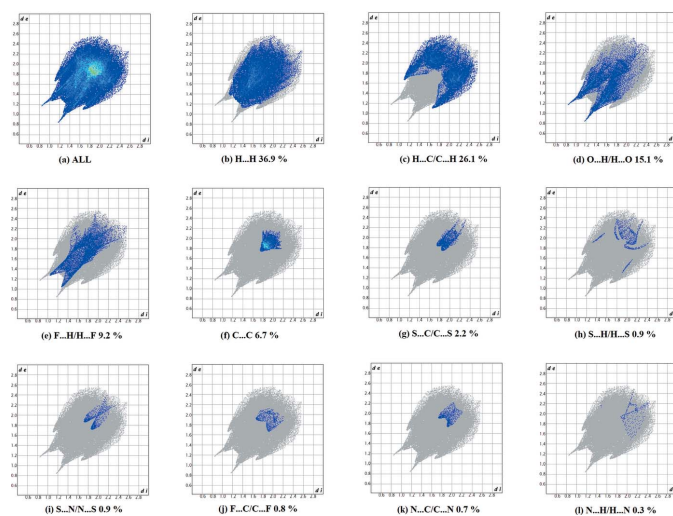


Figure 8
The full two-dimensional fingerprint plot for compound **I**, and fingerprint plots delineated into (b) H...H, (c) O...H/H...O, (d) C...H/H...C, (e) C...C and (f) N...H/H...N contacts.

with high curvedness tend to divide the surface into contact patches with each neighbouring molecule. The coordination number in the crystal is defined by the curvedness of the Hirshfeld surface (Fig. 6*c* for **I** and Fig. 7*c* for **II**). The nearest neighbour coordination environment of a molecule is identified from the colour patches on the Hirshfeld surface depending on their closeness to adjacent molecules (Fig. 6*d* for **I** and Fig. 7*d* for **II**).

The fingerprint plots are given in Figs. 8 and 9. For compound **I**, they reveal that the principal intermolecular contacts are H...H contacts at 36.9% (Fig. 8*b*), H...C/C...H contacts at 26.1% (Fig. 8*c*), O...H/H...O at 15.1% (Fig. 8*d*), F...H/H...F at 9.2% (Fig. 8*e*), C...C at 6.7% (Fig. 8*f*), S...C/C...S at 2.2% (Fig. 8*g*), S...H/H...S contacts at 0.9% (Fig. 8*h*), F...C/C...F at 0.8% (Fig. 8*j*), N...C/C...N at 0.7% (Fig. 8*k*) and N...H/H...N contacts at 0.3% (Fig. 8*l*).

For compound **II**, they reveal a similar trend, with the principal intermolecular contacts being H...H/H...H at 41.4% (Fig. 9*b*), H...C/C...H contacts at 25.1% (Fig. 9*c*), O...H/H...O at 12.1% (Fig. 9*d*), F...H/H...F at 8.1% C...C at 4.6% (Fig. 9*e*), C...C at 4.7% (Fig. 9*f*), S...H/H...S contacts at 4.5% (Fig. 9*g*), S...C/C...S contacts at 2.1% (Fig. 9*h*), C...O/O...C contacts at 1.0% (Fig. 9*i*), F...S/S...F at 0.9% (Fig. 9*j*) and O...O contacts at 0.3 (Fig. 9*k*). In both compounds, the H...H intermolecular contacts predominate, followed by the C...H/H...C and O...H/H...O contacts.

5. Synthesis and crystallization

Compound I: To a solution of (*E*)-2-(2-(benzo[*b*]thiophen-2-yl)vinyl)-5-fluorobenzenaminium chloride (1.2 g, 3.934 mmol) in dry DCM (10 mL), pyridine (0.47 mL, 5.901 mmol) and PhSO₂Cl (0.6 mL, 4.721 mmol) were added and stirred at

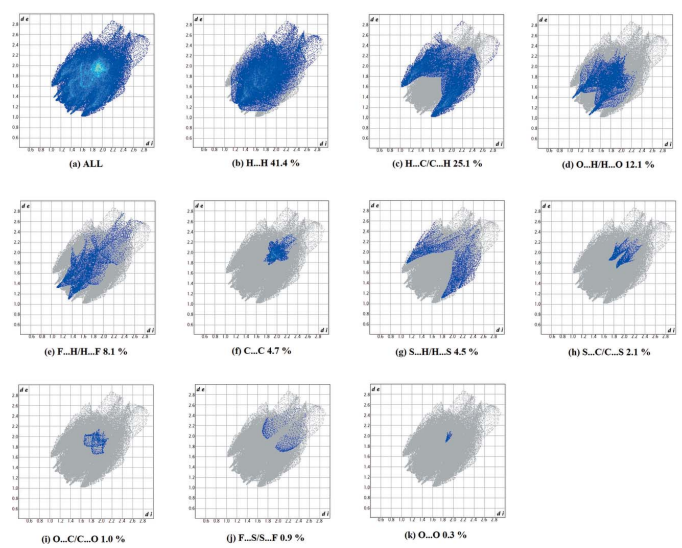


Figure 9
The full two-dimensional fingerprint plot for compound **II**, and fingerprint plots delineated into (b) C...C, (c) C...H/H...C, (d) C...N/N...C, (e) C...O/O...C, (f) H...H, (g) N...H/H...N, (h) O...H/H...O and (i) S...H/H...S contacts.

Table 3
Experimental details.

	I	II
Crystal data		
Chemical formula	C ₂₂ H ₁₆ FNO ₂ S ₂	C ₂₆ H ₂₀ FNO ₂ S ₂
<i>M_r</i>	409.48	461.55
Crystal system, space group	Monoclinic, <i>P2₁/c</i>	Monoclinic, <i>P2₁/c</i>
Temperature (K)	297	297
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.9588 (1), 25.9840 (4), 9.5178 (2)	9.3517 (3), 31.7075 (11), 8.6063 (3)
β (°)	96.853 (1)	115.179 (2)
<i>V</i> (Å ³)	1954.23 (6)	2309.45 (14)
<i>Z</i>	4	4
Radiation type	Cu <i>K</i> α	Cu <i>K</i> α
μ (mm ⁻¹)	2.70	2.35
Crystal size (mm)	0.15 × 0.10 × 0.08	0.11 × 0.07 × 0.02
Data collection		
Diffractometer	Bruker D8 Venture Diffractometer	Bruker D8 Venture Diffractometer
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2016)	Multi-scan (<i>SADABS</i> ; Bruker, 2016)
<i>T_{min}</i> , <i>T_{max}</i>	0.589, 0.753	0.604, 0.753
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	44325, 3597, 2964	39443, 4270, 2098
<i>R_{int}</i>	0.049	0.155
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.604	0.605
Refinement		
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.042, 0.115, 1.03	0.066, 0.232, 1.00
No. of reflections	3597	4270
No. of parameters	272	291
No. of restraints	11	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.21, -0.28	0.33, -0.38

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXS2018/3* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020), *pubCIF* (Westrip, 2010) and *PLATON* (Spek, 2020).

room temperature for 12 h. After completion of the reaction (monitored by TLC), it was poured into crushed ice (50 g) containing conc. HCl (5 mL), extracted with DCM (2 × 20 mL) then washed with water (2 × 20 mL) and dried (Na₂SO₄). Removal of solvent *in vacuo* followed by crystallization from diethylether (4 mL) afforded (*E*)-*N*-[2-[2-(benzo[*b*]thiophen-2-yl)ethenyl]-5-fluorophenyl]benzenesulfonamide as a white solid.

Compound II: To a solution of (*E*)-*N*-[2-[2-(benzo[*b*]thiophen-2-yl)vinyl]-5-fluorophenyl]benzenesulfonamide (0.70 g, 1.711 mmol) in CH₃CN (10 mL), K₂CO₃ (0.35 g, 2.567 mmol) and 1-bromobut-2-yne (0.22 mL, 2.567 mmol) were added and stirred at room temperature for 12 h. After completion of the reaction (monitored by TLC), it was poured into crushed ice (50 g) containing conc. HCl (5 mL), extracted with ethyl acetate (2 × 20 mL) then washed with water (2 × 20 mL) and dried (Na₂SO₄). Removal of solvent *in vacuo* followed by crystallization from methanol (4 mL) afforded (*E*)-*N*-[2-[2-(benzo[*b*]thiophen-2-yl)ethenyl]-5-fluorophenyl]-*N*-(but-2-yn-1-yl)benzenesulfonamide as a white solid.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For compound **I**, the NH H atoms were located in difference-Fourier maps and freely refined. For compound **II**, they were included in calculated positions

and refined as riding: N–H = 0.93 Å with *U*_{iso}(H) = 1.2*U*_{eq}(N). All C-bound H atoms were positioned geometrically and constrained to ride on their parent atoms: C–H = 0.93–0.97 Å with *U*_{iso}(H) = 1.5*U*_{eq}(C-methyl) and 1.2*U*_{eq}(C) for other H atoms. In compound **I**, the thiophene ring is disordered over two positions with a refined occupancy ratio of 0.756 (4):0.244 (3). The geometries were regularized using soft restraints.

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Computing details

For both structures, data collection: *APEX2* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXS2018/3* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *pubCIF* (Westrip, 2010) and *PLATON* (Spek, 2020).

(*E*)-*N*-{2-[2-(Benzo[*b*]thiophen-2-yl)ethenyl]-5-fluorophenyl}benzenesulfonamide (I)

Crystal data

$C_{22}H_{16}FNO_2S_2$	$F(000) = 848$
$M_r = 409.48$	$D_x = 1.392 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
$a = 7.9588 (1) \text{ \AA}$	Cell parameters from 9457 reflections
$b = 25.9840 (4) \text{ \AA}$	$\theta = 3.4\text{--}68.6^\circ$
$c = 9.5178 (2) \text{ \AA}$	$\mu = 2.70 \text{ mm}^{-1}$
$\beta = 96.853 (1)^\circ$	$T = 297 \text{ K}$
$V = 1954.23 (6) \text{ \AA}^3$	Block, brown
$Z = 4$	$0.15 \times 0.10 \times 0.08 \text{ mm}$

Data collection

Bruker D8 Venture Diffractometer	3597 independent reflections
Radiation source: micro focus sealed tube	2964 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{\text{int}} = 0.049$
Absorption correction: multi-scan	$\theta_{\text{max}} = 68.7^\circ$, $\theta_{\text{min}} = 3.4^\circ$
(<i>SADABS</i> ; Bruker, 2016)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.589$, $T_{\text{max}} = 0.753$	$k = -31 \rightarrow 31$
44325 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	$S = 1.03$
Least-squares matrix: full	3597 reflections
$R[F^2 > 2\sigma(F^2)] = 0.042$	272 parameters
$wR(F^2) = 0.115$	11 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.7846P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.7141 (2)	0.64416 (6)	0.53276 (16)	0.0782 (7)	
C2	0.6743 (3)	0.69557 (7)	0.5055 (2)	0.1055 (10)	
H2	0.611424	0.704923	0.420704	0.127*	
C3	0.7286 (3)	0.73300 (5)	0.6050 (3)	0.1127 (11)	
H3	0.701996	0.767393	0.586823	0.135*	
C4	0.8226 (3)	0.71902 (7)	0.7318 (2)	0.1109 (11)	
H4	0.858902	0.744059	0.798407	0.133*	
C5	0.8623 (3)	0.66761 (8)	0.75906 (17)	0.1018 (9)	
H5	0.925238	0.658254	0.843872	0.122*	
C6	0.8081 (2)	0.63018 (5)	0.65953 (18)	0.0788 (7)	
S1'	0.8669 (7)	0.56832 (19)	0.7105 (5)	0.0855 (14)	0.243 (4)
C7'	0.709 (3)	0.5902 (6)	0.4679 (19)	0.103 (8)	0.243 (4)
H7'	0.649984	0.584659	0.378833	0.124*	0.243 (4)
C8'	0.790 (5)	0.5504 (7)	0.539 (2)	0.051 (5)	0.243 (4)
S1	0.6512 (2)	0.59509 (5)	0.41950 (14)	0.0758 (4)	0.757 (4)
C7	0.8282 (9)	0.5758 (2)	0.6526 (7)	0.0900 (18)	0.757 (4)
H7	0.893320	0.557894	0.724278	0.108*	0.757 (4)
C8	0.7498 (15)	0.5511 (3)	0.5389 (9)	0.067 (3)	0.757 (4)
C9	0.7644 (3)	0.49638 (9)	0.5064 (3)	0.0754 (6)	
H9	0.808242	0.474482	0.579001	0.090*	
C10	0.6922 (3)	0.47259 (9)	0.3953 (3)	0.0741 (6)	
H10	0.632873	0.492988	0.325994	0.089*	
C11	0.6936 (3)	0.41711 (8)	0.3671 (2)	0.0673 (6)	
C12	0.7752 (4)	0.38326 (10)	0.4678 (3)	0.0976 (9)	
H12	0.829122	0.396833	0.551708	0.117*	
C13	0.7790 (5)	0.33108 (10)	0.4481 (3)	0.1019 (10)	
H13	0.835045	0.309475	0.516146	0.122*	
C14	0.6980 (4)	0.31212 (9)	0.3256 (3)	0.0837 (7)	
C15	0.6143 (3)	0.34215 (8)	0.2231 (3)	0.0711 (6)	
H15	0.557999	0.327509	0.141557	0.085*	
C16	0.6145 (3)	0.39533 (7)	0.2428 (2)	0.0578 (5)	
C17	0.6983 (2)	0.40434 (7)	-0.0853 (2)	0.0545 (5)	
C18	0.8053 (3)	0.44596 (9)	-0.0912 (3)	0.0739 (6)	
H18	0.770751	0.478886	-0.069161	0.089*	

C19	0.9636 (3)	0.43766 (13)	-0.1303 (3)	0.0927 (8)
H19	1.037422	0.465199	-0.134587	0.111*
C20	1.0139 (3)	0.38892 (15)	-0.1632 (3)	0.0947 (9)
H20	1.121259	0.383777	-0.189882	0.114*
C21	0.9072 (4)	0.34806 (12)	-0.1569 (3)	0.0888 (8)
H21	0.942294	0.315210	-0.179119	0.107*
C22	0.7481 (3)	0.35538 (9)	-0.1179 (2)	0.0689 (6)
H22	0.675016	0.327657	-0.113642	0.083*
N1	0.5283 (2)	0.42741 (6)	0.1368 (2)	0.0616 (4)
O1	0.40697 (18)	0.36642 (5)	-0.05058 (18)	0.0706 (4)
O2	0.42235 (19)	0.45927 (5)	-0.09632 (17)	0.0674 (4)
F1	0.6977 (3)	0.26050 (5)	0.3036 (2)	0.1171 (6)
S2	0.49738 (6)	0.41360 (2)	-0.03136 (6)	0.05557 (17)
H1N	0.545 (3)	0.4587 (6)	0.147 (2)	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0989 (18)	0.0723 (15)	0.0687 (14)	-0.0213 (13)	0.0318 (13)	-0.0024 (12)
C2	0.132 (3)	0.0839 (19)	0.103 (2)	-0.0145 (18)	0.0231 (19)	0.0204 (17)
C3	0.135 (3)	0.0621 (16)	0.149 (3)	-0.0154 (17)	0.052 (3)	-0.0014 (19)
C4	0.135 (3)	0.081 (2)	0.126 (3)	-0.0312 (19)	0.054 (2)	-0.0337 (19)
C5	0.124 (2)	0.099 (2)	0.0829 (18)	-0.0240 (19)	0.0139 (17)	-0.0201 (16)
C6	0.0929 (17)	0.0706 (15)	0.0766 (16)	-0.0123 (13)	0.0252 (13)	-0.0080 (12)
S1'	0.104 (3)	0.077 (2)	0.074 (3)	-0.0128 (19)	0.004 (2)	-0.0059 (19)
C7'	0.127 (16)	0.121 (16)	0.059 (10)	-0.069 (13)	0.001 (8)	-0.016 (10)
C8'	0.045 (12)	0.060 (8)	0.050 (8)	-0.004 (5)	0.017 (5)	0.001 (6)
S1	0.1095 (10)	0.0607 (5)	0.0576 (8)	-0.0079 (5)	0.0109 (6)	-0.0006 (4)
C7	0.111 (4)	0.077 (3)	0.076 (4)	0.003 (2)	-0.010 (3)	0.000 (3)
C8	0.065 (6)	0.067 (3)	0.071 (3)	-0.009 (2)	0.017 (2)	-0.003 (2)
C9	0.0896 (17)	0.0647 (14)	0.0712 (14)	0.0018 (12)	0.0068 (12)	0.0001 (11)
C10	0.1028 (18)	0.0551 (12)	0.0632 (13)	-0.0022 (12)	0.0055 (12)	0.0060 (10)
C11	0.0864 (15)	0.0516 (11)	0.0647 (13)	0.0000 (10)	0.0123 (11)	0.0086 (10)
C12	0.142 (3)	0.0674 (16)	0.0772 (17)	-0.0011 (16)	-0.0111 (17)	0.0139 (13)
C13	0.141 (3)	0.0651 (16)	0.095 (2)	0.0093 (16)	-0.0046 (19)	0.0296 (15)
C14	0.114 (2)	0.0459 (12)	0.0930 (19)	0.0051 (12)	0.0186 (16)	0.0146 (12)
C15	0.0888 (16)	0.0472 (11)	0.0783 (15)	0.0022 (11)	0.0142 (12)	0.0065 (10)
C16	0.0645 (12)	0.0457 (10)	0.0658 (12)	0.0025 (9)	0.0186 (10)	0.0083 (9)
C17	0.0545 (10)	0.0502 (10)	0.0561 (11)	-0.0008 (8)	-0.0041 (8)	-0.0033 (8)
C18	0.0654 (13)	0.0673 (14)	0.0871 (16)	-0.0139 (11)	0.0014 (12)	-0.0091 (12)
C19	0.0671 (15)	0.116 (2)	0.0935 (19)	-0.0253 (16)	0.0020 (14)	-0.0039 (17)
C20	0.0562 (14)	0.147 (3)	0.0796 (17)	0.0120 (17)	0.0026 (12)	-0.0036 (18)
C21	0.0794 (17)	0.096 (2)	0.0904 (19)	0.0269 (15)	0.0098 (14)	-0.0087 (15)
C22	0.0724 (14)	0.0582 (12)	0.0752 (14)	0.0077 (10)	0.0049 (11)	-0.0050 (11)
N1	0.0745 (11)	0.0401 (8)	0.0700 (11)	0.0070 (8)	0.0081 (9)	0.0009 (8)
O1	0.0613 (8)	0.0459 (7)	0.1008 (12)	-0.0087 (6)	-0.0061 (8)	-0.0028 (7)
O2	0.0711 (9)	0.0437 (7)	0.0826 (10)	0.0098 (6)	-0.0111 (7)	0.0015 (7)
F1	0.1731 (17)	0.0454 (8)	0.1300 (14)	0.0126 (9)	0.0067 (12)	0.0189 (8)

S2	0.0546 (3)	0.0379 (2)	0.0718 (3)	0.00112 (18)	-0.0029 (2)	-0.0018 (2)
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Geometric parameters (Å, °)

C1—C2	1.3900	C11—C12	1.402 (3)
C1—C6	1.3900	C12—C13	1.369 (4)
C1—C7'	1.531 (14)	C12—H12	0.9300
C1—S1	1.7058 (18)	C13—C14	1.356 (4)
C2—C3	1.3900	C13—H13	0.9300
C2—H2	0.9300	C14—F1	1.358 (3)
C3—C4	1.3900	C14—C15	1.360 (3)
C3—H3	0.9300	C15—C16	1.394 (3)
C4—C5	1.3900	C15—H15	0.9300
C4—H4	0.9300	C16—N1	1.421 (3)
C5—C6	1.3900	C17—C22	1.379 (3)
C5—H5	0.9300	C17—C18	1.381 (3)
C6—C7	1.426 (6)	C17—S2	1.754 (2)
C6—S1'	1.727 (5)	C18—C19	1.373 (4)
S1'—C8'	1.738 (17)	C18—H18	0.9300
C7'—C8'	1.356 (18)	C19—C20	1.375 (4)
C7'—H7'	0.9300	C19—H19	0.9300
C8'—C9	1.446 (17)	C20—C21	1.365 (4)
S1—C8	1.732 (7)	C20—H20	0.9300
C7—C8	1.345 (8)	C21—C22	1.375 (4)
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.463 (7)	C22—H22	0.9300
C9—C10	1.298 (3)	N1—S2	1.6301 (19)
C9—H9	0.9300	N1—H1N	0.828 (16)
C10—C11	1.467 (3)	O1—S2	1.4222 (14)
C10—H10	0.9300	O2—S2	1.4348 (14)
C11—C16	1.393 (3)		
C2—C1—C6	120.0	C16—C11—C10	122.8 (2)
C2—C1—C7'	144.2 (7)	C12—C11—C10	120.3 (2)
C6—C1—C7'	95.5 (7)	C13—C12—C11	122.9 (3)
C2—C1—S1	123.88 (12)	C13—C12—H12	118.5
C6—C1—S1	116.11 (12)	C11—C12—H12	118.5
C3—C2—C1	120.0	C14—C13—C12	117.5 (3)
C3—C2—H2	120.0	C14—C13—H13	121.3
C1—C2—H2	120.0	C12—C13—H13	121.3
C2—C3—C4	120.0	C13—C14—F1	118.9 (2)
C2—C3—H3	120.0	C13—C14—C15	123.4 (2)
C4—C3—H3	120.0	F1—C14—C15	117.7 (3)
C5—C4—C3	120.0	C14—C15—C16	118.6 (2)
C5—C4—H4	120.0	C14—C15—H15	120.7
C3—C4—H4	120.0	C16—C15—H15	120.7
C4—C5—C6	120.0	C11—C16—C15	120.7 (2)
C4—C5—H5	120.0	C11—C16—N1	119.74 (18)

C6—C5—H5	120.0	C15—C16—N1	119.6 (2)
C5—C6—C1	120.0	C22—C17—C18	121.2 (2)
C5—C6—C7	134.3 (3)	C22—C17—S2	119.30 (17)
C1—C6—C7	105.7 (3)	C18—C17—S2	119.49 (17)
C5—C6—S1'	114.1 (2)	C19—C18—C17	118.5 (2)
C1—C6—S1'	125.9 (2)	C19—C18—H18	120.7
C6—S1'—C8'	86.1 (6)	C17—C18—H18	120.7
C8'—C7'—C1	120.6 (13)	C18—C19—C20	120.5 (3)
C8'—C7'—H7'	119.7	C18—C19—H19	119.7
C1—C7'—H7'	119.7	C20—C19—H19	119.7
C7'—C8'—C9	126.0 (15)	C21—C20—C19	120.5 (3)
C7'—C8'—S1'	110.9 (13)	C21—C20—H20	119.8
C9—C8'—S1'	119.1 (13)	C19—C20—H20	119.8
C1—S1—C8	90.1 (2)	C20—C21—C22	120.1 (3)
C8—C7—C6	117.7 (6)	C20—C21—H21	119.9
C8—C7—H7	121.1	C22—C21—H21	119.9
C6—C7—H7	121.1	C21—C22—C17	119.2 (2)
C7—C8—C9	126.3 (6)	C21—C22—H22	120.4
C7—C8—S1	110.1 (5)	C17—C22—H22	120.4
C9—C8—S1	122.9 (5)	C16—N1—S2	124.85 (14)
C10—C9—C8'	132.4 (8)	C16—N1—H1N	116.0 (16)
C10—C9—C8	126.6 (4)	S2—N1—H1N	109.5 (16)
C10—C9—H9	113.8	O1—S2—O2	118.64 (9)
C8'—C9—H9	113.8	O1—S2—N1	109.32 (10)
C9—C10—C11	127.2 (2)	O2—S2—N1	104.32 (9)
C9—C10—H10	116.4	O1—S2—C17	108.01 (9)
C11—C10—H10	116.4	O2—S2—C17	109.55 (10)
C16—C11—C12	116.8 (2)	N1—S2—C17	106.35 (9)
C6—C1—C2—C3	0.0	C8'—C9—C10—C11	171 (2)
C7'—C1—C2—C3	-171.5 (14)	C8—C9—C10—C11	-174.3 (7)
S1—C1—C2—C3	178.91 (16)	C9—C10—C11—C16	-178.7 (3)
C1—C2—C3—C4	0.0	C9—C10—C11—C12	2.1 (4)
C2—C3—C4—C5	0.0	C16—C11—C12—C13	-0.1 (5)
C3—C4—C5—C6	0.0	C10—C11—C12—C13	179.2 (3)
C4—C5—C6—C1	0.0	C11—C12—C13—C14	-0.7 (5)
C4—C5—C6—C7	178.8 (4)	C12—C13—C14—F1	-179.2 (3)
C4—C5—C6—S1'	-179.6 (2)	C12—C13—C14—C15	-0.1 (5)
C2—C1—C6—C5	0.0	C13—C14—C15—C16	1.5 (4)
C7'—C1—C6—C5	175.0 (8)	F1—C14—C15—C16	-179.3 (2)
S1—C1—C6—C5	-178.99 (15)	C12—C11—C16—C15	1.6 (4)
C2—C1—C6—C7	-179.1 (3)	C10—C11—C16—C15	-177.7 (2)
S1—C1—C6—C7	1.9 (3)	C12—C11—C16—N1	179.5 (2)
C2—C1—C6—S1'	179.5 (3)	C10—C11—C16—N1	0.2 (3)
C7'—C1—C6—S1'	-5.5 (8)	C14—C15—C16—C11	-2.3 (4)
C5—C6—S1'—C8'	-171.8 (13)	C14—C15—C16—N1	179.8 (2)
C1—C6—S1'—C8'	8.7 (14)	C22—C17—C18—C19	-0.1 (4)
C2—C1—C7'—C8'	171 (2)	S2—C17—C18—C19	178.41 (19)

C6—C1—C7'—C8'	-2 (3)	C17—C18—C19—C20	0.2 (4)
C1—C7'—C8'—C9	165 (2)	C18—C19—C20—C21	-0.2 (4)
C1—C7'—C8'—S1'	8 (4)	C19—C20—C21—C22	0.2 (4)
C6—S1'—C8'—C7'	-8 (2)	C20—C21—C22—C17	-0.1 (4)
C6—S1'—C8'—C9	-167 (3)	C18—C17—C22—C21	0.0 (4)
C2—C1—S1—C8	-178.8 (5)	S2—C17—C22—C21	-178.48 (19)
C6—C1—S1—C8	0.1 (5)	C11—C16—N1—S2	153.99 (18)
C5—C6—C7—C8	177.3 (7)	C15—C16—N1—S2	-28.1 (3)
C1—C6—C7—C8	-3.8 (9)	C16—N1—S2—O1	58.1 (2)
C6—C7—C8—C9	175.1 (8)	C16—N1—S2—O2	-174.05 (17)
C6—C7—C8—S1	4.0 (11)	C16—N1—S2—C17	-58.28 (19)
C1—S1—C8—C7	-2.2 (8)	C22—C17—S2—O1	-8.2 (2)
C1—S1—C8—C9	-173.7 (9)	C18—C17—S2—O1	173.24 (18)
C7'—C8'—C9—C10	15 (5)	C22—C17—S2—O2	-138.77 (17)
S1'—C8'—C9—C10	170.8 (10)	C18—C17—S2—O2	42.7 (2)
C7—C8—C9—C10	-178.3 (8)	C22—C17—S2—N1	109.03 (18)
S1—C8—C9—C10	-8.4 (13)	C18—C17—S2—N1	-69.51 (19)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15—H15 \cdots O1	0.93	2.30	2.980 (3)	130
C10—H10 \cdots O2 ⁱ	0.93	2.51	3.383 (3)	157
N1—H1N \cdots O2 ⁱ	0.83 (2)	2.21 (2)	3.001 (2)	161 (2)
C22—H22 \cdots F1 ⁱⁱ	0.93	2.44	3.116 (3)	130

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x, -y+1/2, z-1/2$.*(E)-N*-{2-[2-(Benzo[*b*]thiophen-2-yl)ethenyl]-5-fluorophenyl}-*N*-(but-2-yn-1-yl)benzenesulfonamide (II)

Crystal data

 $C_{26}H_{20}FNO_2S_2$ $M_r = 461.55$ Monoclinic, $P2_1/c$ $a = 9.3517$ (3) \AA $b = 31.7075$ (11) \AA $c = 8.6063$ (3) \AA $\beta = 115.179$ (2) $^\circ$ $V = 2309.45$ (14) \AA^3 $Z = 4$ $F(000) = 960$ $D_x = 1.327$ Mg m^{-3} Cu $K\alpha$ radiation, $\lambda = 1.54178$ \AA

Cell parameters from 3616 reflections

 $\theta = 2.8\text{--}65.4^\circ$ $\mu = 2.35$ mm^{-1} $T = 297$ K

Solid, white

 $0.11 \times 0.07 \times 0.02$ mm

Data collection

Bruker D8 Venture Diffractometer

Radiation source: micro focus sealed tube

 ω and ϕ scans

Absorption correction: multi-scan

(SADABS; Bruker, 2016)

 $T_{\min} = 0.604$, $T_{\max} = 0.753$

39443 measured reflections

4270 independent reflections

2098 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.155$ $\theta_{\text{max}} = 68.8^\circ$, $\theta_{\text{min}} = 5.2^\circ$ $h = -11 \rightarrow 11$ $k = -37 \rightarrow 38$ $l = -10 \rightarrow 10$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.066$ $wR(F^2) = 0.232$ $S = 1.00$

4270 reflections

291 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.1325P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$ Extinction correction: SHELXL-2018/3
(Sheldrick 2015), $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0040 (6)

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2549 (6)	0.32808 (15)	-0.0285 (6)	0.0669 (12)
C2	0.2360 (6)	0.33934 (17)	-0.1918 (6)	0.0778 (14)
H2	0.311900	0.355578	-0.207042	0.093*
C3	0.1029 (7)	0.32600 (17)	-0.3309 (7)	0.0825 (15)
H3	0.089065	0.333320	-0.441041	0.099*
C4	-0.0110 (6)	0.30184 (16)	-0.3096 (6)	0.0763 (14)
H4	-0.100010	0.293249	-0.405677	0.092*
C5	0.0054 (6)	0.29044 (15)	-0.1498 (6)	0.0722 (13)
H5	-0.071951	0.274308	-0.137015	0.087*
C6	0.1408 (5)	0.30337 (14)	-0.0042 (5)	0.0626 (11)
C7	0.1836 (6)	0.29535 (14)	0.1732 (6)	0.0673 (12)
H7	0.122120	0.279321	0.212083	0.081*
C8	0.3227 (5)	0.31338 (13)	0.2798 (5)	0.0609 (11)
C9	0.3969 (6)	0.31034 (15)	0.4648 (6)	0.0682 (12)
H9	0.350312	0.292242	0.514847	0.082*
C10	0.5265 (6)	0.33107 (14)	0.5712 (6)	0.0633 (12)
H10	0.571084	0.350331	0.523168	0.076*
C11	0.6030 (5)	0.32555 (13)	0.7581 (5)	0.0586 (11)
C12	0.5852 (6)	0.28800 (14)	0.8336 (6)	0.0659 (12)
H12	0.521274	0.266825	0.763600	0.079*
C13	0.6595 (6)	0.28137 (15)	1.0084 (6)	0.0702 (13)
H13	0.646816	0.256223	1.056735	0.084*
C14	0.7527 (6)	0.31322 (16)	1.1085 (6)	0.0718 (13)
C15	0.7743 (6)	0.35085 (15)	1.0435 (6)	0.0694 (13)
H15	0.836300	0.371959	1.115842	0.083*
C16	0.7016 (5)	0.35672 (13)	0.8677 (5)	0.0585 (11)
C17	0.6526 (6)	0.45543 (14)	0.9821 (6)	0.0688 (13)
C18	0.5818 (8)	0.43930 (18)	1.0789 (7)	0.0899 (17)

H18	0.505581	0.418355	1.033546	0.108*
C19	0.6226 (9)	0.4539 (2)	1.2444 (9)	0.106 (2)
H19	0.574503	0.442786	1.310278	0.128*
C20	0.7344 (9)	0.4848 (2)	1.3093 (9)	0.109 (2)
H20	0.762946	0.494415	1.420623	0.131*
C21	0.8042 (9)	0.5017 (2)	1.2151 (9)	0.109 (2)
H21	0.878624	0.523052	1.260868	0.130*
C22	0.7647 (7)	0.48710 (16)	1.0491 (7)	0.0872 (16)
H22	0.812980	0.498474	0.983836	0.105*
C23	0.8877 (6)	0.40504 (16)	0.8143 (7)	0.0763 (14)
H23A	0.925473	0.380835	0.773623	0.092*
H23B	0.882648	0.428675	0.740500	0.092*
C24	1.0039 (6)	0.41494 (15)	0.9891 (7)	0.0764 (14)
C25	1.0953 (7)	0.42202 (17)	1.1328 (8)	0.0886 (17)
C26	1.2031 (8)	0.4310 (2)	1.3114 (8)	0.117 (2)
H26A	1.143024	0.438114	1.374590	0.175*
H26B	1.270375	0.454214	1.315234	0.175*
H26C	1.266516	0.406545	1.361637	0.175*
N1	0.7255 (4)	0.39583 (10)	0.7947 (5)	0.0613 (10)
O1	0.4505 (4)	0.41733 (11)	0.7156 (4)	0.0851 (11)
O2	0.6400 (5)	0.46681 (11)	0.6790 (5)	0.0949 (12)
S1	0.40923 (16)	0.34048 (5)	0.16627 (16)	0.0776 (5)
S2	0.60508 (16)	0.43535 (4)	0.77698 (15)	0.0715 (4)
F1	0.8245 (4)	0.30760 (10)	1.2817 (3)	0.0982 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.060 (3)	0.078 (3)	0.063 (3)	−0.003 (2)	0.026 (2)	−0.005 (2)
C2	0.073 (3)	0.097 (4)	0.066 (3)	−0.005 (3)	0.033 (3)	0.000 (3)
C3	0.080 (4)	0.107 (4)	0.059 (3)	0.005 (3)	0.029 (3)	−0.003 (3)
C4	0.074 (3)	0.089 (3)	0.062 (3)	0.001 (3)	0.025 (3)	−0.013 (2)
C5	0.063 (3)	0.079 (3)	0.066 (3)	−0.008 (2)	0.019 (2)	−0.013 (2)
C6	0.060 (3)	0.071 (3)	0.056 (2)	−0.001 (2)	0.024 (2)	−0.008 (2)
C7	0.065 (3)	0.072 (3)	0.065 (3)	−0.015 (2)	0.028 (2)	−0.005 (2)
C8	0.063 (3)	0.064 (2)	0.057 (2)	−0.005 (2)	0.027 (2)	−0.003 (2)
C9	0.068 (3)	0.071 (3)	0.061 (3)	−0.007 (2)	0.023 (2)	−0.004 (2)
C10	0.064 (3)	0.065 (3)	0.059 (2)	−0.001 (2)	0.025 (2)	0.000 (2)
C11	0.057 (3)	0.061 (2)	0.057 (2)	0.000 (2)	0.024 (2)	0.0004 (19)
C12	0.068 (3)	0.064 (3)	0.066 (3)	−0.003 (2)	0.029 (2)	0.000 (2)
C13	0.076 (3)	0.070 (3)	0.067 (3)	0.000 (3)	0.034 (3)	0.007 (2)
C14	0.079 (3)	0.081 (3)	0.049 (2)	0.007 (3)	0.021 (2)	0.009 (2)
C15	0.070 (3)	0.070 (3)	0.060 (3)	−0.001 (2)	0.020 (2)	−0.001 (2)
C16	0.062 (3)	0.056 (2)	0.057 (2)	0.002 (2)	0.025 (2)	0.0017 (18)
C17	0.076 (3)	0.063 (3)	0.070 (3)	0.003 (2)	0.033 (3)	−0.001 (2)
C18	0.107 (5)	0.085 (3)	0.081 (4)	−0.009 (3)	0.044 (3)	−0.010 (3)
C19	0.132 (6)	0.106 (4)	0.096 (5)	0.003 (4)	0.063 (4)	−0.003 (4)
C20	0.134 (6)	0.110 (5)	0.079 (4)	0.016 (5)	0.042 (4)	−0.019 (4)

C21	0.119 (5)	0.096 (4)	0.099 (5)	-0.019 (4)	0.034 (4)	-0.035 (4)
C22	0.099 (4)	0.072 (3)	0.088 (4)	-0.016 (3)	0.038 (3)	-0.014 (3)
C23	0.074 (3)	0.076 (3)	0.081 (3)	-0.009 (3)	0.035 (3)	-0.005 (2)
C24	0.068 (3)	0.068 (3)	0.090 (4)	-0.008 (3)	0.031 (3)	-0.005 (3)
C25	0.081 (4)	0.075 (3)	0.101 (4)	-0.008 (3)	0.030 (3)	-0.008 (3)
C26	0.102 (5)	0.123 (5)	0.093 (4)	-0.012 (4)	0.010 (4)	-0.015 (4)
N1	0.064 (2)	0.0555 (19)	0.061 (2)	-0.0017 (17)	0.0238 (18)	0.0022 (16)
O1	0.062 (2)	0.084 (2)	0.088 (2)	0.0006 (18)	0.0117 (18)	-0.0075 (18)
O2	0.139 (3)	0.0680 (19)	0.077 (2)	0.000 (2)	0.045 (2)	0.0174 (17)
S1	0.0655 (8)	0.0998 (9)	0.0656 (7)	-0.0180 (7)	0.0261 (6)	-0.0056 (6)
S2	0.0822 (9)	0.0616 (6)	0.0625 (7)	0.0020 (6)	0.0229 (6)	0.0030 (5)
F1	0.114 (2)	0.107 (2)	0.0552 (16)	-0.0063 (19)	0.0187 (16)	0.0166 (15)

Geometric parameters (Å, °)

C1—C2	1.387 (7)	C15—C16	1.382 (6)
C1—C6	1.409 (7)	C15—H15	0.9300
C1—S1	1.729 (5)	C16—N1	1.450 (5)
C2—C3	1.376 (7)	C17—C18	1.365 (7)
C2—H2	0.9300	C17—C22	1.387 (7)
C3—C4	1.386 (7)	C17—S2	1.747 (5)
C3—H3	0.9300	C18—C19	1.388 (8)
C4—C5	1.367 (7)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.368 (9)
C5—C6	1.411 (6)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.349 (9)
C6—C7	1.426 (6)	C20—H20	0.9300
C7—C8	1.358 (6)	C21—C22	1.394 (8)
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.444 (6)	C22—H22	0.9300
C8—S1	1.738 (5)	C23—C24	1.467 (7)
C9—C10	1.340 (6)	C23—N1	1.483 (6)
C9—H9	0.9300	C23—H23A	0.9700
C10—C11	1.466 (6)	C23—H23B	0.9700
C10—H10	0.9300	C24—C25	1.188 (7)
C11—C12	1.400 (6)	C25—C26	1.464 (8)
C11—C16	1.406 (6)	C26—H26A	0.9600
C12—C13	1.378 (6)	C26—H26B	0.9600
C12—H12	0.9300	C26—H26C	0.9600
C13—C14	1.372 (7)	N1—S2	1.648 (4)
C13—H13	0.9300	O1—S2	1.431 (4)
C14—F1	1.361 (5)	O2—S2	1.431 (4)
C14—C15	1.369 (7)		
C2—C1—C6	121.0 (4)	C15—C16—C11	121.1 (4)
C2—C1—S1	128.2 (4)	C15—C16—N1	119.7 (4)
C6—C1—S1	110.8 (3)	C11—C16—N1	119.2 (4)
C3—C2—C1	118.7 (5)	C18—C17—C22	119.6 (5)

C3—C2—H2	120.6	C18—C17—S2	119.9 (4)
C1—C2—H2	120.6	C22—C17—S2	120.4 (4)
C2—C3—C4	121.1 (5)	C17—C18—C19	120.6 (6)
C2—C3—H3	119.4	C17—C18—H18	119.7
C4—C3—H3	119.4	C19—C18—H18	119.7
C5—C4—C3	121.0 (5)	C20—C19—C18	119.1 (7)
C5—C4—H4	119.5	C20—C19—H19	120.4
C3—C4—H4	119.5	C18—C19—H19	120.4
C4—C5—C6	119.4 (5)	C21—C20—C19	121.4 (6)
C4—C5—H5	120.3	C21—C20—H20	119.3
C6—C5—H5	120.3	C19—C20—H20	119.3
C1—C6—C5	118.7 (4)	C20—C21—C22	119.9 (6)
C1—C6—C7	111.9 (4)	C20—C21—H21	120.0
C5—C6—C7	129.5 (5)	C22—C21—H21	120.0
C8—C7—C6	113.6 (4)	C17—C22—C21	119.3 (6)
C8—C7—H7	123.2	C17—C22—H22	120.3
C6—C7—H7	123.2	C21—C22—H22	120.3
C7—C8—C9	126.1 (4)	C24—C23—N1	115.7 (4)
C7—C8—S1	111.7 (3)	C24—C23—H23A	108.3
C9—C8—S1	122.2 (3)	N1—C23—H23A	108.3
C10—C9—C8	126.3 (5)	C24—C23—H23B	108.3
C10—C9—H9	116.9	N1—C23—H23B	108.3
C8—C9—H9	116.9	H23A—C23—H23B	107.4
C9—C10—C11	124.7 (5)	C25—C24—C23	177.7 (6)
C9—C10—H10	117.7	C24—C25—C26	177.9 (7)
C11—C10—H10	117.7	C25—C26—H26A	109.5
C12—C11—C16	117.4 (4)	C25—C26—H26B	109.5
C12—C11—C10	120.8 (4)	H26A—C26—H26B	109.5
C16—C11—C10	121.8 (4)	C25—C26—H26C	109.5
C13—C12—C11	122.1 (4)	H26A—C26—H26C	109.5
C13—C12—H12	118.9	H26B—C26—H26C	109.5
C11—C12—H12	118.9	C16—N1—C23	117.3 (4)
C14—C13—C12	117.6 (4)	C16—N1—S2	117.7 (3)
C14—C13—H13	121.2	C23—N1—S2	119.1 (3)
C12—C13—H13	121.2	C1—S1—C8	92.1 (2)
F1—C14—C15	118.2 (4)	O2—S2—O1	120.6 (2)
F1—C14—C13	118.5 (4)	O2—S2—N1	105.5 (2)
C15—C14—C13	123.3 (4)	O1—S2—N1	105.9 (2)
C14—C15—C16	118.4 (4)	O2—S2—C17	108.5 (2)
C14—C15—H15	120.8	O1—S2—C17	107.5 (2)
C16—C15—H15	120.8	N1—S2—C17	108.3 (2)
C6—C1—C2—C3	0.2 (8)	C10—C11—C16—N1	1.5 (7)
S1—C1—C2—C3	180.0 (4)	C22—C17—C18—C19	-0.9 (9)
C1—C2—C3—C4	0.1 (8)	S2—C17—C18—C19	177.7 (5)
C2—C3—C4—C5	-0.1 (8)	C17—C18—C19—C20	0.3 (10)
C3—C4—C5—C6	-0.2 (8)	C18—C19—C20—C21	0.8 (11)
C2—C1—C6—C5	-0.5 (7)	C19—C20—C21—C22	-1.1 (11)

S1—C1—C6—C5	179.7 (4)	C18—C17—C22—C21	0.6 (9)
C2—C1—C6—C7	179.8 (5)	S2—C17—C22—C21	-178.0 (5)
S1—C1—C6—C7	-0.1 (5)	C20—C21—C22—C17	0.5 (10)
C4—C5—C6—C1	0.5 (7)	C15—C16—N1—C23	64.9 (6)
C4—C5—C6—C7	-179.8 (5)	C11—C16—N1—C23	-115.9 (5)
C1—C6—C7—C8	0.6 (6)	C15—C16—N1—S2	-87.9 (5)
C5—C6—C7—C8	-179.0 (5)	C11—C16—N1—S2	91.3 (5)
C6—C7—C8—C9	-179.2 (4)	C24—C23—N1—C16	-69.7 (5)
C6—C7—C8—S1	-0.9 (5)	C24—C23—N1—S2	82.7 (5)
C7—C8—C9—C10	-173.6 (5)	C2—C1—S1—C8	179.8 (5)
S1—C8—C9—C10	8.3 (7)	C6—C1—S1—C8	-0.4 (4)
C8—C9—C10—C11	-176.8 (4)	C7—C8—S1—C1	0.7 (4)
C9—C10—C11—C12	24.6 (7)	C9—C8—S1—C1	179.1 (4)
C9—C10—C11—C16	-158.0 (5)	C16—N1—S2—O2	-171.5 (3)
C16—C11—C12—C13	0.5 (7)	C23—N1—S2—O2	36.2 (4)
C10—C11—C12—C13	178.0 (5)	C16—N1—S2—O1	-42.6 (4)
C11—C12—C13—C14	0.2 (7)	C23—N1—S2—O1	165.2 (3)
C12—C13—C14—F1	178.7 (4)	C16—N1—S2—C17	72.5 (4)
C12—C13—C14—C15	0.4 (8)	C23—N1—S2—C17	-79.8 (4)
F1—C14—C15—C16	-180.0 (4)	C18—C17—S2—O2	156.6 (5)
C13—C14—C15—C16	-1.6 (8)	C22—C17—S2—O2	-24.9 (5)
C14—C15—C16—C11	2.4 (7)	C18—C17—S2—O1	24.6 (5)
C14—C15—C16—N1	-178.4 (4)	C22—C17—S2—O1	-156.9 (4)
C12—C11—C16—C15	-1.8 (7)	C18—C17—S2—N1	-89.4 (5)
C10—C11—C16—C15	-179.3 (4)	C22—C17—S2—N1	89.1 (4)
C12—C11—C16—N1	179.0 (4)		

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C1—C6 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O1 ⁱ	0.93	2.59	3.483 (7)	162
C4—H4...F1 ⁱⁱ	0.93	2.52	3.188 (6)	130
C18—H18...S1 ⁱⁱⁱ	0.93	3.01	3.744 (6)	137
C23—H23 <i>A</i> ...Cg1 ^{iv}	0.93	2.69	3.566 (6)	151

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