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[3-Amino-5-(3,5-dimethylanilino)-4-phenylsulfonyl-2-thienyl]phenylmethanone

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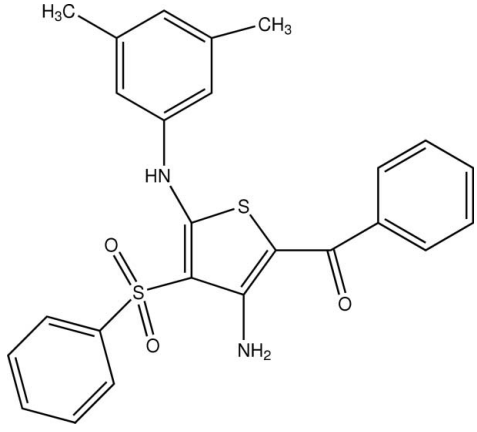
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.043; wR factor = 0.108; data-to-parameter ratio = 12.6.

In the title molecule, $C_{25}H_{22}N_2O_3S_2$, the two C—S bond lengths of the thiophene ring are significantly different, at 1.719 (2) and 1.758 (2) Å. In the crystal structure, molecules form centrosymmetric dimers *via* intermolecular N—H···O hydrogen bonds.

Related literature

For a comparison of the Csp^2—S bond lengths in other related crystal structures, see: Apinitis *et al.* (1984); Xu *et al.* (2004).

For related literature, see: Bürgi & Dunitz (1994); Kovalenko & Victorova (2005); Dorwald (2000); Vlasenko *et al.* (2005); Zefirov & Zorky (1995).



Experimental

Crystal data

$C_{25}H_{22}N_2O_3S_2$
M_r = 462.57
Triclinic, $P\overline{1}$
a = 10.497 (3) Å
b = 11.451 (3) Å
c = 11.863 (3) Å
α = 65.65 (2)°
β = 69.654 (19)°
γ = 70.18 (2)°
V = 1185.6 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 293 (2) K
0.40 × 0.20 × 0.20 mm

Data collection

Siemens $P3$/PC diffractometer
Absorption correction: none
4246 measured reflections
4042 independent reflections
3150 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
2 standard reflections
every 98 reflections
intensity decay: 5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.108
S = 1.02
4042 reflections
322 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1NA···O3	0.76 (3)	2.06 (3)	2.699 (3)	141 (3)
N1—H1NB···O2	0.95 (3)	2.22 (3)	2.864 (3)	124 (2)
N2—H2NA···O1	0.78 (3)	2.25 (3)	2.820 (3)	130 (2)
N1—H1NB···O2^{i}	0.95 (3)	2.19 (3)	2.993 (3)	142 (3)

Symmetry code: (i) $-x+1, -y+1, -z+2$.

Data collection: *P3* (Siemens,1989); cell refinement: *P3*; data reduction: *XDISK* (Siemens, 1991); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2388).

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supplementary materials

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[3-Amino-5-(3,5-dimethylanilino)-4-phenylsulfonyl-2-thienyl]phenylmethanone

I. S. Konovalova, V. N. Baumer, O. V. Shishkin, Y. D. Vlasenko, O. O. Parkhomenko and S. M. Kovalenko

Comment

Thiophene is a very important pharmacophore in many biologically active compounds. Thiophene derivatives are used as antibiotics, anaesthetics, antiparasitics, resolvents, antihelmintic drugs, anticholinergic drugs, antiulcer agents, antihistamines, antitussives (Patent USA, 2000, Kovalenko & Victorova, 2005), therefore investigation of their molecular structure may provide useful information for the understanding of mechanisms of biological activity. In this paper we report the molecular and crystal structure of 2-aroyl-3-amino-4-arylsulfonyl-5-arylamino-thiophene (Fig.1). The carbonyl group is essentially coplanar with the thiophene ring (the C1—C4—C5—O3 torsion angle is 3.1 (4)°). Such a conformation of this group is stabilized by the weak intramolecular hydrogen bond N1—H1NA···O3 H···O 2.06 Å, N—H···O 141°. Atoms N1 and N2 have a planar configuration, the sum of the bond angles, centered at these atoms are 360° in both cases. The phenyl substituent at atom C5 atom is rotated with respect to the C4—C5 bond (the C4—C5—C6—C7 torsion angle is −47.9 (3) °). Such orientation of the phenyl ring indicates an interaction between phenyl ring and atom S1 (the short intramolecular contact C7···S1 is 2.71Å [van der Waals radii sum is 3.01 Å; Zefirov & Zorky (1995)]. The phenyl substituent at the S2 atom has an almost orthogonal orientation relative to the thiophene ring (the C20—S2—C2—C3 torsion angle is −84.4 (2) °) and with respect to the C2—S2 bond (the C2—S2—C20—C25 torsion angle is −83.3 (2)°). The conformation of sulfonyl group is stabilized by weak intramolecular hydrogen bonds N1—H1NB···O2 H···O 2.22 Å, N—H···O 124° and N2—H2NA···O1 H···O 2.25 Å, N—H···O 130°, respectively. The dimethylphenylamino substituent adopts an *sp*-conformation relative to the C3—S1 bond (the S1—C3—N2—C12 torsion angle is −3.9 (4) °) and it is rotated with respect to the C3—N2 bond (the C3—N2—C12—C17 torsion angle is 64.5 (4) °). The most interesting feature of the structure is difference in the S—C bond lengths within thiophene ring. The C4—S1 bond (1.758 (2) Å) is significantly longer than the S1—C3 bond (1.719 (2) Å) and the reported mean value is 1.712 Å (Bürgi & Dunitz, 1994). Comparison of bond lengths within the thiophene ring in the title compound and other 2,5-disubstituted thiophene compounds (Apinitis *et al.*, 1984; Xu *et al.*, 2004) indicates that elongation of the S1—C4 bond is observed when an electron-withdrawing substituent is at atom C4. This may lead to considerable asymmetry in conjugation interactions within the C—S—C fragment of thiophene ring. In the crystal structure, molecules of title compound form centrosymmetric dimers due to intermolecular hydrogen bond N1—H1NB···O2' (symmetry code (') $-x + 1, -y + 1, -z + 2$) H···O' 2.19 Å, N—H···O' 142 °.

Experimental

The title compound was obtained by means of one pot method of synthesis, applying Thorpe-Ziegler-cyclization. The reaction was carried out in the methanol solution of potassium hydroxide (1.99 mmol), in which arylsulfonylacetonitrile (1.66 mmol) and arylisothiocyanate (1.66 mmol) were dissolved. The solution was treated with phenacylbromide (1.99 mmol) and potassium hydroxide (1.99 mmol). At reation completion the solid was acidified using mineral acid. Crystals for X-ray diffraction study were obtained by evaporation of methanol -dimethyl formamide solution (Vlasenko *et al.*, 2005).

Refinement

All hydrogen atoms were located from electron density difference maps but were included in the refinement in the riding motion approximation with C—H = 0.93–0.96Å and U_{iso} constrained to be 1.5 times the U_{eq} of the carrier atom for the methyl groups and 1.2 times U_{eq} of the carrier atom for the other atoms. The hydrogen atoms which are take part in the formation of hydrogen bonds were refined isotropically.

Figures

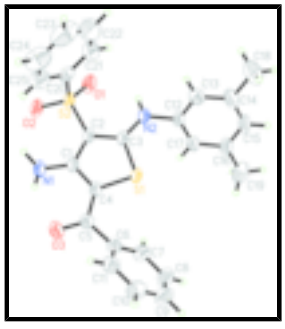

Fig. 1. View of the molecular structure of (I) with atomic numbering. All atoms are shown with displacement ellipsoids drawn at the 50% probability level.

[3-Amino-5-(3,5-dimethylanilino)-4-phenylsulfonyl-2-thienyl]phenylmethanone

Crystal data

$C_{25}H_{22}N_2O_3S_2$	$Z = 2$
$M_r = 462.57$	$F_{000} = 484$
Triclinic, $P\overline{1}$	$D_x = 1.296$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.497$ (3) Å	Cell parameters from 36 reflections
$b = 11.451$ (3) Å	$\theta = 8$–22º
$c = 11.863$ (3) Å	$\mu = 0.25$ mm^{-1}
$\alpha = 65.65$ (2)º	$T = 293$ (2) K
$\beta = 69.654$ (19)º	Block, colourless
$\gamma = 70.18$ (2)º	0.40 × 0.20 × 0.20 mm
$V = 1185.6$ (6) Å^3	

Data collection

Siemens P3/PC diffractometer	$R_{int} = 0.048$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.0$º
Monochromator: graphite	$\theta_{min} = 2.0$º
$T = 293$(2) K	$h = -11 \rightarrow 12$
θ–2θ scans	$k = -12 \rightarrow 13$
Absorption correction: none	$l = -13 \rightarrow 14$

4246 measured reflections	2 standard reflections
4042 independent reflections	every 98 reflections
3150 reflections with $I > 2\sigma(I)$	intensity decay: ?

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.2736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
4042 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
322 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.47589 (6)	0.72106 (6)	0.46973 (5)	0.04259 (18)
S2	0.30992 (6)	0.69038 (6)	0.85957 (5)	0.03452 (16)
N1	0.6086 (3)	0.5073 (2)	0.7787 (2)	0.0498 (6)
H1NA	0.681 (3)	0.473 (3)	0.750 (3)	0.046 (8)*
H1NB	0.575 (3)	0.501 (3)	0.866 (3)	0.070 (9)*
N2	0.2320 (2)	0.8339 (2)	0.5927 (2)	0.0473 (6)
H2NA	0.177 (3)	0.849 (3)	0.653 (3)	0.047 (8)*
O1	0.16388 (16)	0.73500 (19)	0.86151 (15)	0.0497 (5)
O2	0.35524 (18)	0.57316 (16)	0.95816 (14)	0.0443 (4)
O3	0.81054 (17)	0.46304 (18)	0.57554 (16)	0.0525 (5)
C1	0.5382 (2)	0.5893 (2)	0.6897 (2)	0.0329 (5)
C2	0.4011 (2)	0.6711 (2)	0.71376 (19)	0.0332 (5)
C3	0.3543 (2)	0.7472 (2)	0.6033 (2)	0.0350 (5)
C4	0.5941 (2)	0.6049 (2)	0.5602 (2)	0.0355 (5)
C5	0.7306 (2)	0.5429 (2)	0.5067 (2)	0.0365 (5)

C6	0.7839 (2)	0.5752 (2)	0.3652 (2)	0.0347 (5)
C7	0.7075 (3)	0.5789 (2)	0.2888 (2)	0.0420 (6)
H7	0.6175	0.5651	0.3244	0.052 (8)*
C8	0.7649 (3)	0.6031 (3)	0.1598 (2)	0.0517 (7)
H8	0.7140	0.6038	0.1091	0.051 (7)*
C9	0.8971 (3)	0.6262 (3)	0.1057 (3)	0.0547 (7)
H9	0.9347	0.6440	0.0184	0.067 (9)*
C10	0.9727 (3)	0.6230 (3)	0.1805 (3)	0.0551 (7)
H10	1.0619	0.6388	0.1439	0.056 (8)*
C11	0.9177 (3)	0.5966 (2)	0.3100 (2)	0.0466 (6)
H11	0.9706	0.5931	0.3605	0.064 (9)*
C12	0.1956 (2)	0.9153 (2)	0.4746 (2)	0.0398 (6)
C13	0.1705 (3)	1.0494 (3)	0.4418 (3)	0.0490 (6)
H13	0.1802	1.0854	0.4950	0.057 (8)*
C14	0.1303 (3)	1.1318 (3)	0.3284 (3)	0.0559 (7)
C15	0.1194 (3)	1.0741 (3)	0.2517 (2)	0.0522 (7)
H15	0.0926	1.1281	0.1762	0.090 (11)*
C16	0.1467 (3)	0.9397 (3)	0.2822 (2)	0.0484 (6)
C17	0.1831 (3)	0.8601 (3)	0.3971 (2)	0.0447 (6)
H17	0.1989	0.7691	0.4215	0.056 (8)*
C18	0.1001 (5)	1.2791 (3)	0.2929 (4)	0.0915 (12)
H18B	0.0676	1.3021	0.3690	0.17 (2)*
H18A	0.0297	1.3198	0.2454	0.132 (17)*
H18C	0.1838	1.3093	0.2418	0.17 (2)*
C19	0.1363 (5)	0.8786 (4)	0.1955 (4)	0.0811 (11)
H19A	0.0981	0.9464	0.1269	0.16 (2)*
H19C	0.0765	0.8178	0.2432	0.19 (3)*
H19B	0.2275	0.8326	0.1615	0.144 (19)*
C20	0.3623 (3)	0.8199 (2)	0.8620 (2)	0.0411 (6)
C21	0.2846 (4)	0.9460 (3)	0.8255 (3)	0.0666 (9)
H21	0.2015	0.9635	0.8038	0.086 (11)*
C22	0.3316 (6)	1.0473 (4)	0.8215 (4)	0.0931 (13)
H22	0.2794	1.1334	0.7972	0.125 (16)*
C23	0.4522 (6)	1.0221 (4)	0.8525 (4)	0.0916 (13)
H23	0.4838	1.0912	0.8473	0.116 (14)*
C24	0.5291 (4)	0.8953 (4)	0.8917 (4)	0.0811 (10)
H24	0.6113	0.8788	0.9146	0.103 (13)*
C25	0.4848 (3)	0.7929 (3)	0.8970 (3)	0.0599 (8)
H25	0.5362	0.7068	0.9237	0.071 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0381 (3)	0.0532 (4)	0.0214 (3)	0.0055 (3)	−0.0114 (2)	−0.0074 (3)
S2	0.0337 (3)	0.0432 (3)	0.0204 (3)	−0.0070 (2)	−0.0074 (2)	−0.0055 (2)
N1	0.0429 (14)	0.0621 (15)	0.0295 (12)	0.0092 (11)	−0.0175 (10)	−0.0107 (11)
N2	0.0400 (12)	0.0579 (14)	0.0252 (10)	0.0110 (10)	−0.0115 (9)	−0.0107 (10)
O1	0.0325 (9)	0.0755 (13)	0.0309 (9)	−0.0087 (8)	−0.0057 (7)	−0.0127 (9)

O2	0.0539 (10)	0.0470 (10)	0.0246 (8)	−0.0116 (8)	−0.0145 (7)	−0.0010 (7)
O3	0.0383 (10)	0.0603 (11)	0.0418 (10)	0.0065 (8)	−0.0169 (8)	−0.0092 (9)
C1	0.0341 (12)	0.0349 (12)	0.0264 (11)	−0.0047 (9)	−0.0127 (9)	−0.0051 (9)
C2	0.0373 (12)	0.0362 (12)	0.0232 (11)	−0.0057 (9)	−0.0117 (9)	−0.0057 (9)
C3	0.0357 (12)	0.0400 (12)	0.0248 (11)	−0.0035 (10)	−0.0101 (9)	−0.0083 (10)
C4	0.0336 (12)	0.0413 (13)	0.0265 (11)	−0.0012 (10)	−0.0132 (9)	−0.0076 (10)
C5	0.0343 (12)	0.0382 (12)	0.0351 (12)	−0.0048 (10)	−0.0123 (10)	−0.0098 (10)
C6	0.0342 (12)	0.0315 (11)	0.0336 (12)	−0.0039 (9)	−0.0065 (10)	−0.0105 (10)
C7	0.0418 (14)	0.0473 (14)	0.0403 (13)	−0.0136 (11)	−0.0067 (11)	−0.0180 (11)
C8	0.0677 (18)	0.0548 (16)	0.0406 (14)	−0.0151 (13)	−0.0179 (13)	−0.0185 (13)
C9	0.0657 (18)	0.0517 (16)	0.0369 (15)	−0.0149 (14)	−0.0010 (13)	−0.0135 (12)
C10	0.0426 (15)	0.0651 (18)	0.0445 (15)	−0.0172 (13)	0.0035 (12)	−0.0135 (14)
C11	0.0368 (13)	0.0521 (15)	0.0470 (15)	−0.0066 (11)	−0.0096 (11)	−0.0161 (12)
C12	0.0317 (12)	0.0470 (14)	0.0269 (11)	0.0058 (10)	−0.0112 (9)	−0.0078 (10)
C13	0.0435 (14)	0.0503 (15)	0.0478 (15)	0.0006 (11)	−0.0157 (12)	−0.0164 (13)
C14	0.0486 (16)	0.0439 (15)	0.0528 (17)	0.0011 (12)	−0.0166 (13)	−0.0006 (13)
C15	0.0424 (14)	0.0574 (17)	0.0352 (14)	0.0009 (12)	−0.0178 (11)	0.0020 (13)
C16	0.0403 (14)	0.0619 (17)	0.0349 (13)	−0.0016 (12)	−0.0154 (11)	−0.0112 (12)
C17	0.0422 (14)	0.0439 (14)	0.0363 (13)	0.0034 (11)	−0.0148 (11)	−0.0083 (11)
C18	0.111 (3)	0.0471 (19)	0.096 (3)	−0.003 (2)	−0.042 (3)	−0.0024 (19)
C19	0.096 (3)	0.096 (3)	0.063 (2)	−0.008 (2)	−0.042 (2)	−0.030 (2)
C20	0.0474 (14)	0.0486 (14)	0.0244 (11)	−0.0107 (11)	−0.0053 (10)	−0.0125 (10)
C21	0.091 (2)	0.0486 (17)	0.0590 (19)	−0.0016 (15)	−0.0334 (17)	−0.0154 (14)
C22	0.158 (4)	0.048 (2)	0.072 (2)	−0.020 (2)	−0.039 (3)	−0.0120 (17)
C23	0.146 (4)	0.085 (3)	0.060 (2)	−0.068 (3)	−0.006 (2)	−0.022 (2)
C24	0.079 (2)	0.103 (3)	0.084 (3)	−0.044 (2)	−0.008 (2)	−0.044 (2)
C25	0.0550 (17)	0.071 (2)	0.0635 (19)	−0.0158 (15)	−0.0109 (15)	−0.0333 (16)

Geometric parameters (Å, °)

S1—C3	1.719 (2)	C12—C17	1.371 (3)
S1—C4	1.758 (2)	C12—C13	1.372 (4)
S2—O2	1.4337 (17)	C13—C14	1.399 (4)
S2—O1	1.4372 (17)	C13—H13	0.9300
S2—C2	1.726 (2)	C14—C15	1.377 (4)
S2—C20	1.761 (3)	C14—C18	1.506 (4)
N1—C1	1.340 (3)	C15—C16	1.376 (4)
N1—H1NA	0.76 (3)	C15—H15	0.9300
N1—H1NB	0.95 (3)	C16—C17	1.391 (3)
N2—C3	1.340 (3)	C16—C19	1.511 (4)
N2—C12	1.425 (3)	C17—H17	0.9300
N2—H2NA	0.78 (3)	C18—H18B	0.9600
O3—C5	1.244 (3)	C18—H18A	0.9600
C1—C4	1.398 (3)	C18—H18C	0.9600
C1—C2	1.432 (3)	C19—H19A	0.9600
C2—C3	1.391 (3)	C19—H19C	0.9600
C4—C5	1.418 (3)	C19—H19B	0.9600
C5—C6	1.497 (3)	C20—C21	1.367 (4)
C6—C7	1.385 (3)	C20—C25	1.385 (4)

C6—C11	1.386 (3)	C21—C22	1.384 (5)
C7—C8	1.380 (3)	C21—H21	0.9300
C7—H7	0.9300	C22—C23	1.345 (6)
C8—C9	1.378 (4)	C22—H22	0.9300
C8—H8	0.9300	C23—C24	1.373 (6)
C9—C10	1.365 (4)	C23—H23	0.9300
C9—H9	0.9300	C24—C25	1.372 (4)
C10—C11	1.380 (4)	C24—H24	0.9300
C10—H10	0.9300	C25—H25	0.9300
C11—H11	0.9300		
C3—S1—C4	92.08 (11)	C17—C12—N2	120.3 (2)
O2—S2—O1	118.85 (11)	C13—C12—N2	118.6 (2)
O2—S2—C2	108.58 (11)	C12—C13—C14	119.8 (3)
O1—S2—C2	108.25 (10)	C12—C13—H13	120.1
O2—S2—C20	107.97 (11)	C14—C13—H13	120.1
O1—S2—C20	107.25 (12)	C15—C14—C13	118.1 (3)
C2—S2—C20	105.11 (11)	C15—C14—C18	121.7 (3)
C1—N1—H1NA	112 (2)	C13—C14—C18	120.2 (3)
C1—N1—H1NB	123.6 (19)	C16—C15—C14	122.7 (2)
H1NA—N1—H1NB	124 (3)	C16—C15—H15	118.6
C3—N2—C12	124.4 (2)	C14—C15—H15	118.6
C3—N2—H2NA	121 (2)	C15—C16—C17	118.0 (2)
C12—N2—H2NA	114 (2)	C15—C16—C19	121.8 (3)
N1—C1—C4	122.4 (2)	C17—C16—C19	120.2 (3)
N1—C1—C2	125.2 (2)	C12—C17—C16	120.3 (2)
C4—C1—C2	112.35 (18)	C12—C17—H17	119.9
C3—C2—C1	112.82 (19)	C16—C17—H17	119.9
C3—C2—S2	122.23 (17)	C14—C18—H18B	109.5
C1—C2—S2	124.52 (16)	C14—C18—H18A	109.5
N2—C3—C2	127.8 (2)	H18B—C18—H18A	109.5
N2—C3—S1	120.20 (17)	C14—C18—H18C	109.5
C2—C3—S1	112.01 (16)	H18B—C18—H18C	109.5
C1—C4—C5	125.2 (2)	H18A—C18—H18C	109.5
C1—C4—S1	110.74 (16)	C16—C19—H19A	109.5
C5—C4—S1	123.93 (17)	C16—C19—H19C	109.5
O3—C5—C4	121.0 (2)	H19A—C19—H19C	109.5
O3—C5—C6	118.2 (2)	C16—C19—H19B	109.5
C4—C5—C6	120.7 (2)	H19A—C19—H19B	109.5
C7—C6—C11	119.0 (2)	H19C—C19—H19B	109.5
C7—C6—C5	122.7 (2)	C21—C20—C25	120.7 (3)
C11—C6—C5	118.2 (2)	C21—C20—S2	120.0 (2)
C8—C7—C6	120.0 (2)	C25—C20—S2	119.3 (2)
C8—C7—H7	120.0	C20—C21—C22	119.1 (3)
C6—C7—H7	120.0	C20—C21—H21	120.5
C9—C8—C7	120.4 (2)	C22—C21—H21	120.5
C9—C8—H8	119.8	C23—C22—C21	120.5 (4)
C7—C8—H8	119.8	C23—C22—H22	119.8
C10—C9—C8	119.8 (2)	C21—C22—H22	119.8
C10—C9—H9	120.1	C22—C23—C24	120.7 (4)

C8—C9—H9	120.1	C22—C23—H23	119.7
C9—C10—C11	120.4 (3)	C24—C23—H23	119.7
C9—C10—H10	119.8	C25—C24—C23	120.1 (4)
C11—C10—H10	119.8	C25—C24—H24	120.0
C10—C11—C6	120.3 (2)	C23—C24—H24	120.0
C10—C11—H11	119.9	C24—C25—C20	118.9 (3)
C6—C11—H11	119.9	C24—C25—H25	120.5
C17—C12—C13	121.0 (2)	C20—C25—H25	120.5
N1—C1—C2—C3	179.4 (2)	C6—C7—C8—C9	−1.3 (4)
C4—C1—C2—C3	0.2 (3)	C7—C8—C9—C10	1.1 (4)
N1—C1—C2—S2	6.8 (4)	C8—C9—C10—C11	0.1 (4)
C4—C1—C2—S2	−172.34 (17)	C9—C10—C11—C6	−1.1 (4)
O2—S2—C2—C3	160.23 (19)	C7—C6—C11—C10	0.9 (4)
O1—S2—C2—C3	29.9 (2)	C5—C6—C11—C10	178.2 (2)
C20—S2—C2—C3	−84.4 (2)	C3—N2—C12—C17	64.5 (4)
O2—S2—C2—C1	−27.9 (2)	C3—N2—C12—C13	−116.9 (3)
O1—S2—C2—C1	−158.18 (19)	C17—C12—C13—C14	0.6 (4)
C20—S2—C2—C1	87.5 (2)	N2—C12—C13—C14	−178.0 (2)
C12—N2—C3—C2	175.3 (2)	C12—C13—C14—C15	−1.0 (4)
C12—N2—C3—S1	−3.9 (4)	C12—C13—C14—C18	178.9 (3)
C1—C2—C3—N2	−179.6 (2)	C13—C14—C15—C16	−0.1 (4)
S2—C2—C3—N2	−6.9 (4)	C18—C14—C15—C16	179.9 (3)
C1—C2—C3—S1	−0.3 (3)	C14—C15—C16—C17	1.7 (4)
S2—C2—C3—S1	172.41 (13)	C14—C15—C16—C19	−179.0 (3)
C4—S1—C3—N2	179.6 (2)	C13—C12—C17—C16	1.1 (4)
C4—S1—C3—C2	0.29 (19)	N2—C12—C17—C16	179.6 (2)
N1—C1—C4—C5	−3.0 (4)	C15—C16—C17—C12	−2.2 (4)
C2—C1—C4—C5	176.2 (2)	C19—C16—C17—C12	178.6 (3)
N1—C1—C4—S1	−179.2 (2)	O2—S2—C20—C21	−149.6 (2)
C2—C1—C4—S1	0.0 (3)	O1—S2—C20—C21	−20.4 (2)
C3—S1—C4—C1	−0.16 (19)	C2—S2—C20—C21	94.6 (2)
C3—S1—C4—C5	−176.4 (2)	O2—S2—C20—C25	32.5 (2)
C1—C4—C5—O3	3.1 (4)	O1—S2—C20—C25	161.7 (2)
S1—C4—C5—O3	178.77 (19)	C2—S2—C20—C25	−83.3 (2)
C1—C4—C5—C6	−175.0 (2)	C25—C20—C21—C22	1.3 (4)
S1—C4—C5—C6	0.7 (3)	S2—C20—C21—C22	−176.5 (3)
O3—C5—C6—C7	134.0 (2)	C20—C21—C22—C23	0.3 (6)
C4—C5—C6—C7	−47.9 (3)	C21—C22—C23—C24	−1.6 (6)
O3—C5—C6—C11	−43.2 (3)	C22—C23—C24—C25	1.4 (6)
C4—C5—C6—C11	134.9 (2)	C23—C24—C25—C20	0.2 (5)
C11—C6—C7—C8	0.3 (4)	C21—C20—C25—C24	−1.6 (4)
C5—C6—C7—C8	−176.9 (2)	S2—C20—C25—C24	176.3 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1NA···O3	0.76 (3)	2.06 (3)	2.699 (3)	141 (3)
N1—H1NB···O2	0.95 (3)	2.22 (3)	2.864 (3)	124 (2)
N2—H2NA···O1	0.78 (3)	2.25 (3)	2.820 (3)	130 (2)

N1—H1NB···O2^{i}	0.95 (3)	2.19 (3)	2.993 (3)	142 (3)

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

Fig. 1