Synthesis and crystal structure of *N*-phenyl-2-(phenylsulfanyl)acetamide

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N-Phenyl-2-(phenylsulfanyl)acetamide, $C_{14}H_{13}NOS$, was synthesized and structurally characterized. In the crystal, N—H⋯O hydrogen bonding leads to the formation of chains of molecules along the [100] direction. The chains are linked by C—H⋯π interactions, forming a three-dimensional network. The crystal studied was twinned by a twofold rotation around [100].

1. Chemical context

The acetamide moiety possesses therapeutic potential for targeting various diseases. Acetamide-containing drugs are used for inflammation control, cyclooxygenase (COX) enzyme inhibition, and as antiviral drugs (Agrawal *et al.*, 2010; Orzalesi *et al.*, 1977). Recently, starting from acetamides, we have synthesized various heterocyclic compounds that exhibit diverse activities, including anti-SARS CoV-2 (Mohamed-Ezzat & Elgemeie, 2023), antimicrobial (Elgemeie *et al.*, 2017*a,b*), antitumor properties (Elgemeie & Mohamed-Ezzat, 2022; Mohamed-Ezzat *et al.*, 2023*a,b*), as well as potential for other applications (Elgemeie *et al.*, 2015, 2017*a,b*, 2019; Mohamed-Ezzat *et al.*, 2021, 2023*a,b*).

Additionally, the evolution of the pharmaceutical industry has been greatly aided by the discovery of sulfur-based therapies. Sulfur-derived functional groups can be found in a broad range of natural products and pharmaceuticals. Sulfur remains the dominant heteroatom integrated into a variety of FDA-approved sulfur-containing medications (Feng *et al.*, 2016).

Sulfides have been presented *inter alia* as precursors for sulfonyl chloride synthesis (Langler *et al.*, 1979). Advanced methods previously reported for the transformation of sulfides include, for example, using sulfate-modified multi-walled carbon nanotubes (S-MWCNT) and mesoporous carbon (S-MC) as heterogenous catalysts to facilitate the synthesis of acetamide derivatives (Minchitha *et al.*, 2018).

Herein, we report the first synthesis of a sulfide from a sulfonyl derivative *via* an alternative new, direct and efficient approach. Upon reaction of the sulfonylguanidine derivative with 2-chloro-*N*-phenylacetamide, the title compound *N*-phenyl-2-(phenylsulfanyl)acetamide (**3**) is formed. Its
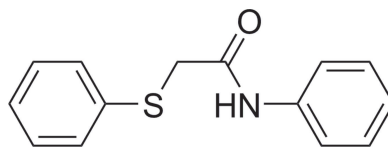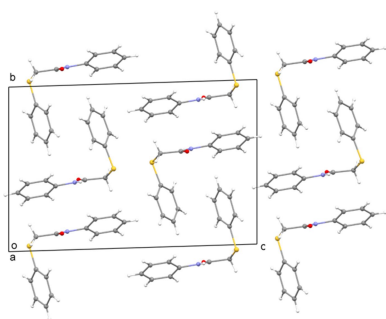
chemical structure was confirmed by spectroscopic techniques and elemental analysis. The ^{1}H NMR spectrum has a singlet signal of the methylene group at δ 3.84 ppm, the multiplet aromatic protons at δ 7.30 ppm, as well as the amine proton at δ 9.15 ppm, which is roughly in accordance with previously reported data (Motherwell et al., 2002). Confirmation of the molecular structure is provided by means of single crystal X-ray diffraction structural analysis which provides the first crystal structure and geometric parameters for the title compound.

2. Structural commentary

The asymmetric unit of the crystal structure is composed of two independent molecules of the title compound (Fig. 1). The molecules of **3** consist of three planar segments, namely sulfanylbenzene [**sb$_1$** (C1–C6/S1) and **sb$_2$** (C15–C21/S2)], acetamide [**ac$_1$** (C7/C8/N1/O1) and **ac$_2$** (C22/C23/N2/O2)], and phenyl [**ph$_1$** (C9–C14) and **ph$_2$** (C24–C29)] groups. The conformations of the two independent molecules in the structure are similar but not identical. The twist angles **sb/ac** are 85.12 (11) and 77.58 (11)° for molecules **1** and **2**, respectively, and twist angles **sb/ph** are 28.30 (10) and 30.60 (10)° for molecules **1** and **2**, respectively. Thus, the phenyl and acetamide groups are almost coplanar whereas the sulfanylbenzene groups are almost perpendicular to this plane. The C_{phenyl}—S-C—$C_{carbonyl}$ torsion angles are 72.1 (3)° for C1—S1—C7—C8 and −65.13 (3)° for C15—S2—C22—C23. A similar molecular conformation is observed in the crystal structures of the related compounds N-(2-hydroxy-5-chlorophenyl)thiophenylacetamide (Tarimci et al., 1998) and 2-[(2-aminophenyl)sulfanyl]-N-(2-nitrophenyl)acetamide (Murtaza et al., 2019) in which the C_{phenyl}—S—C—$C_{carbonyl}$ torsion angles are ca 80°.

3. Supramolecular features

The packing in the crystal structure of **3** is shown in Fig. 2a. In the crystal, the acetamide groups of each set of independent
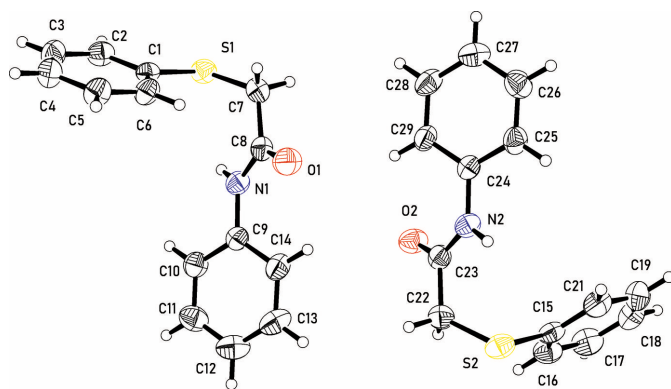
Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯O1^i	0.86 (3)	2.70 (3)	3.477 (3)	152 (3)
N2—H2A⋯O2^{ii}	0.83 (3)	2.71 (4)	3.456 (3)	150 (3)

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

molecules interact through weak N—H⋯O contacts (Table 1), forming chains parallel to [100] (Fig. 2b).

Adjacent chains are linked by weak C—H⋯π contacts between methylene and phenyl groups. The rings involved in the contacts are **ph$_1$** (C9–C14, Cg1) and **ph$_2$**$^{\#}$ (C24–C29, Cg2$^{\#}$) where # is $x + 1$, y, z. The associated H⋯π distances H7A⋯**ph$_2$**$^{\#}$, and H22B⋯**ph$_1$** are 2.80 Å and 2.94 Å, respectively. The H⋯centroid distances H7A⋯Cg2$^{\#}$ and H22B⋯Cg1 are 3.00 and 3.10 Å, respectively. The C—H⋯centroid angles for C7—H7A⋯Cg2$^{\#}$ and C22—H22B⋯Cg1 are 129 and 128°, respectively.

(a)

(b)

Figure 1
The asymmetric unit and molecular structures of the two independent molecules of N-phenyl-2-(phenylsulfanyl)acetamide (**3**) showing displacement ellipsoids at the 50% probability level.
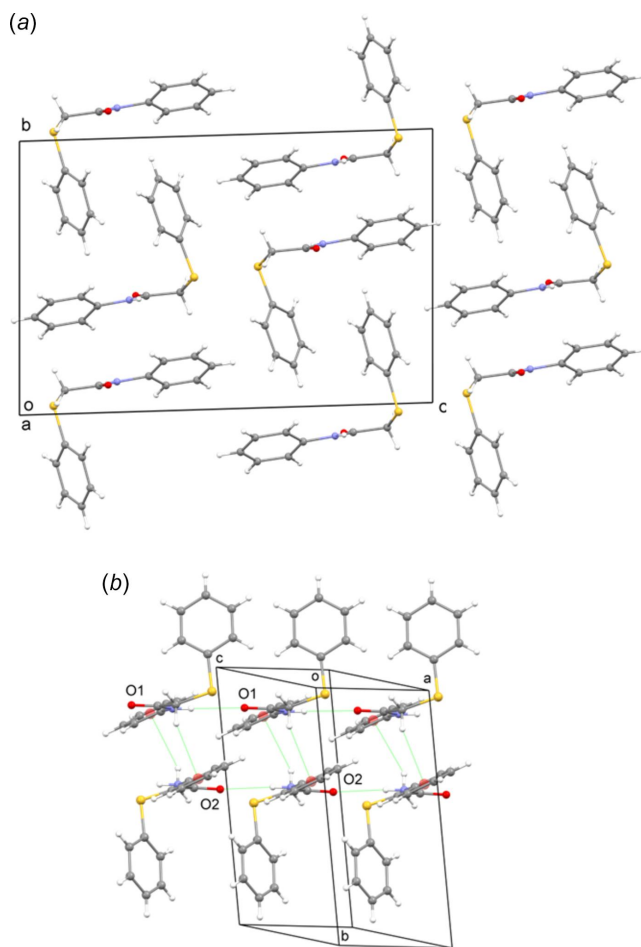
Figure 2
(a) Crystal packing in the crystal structure of N-phenyl-2-(phenylsulfanyl)acetamide (**3**). (b) A segment of the crystal structure of compound **3** showing the N—H⋯O and C—H⋯π intermolecular contacts as green dotted lines.
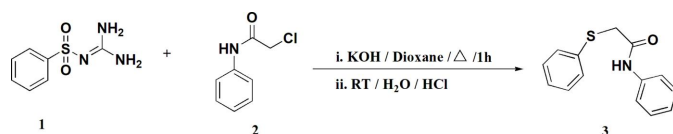
Figure 3
The synthesis of compound **3** from sulfonylguanidine.

4. Database survey

A search of the CSD (version 5.44, April 2023; Groom *et al.*, 2016) using the routine ConQuest (Bruno *et al.*, 2002) for crystal structures containing the *N*-phenyl-2-(phenylsulfanyl)acetamide fragment returned *N*-(2-hydroxy-5-chlorophenyl)thiophenylacetamide (NILWEK; Tarimci *et al.*, 1998) and 2-[(2-aminophenyl)sulfanyl]-*N*-(2-nitrophenyl)acetamide (NULZOM; Murtaza *et al.*, 2019), which both have similar conformational geometries to compound **3**. In contrast, 2-[(2-aminophenyl)sulfanyl]-*N*-(4-methoxyphenyl)acetamide (PAXTEP; Murtaza *et al.*, 2012) has a C_{phenyl}—S—C—$C_{carbonyl}$ torsion angle of 159° compared to the values of *ca* 80° in NILWEK and NULZOM and even more acute ones are observed in the crystal of the title compound.

5. Synthesis and crystallization

A mixture of benzenesulfonylguanidine (**1**) (0.01 mol) with 2-chloro-*N*-phenylacetamide **2** (0.01 mol) in dry 1,4-dioxane (20 mL) containing potassium hydroxide (0.015 mol) was refluxed for 1 h. The reaction mixture was poured onto ice–water and then neutralized using hydrochloric acid (Fig. 3).

The solid precipitate that formed was then filtered, washed thoroughly with water and left in the open to dry at room temperature. The solid obtained was recrystallized from water to afford colorless crystals of compound **3** in 83% yield; mp > 573 K; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.84 (*s*, 2H, CH$_2$), 7.30 (*m*, 10H, Ar-H), 9.15 (*s*, 1H, NH); analysis calculated for C$_{14}$H$_{13}$NOS (243.32): C, 69.11; H, 5.39; N, 5.76; S, 13.18. Found: C, 69.07; H, 5.35; N, 5.75; S, 13.16.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was twinned by a twofold rotation around [100]. This problem was addressed using a HKLF5 file for refinement. The N-bound hydrogen atoms were refined with regard to location while the displacement parameters were constrained to those of their parent atoms [$U_{iso}(H) = 1.2U_{eq}(N)$]. All other hydrogen atoms were placed in idealized positions (C—H = 0.93–0.97 Å) and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

Acknowledgements

Table 2
Experimental details.

Crystal data	
Chemical formula	C$_{14}$H$_{13}$NOS
M_r	243.31
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, b, c (Å)	5.6768 (3), 12.0747 (6), 18.1912 (9)
α, β, γ (°)	87.071 (4), 82.110 (4), 81.110 (4)
V (Å^3)	1219.72 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.25
Crystal size (mm)	0.54 × 0.17 × 0.09
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at home/near, Atlas
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.662, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7742, 7742, 5708
R_{int}	0.040
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.697
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.162, 1.03
No. of reflections	7742
No. of parameters	314
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.23, −0.23

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012).

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supporting information

Synthesis and crystal structure of *N*-phenyl-2-(phenylsulfanyl)acetamide

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Computing details

N-**Phenyl-2-(phenylsulfanyl)acetamide**

Crystal data

$C_{14}H_{13}NOS$	$Z = 4$
$M_r = 243.31$	$F(000) = 512$
Triclinic, $P\bar{1}$	$D_x = 1.325$ Mg m^{-3}
$a = 5.6768$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 12.0747$ (6) Å	Cell parameters from 3492 reflections
$c = 18.1912$ (9) Å	$\theta = 3.7–28.1°$
$\alpha = 87.071$ (4)°	$\mu = 0.25$ mm^{-1}
$\beta = 82.110$ (4)°	$T = 293$ K
$\gamma = 81.110$ (4)°	Needle, yellow
$V = 1219.72$ (11) Å^3	$0.54 \times 0.17 \times 0.09$ mm

Data collection

Agilent SuperNova, Dual, Cu at home/near, Atlas diffractometer	7742 independent reflections
	5708 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.040$
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2023)	$\theta_{max} = 29.7°$, $\theta_{min} = 3.4°$
	$h = -7 \rightarrow 6$
$T_{min} = 0.662$, $T_{max} = 1.000$	$k = -15 \rightarrow 15$
7742 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.058$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.162$	
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 0.551P]$
7742 reflections	where $P = (F_o^2 + 2F_c^2)/3$
314 parameters	$(\Delta/\sigma)_{max} = 0.001$
0 restraints	$\Delta\rho_{max} = 0.23$ e Å^{-3}
	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Experimental. Single-crystal XRD data were collected at room temperature on an Agilent SuperNova Dual Atlas diffractometer using mirror-monochromated Mo K*α* radiation.

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.

Refinement. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.1641 (5)	−0.1130 (2)	0.11013 (13)	0.0415 (6)
C2	1.3815 (5)	−0.1806 (3)	0.08899 (15)	0.0532 (7)
H2	1.506625	−0.150022	0.060835	0.064*
C3	1.4122 (6)	−0.2916 (3)	0.10934 (17)	0.0600 (8)
H3	1.558973	−0.335965	0.095112	0.072*
C4	1.2294 (6)	−0.3390 (3)	0.15062 (17)	0.0591 (8)
H4	1.251613	−0.414900	0.164104	0.071*
C5	1.0147 (6)	−0.2730 (3)	0.17151 (17)	0.0560 (8)
H5	0.890629	−0.304415	0.199571	0.067*
C6	0.9792 (5)	−0.1608 (2)	0.15170 (15)	0.0512 (7)
H6	0.831850	−0.116989	0.166072	0.061*
C7	0.8387 (6)	0.0859 (3)	0.10985 (15)	0.0551 (8)
H7A	0.807561	0.158969	0.085390	0.066*
H7B	0.741087	0.037878	0.090528	0.066*
C8	0.7505 (6)	0.0994 (2)	0.19250 (15)	0.0480 (7)
C9	0.8784 (5)	0.1283 (2)	0.31338 (14)	0.0434 (6)
C10	1.0655 (5)	0.0928 (3)	0.35418 (16)	0.0534 (7)
H10	1.212546	0.058503	0.330670	0.064*
C11	1.0350 (7)	0.1082 (3)	0.42985 (17)	0.0648 (9)
H11	1.161619	0.084293	0.457099	0.078*
C12	0.8180 (7)	0.1586 (3)	0.46490 (18)	0.0689 (10)
H12	0.796532	0.167685	0.515957	0.083*
C13	0.6343 (6)	0.1953 (3)	0.42445 (18)	0.0658 (9)
H13	0.488293	0.230248	0.448232	0.079*
C14	0.6618 (6)	0.1812 (2)	0.34868 (17)	0.0557 (7)
H14	0.535726	0.207188	0.321611	0.067*
C15	0.6954 (5)	0.6251 (2)	0.38739 (14)	0.0483 (7)
C16	0.8379 (6)	0.6999 (3)	0.40561 (17)	0.0594 (8)
H16	0.958419	0.676480	0.435258	0.071*
C17	0.8000 (7)	0.8093 (3)	0.37954 (19)	0.0677 (9)
H17	0.897550	0.859209	0.391344	0.081*
C18	0.6223 (6)	0.8462 (3)	0.33670 (19)	0.0655 (9)
H18	0.598021	0.920754	0.320109	0.079*
C19	0.4793 (6)	0.7723 (3)	0.31825 (19)	0.0667 (9)
H19	0.357922	0.796749	0.289068	0.080*
C21	0.5166 (6)	0.6616 (3)	0.34325 (17)	0.0579 (8)

H21	0.421285	0.611422	0.330344	0.069*
C22	1.0326 (6)	0.4309 (3)	0.38916 (15)	0.0568 (8)
H22A	1.133364	0.478430	0.407477	0.068*
H22B	1.070250	0.356802	0.411605	0.068*
C23	1.1052 (6)	0.4220 (2)	0.30651 (15)	0.0467 (7)
C24	0.9628 (5)	0.3906 (2)	0.18839 (14)	0.0405 (6)
C25	0.7707 (5)	0.4253 (3)	0.14992 (16)	0.0529 (7)
H25	0.626080	0.460022	0.174787	0.063*
C26	0.7913 (6)	0.4091 (3)	0.07505 (18)	0.0619 (8)
H26	0.661178	0.434012	0.049420	0.074*
C27	1.0032 (6)	0.3561 (3)	0.03737 (16)	0.0604 (8)
H27	1.017265	0.344880	−0.013342	0.072*
C28	1.1923 (6)	0.3204 (3)	0.07640 (17)	0.0596 (8)
H28	1.335639	0.284254	0.051660	0.071*
C29	1.1747 (5)	0.3368 (2)	0.15161 (16)	0.0508 (7)
H29	1.304784	0.311726	0.177232	0.061*
N1	0.9169 (5)	0.1113 (2)	0.23607 (13)	0.0484 (6)
H1	1.062 (6)	0.103 (3)	0.2146 (16)	0.058*
N2	0.9320 (5)	0.4085 (2)	0.26590 (13)	0.0483 (6)
H2A	0.790 (6)	0.419 (3)	0.2863 (17)	0.058*
O1	0.5380 (4)	0.1003 (2)	0.21474 (12)	0.0656 (6)
O2	1.3142 (4)	0.4238 (2)	0.28135 (11)	0.0618 (6)
S1	1.14801 (15)	0.03015 (6)	0.08281 (4)	0.0539 (2)
S2	0.72463 (16)	0.48404 (7)	0.42268 (4)	0.0584 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0422 (15)	0.0485 (15)	0.0349 (12)	−0.0088 (13)	−0.0048 (11)	−0.0066 (11)
C2	0.0443 (17)	0.0652 (19)	0.0493 (15)	−0.0133 (15)	0.0039 (13)	−0.0050 (14)
C3	0.0466 (18)	0.061 (2)	0.0661 (18)	0.0059 (16)	0.0017 (15)	−0.0047 (15)
C4	0.057 (2)	0.0507 (17)	0.0667 (19)	−0.0023 (16)	−0.0053 (16)	−0.0001 (14)
C5	0.0492 (18)	0.0543 (18)	0.0622 (18)	−0.0114 (15)	0.0047 (15)	−0.0020 (14)
C6	0.0398 (16)	0.0535 (17)	0.0564 (16)	−0.0038 (14)	0.0059 (13)	−0.0061 (13)
C7	0.0588 (19)	0.0538 (17)	0.0507 (16)	−0.0015 (15)	−0.0099 (14)	0.0036 (13)
C8	0.0507 (18)	0.0408 (15)	0.0500 (15)	−0.0009 (14)	−0.0054 (14)	0.0007 (12)
C9	0.0444 (16)	0.0380 (14)	0.0481 (14)	−0.0100 (12)	−0.0025 (12)	−0.0018 (11)
C10	0.0424 (16)	0.0593 (18)	0.0573 (16)	−0.0067 (14)	−0.0027 (14)	−0.0027 (13)
C11	0.063 (2)	0.080 (2)	0.0559 (17)	−0.0175 (19)	−0.0163 (17)	−0.0002 (16)
C12	0.069 (2)	0.090 (3)	0.0513 (17)	−0.031 (2)	0.0012 (17)	−0.0101 (17)
C13	0.056 (2)	0.077 (2)	0.065 (2)	−0.0172 (18)	0.0091 (17)	−0.0246 (17)
C14	0.0471 (17)	0.0543 (18)	0.0642 (18)	−0.0019 (15)	−0.0043 (15)	−0.0125 (14)
C15	0.0422 (16)	0.0599 (17)	0.0417 (13)	−0.0109 (14)	0.0069 (12)	−0.0134 (12)
C16	0.058 (2)	0.070 (2)	0.0545 (17)	−0.0202 (17)	−0.0063 (15)	−0.0116 (15)
C17	0.073 (2)	0.065 (2)	0.070 (2)	−0.0277 (19)	−0.0017 (18)	−0.0116 (17)
C18	0.060 (2)	0.0559 (19)	0.074 (2)	−0.0052 (17)	0.0098 (18)	−0.0068 (16)
C19	0.0473 (19)	0.076 (2)	0.073 (2)	0.0004 (18)	−0.0070 (17)	−0.0035 (18)
C21	0.0455 (17)	0.067 (2)	0.0643 (18)	−0.0162 (16)	−0.0031 (15)	−0.0167 (16)

C22	0.0571 (19)	0.0625 (19)	0.0470 (16)	−0.0046 (16)	0.0001 (14)	0.0019 (14)
C23	0.0483 (17)	0.0410 (15)	0.0475 (15)	−0.0046 (13)	0.0011 (14)	0.0025 (12)
C24	0.0411 (15)	0.0329 (13)	0.0468 (14)	−0.0094 (12)	0.0013 (12)	−0.0017 (10)
C25	0.0381 (16)	0.0572 (18)	0.0602 (18)	−0.0038 (14)	0.0000 (14)	0.0000 (14)
C26	0.0539 (19)	0.073 (2)	0.0614 (19)	−0.0130 (17)	−0.0140 (16)	0.0021 (16)
C27	0.063 (2)	0.074 (2)	0.0471 (15)	−0.0232 (18)	0.0012 (15)	−0.0110 (14)
C28	0.0445 (18)	0.066 (2)	0.0653 (19)	−0.0062 (16)	0.0060 (15)	−0.0216 (15)
C29	0.0419 (16)	0.0496 (16)	0.0593 (17)	0.0012 (14)	−0.0058 (14)	−0.0126 (13)
N1	0.0421 (14)	0.0522 (14)	0.0491 (13)	−0.0056 (12)	−0.0002 (11)	−0.0045 (11)
N2	0.0395 (13)	0.0554 (14)	0.0475 (13)	−0.0088 (12)	0.0058 (11)	−0.0037 (10)
O1	0.0461 (13)	0.0878 (16)	0.0626 (13)	−0.0066 (12)	−0.0069 (11)	−0.0105 (11)
O2	0.0508 (13)	0.0819 (15)	0.0526 (11)	−0.0155 (12)	0.0021 (10)	−0.0084 (10)
S1	0.0569 (5)	0.0547 (4)	0.0488 (4)	−0.0124 (4)	0.0008 (4)	0.0004 (3)
S2	0.0579 (5)	0.0655 (5)	0.0487 (4)	−0.0162 (4)	0.0119 (4)	−0.0027 (3)

Geometric parameters (Å, º)

C1—C2	1.388 (4)	C15—C21	1.385 (4)
C1—C6	1.389 (4)	C15—S2	1.781 (3)
C1—S1	1.767 (3)	C16—C17	1.375 (5)
C2—C3	1.363 (4)	C16—H16	0.9300
C2—H2	0.9300	C17—C18	1.366 (5)
C3—C4	1.376 (5)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.378 (5)
C4—C5	1.368 (4)	C18—H18	0.9300
C4—H4	0.9300	C19—C21	1.385 (5)
C5—C6	1.375 (4)	C19—H19	0.9300
C5—H5	0.9300	C21—H21	0.9300
C6—H6	0.9300	C22—C23	1.508 (4)
C7—C8	1.527 (4)	C22—S2	1.800 (3)
C7—S1	1.791 (3)	C22—H22A	0.9700
C7—H7A	0.9700	C22—H22B	0.9700
C7—H7B	0.9700	C23—O2	1.215 (4)
C8—O1	1.217 (4)	C23—N2	1.342 (4)
C8—N1	1.342 (4)	C24—C25	1.376 (4)
C9—C10	1.380 (4)	C24—C29	1.378 (4)
C9—C14	1.384 (4)	C24—N2	1.420 (3)
C9—N1	1.414 (3)	C25—C26	1.373 (4)
C10—C11	1.382 (4)	C25—H25	0.9300
C10—H10	0.9300	C26—C27	1.381 (5)
C11—C12	1.373 (5)	C26—H26	0.9300
C11—H11	0.9300	C27—C28	1.370 (5)
C12—C13	1.364 (5)	C27—H27	0.9300
C12—H12	0.9300	C28—C29	1.380 (4)
C13—C14	1.382 (4)	C28—H28	0.9300
C13—H13	0.9300	C29—H29	0.9300
C14—H14	0.9300	N1—H1	0.86 (3)
C15—C16	1.382 (4)	N2—H2A	0.83 (3)

C2—C1—C6	118.9 (3)	C17—C16—H16	120.3
C2—C1—S1	116.2 (2)	C15—C16—H16	120.3
C6—C1—S1	124.9 (2)	C18—C17—C16	121.5 (3)
C3—C2—C1	120.2 (3)	C18—C17—H17	119.3
C3—C2—H2	119.9	C16—C17—H17	119.3
C1—C2—H2	119.9	C17—C18—C19	119.5 (3)
C2—C3—C4	121.0 (3)	C17—C18—H18	120.2
C2—C3—H3	119.5	C19—C18—H18	120.2
C4—C3—H3	119.5	C18—C19—C21	119.8 (3)
C5—C4—C3	119.0 (3)	C18—C19—H19	120.1
C5—C4—H4	120.5	C21—C19—H19	120.1
C3—C4—H4	120.5	C19—C21—C15	120.2 (3)
C4—C5—C6	121.1 (3)	C19—C21—H21	119.9
C4—C5—H5	119.5	C15—C21—H21	119.9
C6—C5—H5	119.5	C23—C22—S2	118.5 (2)
C5—C6—C1	119.8 (3)	C23—C22—H22A	107.7
C5—C6—H6	120.1	S2—C22—H22A	107.7
C1—C6—H6	120.1	C23—C22—H22B	107.7
C8—C7—S1	118.2 (2)	S2—C22—H22B	107.7
C8—C7—H7A	107.8	H22A—C22—H22B	107.1
S1—C7—H7A	107.8	O2—C23—N2	124.4 (3)
C8—C7—H7B	107.8	O2—C23—C22	118.9 (3)
S1—C7—H7B	107.8	N2—C23—C22	116.6 (3)
H7A—C7—H7B	107.1	C25—C24—C29	119.6 (3)
O1—C8—N1	124.2 (3)	C25—C24—N2	118.3 (2)
O1—C8—C7	119.3 (3)	C29—C24—N2	122.2 (3)
N1—C8—C7	116.5 (3)	C26—C25—C24	120.4 (3)
C10—C9—C14	119.4 (3)	C26—C25—H25	119.8
C10—C9—N1	118.5 (3)	C24—C25—H25	119.8
C14—C9—N1	122.0 (3)	C25—C26—C27	120.7 (3)
C9—C10—C11	120.2 (3)	C25—C26—H26	119.7
C9—C10—H10	119.9	C27—C26—H26	119.7
C11—C10—H10	119.9	C28—C27—C26	118.5 (3)
C12—C11—C10	120.1 (3)	C28—C27—H27	120.8
C12—C11—H11	119.9	C26—C27—H27	120.8
C10—C11—H11	119.9	C27—C28—C29	121.5 (3)
C13—C12—C11	119.7 (3)	C27—C28—H28	119.3
C13—C12—H12	120.2	C29—C28—H28	119.3
C11—C12—H12	120.2	C24—C29—C28	119.4 (3)
C12—C13—C14	121.0 (3)	C24—C29—H29	120.3
C12—C13—H13	119.5	C28—C29—H29	120.3
C14—C13—H13	119.5	C8—N1—C9	127.0 (3)
C13—C14—C9	119.5 (3)	C8—N1—H1	115 (2)
C13—C14—H14	120.2	C9—N1—H1	118 (2)
C9—C14—H14	120.2	C23—N2—C24	126.2 (2)
C16—C15—C21	119.5 (3)	C23—N2—H2A	118 (2)
C16—C15—S2	121.9 (2)	C24—N2—H2A	115 (2)

C21—C15—S2	118.5 (2)	C1—S1—C7	103.55 (14)
C17—C16—C15	119.4 (3)	C15—S2—C22	102.38 (14)
C6—C1—C2—C3	−0.5 (4)	S2—C15—C21—C19	176.3 (2)
S1—C1—C2—C3	178.3 (2)	S2—C22—C23—O2	155.3 (3)
C1—C2—C3—C4	0.4 (5)	S2—C22—C23—N2	−27.0 (4)
C2—C3—C4—C5	−0.3 (5)	C29—C24—C25—C26	−1.6 (4)
C3—C4—C5—C6	0.3 (5)	N2—C24—C25—C26	−179.5 (3)
C4—C5—C6—C1	−0.4 (5)	C24—C25—C26—C27	1.1 (5)
C2—C1—C6—C5	0.5 (4)	C25—C26—C27—C28	−0.1 (5)
S1—C1—C6—C5	−178.2 (2)	C26—C27—C28—C29	−0.3 (5)
S1—C7—C8—O1	−155.7 (3)	C25—C24—C29—C28	1.2 (4)
S1—C7—C8—N1	25.3 (4)	N2—C24—C29—C28	179.0 (3)
C14—C9—C10—C11	1.3 (4)	C27—C28—C29—C24	−0.2 (5)
N1—C9—C10—C11	179.9 (3)	O1—C8—N1—C9	−0.9 (5)
C9—C10—C11—C12	0.1 (5)	C7—C8—N1—C9	178.0 (2)
C10—C11—C12—C13	−1.2 (5)	C10—C9—N1—C8	153.0 (3)
C11—C12—C13—C14	0.8 (5)	C14—C9—N1—C8	−28.4 (4)
C12—C13—C14—C9	0.6 (5)	O2—C23—N2—C24	2.1 (5)
C10—C9—C14—C13	−1.6 (4)	C22—C23—N2—C24	−175.4 (2)
N1—C9—C14—C13	179.8 (3)	C25—C24—N2—C23	−152.4 (3)
C21—C15—C16—C17	−0.1 (4)	C29—C24—N2—C23	29.7 (4)
S2—C15—C16—C17	−177.0 (2)	C2—C1—S1—C7	173.7 (2)
C15—C16—C17—C18	0.8 (5)	C6—C1—S1—C7	−7.6 (3)
C16—C17—C18—C19	−0.8 (5)	C8—C7—S1—C1	72.1 (3)
C17—C18—C19—C21	0.0 (5)	C16—C15—S2—C22	−59.3 (3)
C18—C19—C21—C15	0.7 (5)	C21—C15—S2—C22	123.7 (2)
C16—C15—C21—C19	−0.7 (4)	C23—C22—S2—C15	−65.1 (3)

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯O1[i]	0.86 (3)	2.70 (3)	3.477 (3)	152 (3)
N2—H2A⋯O2[ii]	0.83 (3)	2.71 (4)	3.456 (3)	150 (3)

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