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Synthesis, crystal structure and Hirshfeld surface analysis of 3-ethyl-2-(methylsulfanyl)-5,5-diphenyl-3*H*-imidazol-4(5*H*)-one (Thiophenytoin analogue)

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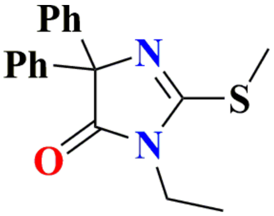
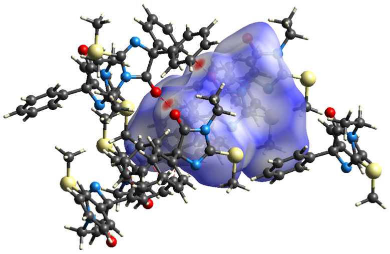
In the title molecule, 3-ethyl-2-(methylsulfanyl)-5,5-diphenyl-3*H*-imidazol-4(5*H*)-one, $C_{18}H_{18}N_2OS$, the two substituent phenyl rings are inclined of 59.50 (7) and 83.53 (8)° with respect to the plane of the five-membered ring. The *S*-methyl group lies in this plane while the ethyl group is nearly perpendicular to it. In the crystal, weak C—H···O hydrogen bonds form inversion dimers, which pack *via* conventional van der Waals contacts. A Hirshfeld surface analysis was performed, showing the predominance of H···H and C···H/H···C contacts.

1. Chemical context

Hydantoin (imidazolidine-2,4-dione) represents a highly valuable and widely utilized heterocyclic scaffold in medicinal chemistry, as demonstrated by its presence in several clinically approved drugs, including phenytoin, nitrofurantoin, and enzalutamide (El Moutaouakil Ala Allah, Guerrab *et al.*, 2024). The hydantoin scaffold exhibits a wide range of pharmacological and biological properties, including antibacterial (Allah *et al.*, 2024), antiepileptic (El Moutaouakil Ala Allah, Guerrab *et al.*, 2024), antidiabetic (Guerrab *et al.*, 2025; El Moutaouakil Ala Allah *et al.*, 2025), anticancer (Shankaraiah *et al.*, 2014), and anti-inflammatory (Asim Kaplancikli *et al.*, 2012) activities. Furthermore, hydantoin derivatives are well known for their broad activity in corrosion prevention (AlObaid *et al.*, 2024; Ait Mansour *et al.*, 2025), and several of them have demonstrated high corrosion inhibition efficiency (Ettahiri *et al.*, 2025; El Kaouahi *et al.*, 2025).



As part of our ongoing research on heterocyclic scaffolds (El Moutaouakil Ala Allah, Kariuki *et al.* 2024, El Moutaouakil Ala Allah *et al.*, 2025; Guerrab *et al.*, 2022), we report the synthesis of 3-ethyl-2-(methylsulfanyl)-5,5-diphenyl-3*H*-imidazol-4(5*H*)-one, **3**, *via* an *N*-alkylation reaction of 2-(methylsulfanyl)-5,5-diphenyl-3*H*-imidazol-4(5*H*)-one.



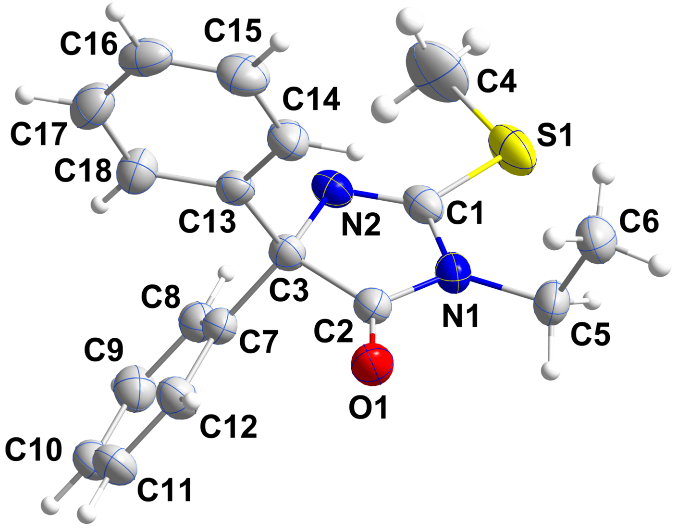


Figure 1
Perspective view of the title molecule with labeling scheme and 50% probability ellipsoids.

2. Structural commentary

The title molecule crystallizes in the monoclinic space group $P2_1/n$ (Fig. 1). The dihedral angles between the mean plane of the five-membered ring and the planes of the C7–C12 and the C13–C18 phenyl rings are 59.50 (7) and 83.53 (8)°, respectively, which is one of the larger differences in the dihedral angles found in related molecules (*vide infra*). The five-membered ring is planar to within 0.007 (1) Å (r.m.s. deviation of the fitted atoms = 0.001 Å) and the C4—S1 group lies within its plane as the C4—S1—C1—N1 torsion angle is −179.47 (13)°. In contrast, the ethyl group is nearly perpendicular to the aforementioned plane as the C1—N1—C5—C6 torsion angle is 87.81 (19)°.

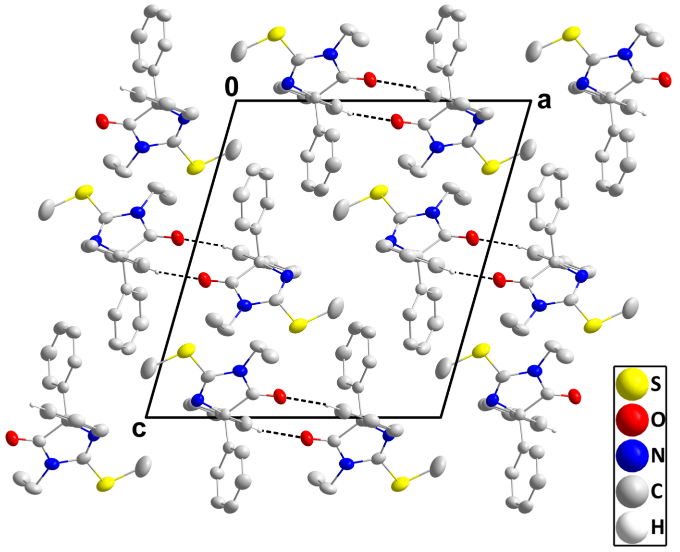


Figure 2
Packing viewed along the *b*-axis direction with C—H⋯O hydrogen bonds depicted by dashed lines and hydrogen atoms not participating in these interactions omitted for clarity.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C11—H11⋯O1^{i}	0.95	2.49	3.434 (2)	171

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

3. Supramolecular features

In the crystal, weak C11—H11⋯O1^{i} hydrogen bonds (Table 1) form centrosymmetric dimers, which, in turn, pack *via* conventional van der Waals contacts (Fig. 2).

4. Database survey

A search of the Cambridge Structural Database (CSD, updated to May 2025 (Groom *et al.*, 2016) with the fragment shown in Fig. 3, where *R* = *R*′ = no substituent, yielded nine hits. Included molecules have *R*,*R*′ = $-CH_2CH_2-$ (DIYRAE; Karolak-Wojciechowska *et al.*, 1985), $-CH_2CH(COOEt)-$ (FURFED; Karolak-Wojciechowska & Kieć-Kononowicz, 1987), $-CH_2CH_2CH_2-$ (IMTHZN; Kieć-Kononowicz *et al.*, 1981 and IMTHZN01; Guerrab *et al.*, 2019), and $-CH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2-$ (LIGWOR; Guerrab *et al.*, 2023) as well as *R* = *R*′ = benzyl (RAHGUF; Akrad *et al.*, 2017), *R* = *R*′ = *n*-propyl (RIJZIW; Akrad *et al.*, 2018), *R* = *R*′ = methyl (YEYYUA; El Moutaouakil Ala Allah *et al.*, 2023) and *R* = *R*′ = ethyl (HOPQAI; El Moutaouakil Ala Allah, Guerrab *et al.*, 2024). The dihedral angles between the planes of the two phenyl rings attached directly to the 4,5-dihydro-1*H*-imidazol-5-one ring vary over the range 47.89° to 89.59° due to the differing packings resulting from the varied sizes and shapes of the *R* and *R*′ substituents. In most instances, the two angles differ by *ca.* 15° but in LIGWOR they are nearly equal, being 62.10 (11) and 61.35 (11)°. As in the title molecule, the packing in RAHGOF and HOPQAI involves the formation of centrosymmetric dimers through weak C—H⋯O hydrogen bonds, with dimers associated through van der Waals interactions. In all of the other compounds, except for IMTHZN and IMTHZN01, chains of molecules parallel to crystallographic *a* axis are generated by weak C—H⋯O hydrogen bonds. In the exceptions, the chain is formed by weak C—H⋯N hydrogen bonds and the chains are linked by weak C—H⋯O hydrogen bonds and C—H⋯*π*(ring) interactions.

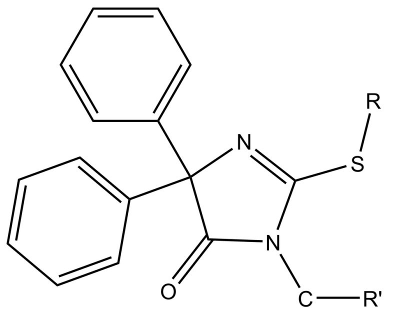


Figure 3
The fragment used in the Cambridge Structural Database search.

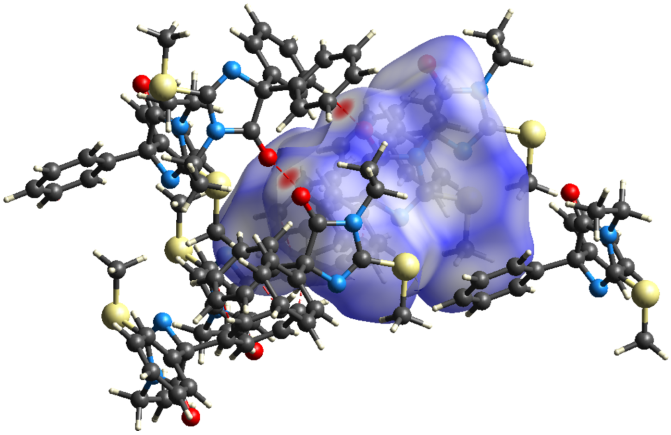
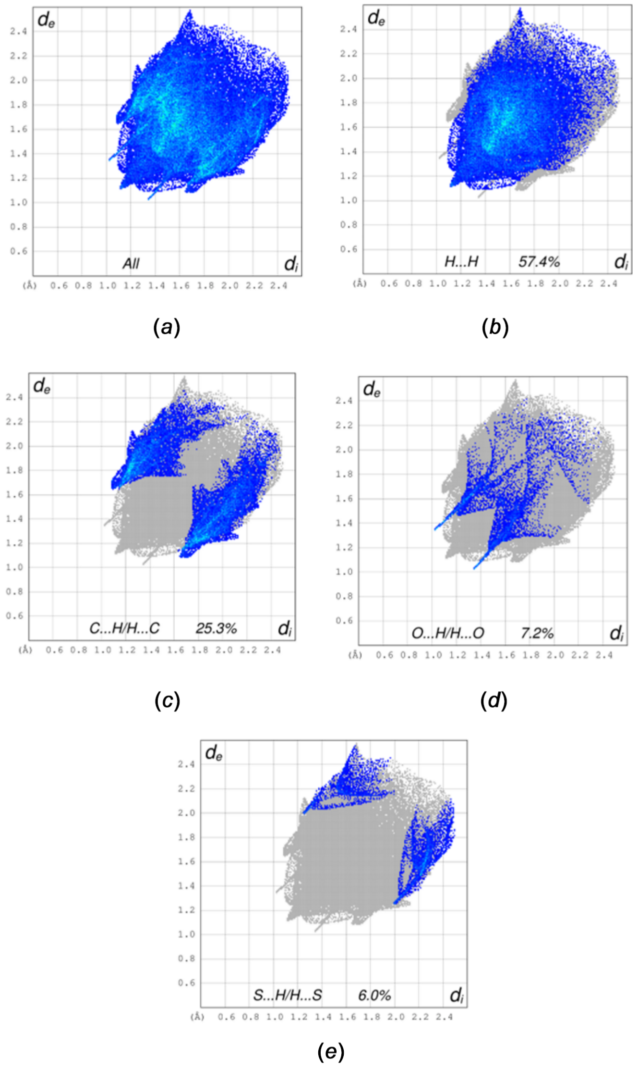


Figure 4
The Hirshfeld d_{norm} surface of the title compound with several neighboring molecules. The C—H$\cdots$O hydrogen bonds are depicted by red dashed lines.



(*a*) (*b*) (*c*) (*d*) (*e*)

Figure 5
The 2-D fingerprint plots showing all intermolecular contacts (*a*) and those delineated into H$\cdots$H (*b*), C$\cdots$H/H$\cdots$C (*c*), O$\cdots$H/H$\cdots$O (*d*) and S$\cdots$H/H$\cdots$S (***e***) contacts.

5. Hirshfeld surface analysis

The d_{norm} surface and 2-D fingerprint plots for the title molecule were calculated with *CrystalExplorer* (Spackman *et al.*, 2021) and full descriptions of the methods and interpretations of the results have been published by Tan *et al.* (2019). The d_{norm} surface together with several neighboring molecules is shown in Fig. 4, in which the C—H$\cdots$O hydrogen bonds are shown as red dashed lines passing through the dark red spots on the surface (indicating contacts shorter than the sum of the van der Waals radii). Fig. 5 shows the 2-D fingerprint plots for all intermolecular interactions (*a*) and those delineated into contacts between specific atom types (*b*)–(*e*). The H$\cdots$H contacts (*b*) account for 57.4% of the total, which is expected as the periphery of the molecule consists largely of hydrogen atoms. Most are bound to phenyl and methyl groups, which are directed outwards from the center of gravity and so will be the first to contact neighboring molecules. It is perhaps surprising that the C$\cdots$H/H$\cdots$C contacts (*c*), which contribute 25.3% of the total, are more prevalent than the O$\cdots$H/H$\cdots$O contacts (*d*, 7.2%), despite the latter being the only interactions in the packing that can be regarded as directional (*vide supra*). However, the geometrical analysis carried out with *PLATON* (Spek, 2020) shows a contact of 2.94 Å between H5*B* and the centroid *Cg* of the C7–C12 phenyl ring at $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$. Nevertheless, the C5—H5*B*$\cdots$*Cg*1 angle of 127° is quite small for the contact to be considered a definite C—H$\cdots\pi$(ring) interaction. Several other C$\cdots$H distances approximately equal to the sum of the two van der Waals radii are listed, which can account for this high percentage contribution. As noted, the O$\cdots$H/H$\cdots$O contacts come primarily from the weak C—H$\cdots$O hydrogen bonds described in Table 1. Although the S$\cdots$H/H$\cdots$S interactions contribute almost as much, there does not appear to be any obvious C—H$\cdots$S hydrogen bond.

6. Synthesis and crystallization

The title compound was obtained according to the reaction scheme shown in Fig. 6. To a solution of 2-(methylsulfanyl)-5,5-diphenyl-3*H*-imidazol-4(5*H*)-one (**1**) (0.5 g, 1.7 mmol) in DMF (10 mL), iodoethane (**2**) (2.10 mmol) was added in the presence of K_2CO_3 (1.8 mmol) and a catalytic amount of BTBA (10%). The reaction mixture was stirred at room temperature for 3 h (El Moutaouakil Ala Allah *et al.*, 2023; Guerrab *et al.*, 2023; El Moutaouakil Ala Allah, Kariuki, Alsubari *et al.*, 2024). After filtration of the inorganic salts, the solvent was evaporated under reduced pressure, and the crude

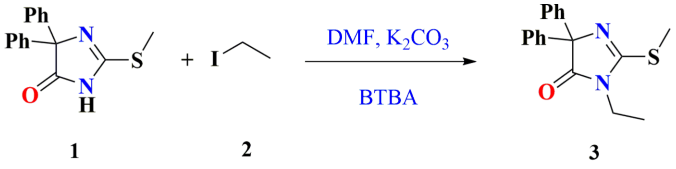


Figure 6
Synthesis of the title compound.

residue was purified by recrystallization from ethanol, affording 3-ethyl-2-(methylsulfanyl)-5,5-diphenyl-3*H*-imidazol-4(5*H*)-one (**3**) in 96% yield, m.p. = 394–396 K. **FT-IR** (ATR, ν, cm^{-1}): 3061 (C—H Ar), 2980 (–CH$_3$), 2854 (C—H Aliphatic), 1726 (C═O); **^{1}H NMR** (500 MHz, CDCl$_3$): δ ppm 1.24 (*t*, 3H, N—CH$_2$—CH$_3$), 2.70 (*s*, 3H, S—CH$_3$), 3.56 (*q*, 2H, N—CH$_2$—CH$_3$), 7.25–7.56 (*m*, 10H, Ar H); **^{13}C NMR** (125 MHz, CDCl$_3$); 12.85 (N—CH$_2$—CH$_3$), 14.29 (S—CH$_3$), 35.96 (N—CH$_2$—CH$_3$), 78.47 (C—2Ph); 127.24, 127.73, 128.48, 140.67 (C—Ar), 161.67 (C═N), 180,67 (C═O); **HRMS** (ESI-MS) (*m*/*z*) calculated for $C_{18}H_{18}N_2OS$ 311.1140; found 311.12036.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The carbon-bound H atoms were placed in calculated positions and refined isotropically using the riding model, with C—H distances ranging from 0.95 to 0.99 Å and $U_{\rm iso}$(H) set to 1.2–1.5 $U_{\rm eq}$(C).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{18}N_2OS$
M_r	310.40
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	200
a, b, c (Å)	12.6759 (2), 9.2109 (2), 14.1568 (3)
β (°)	105.915 (1)
V (Å^3)	1589.54 (5)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.82
Crystal size (mm)	0.19 × 0.15 × 0.14
Data collection	
Diffractometer	Bruker D8 Venture PhotonII
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{\rm min}$, $T_{\rm max}$	0.58, 0.75
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15894, 3237, 2875
$R_{\rm int}$	0.047
(sin $\theta/\lambda)_{\rm max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.101, 1.05
No. of reflections	3237
No. of parameters	202
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.23, −0.33

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012), *WinGX* (Farrugia, 2012), *publCIF* (Westrip, 2010) and *enCIFer* (Allen *et al.*, 2004).

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Computing details

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Crystal data

$C_{18}H_{18}N_2OS$
$M_r = 310.40$
Monoclinic, $P2_1/n$
$a = 12.6759$ (2) Å
$b = 9.2109$ (2) Å
$c = 14.1568$ (3) Å
$\beta = 105.915$ (1)°
$V = 1589.54$ (5) Å^3
$Z = 4$
$F(000) = 656$
$D_x = 1.297$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 438 reflections
$\theta = 4.2$–74.6°
$\mu = 1.82$ mm^{-1}
$T = 200$ K
Prism, colourless
0.19 × 0.15 × 0.14 mm

Data collection

Bruker D8 Venture PhotonII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi & ω scan
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.58$, $T_{max} = 0.75$
15894 measured reflections
3237 independent reflections
2875 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 74.6°$, $\theta_{min} = 4.2°$
$h = -15 \rightarrow 15$
$k = -11 \rightarrow 10$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.101$
$S = 1.05$
3237 reflections
202 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.4531P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Extinction correction: SHELXL-2019/2 (Sheldrick 2019), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0025 (4)

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 (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
S1	0.42759 (4)	1.04706 (4)	0.71077 (3)	0.05142 (16)
O1	0.06602 (8)	0.81371 (11)	0.56610 (8)	0.0416 (3)
N2	0.34143 (9)	0.87359 (12)	0.55450 (8)	0.0325 (3)
N1	0.22587 (10)	0.92996 (13)	0.64679 (8)	0.0356 (3)
C13	0.19033 (10)	0.85995 (14)	0.40490 (9)	0.0292 (3)
C3	0.23515 (10)	0.80042 (14)	0.50922 (9)	0.0287 (3)
C7	0.24828 (10)	0.63546 (14)	0.51131 (9)	0.0295 (3)
C2	0.16102 (11)	0.84460 (14)	0.57434 (10)	0.0317 (3)
C1	0.32858 (11)	0.94226 (14)	0.62915 (10)	0.0337 (3)
C8	0.35072 (11)	0.57087 (15)	0.54165 (10)	0.0337 (3)
H8	0.414523	0.629466	0.562886	0.040*
C18	0.20459 (12)	0.78517 (17)	0.32453 (10)	0.0396 (3)
H18	0.236884	0.691312	0.333256	0.047*
C12	0.15565 (12)	0.54770 (16)	0.48046 (12)	0.0390 (3)
H12	0.085017	0.590867	0.459211	0.047*
C10	0.26845 (13)	0.33415 (16)	0.51073 (11)	0.0416 (3)
H10	0.275616	0.231491	0.510549	0.050*
C9	0.36044 (13)	0.42047 (16)	0.54111 (11)	0.0400 (3)
H9	0.430967	0.376892	0.561814	0.048*
C14	0.14038 (12)	0.99562 (16)	0.39013 (11)	0.0391 (3)
H14	0.128113	1.047293	0.444221	0.047*
C17	0.17226 (13)	0.84580 (19)	0.23138 (11)	0.0454 (4)
H17	0.182748	0.793562	0.176805	0.054*
C11	0.16586 (13)	0.39736 (17)	0.48057 (12)	0.0442 (4)
H11	0.102309	0.338169	0.459910	0.053*
C5	0.18677 (15)	0.99957 (17)	0.72403 (11)	0.0437 (4)
H5B	0.248783	1.009702	0.783927	0.052*
H5A	0.130796	0.936822	0.740302	0.052*
C16	0.12491 (12)	0.98171 (19)	0.21774 (11)	0.0447 (4)
H16	0.103796	1.023941	0.154098	0.054*
C15	0.10842 (14)	1.05583 (18)	0.29694 (13)	0.0477 (4)
H15	0.074882	1.148914	0.287611	0.057*
C6	0.13762 (15)	1.14777 (17)	0.69332 (12)	0.0493 (4)
H6A	0.079291	1.139169	0.631694	0.074*
H6C	0.194766	1.213302	0.683826	0.074*
H6B	0.107005	1.186788	0.744561	0.074*
C4	0.53801 (16)	1.0279 (3)	0.65510 (19)	0.0739 (6)
H4C	0.519234	1.078181	0.591672	0.111*
H4B	0.550231	0.924663	0.644994	0.111*

H4A	0.604906	1.070302	0.698209	0.111*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0557 (3)	0.0418 (2)	0.0454 (2)	−0.01332 (17)	−0.00529 (18)	−0.00844 (16)
O1	0.0385 (5)	0.0426 (6)	0.0487 (6)	−0.0066 (4)	0.0205 (4)	−0.0076 (5)
N2	0.0308 (5)	0.0286 (6)	0.0351 (6)	−0.0050 (4)	0.0042 (4)	−0.0001 (5)
N1	0.0449 (6)	0.0318 (6)	0.0299 (6)	−0.0034 (5)	0.0098 (5)	−0.0047 (5)
C13	0.0271 (6)	0.0298 (6)	0.0304 (6)	−0.0048 (5)	0.0075 (5)	0.0000 (5)
C3	0.0279 (6)	0.0279 (6)	0.0299 (6)	−0.0031 (5)	0.0071 (5)	−0.0024 (5)
C7	0.0348 (6)	0.0286 (6)	0.0258 (6)	−0.0027 (5)	0.0096 (5)	−0.0013 (5)
C2	0.0379 (7)	0.0270 (6)	0.0308 (6)	−0.0016 (5)	0.0107 (5)	−0.0002 (5)
C1	0.0385 (7)	0.0264 (6)	0.0312 (7)	−0.0038 (5)	0.0008 (5)	0.0018 (5)
C8	0.0370 (7)	0.0328 (7)	0.0306 (6)	−0.0016 (5)	0.0080 (5)	−0.0013 (5)
C18	0.0423 (8)	0.0423 (8)	0.0350 (7)	0.0047 (6)	0.0121 (6)	−0.0012 (6)
C12	0.0361 (7)	0.0339 (7)	0.0473 (8)	−0.0045 (5)	0.0119 (6)	−0.0053 (6)
C10	0.0604 (9)	0.0275 (7)	0.0385 (7)	−0.0016 (6)	0.0161 (7)	0.0004 (6)
C9	0.0460 (8)	0.0357 (7)	0.0363 (7)	0.0063 (6)	0.0075 (6)	0.0010 (6)
C14	0.0480 (8)	0.0296 (7)	0.0393 (7)	−0.0004 (6)	0.0114 (6)	0.0000 (6)
C17	0.0473 (8)	0.0577 (10)	0.0318 (7)	−0.0036 (7)	0.0120 (6)	−0.0009 (7)
C11	0.0481 (8)	0.0347 (8)	0.0514 (9)	−0.0126 (6)	0.0166 (7)	−0.0069 (7)
C5	0.0641 (10)	0.0384 (8)	0.0314 (7)	−0.0014 (7)	0.0177 (7)	−0.0058 (6)
C16	0.0404 (8)	0.0540 (9)	0.0358 (7)	−0.0114 (7)	0.0037 (6)	0.0126 (7)
C15	0.0531 (9)	0.0372 (8)	0.0500 (9)	0.0012 (7)	0.0093 (7)	0.0116 (7)
C6	0.0661 (10)	0.0375 (8)	0.0469 (9)	−0.0004 (7)	0.0200 (8)	−0.0072 (7)
C4	0.0447 (10)	0.0732 (14)	0.0939 (16)	−0.0214 (9)	0.0023 (10)	−0.0164 (12)

Geometric parameters (Å, º)

S1—C1	1.7455 (14)	C10—C9	1.379 (2)
S1—C4	1.793 (2)	C10—C11	1.381 (2)
O1—C2	1.2116 (16)	C10—H10	0.9500
N2—C1	1.2797 (18)	C9—H9	0.9500
N2—C3	1.4855 (16)	C14—C15	1.385 (2)
N1—C2	1.3723 (17)	C14—H14	0.9500
N1—C1	1.3960 (19)	C17—C16	1.379 (2)
N1—C5	1.4663 (18)	C17—H17	0.9500
C13—C18	1.3837 (19)	C11—H11	0.9500
C13—C14	1.3906 (19)	C5—C6	1.514 (2)
C13—C3	1.5311 (17)	C5—H5B	0.9900
C3—C7	1.5279 (18)	C5—H5A	0.9900
C3—C2	1.5405 (18)	C16—C15	1.377 (2)
C7—C8	1.3851 (19)	C16—H16	0.9500
C7—C12	1.3934 (19)	C15—H15	0.9500
C8—C9	1.391 (2)	C6—H6A	0.9800
C8—H8	0.9500	C6—H6C	0.9800
C18—C17	1.386 (2)	C6—H6B	0.9800

C18—H18	0.9500	C4—H4C	0.9800
C12—C11	1.391 (2)	C4—H4B	0.9800
C12—H12	0.9500	C4—H4A	0.9800

C1—S1—C4	99.25 (8)	C10—C9—H9	119.8
C1—N2—C3	105.96 (11)	C8—C9—H9	119.8
C2—N1—C1	108.04 (11)	C15—C14—C13	120.35 (14)
C2—N1—C5	123.52 (13)	C15—C14—H14	119.8
C1—N1—C5	128.35 (12)	C13—C14—H14	119.8
C18—C13—C14	118.71 (13)	C16—C17—C18	120.18 (14)
C18—C13—C3	121.15 (12)	C16—C17—H17	119.9
C14—C13—C3	120.01 (12)	C18—C17—H17	119.9
N2—C3—C7	111.21 (10)	C10—C11—C12	119.97 (14)
N2—C3—C13	107.85 (10)	C10—C11—H11	120.0
C7—C3—C13	112.61 (10)	C12—C11—H11	120.0
N2—C3—C2	104.58 (10)	N1—C5—C6	112.13 (12)
C7—C3—C2	109.41 (10)	N1—C5—H5B	109.2
C13—C3—C2	110.90 (10)	C6—C5—H5B	109.2
C8—C7—C12	119.06 (13)	N1—C5—H5A	109.2
C8—C7—C3	121.40 (11)	C6—C5—H5A	109.2
C12—C7—C3	119.53 (12)	H5B—C5—H5A	107.9
O1—C2—N1	125.61 (12)	C15—C16—C17	119.58 (14)
O1—C2—C3	129.32 (12)	C15—C16—H16	120.2
N1—C2—C3	105.07 (11)	C17—C16—H16	120.2
N2—C1—N1	116.34 (12)	C16—C15—C14	120.46 (15)
N2—C1—S1	126.07 (11)	C16—C15—H15	119.8
N1—C1—S1	117.58 (10)	C14—C15—H15	119.8
C7—C8—C9	120.20 (13)	C5—C6—H6A	109.5
C7—C8—H8	119.9	C5—C6—H6C	109.5
C9—C8—H8	119.9	H6A—C6—H6C	109.5
C13—C18—C17	120.69 (14)	C5—C6—H6B	109.5
C13—C18—H18	119.7	H6A—C6—H6B	109.5
C17—C18—H18	119.7	H6C—C6—H6B	109.5
C11—C12—C7	120.47 (14)	S1—C4—H4C	109.5
C11—C12—H12	119.8	S1—C4—H4B	109.5
C7—C12—H12	119.8	H4C—C4—H4B	109.5
C9—C10—C11	119.82 (14)	S1—C4—H4A	109.5
C9—C10—H10	120.1	H4C—C4—H4A	109.5
C11—C10—H10	120.1	H4B—C4—H4A	109.5
C10—C9—C8	120.48 (14)		

C1—N2—C3—C7	−117.50 (12)	C3—N2—C1—S1	179.54 (10)
C1—N2—C3—C13	118.57 (12)	C2—N1—C1—N2	−1.10 (16)
C1—N2—C3—C2	0.48 (13)	C5—N1—C1—N2	−177.81 (13)
C18—C13—C3—N2	98.09 (14)	C2—N1—C1—S1	179.61 (9)
C14—C13—C3—N2	−77.78 (14)	C5—N1—C1—S1	2.90 (19)
C18—C13—C3—C7	−24.99 (17)	C4—S1—C1—N2	1.33 (15)
C14—C13—C3—C7	159.15 (12)	C4—S1—C1—N1	−179.47 (13)

C18—C13—C3—C2	−147.96 (12)	C12—C7—C8—C9	0.0 (2)
C14—C13—C3—C2	36.17 (16)	C3—C7—C8—C9	−178.82 (12)
N2—C3—C7—C8	−7.14 (16)	C14—C13—C18—C17	1.6 (2)
C13—C3—C7—C8	114.04 (13)	C3—C13—C18—C17	−174.32 (13)
C2—C3—C7—C8	−122.16 (13)	C8—C7—C12—C11	0.3 (2)
N2—C3—C7—C12	174.01 (12)	C3—C7—C12—C11	179.17 (13)
C13—C3—C7—C12	−64.81 (15)	C11—C10—C9—C8	0.0 (2)
C2—C3—C7—C12	58.99 (15)	C7—C8—C9—C10	−0.2 (2)
C1—N1—C2—O1	−178.57 (13)	C18—C13—C14—C15	−1.7 (2)
C5—N1—C2—O1	−1.7 (2)	C3—C13—C14—C15	174.24 (13)
C1—N1—C2—C3	1.28 (14)	C13—C18—C17—C16	−0.3 (2)
C5—N1—C2—C3	178.18 (12)	C9—C10—C11—C12	0.3 (2)
N2—C3—C2—O1	178.75 (14)	C7—C12—C11—C10	−0.5 (2)
C7—C3—C2—O1	−62.04 (18)	C2—N1—C5—C6	−88.44 (17)
C13—C3—C2—O1	62.76 (18)	C1—N1—C5—C6	87.81 (19)
N2—C3—C2—N1	−1.09 (13)	C18—C17—C16—C15	−1.0 (2)
C7—C3—C2—N1	118.11 (11)	C17—C16—C15—C14	0.9 (2)
C13—C3—C2—N1	−117.09 (11)	C13—C14—C15—C16	0.5 (2)
C3—N2—C1—N1	0.33 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.95	2.49	3.434 (2)	171

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