



1-Ethenyl-2-(methylsulfanyl)-4,4-diphenyl-4,5-dihydro-1*H*-imidazol-5-one (Thiophenytol analogue): synthesis, structure and Hirshfeld surface analysis

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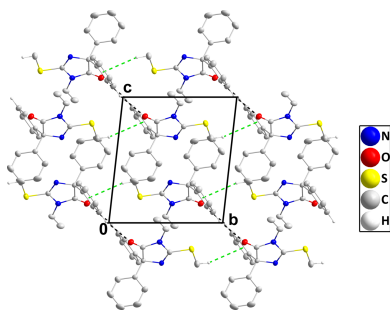
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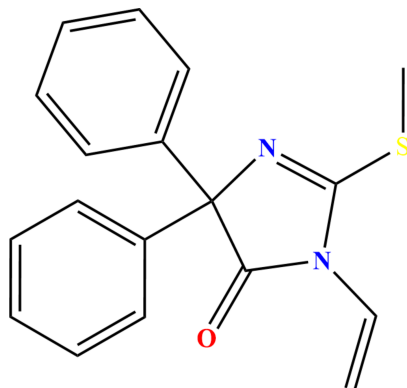
The title molecule, C₁₈H₁₆N₂OS, exhibits a slight ‘ruffling’ of the imidazolone ring, and the lone pair on the tricoordinate nitrogen atom is involved in N→C π-bonding within the ring. Both the methyl group bonded to sulfur and the vinyl substituent lie very close to the plane of the five-membered ring. In the crystal, C—H···O hydrogen bonds form inversion dimers, which are linked into chains extending along the *b*-axis direction by C—H···π(ring) interactions. Hirshfeld surface analysis indicates that H···H interactions account for more than half of the intermolecular contacts, with C—H···π(ring) interactions contributing a further quarter of the total.

1. Chemical context

Heterocycles incorporating both sulfur and nitrogen atoms constitute a class of compounds of great interest in organic and medicinal chemistry, owing to the richness of their physicochemical properties and the diversity of their biological activities (El Moutaouakil Ala Allah *et al.*, 2024a; Ettahiri *et al.*, 2024; Guerrab *et al.*, 2025). Among them, thiohydantoin, a sulfur-containing heterocycle structurally related to hydantoin and characterized by the presence of a thioxo (C=S) group, has emerged as a privileged scaffold in medicinal chemistry (Gupta *et al.*, 2025). Its distinctive electronic and structural features enable a wide range of chemical modifications and promote strong interactions with various biological targets (El Moutaouakil Ala Allah *et al.*, 2024b). Consequently, numerous thiohydantoin derivatives have demonstrated significant pharmacological activities, including antidiabetic (Ala Allah *et al.*, 2025c), anticancer (Mezoughi *et al.*, 2021), and antimicrobial effects (El Moutaouakil Ala Allah *et al.*, 2024c). In addition, some derivatives have shown promising performance as corrosion inhibitors (Ala Allah *et al.*, 2024; AlObaid *et al.*, 2024; El Moutaouakil Ala Allah *et al.*, 2024d). In a continuation of our research on thiohydantoin derivatives (Ramli *et al.*, 2017; Guerrab *et al.*, 2023a,,b, 2022; El Moutaouakil Ala Allah *et al.*, 2024e), we report herein the synthesis of 2-(methylthio)-5,5-diphenyl-3-vinyl-3,5-dihydro-4*H*-imidazol-4-one (Fig. 1) *via* an E2 elimination from 3-(2-bromoethyl)-2-(methylthio)-5,5-diphenyl-3,5-dihydro-4*H*-imidazol-4-one, a secondary halide, under conditions



promoting unimolecular elimination in the presence of diethylamine [(Et)₂NH] as the base and DMF as the solvent.



2. Structural commentary

The dihydroimidazolone ring is essentially planar, with a maximum deviation of 0.035 (1) Å from the mean plane (r.m.s. deviation of the fitted atoms = 0.001 Å). Atom C3 lies 0.035 (1) Å on one side of this plane, while C2 is displaced by 0.034 (1) Å on the opposite side. This slight out-of-plane displacement gives the ring a slight ‘ruffled’ conformation. The mean planes of the C7–C12 and C13–C18 rings are inclined to that of the dihydroimidazolone ring by 70.15 (9) and 66.01 (8)°, respectively. Atoms C4 and C6 both lie close to the plane of the dihydroimidazolone ring, as indicated by the C4–S1–C1–N2 and the C2–N1–C5–C6 torsion angles of –3.4 (2) and –1.8 (3)°, respectively. The sum of the bond angles about N1 is 360° within experimental error, indicating that its lone pair is involved in N→C π-bonding. Although all the bonds to N1 are shorter than expected for formal single bonds, the N1–C2 distance of 1.387 (2) Å is the shortest,

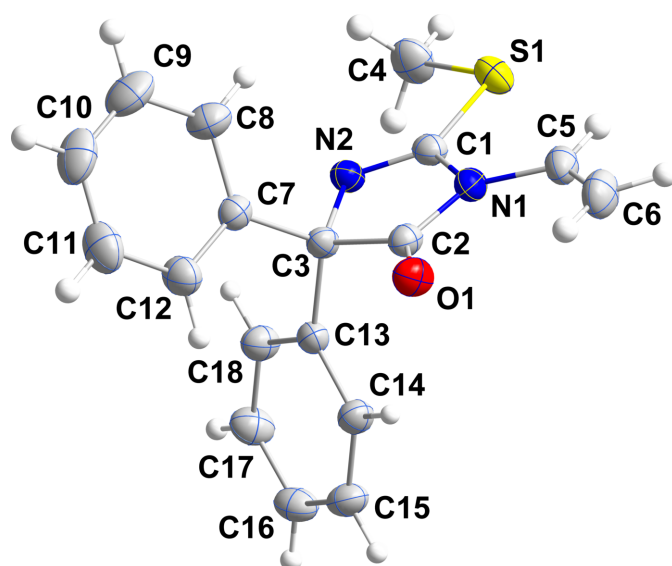


Figure 1
Perspective view of the title molecule with labeling scheme and 30% probability ellipsoids.

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

Cg3 is the centroid of the C13–C18 benzene 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>
C4–H4B···Cg3 ⁱ	0.96	2.90	3.815 (2)	160
C15–H15···O1 ⁱⁱ	0.93	2.53	3.434 (2)	166

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

suggesting that the lone-pair interaction is strongest in this bond.

3. Supramolecular features

In the crystal, inversion dimers are generated by weak C15–H15···O1ⁱⁱ hydrogen bonds and these are connected into chains extending along the *b*-axis direction by C4–H4B···Cg3ⁱ interactions (Table 1; Cg3 is the centroid of the C13–C18 benzene ring). The chains pack with normal van der Waals contacts (Fig. 2).

4. Database survey

A search of the Cambridge Structural Database (CSD, updated to January 2026; Groom *et al.*, 2016) with the search fragment shown in Fig. 3 (*R* = *R*') gave nine hits, all of which are similar to the title compound. One group has *R* = *R*' = Me (YEYYUA; El Moutaouakil Ala Allah *et al.*, 2023), Et (HOPQAI; El Moutaouakil Ala Allah *et al.*, 2024a), *n*-Pr (RIJZIW; Akrad *et al.*, 2018) and benzyl (RAHGUF; Akrad *et al.*, 2017). In the second group, the nitrogen and sulfur atoms are part of an exocyclic ring fused to the dihydroimidazolone ring, with *R*, *R*' = –CH₂CH₂– (DIYRAE; Karolak-Wojciechowska *et al.*, 1985), –CH(CO₂Et)CH₂– (FURFED; Karolak-

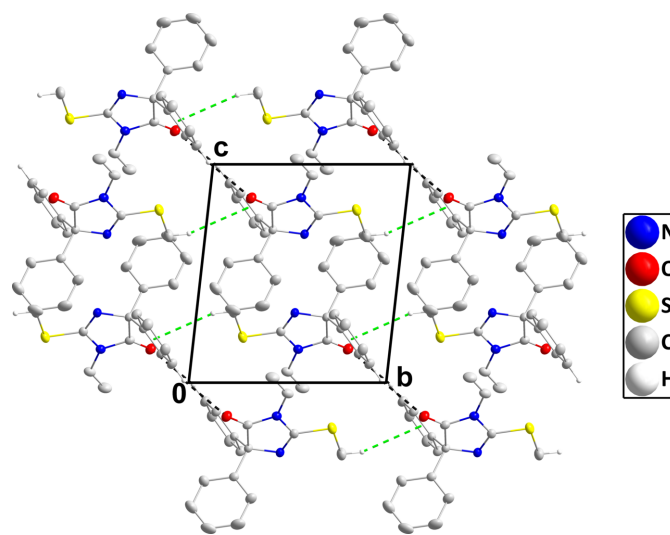


Figure 2
Packing viewed along the *a*-axis direction with C–H···O hydrogen bonds and C–H···π(ring) interactions depicted, respectively, by black and green dashed lines. Hydrogen atoms not involved in these interactions are omitted for clarity.

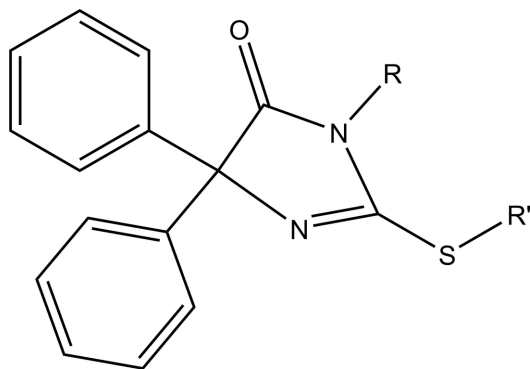


Figure 3
The search fragment used in the database survey.

Wojciechowska & Kieć-Kononowicz, 1987), $-(\text{CH}_2)_3-$ (IMTHZN; Kieć-Kononowicz *et al.*, 1981 and IMTHZN01; Guerrab *et al.*, 2019) and $-(\text{CH}_2)_2\text{O}(\text{CH}_2)_2\text{O}(\text{CH}_2)_2\text{O}(\text{CH}_2)_2-$ (LIGWOR; Guerrab *et al.*, 2023b). In all cases, the sum of the angles about the tri-coordinate nitrogen atom in the five-membered ring is 360° within experimental error, indicating participation of the nitrogen lone pair $\text{N} \rightarrow \text{C} \pi$ -bonding. With the exception of DIYRAE, the $\text{N}-\text{C}$ bond to the carbonyl carbon is the shortest of the three bonds involving this nitrogen atom, as in the title compound; the corresponding distances range from 1.362 (2) Å in FURFED to 1.380 (2) Å in RAHGUF. In DIYRAE, the $\text{N}-\text{C}$ bond to the carbonyl carbon is 1.383 (11) Å, whereas the other endocyclic $\text{N}-\text{C}$ bond is 1.363 (11) Å. The reason for this variation is unclear; however, the associated standard uncertainties are relatively large, so the difference may not be significant. In all examples, the $\text{S}-\text{C}$ bond corresponding to C_4-S_1 in the title molecule lies close to the mean plane of the five-membered ring. The largest torsion angle (corresponding to the $\text{C}_5-\text{S}_1-\text{C}_1-\text{N}_2$ angle in the title molecule) is $\text{C}_5-\text{S}_1-\text{C}_1-\text{N}_1$ in FURFED [-17.41 (15°)]. This is likely due to the constraints imposed by the ring attached to the dihydroimidazolone moiety. For $R = \text{Et}$, $n\text{-Pr}$ and benzyl (Fig. 3), the carbon bonded to the nitrogen atom lies in the plane of the dihydroimidazolone moiety, but the rest of the substituent is rotated well out of this plane. In the remaining derivatives, a similar twist is observed, but only to the extent allowed by the geometry of the pendant ring.

5. Hirshfeld surface analysis

The Hirshfeld surface analysis of the intermolecular interactions in the crystal of the title molecule was performed with *CrystalExplorer* (Spackman *et al.*, 2021). Descriptions of the plots obtained and their interpretations have been previously published (Tan *et al.*, 2019). Fig. 4a shows the d_{norm} surface with several neighboring molecules included. In the lower right of the figure, one of the inversion dimers formed by the $\text{C}-\text{H} \cdots \text{O}$ hydrogen bond listed in Table 1 (red dashed lines) is shown. In the upper right of the figure, the $\text{S}-\text{CH}_3$ group forms a $\text{C}-\text{H} \cdots \pi(\text{ring})$ interaction with the phenyl group directly beneath it. Fig. 4b shows the Hirshfeld surface mapped over the shape-index function; the absence of orange

triangle motifs indicates that significant $\pi-\pi$ stacking interactions are not present. Fig. 5 presents the two-dimensional fingerprint plots for all interactions (a) and those limited to specific interaction types. Fig. 5b shows that $\text{H} \cdots \text{H}$ interactions comprise 54.5% of the total, consistent with the molecule's periphery being dominated by hydrogen atoms. Next, contributing 25.8% of the total, are the $\text{C} \cdots \text{H}/\text{H} \cdots \text{C}$ interactions (Fig. 5c). These appear as diffuse regions with a superimposed pair of blunt peaks. The peaks can be ascribed to the $\text{C}-\text{H} \cdots \pi(\text{ring})$ interactions (Table 1), whereas the diffuse regions represent a range of van der Waals contacts. The $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds are reflected in the $\text{O} \cdots \text{H}/\text{H} \cdots \text{O}$ interactions, which appear as a pair of relatively sharp peaks in Fig. 5d and comprise 6.7% of the total. Finally, the $\text{S} \cdots \text{H}/\text{H} \cdots \text{S}$ interactions, which account for 6.6% of the total, appear in Fig. 5e as a pair of blunt peaks with a superimposed pair of sharper peaks. Although this might suggest $\text{C}-\text{H} \cdots \text{S}$ hydrogen bonding, the $d_e + d_i$ distance of ≈ 3.1 Å indicates that it is simply a normal van der Waals contact.

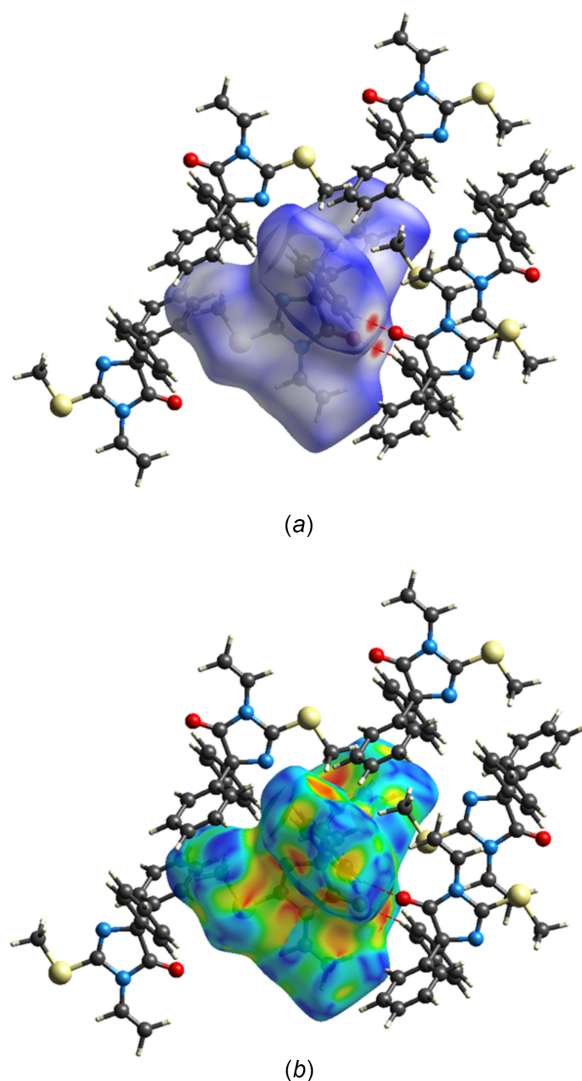
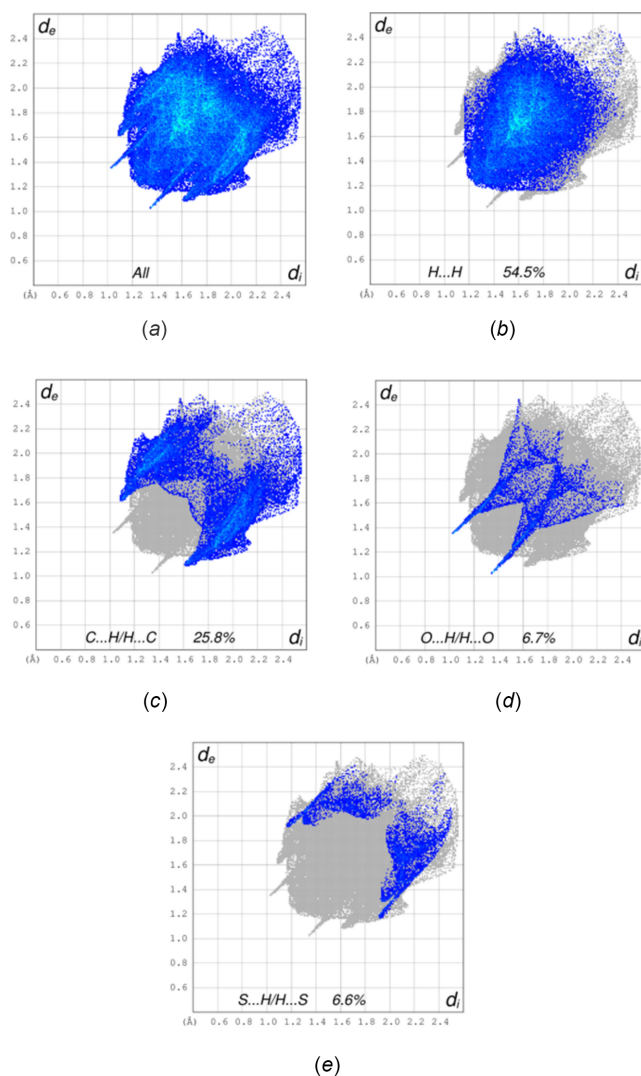


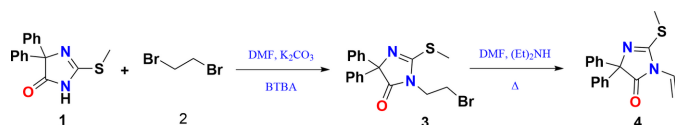
Figure 4
The Hirshfeld d_{norm} surface (a) and the Hirshfeld surface mapped over shape-index (b) showing several added neighboring molecules.


Figure 5

Two-dimensional fingerprint plots showing all intermolecular contacts (a) and those limited to H...H contacts (b), C...H/H...C contacts (c), O...H/H...O contacts (d) and S...H/H...S contacts (e).

6. Synthesis and crystallization

To a solution of 2-(methylthio)-5,5-diphenyl-3,5-dihydro-4H-imidazol-4-one (**1**) (0.5 g, 1.2 mmol) in DMF (10 mL), half an equivalent of 1,2-dibromoethane (**2**) (0.6 mmol) was added in the presence of K_2CO_3 (1.8 mmol) and a catalytic amount of benzyltributylammonium bromide (BTBA, 10%). The reaction mixture was stirred at room temperature for 4h, as described in our previous work (El Moutaouakil Ala Allah *et al.*, 2023; El Moutaouakil Ala Allah *et al.*, 2025b; El Moutaouakil Ala Allah *et al.*, 2024c; El Moutaouakil Ala


Figure 6

Synthesis of the title compound.

Table 2

Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{16}N_2OS$
M_r	308.39
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	295
a, b, c (Å)	8.9481 (3), 9.0321 (2), 10.6253 (3)
α, β, γ (°)	81.333 (1), 69.520 (1), 82.227 (1)
V (Å ³)	792.11 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.21
Crystal size (mm)	0.20 × 0.18 × 0.17
Data collection	
Diffractometer	Bruker D8 Venture PhotonIII
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
T_{min}, T_{max}	0.723, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29667, 3209, 2950
R_{int}	0.036
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.041, 0.111, 1.04
No. of reflections	3209
No. of parameters	212
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, -0.41

Computer programs: *APEX5* (and *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020), *WinGX* (Farrugia, 2012), *publCIF* (Westrip, 2010) and *enCIFer* (Allen *et al.*, 2004).

Allah *et al.*, 2025a). The resulting compound (**3**) was subsequently refluxed in DMF in the presence of diethylamine, affording 2-(methylthio)-5,5-diphenyl-3-vinyl-3,5-dihydro-4H-imidazol-4-one (**4**) via an elimination reaction (Fig. 6).

2-(Methylthio)-5,5-diphenyl-3-vinyl-3,5-dihydro-4H-imidazol-4-one (4) Yield = 68%; m.p. = 391–393K; Appearance: White powder; FT-IR (ATR, cm^{-1}): 3062 (C–H Ar), 2985 (–CH₃), 2852 (C–H Aliphatic), 1728 (C=O); ¹H NMR (500 MHz, CDCl₃): δ ppm 1.24–2.72 (s, 3H, S–CH₃), 5.54 (dd, 2H, –CH₂), 6.80 (m, 1H, CH), 7.20–7.30 (m, 10H, Ar H); ¹³C NMR (125 MHz, CDCl₃): 14.18 (S–CH₃), 76.20 (C–2Ph), 118.22 (–CH₂), 130.14 (CH), 124.20, 126.23, 128.40, 140.62 (C–Ar), 162.57 (C=N), 178.12 (C=O).

7. Refinement details

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 0.93 to 0.99 Å and $U_{iso}(H)$ set to 1.2–1.5 $U_{eq}(C)$.

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supporting information

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1-Ethenyl-2-(methylsulfanyl)-4,4-diphenyl-4,5-dihydro-1*H*-imidazol-5-one (Thiophenytoin analogue): synthesis, structure and Hirshfeld surface analysis

**Abderrazzak El Moutaouakil Ala Allah, Chiara Massera, Joel T. Mague, Abdulsalam Alsubari
and Youssef Ramli**

Computing details

1-Ethenyl-2-(methylsulfanyl)-4,4-diphenyl-4,5-dihydro-1*H*-imidazol-5-one

Crystal data

$C_{18}H_{16}N_2OS$

$M_r = 308.39$

Triclinic, $P\bar{1}$

$a = 8.9481$ (3) Å

$b = 9.0321$ (2) Å

$c = 10.6253$ (3) Å

$\alpha = 81.333$ (1)°

$\beta = 69.520$ (1)°

$\gamma = 82.227$ (1)°

$V = 792.11$ (4) Å³

$Z = 2$

$F(000) = 324$

$D_x = 1.293$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1561 reflections

$\theta = 2.1$ – 26.0 °

$\mu = 0.21$ mm⁻¹

$T = 295$ K

Prismatic, colourless

$0.20 \times 0.18 \times 0.17$ mm

Data collection

Bruker D8 Venture PhotonIII

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi & ω scan

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.723$, $T_{\max} = 0.745$

29667 measured reflections

3209 independent reflections

2950 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 2.1$ °

$h = -11 \rightarrow 10$

$k = -11 \rightarrow 10$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.111$

$S = 1.04$

3209 reflections

212 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 0.2157P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.23$ e Å⁻³

$\Delta\rho_{\min} = -0.41$ e Å⁻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>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.30806 (14)	0.53530 (14)	0.15287 (12)	0.0456 (3)
N2	0.41715 (14)	0.49764 (13)	0.32000 (12)	0.0437 (3)
O1	0.21905 (14)	0.78849 (13)	0.15425 (12)	0.0576 (3)
S1	0.42204 (5)	0.24750 (4)	0.20897 (5)	0.05768 (16)
C1	0.38291 (16)	0.43747 (16)	0.23382 (14)	0.0438 (3)
C2	0.28861 (16)	0.67747 (16)	0.19379 (14)	0.0441 (3)
C3	0.37180 (16)	0.66082 (15)	0.30036 (13)	0.0403 (3)
C4	0.5259 (3)	0.1856 (2)	0.3269 (2)	0.0708 (5)
H4A	0.611516	0.247781	0.309316	0.106*
H4B	0.569044	0.083047	0.317336	0.106*
H4C	0.452827	0.192825	0.417262	0.106*
C5	0.2620 (2)	0.4928 (2)	0.04959 (16)	0.0565 (4)
C6	0.1893 (3)	0.5785 (3)	−0.0238 (2)	0.0745 (5)
C7	0.25522 (16)	0.71697 (16)	0.43112 (14)	0.0437 (3)
C8	0.1613 (2)	0.6187 (2)	0.53057 (18)	0.0634 (4)
H8	0.169625	0.517770	0.518152	0.076*
C9	0.0550 (2)	0.6700 (3)	0.6487 (2)	0.0846 (6)
H9	−0.007131	0.602963	0.715446	0.101*
C10	0.0403 (2)	0.8174 (3)	0.6681 (2)	0.0848 (7)
H10	−0.031074	0.850703	0.748042	0.102*
C11	0.1310 (2)	0.9168 (3)	0.5695 (2)	0.0788 (6)
H11	0.120184	1.017900	0.582140	0.095*
C12	0.2388 (2)	0.8667 (2)	0.45097 (19)	0.0614 (4)
H12	0.300294	0.934462	0.384488	0.074*
C13	0.52751 (16)	0.73904 (15)	0.24654 (13)	0.0401 (3)
C14	0.56481 (18)	0.84435 (17)	0.13351 (15)	0.0482 (3)
H14	0.491099	0.874571	0.088924	0.058*
C15	0.7120 (2)	0.90521 (19)	0.08628 (17)	0.0578 (4)
H15	0.736437	0.975100	0.009807	0.069*
C16	0.82111 (19)	0.86263 (19)	0.15194 (19)	0.0597 (4)
H16	0.919585	0.902990	0.120003	0.072*
C17	0.7836 (2)	0.7593 (2)	0.26591 (19)	0.0612 (4)
H17	0.856806	0.730985	0.311200	0.073*
C18	0.63817 (19)	0.69766 (18)	0.31316 (16)	0.0525 (4)
H18	0.614243	0.628148	0.389912	0.063*
H6A	0.169 (3)	0.530 (3)	−0.092 (2)	0.090 (7)*
H6B	0.151 (3)	0.684 (3)	−0.007 (3)	0.103 (8)*
H5	0.293 (3)	0.386 (3)	0.034 (3)	0.103 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0450 (6)	0.0517 (7)	0.0435 (6)	-0.0105 (5)	-0.0168 (5)	-0.0055 (5)
N2	0.0481 (6)	0.0381 (6)	0.0467 (6)	-0.0065 (5)	-0.0182 (5)	-0.0020 (5)
O1	0.0607 (7)	0.0557 (6)	0.0628 (7)	-0.0048 (5)	-0.0336 (5)	0.0049 (5)
S1	0.0605 (3)	0.0467 (2)	0.0703 (3)	-0.00652 (17)	-0.0231 (2)	-0.01581 (18)
C1	0.0400 (7)	0.0441 (7)	0.0459 (7)	-0.0090 (5)	-0.0112 (6)	-0.0040 (6)
C2	0.0416 (7)	0.0508 (8)	0.0410 (7)	-0.0099 (6)	-0.0157 (6)	0.0015 (6)
C3	0.0446 (7)	0.0379 (6)	0.0406 (7)	-0.0057 (5)	-0.0181 (6)	0.0001 (5)
C4	0.0841 (13)	0.0495 (9)	0.0846 (13)	0.0050 (9)	-0.0378 (11)	-0.0119 (9)
C5	0.0525 (9)	0.0746 (11)	0.0476 (8)	-0.0166 (8)	-0.0166 (7)	-0.0137 (7)
C6	0.0723 (12)	0.1042 (17)	0.0591 (11)	-0.0116 (11)	-0.0334 (9)	-0.0147 (11)
C7	0.0401 (7)	0.0504 (8)	0.0422 (7)	-0.0038 (6)	-0.0170 (6)	-0.0022 (6)
C8	0.0548 (9)	0.0658 (10)	0.0592 (10)	-0.0092 (8)	-0.0089 (8)	0.0032 (8)
C9	0.0618 (11)	0.1100 (18)	0.0605 (11)	-0.0099 (11)	0.0017 (9)	0.0029 (11)
C10	0.0556 (11)	0.130 (2)	0.0620 (11)	0.0081 (12)	-0.0082 (9)	-0.0347 (12)
C11	0.0651 (11)	0.0857 (14)	0.0867 (14)	0.0062 (10)	-0.0188 (10)	-0.0414 (12)
C12	0.0581 (9)	0.0581 (9)	0.0646 (10)	-0.0058 (7)	-0.0128 (8)	-0.0154 (8)
C13	0.0427 (7)	0.0388 (6)	0.0394 (6)	-0.0043 (5)	-0.0138 (5)	-0.0060 (5)
C14	0.0512 (8)	0.0468 (8)	0.0465 (7)	-0.0069 (6)	-0.0178 (6)	0.0004 (6)
C15	0.0584 (9)	0.0523 (9)	0.0549 (9)	-0.0137 (7)	-0.0101 (7)	0.0039 (7)
C16	0.0462 (8)	0.0554 (9)	0.0734 (11)	-0.0132 (7)	-0.0123 (8)	-0.0062 (8)
C17	0.0512 (9)	0.0627 (10)	0.0768 (11)	-0.0098 (7)	-0.0312 (8)	-0.0013 (8)
C18	0.0529 (8)	0.0545 (8)	0.0538 (8)	-0.0114 (7)	-0.0247 (7)	0.0047 (7)

Geometric parameters (Å, °)

N1—C2	1.3868 (19)	C8—C9	1.384 (3)
N1—C1	1.4082 (19)	C8—H8	0.9300
N1—C5	1.4170 (19)	C9—C10	1.360 (3)
N2—C1	1.2724 (18)	C9—H9	0.9300
N2—C3	1.4782 (17)	C10—C11	1.371 (4)
O1—C2	1.2068 (18)	C10—H10	0.9300
S1—C1	1.7452 (14)	C11—C12	1.387 (3)
S1—C4	1.792 (2)	C11—H11	0.9300
C2—C3	1.5386 (18)	C12—H12	0.9300
C3—C7	1.5267 (19)	C13—C14	1.385 (2)
C3—C13	1.5344 (18)	C13—C18	1.390 (2)
C4—H4A	0.9600	C14—C15	1.392 (2)
C4—H4B	0.9600	C14—H14	0.9300
C4—H4C	0.9600	C15—C16	1.372 (2)
C5—C6	1.291 (3)	C15—H15	0.9300
C5—H5	0.99 (3)	C16—C17	1.382 (3)
C6—H6A	0.98 (2)	C16—H16	0.9300
C6—H6B	0.99 (3)	C17—C18	1.382 (2)
C7—C12	1.381 (2)	C17—H17	0.9300
C7—C8	1.381 (2)	C18—H18	0.9300

C2—N1—C1	107.34 (11)	C7—C8—H8	119.9
C2—N1—C5	127.43 (14)	C9—C8—H8	119.9
C1—N1—C5	125.23 (14)	C10—C9—C8	120.7 (2)
C1—N2—C3	107.02 (11)	C10—C9—H9	119.6
C1—S1—C4	98.78 (8)	C8—C9—H9	119.6
N2—C1—N1	115.82 (13)	C9—C10—C11	119.80 (18)
N2—C1—S1	125.42 (11)	C9—C10—H10	120.1
N1—C1—S1	118.76 (11)	C11—C10—H10	120.1
O1—C2—N1	126.56 (13)	C10—C11—C12	120.1 (2)
O1—C2—C3	128.33 (14)	C10—C11—H11	120.0
N1—C2—C3	105.10 (11)	C12—C11—H11	120.0
N2—C3—C7	111.22 (11)	C7—C12—C11	120.39 (18)
N2—C3—C13	107.03 (11)	C7—C12—H12	119.8
C7—C3—C13	112.69 (11)	C11—C12—H12	119.8
N2—C3—C2	104.32 (11)	C14—C13—C18	118.84 (13)
C7—C3—C2	109.81 (11)	C14—C13—C3	123.49 (12)
C13—C3—C2	111.43 (11)	C18—C13—C3	117.64 (12)
S1—C4—H4A	109.5	C13—C14—C15	120.39 (14)
S1—C4—H4B	109.5	C13—C14—H14	119.8
H4A—C4—H4B	109.5	C15—C14—H14	119.8
S1—C4—H4C	109.5	C16—C15—C14	120.35 (15)
H4A—C4—H4C	109.5	C16—C15—H15	119.8
H4B—C4—H4C	109.5	C14—C15—H15	119.8
C6—C5—N1	126.82 (19)	C15—C16—C17	119.49 (15)
C6—C5—H5	119.8 (15)	C15—C16—H16	120.3
N1—C5—H5	113.4 (15)	C17—C16—H16	120.3
C5—C6—H6A	115.8 (14)	C18—C17—C16	120.60 (15)
C5—C6—H6B	121.4 (15)	C18—C17—H17	119.7
H6A—C6—H6B	123 (2)	C16—C17—H17	119.7
C12—C7—C8	118.82 (15)	C17—C18—C13	120.31 (14)
C12—C7—C3	120.90 (13)	C17—C18—H18	119.8
C8—C7—C3	120.26 (14)	C13—C18—H18	119.8
C7—C8—C9	120.17 (19)		
C3—N2—C1—N1	-3.01 (16)	N2—C3—C7—C8	-23.74 (18)
C3—N2—C1—S1	176.66 (10)	C13—C3—C7—C8	-143.93 (14)
C2—N1—C1—N2	-1.21 (16)	C2—C3—C7—C8	91.21 (16)
C5—N1—C1—N2	178.98 (13)	C12—C7—C8—C9	-1.1 (3)
C2—N1—C1—S1	179.09 (9)	C3—C7—C8—C9	-179.58 (16)
C5—N1—C1—S1	-0.71 (19)	C7—C8—C9—C10	0.5 (3)
C4—S1—C1—N2	-3.39 (15)	C8—C9—C10—C11	0.4 (3)
C4—S1—C1—N1	176.27 (12)	C9—C10—C11—C12	-0.8 (3)
C1—N1—C2—O1	-174.50 (14)	C8—C7—C12—C11	0.7 (3)
C5—N1—C2—O1	5.3 (2)	C3—C7—C12—C11	179.19 (16)
C1—N1—C2—C3	4.63 (14)	C10—C11—C12—C7	0.2 (3)
C5—N1—C2—C3	-175.57 (13)	N2—C3—C13—C14	130.00 (14)
C1—N2—C3—C7	123.87 (12)	C7—C3—C13—C14	-107.43 (15)

C1—N2—C3—C13	-112.64 (12)	C2—C3—C13—C14	16.55 (18)
C1—N2—C3—C2	5.56 (14)	N2—C3—C13—C18	-47.95 (16)
O1—C2—C3—N2	172.92 (14)	C7—C3—C13—C18	74.61 (16)
N1—C2—C3—N2	-6.19 (13)	C2—C3—C13—C18	-161.41 (13)
O1—C2—C3—C7	53.65 (19)	C18—C13—C14—C15	1.2 (2)
N1—C2—C3—C7	-125.46 (12)	C3—C13—C14—C15	-176.70 (14)
O1—C2—C3—C13	-71.94 (18)	C13—C14—C15—C16	-0.6 (2)
N1—C2—C3—C13	108.96 (12)	C14—C15—C16—C17	-0.3 (3)
C2—N1—C5—C6	-1.8 (3)	C15—C16—C17—C18	0.7 (3)
C1—N1—C5—C6	177.93 (17)	C16—C17—C18—C13	-0.1 (3)
N2—C3—C7—C12	157.80 (14)	C14—C13—C18—C17	-0.9 (2)
C13—C3—C7—C12	37.61 (18)	C3—C13—C18—C17	177.16 (15)
C2—C3—C7—C12	-87.25 (16)		

Hydrogen-bond geometry (Å, °)

Cg3 is the centroid of the C13–C18 benzene 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>
C4—H4 <i>B</i> ... <i>Cg3</i> ⁱ	0.96	2.90	3.815 (2)	160
C15—H15...O1 ⁱⁱ	0.93	2.53	3.434 (2)	166

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