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Synthesis, crystal structure and Hirshfeld surface analysis of 3-[5-(4-chlorophenyl)-2-sulfanylidene-1,3,4-oxadiazol-3-yl]-3-(4-methylphenyl)-1-(thiophen-2-yl)propan-1-one

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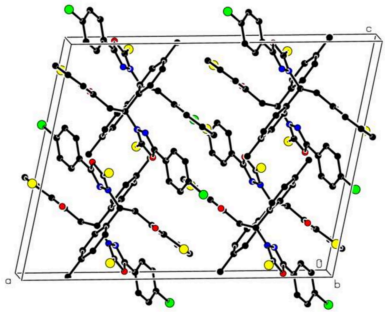
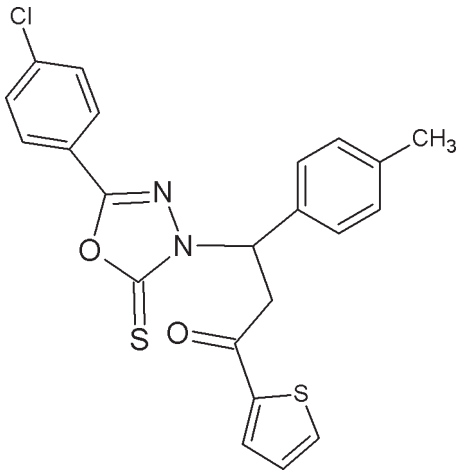
The title thiophene-chalcone derivative, $C_{22}H_{17}ClN_2O_2S_2$, contains a planar oxadiazole, a thiophene and two phenyl rings. The dihedral angle between the oxadiazole and thiophene rings is 27.45 (10)°, and they are oriented with respect to the chlorophenyl and methylphenyl rings at 22.61 (10), 67.07 (8) and 49.16 (10), 87.22 (8)°, respectively, while the phenyl rings are oriented at 51.78 (9)°. In the crystal, π–π stacking interactions and C—H···π(ring) interactions help to consolidate the packing. Hirshfeld surface analysis revealed that the most important contributions to the crystal packing are from H···H (31.6%), H···C/C···H (20.0%), H···S/S···H (14.2%) and H···O/O···H (9.5%) interactions.

1. Chemical context

Oxadiazole is an important structural motif in medicinal chemistry for its role as a pharmacophore and a ligand-binding scaffold (Boström *et al.*, 2012). Among its four isomeric forms, the 1,3,4-oxadiazole ring has attracted considerable attention owing to its broad spectrum of biological activities (Salahuddin *et al.*, 2017; Patel *et al.*, 2014). Numerous 1,3,4- and 1,2,4-oxadiazole derivatives have been reported to exhibit antibacterial, anti-inflammatory, antitubercular, anti-HIV, antifungal, cathepsin K inhibitory, monoamine oxidase inhibitory, antidiabetic, tyrosinase inhibitory, antioxidant and anticancer activities (Palaska *et al.*, 2002; Kadi *et al.*, 2007; Alisi *et al.*, 2020).

In recent years, thiophene-containing chalcone derivatives have emerged as an important class of compounds because of their extended π-conjugated systems and promising applications in medicinal and materials chemistry (Shalaby *et al.*, 2023). Adding heterocyclic moieties to the chalcone scaffold is a well-established approach for modulating molecular geometry and physicochemical properties. In this context, the integration of a 1,3,4-oxadiazole ring with a thiophene-chalcone framework generates conjugated molecular systems of significant structural and potential biological interest. As part of our ongoing research on heterocyclic compounds, the title thiophene-chalcone derivative containing a 1,3,4-oxadiazole unit was synthesized and its crystal structure was elucidated to investigate its molecular conformation and intermolecular interactions governing the crystal packing. Herein, we report the molecular and crystal structures together with a Hirshfeld surface (HS) analysis of the title compound.





2. Structural commentary

The title thiophene-chalcone derivative contains a planar oxadiazole, a thiophene and two phenyl rings (Fig. 1). The phenyl [*A* (C1–C6) and *D* (C16–C21)], oxadiazole [*B* (O1/N1/N2/C7/C8)], and thiophene [*C* (S2/C12–C15)] rings are oriented at dihedral angles of *A*/*B* = 22.61 (10)°, *A*/*C* = 49.16 (10)°, *A*/*D* = 51.78 (9)°, *B*/*C* = 27.45 (10)°, *B*/*D* = 67.07 (8)° and *C*/*D* = 87.22 (8)°. The chlorine atom Cl1 is displaced by −0.0389 (11) Å from the plane of the phenyl ring *A*. Atoms C22 and C9 are only −0.003 (4) Å and −0.002 (3) Å away from phenyl ring *D*. Atoms S1 and C9 are −0.0433 (9) Å and 0.002 (3) Å distant from the oxadiazole, *B*, ring plane, while atom C11 resides 0.016 (3) Å above the thiophene, *C*, ring plane. The specified atoms are, hence, essentially coplanar with the planes of the rings they are attached to. The bond lengths (Allen *et al.*, 1987) and angles are all within normal ranges.

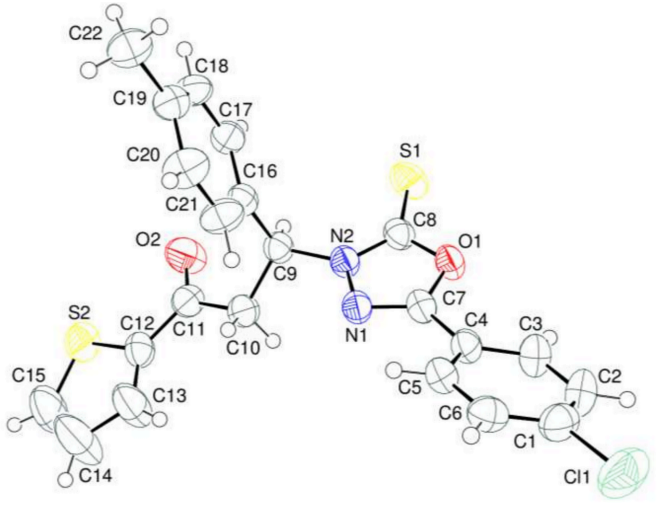


Figure 1
The asymmetric unit with atom-numbering scheme and 50% probability ellipsoids.

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

*Cg*3 and *Cg*4 are the centroids of the C1–C6 and C16–C21 rings.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···*Cg*3^{i}	0.93	2.83	3.726 (3)	164
C22—H22*B*···*Cg*4^{ii}	0.96	2.92	3.671 (4)	136

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

3. Supramolecular features

In the crystal, the thiophene-to-thiophene contacts form pairs, which are arranged along the *c*-axis direction, and adjacent pairs are also essentially arranged in front and behind in the *a*-axis direction, albeit slightly displaced with regard to the *b*-axis direction. The chlorophenyl-to-chlorophenyl contacts also form pairs with contacts arranged along the *a*-axis direction. However, none of these pairs has further contacts that would extend into columns, ribbons or layers (Fig. 2). The π–π stacking interactions involve parallel chlorophenyl rings *A* and approximately parallel thiophene rings *C*. The centroid-to-centroid distances are 3.6612 (18) Å [dihedral angle = 0.00 (16)° slippage = 1.466 Å] and 3.844 (3) Å [dihedral angle = 2.0 (2)°; slippage = 0.871 Å], respectively. Together with the two C—H···π(ring) interactions (Table 1), these contacts help consolidate the overall packing.

The intermolecular interactions in the crystal were further visualized through a Hirshfeld surface (HS) analysis using *CrystalExplorer* 17.5 (Spackman *et al.*, 2021). Fig. 3 shows the Hirshfeld surface for the title molecule plotted over $d_{\rm norm}$. The white surface indicates contacts with distances equal to the sum of van der Waals radii, and the red and blue colours indicate distances shorter and longer than the van der Waals radii, respectively. The π–π stackings and the two C—H···π(ring) interactions are indicated in Fig. 4*a*,*b* by the presence of adjacent red and blue triangles, and Fig. 4*c*,*d* by the presence of red π-holes, respectively.

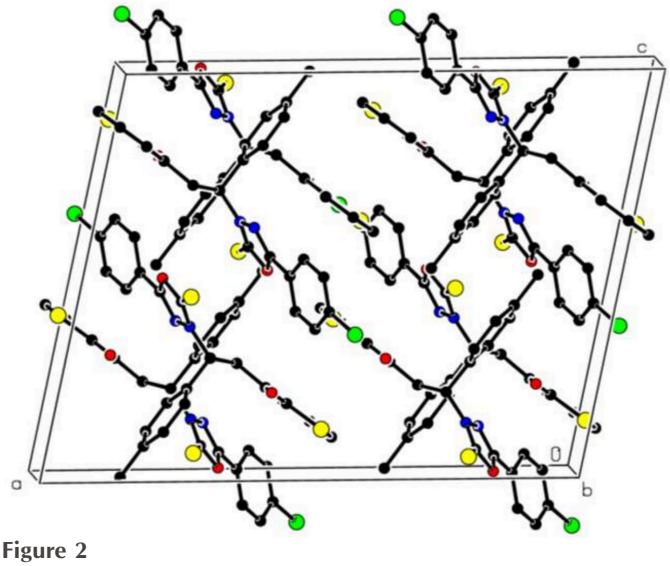


Figure 2
A partial packing diagram viewed down the *b*–axis direction.

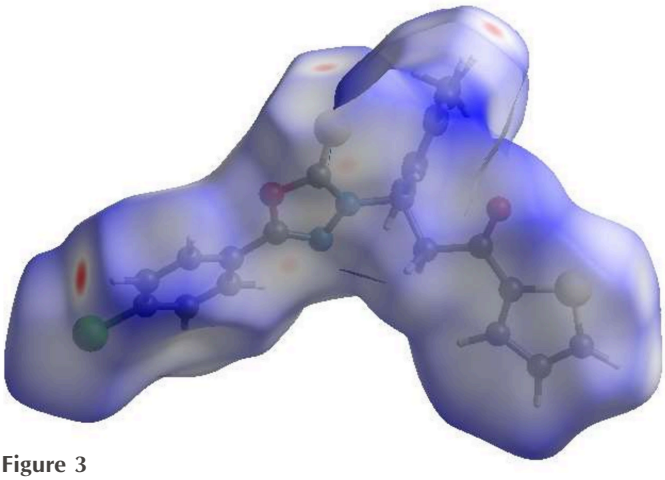


Figure 3
View of the three-dimensional Hirshfeld surface for the title molecule plotted over d_{norm} in the range from −0.2794 to 1.6393 a.u.

The overall two-dimensional fingerprint plot is shown in Fig. 5*a* and those delineated into H···H, H···C/C···H, H···S/S···H, H···O/O···H, H···Cl/Cl···H, C···C, C···Cl/Cl···C, C···S/S···C, O···S/S···O, H···N/N···H, Cl···Cl, O···Cl/Cl···O, N···Cl/Cl···N, N···S/S···N, C···O/O···C, O···O, N···O/O···N and C···N/N···C interactions are illustrated in Fig. 5(*b*)–(*t*), respectively. According to the two-dimensional fingerprint plots the H···H, H···C/C··· H, H···S/S···H and H···O/O···H contacts make the most significant contributions to the Hirshfeld surface, at 31.6%, 20.0%, 14.2% and 9.5%, respectively (Fig. 5).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.01, updated February 2026; Groom *et al.*, 2016) revealed that the crystal structure of the title compound has not been reported previously. However, with the exclusion of

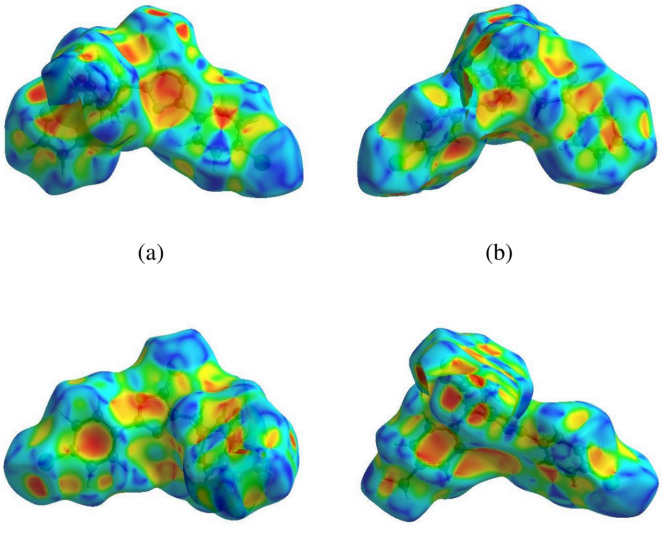


Figure 4
Four orientations of the shape-index showing (*a*) and (*b*) the π–π and (*c*) and (*d*) the C—H···π(ring) interactions.

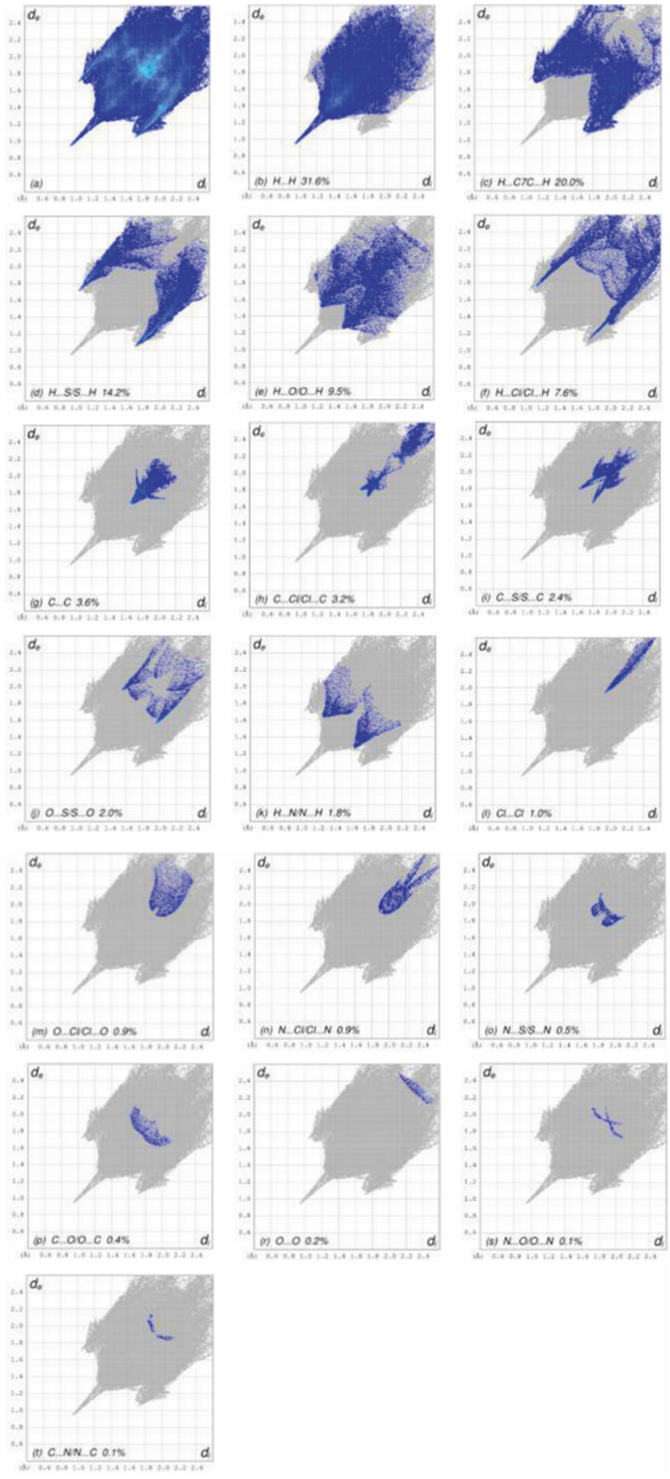


Figure 5
The full two-dimensional fingerprint plots for the title molecule, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···C/C···H, (*d*) H···S/S···H, (*e*) H···O/O···H, (*f*) H···Cl/Cl···H, (*g*) C···C, (*h*) C···Cl/Cl···C, (*i*) C···S/S···C, (*j*) O···S/S···O, (*k*) H···N/N···H, (*l*) Cl···Cl, (*m*) O···Cl/Cl···O, (*n*) N···Cl/Cl···N, (*o*) N···S/S···N, (*p*) C···O/O···C, (*r*) O···O, (*s*) N···O/O···N and (*t*) C···N/N··· C interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

metal containing structures, ten structurally related compounds containing both thiophene and 1,3,4-oxadiazole-2(3*H*)-thione moieties were identified. These are *N*-[2-(2-thienyl)-1-(5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)vinyl]-benzamide (CSD refcode ENOPEE; Sharma *et al.*, 2016), 5-(2-thienyl)-1,3,4-oxadiazole-2(3*H*)-thione (FUSDII; Burcu Arslan *et al.*, 2014), *N*-[1-(5-sulfanylidene-4,5-dihydro-1,3,4-oxadiazol-2-yl)-2-(2-thienyl)vinyl]acetamide (HAJHAF; Karanth *et al.*, 2019), 4-methyl-*N*-[1-(5-sulfanylidene-4,5-dihydro-1,3,4-oxadiazol-2-yl)-2-(thiophen-2-yl)ethenyl]benzamide (HAJHOT; Karanth *et al.*, 2019), 3-[(4-phenylpiperazin-1-yl)methyl]-5-(2-thienyl)-1,3,4-oxadiazole-2(3*H*)-thione (IDOBUA; El-Emam *et al.*, 2013), 3-[(4-phenylpiperidin-1-yl) methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3*H*)-thione (MURSAX; Al-Wahaibi *et al.*, 2025), 3-{[4-(4-fluorophenyl)-piperazin-1-yl]methyl}-5-(2-thienyl)-1,3,4-oxadiazole-2(3*H*)-thione (MUXBAK; Al-Omary *et al.*, 2015*a*), 3-{[4-(2-methoxyphenyl)piperazin-1-yl]methyl}-5-(2-thienyl)-1,3,4-oxadiazole-2(3*H*)-thione (NUZJUP; Al-Alshaikh *et al.*, 2016), 3-[(4-benzylpiperazin-1-yl)methyl]-5-(2-thienyl)-1,3,4-oxadiazole-2(3*H*)-thione (VUBYUO; Al-Omary *et al.*, 2015*b*), and 3-{[methyl(phenyl)amino]methyl}-5-(2-thienyl)-1,3,4-oxadiazole-2(3*H*)-thione (ZAPJIL; El-Emam *et al.*, 2012). Notably, in only three of these structures are the thiophene and oxadiazole moieties not directly linked to each other (ENOPEE, HAJHAF, HAJHOT). Two of these molecules have only the two planar ring systems which comprised the search criteria (FUSDII and HAJHAF), the other eight all have a single additional phenyl ring while none consists of four planar ring systems as the title compound does.

Further thiophene-bearing molecules with structural features resembling those of the title compound include (*E*)-1-(2-aminophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (AFAXUC; Chantrapromma *et al.*, 2013), 1-(4-aminophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (ROTNUN; da Silva *et al.*, 2024), 1-[3-(4-methoxy- phenyl)sydnon-4-yl]-3-(thiophen-2-yl)prop-2-en-1-one (EVAWIH; Shih, 2004), (*E*)-1-(1*H*-pyrrol-2-yl)-3-(thiophen-2-yl) prop-2-en-1-one (RUFLEM; Sweeting *et al.*, 2020), (2*E*)-1-(4-bromophenyl)-3-(thiophen-2-yl)prop-2-en-1-one (GENXED01; Arshad *et al.*, 2017) and 1-(4-methoxyphenyl)-3-(thiophen-2-yl)prop-2-en-1-one (ZOVPOS; Pugh *et al.*, 2019). In addition, compounds incorporating related 1,3,4-oxadiazole frameworks were also found, including 4-hydroxy-3-{[5-(pyridin-3-yl)-1,3,4-oxadiazol-2-yl] sulfanyl}pent-3-en-2-one (CARJIS; Zhang *et al.*, 2021), 5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-ylmethanone (DIPGUI; Bhukta *et al.*, 2023) and 1-(4-chlorophenyl)-2-{[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]sulfanyl}ethan-1-one (GAVMOI; Kumar *et al.*, 2017).

5. Synthesis and crystallization

Methyl 4-chlorobenzoate (15 ml, 0.10 mol) was refluxed with hydrazine hydrate (6 ml, 0.12 mol) in ethanol (10 ml) for 4 h. The reaction mixture was cooled and poured into ice-cold water. The resulting solid was filtered, washed with water and dried to afford 4-chlorobenzohydrazide (91%, m.p. 428 K). 4-Chlorobenzohydrazide (3.41 g, 0.02 mol) was then treated with KOH (0.02 mol) and carbon disulfide (0.04 mol) in ethanol under reflux for 4 h. The reaction mixture was cooled, acidified with dilute HCl, and the precipitated solid was filtered, washed with water, and recrystallized from ethanol to furnish 5-(4-chlorophenyl)-1,3,4-oxadiazole-2-thiol (83%, m.p. 503 K). Subsequently, 5-(4-chlorophenyl)-1,3,4-oxadiazole-2-thiol was refluxed with the (2*Z*)-3-(4-methylphenyl)-1-(thiophen-2-yl)prop-2-en-1-one in ethanol for 4 h. After completion of the reaction, the mixture was cooled and poured into ice-cold water. The precipitated product was filtered, washed thoroughly with water, dried, and recrystallized from ethanol to afford 3-[5-(4-chlorophenyl)-2-thioxo-1,3,4-oxadiazol-3(2*H*)-yl]-3-(4-methylphenyl)-1-(thiophen-2-yl) propan-1-one as a pure solid in 80% yield (m.p. 433 K). IR (KBr) cm^{-1}: 1645 (C═O str.), 1594 (C═N str.), 1214 (C═S str.) and 3069 (Ar. C—H str.).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{17}ClN_2O_2S_2$
M_r	440.94
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	300
a, *b*, *c* (Å)	20.7798 (3), 13.1963 (4), 16.1047 (4)
β (°)	102.440 (3)
V (Å^3)	4312.49 (19)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.39
Crystal size (mm)	0.35 × 0.25 × 0.18
Data collection	
Diffractometer	Bruker D8 Venture Diffractometer
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	53818, 3823, 2660
R_{int}	0.117
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.133, 1.06
No. of reflections	3823
No. of parameters	263
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.34

Computer programs: *APEX4*, *SAINT* and *XPREP* (Bruker, 2021), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *ORTEP-3 for Windows* and *WinGX* publication routines (Farrugia, 2012).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound hydrogen-atom positions were calculated geometrically at distances of 0.93 Å (for aromatic CH), 0.98 Å (for methine CH), 0.97 Å (for methylene CH) and 0.96 Å (for methyl CH) and refined using a riding model by applying the constraint of $U_{iso}(H) = k \times U_{eq}(C)$, where k = 1.5 for methyl H atoms *and* k = 1.2 for the other H atoms. Four reflections, 0 2 0, −2 0 2, 0 0 2 and −1 1 2, were omitted, the first three being affected by the beam stop and the fourth being a clear outlier.

Acknowledgements

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supporting information

Acta Cryst. (2026). E**82** [https://doi.org/10.1107/S2056989026008819]

Synthesis, crystal structure and Hirshfeld surface analysis of 3-[5-(4-chlorophenyl)-2-sulfanylidene-1,3,4-oxadiazol-3-yl]-3-(4-methylphenyl)-1-(thiophen-2-yl)propan-1-one

Shailakshi Jain, Sharatha Kumar and Tuncer Hökelek

Computing details

3-[5-(4-Chlorophenyl)-2-sulfanylidene-1,3,4-oxadiazol-3-yl]-3-(4-methylphenyl)-1-(thiophen-2-yl)propan-1-one

Crystal data

$C_{22}H_{17}ClN_2O_2S_2$
$M_r = 440.94$
Monoclinic, $C2/c$
$a = 20.7798$ (3) Å
$b = 13.1963$ (4) Å
$c = 16.1047$ (4) Å
$\beta = 102.440$ (3)°
$V = 4312.49$ (19) Å^3
$Z = 8$
$F(000) = 1824$
$D_x = 1.358$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9893 reflections
$\theta = 2.9$–24.4°
$\mu = 0.39$ mm^{-1}
$T = 300$ K
Block, colourless
0.35 × 0.25 × 0.18 mm

Data collection

Bruker D8 Venture Diffractometer
φ and ω scans
53818 measured reflections
3823 independent reflections
2660 reflections with $I > 2\sigma(I)$
$R_{int} = 0.117$
$\theta_{max} = 25.1°$, $\theta_{min} = 3.4°$
$h = -24\rightarrow24$
$k = -15\rightarrow15$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.133$
$S = 1.06$
3823 reflections
263 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 5.5114P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.02304 (5)	0.68488 (8)	0.36140 (7)	0.0940 (4)
S1	0.21099 (4)	0.09611 (6)	0.55083 (6)	0.0646 (3)
S2	0.51040 (4)	0.33068 (8)	0.88521 (6)	0.0716 (3)
O1	0.15497 (9)	0.27611 (14)	0.50923 (12)	0.0492 (5)
O2	0.40086 (11)	0.20490 (18)	0.79037 (17)	0.0766 (7)
N1	0.19842 (11)	0.37647 (17)	0.61720 (14)	0.0444 (6)
N2	0.22459 (11)	0.27964 (17)	0.62889 (14)	0.0433 (6)
C1	0.03143 (15)	0.5946 (3)	0.4151 (2)	0.0606 (9)
C2	0.04901 (17)	0.5143 (3)	0.3706 (2)	0.0698 (10)
H2	0.032596	0.509239	0.312306	0.084*
C3	0.09082 (16)	0.4415 (3)	0.41243 (19)	0.0586 (8)
H3	0.102859	0.386888	0.382601	0.070*
C4	0.11520 (13)	0.4497 (2)	0.49971 (18)	0.0459 (7)
C5	0.09805 (14)	0.5322 (2)	0.54302 (19)	0.0497 (7)
H5	0.115268	0.538910	0.601040	0.060*
C6	0.05581 (15)	0.6043 (2)	0.5010 (2)	0.0548 (8)
H6	0.043768	0.659303	0.530460	0.066*
C7	0.15780 (13)	0.3708 (2)	0.54492 (17)	0.0435 (7)
C8	0.19816 (14)	0.2172 (2)	0.56537 (18)	0.0460 (7)
C9	0.27418 (13)	0.2523 (2)	0.70549 (17)	0.0437 (7)
H9	0.294754	0.188761	0.693418	0.052*
C10	0.32768 (14)	0.3332 (2)	0.72144 (19)	0.0506 (7)
H10A	0.337773	0.353284	0.667709	0.061*
H10B	0.311617	0.392485	0.746326	0.061*
C11	0.38986 (14)	0.2951 (2)	0.78047 (19)	0.0508 (7)
C12	0.43695 (14)	0.3706 (2)	0.82279 (19)	0.0526 (8)
C13	0.43258 (19)	0.4740 (3)	0.8214 (3)	0.0882 (13)
H13	0.396509	0.510482	0.791966	0.106*
C14	0.4906 (3)	0.5181 (4)	0.8709 (4)	0.126 (2)
H14	0.497143	0.587718	0.877001	0.151*
C15	0.5353 (2)	0.4492 (3)	0.9083 (3)	0.0953 (14)
H15	0.575662	0.465943	0.943140	0.114*
C16	0.24206 (13)	0.2332 (2)	0.77969 (17)	0.0424 (6)
C17	0.24210 (15)	0.1367 (2)	0.81390 (19)	0.0488 (7)
H17	0.262005	0.083791	0.790687	0.059*
C18	0.21309 (15)	0.1179 (2)	0.8818 (2)	0.0542 (8)
H18	0.213774	0.052413	0.903324	0.065*
C19	0.18314 (14)	0.1939 (2)	0.91841 (19)	0.0498 (7)
C20	0.18410 (17)	0.2903 (2)	0.8847 (2)	0.0639 (9)
H20	0.164964	0.343337	0.908721	0.077*
C21	0.21262 (17)	0.3099 (2)	0.8164 (2)	0.0597 (8)
H21	0.211976	0.375448	0.795043	0.072*
C22	0.15170 (17)	0.1746 (3)	0.9930 (2)	0.0653 (9)
H22A	0.104615	0.174914	0.974141	0.098*
H22B	0.164729	0.226663	1.034900	0.098*

H22C	0.165739	0.109833	1.017591	0.098*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0765 (7)	0.0946 (7)	0.1055 (8)	0.0220 (6)	0.0074 (6)	0.0429 (6)
S1	0.0683 (6)	0.0478 (5)	0.0757 (6)	−0.0032 (4)	0.0109 (5)	−0.0161 (4)
S2	0.0460 (5)	0.0927 (7)	0.0693 (6)	−0.0034 (4)	−0.0026 (4)	0.0089 (5)
O1	0.0486 (12)	0.0504 (12)	0.0448 (11)	−0.0060 (9)	0.0013 (9)	−0.0091 (9)
O2	0.0548 (14)	0.0589 (15)	0.105 (2)	0.0017 (11)	−0.0062 (13)	0.0120 (14)
N1	0.0457 (13)	0.0436 (13)	0.0407 (13)	−0.0005 (11)	0.0023 (11)	−0.0026 (10)
N2	0.0441 (13)	0.0417 (13)	0.0417 (13)	−0.0007 (10)	0.0044 (11)	−0.0039 (10)
C1	0.0454 (18)	0.063 (2)	0.071 (2)	0.0015 (15)	0.0070 (16)	0.0187 (18)
C2	0.066 (2)	0.088 (3)	0.0461 (19)	0.006 (2)	−0.0075 (17)	0.0044 (18)
C3	0.058 (2)	0.070 (2)	0.0438 (18)	0.0051 (16)	0.0020 (15)	−0.0057 (15)
C4	0.0380 (16)	0.0526 (17)	0.0444 (17)	−0.0045 (13)	0.0032 (13)	−0.0002 (13)
C5	0.0446 (17)	0.0534 (18)	0.0477 (17)	−0.0074 (14)	0.0022 (14)	−0.0024 (14)
C6	0.0496 (18)	0.0501 (18)	0.066 (2)	−0.0033 (14)	0.0149 (16)	0.0018 (16)
C7	0.0385 (15)	0.0487 (16)	0.0418 (16)	−0.0037 (13)	0.0057 (13)	−0.0057 (13)
C8	0.0398 (16)	0.0513 (17)	0.0473 (17)	−0.0056 (13)	0.0102 (13)	−0.0028 (14)
C9	0.0413 (16)	0.0424 (15)	0.0451 (16)	0.0017 (12)	0.0040 (13)	0.0005 (13)
C10	0.0411 (16)	0.0544 (17)	0.0534 (18)	−0.0026 (13)	0.0036 (14)	0.0057 (14)
C11	0.0439 (17)	0.0567 (19)	0.0519 (18)	0.0007 (14)	0.0102 (14)	0.0055 (15)
C12	0.0431 (17)	0.064 (2)	0.0477 (17)	−0.0010 (14)	0.0028 (14)	−0.0016 (15)
C13	0.074 (3)	0.064 (2)	0.107 (3)	−0.0009 (19)	−0.025 (2)	−0.016 (2)
C14	0.102 (4)	0.076 (3)	0.167 (5)	−0.008 (3)	−0.040 (3)	−0.038 (3)
C15	0.064 (3)	0.106 (3)	0.099 (3)	−0.012 (2)	−0.017 (2)	−0.017 (3)
C16	0.0370 (15)	0.0421 (15)	0.0457 (16)	0.0013 (12)	0.0036 (12)	−0.0011 (13)
C17	0.0560 (18)	0.0391 (15)	0.0517 (18)	0.0030 (13)	0.0122 (15)	−0.0035 (13)
C18	0.064 (2)	0.0408 (16)	0.0592 (19)	−0.0011 (14)	0.0158 (16)	0.0079 (14)
C19	0.0435 (16)	0.0520 (17)	0.0546 (18)	0.0028 (14)	0.0121 (14)	0.0045 (14)
C20	0.071 (2)	0.0532 (19)	0.075 (2)	0.0200 (16)	0.0325 (19)	0.0060 (17)
C21	0.072 (2)	0.0445 (17)	0.068 (2)	0.0130 (16)	0.0276 (18)	0.0105 (16)
C22	0.066 (2)	0.067 (2)	0.069 (2)	0.0035 (17)	0.0272 (18)	0.0094 (17)

Geometric parameters (Å, º)

Cl1—C1	1.740 (3)	C10—C11	1.516 (4)
S1—C8	1.644 (3)	C10—H10A	0.9700
S2—C15	1.664 (4)	C10—H10B	0.9700
S2—C12	1.719 (3)	C11—C12	1.458 (4)
O1—C8	1.371 (3)	C12—C13	1.368 (5)
O1—C7	1.371 (3)	C13—C14	1.420 (5)
O2—C11	1.216 (3)	C13—H13	0.9300
N1—C7	1.284 (3)	C14—C15	1.345 (6)
N1—N2	1.386 (3)	C14—H14	0.9300
N2—C8	1.336 (3)	C15—H15	0.9300
N2—C9	1.472 (3)	C16—C21	1.381 (4)

C1—C2	1.373 (5)	C16—C17	1.387 (4)
C1—C6	1.373 (5)	C17—C18	1.380 (4)
C2—C3	1.370 (4)	C17—H17	0.9300
C2—H2	0.9300	C18—C19	1.378 (4)
C3—C4	1.392 (4)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.384 (4)
C4—C5	1.381 (4)	C19—C22	1.508 (4)
C4—C7	1.457 (4)	C20—C21	1.381 (4)
C5—C6	1.370 (4)	C20—H20	0.9300
C5—H5	0.9300	C21—H21	0.9300
C6—H6	0.9300	C22—H22A	0.9600
C9—C16	1.510 (4)	C22—H22B	0.9600
C9—C10	1.523 (4)	C22—H22C	0.9600
C9—H9	0.9800		

C15—S2—C12	92.10 (19)	H10A—C10—H10B	108.0
C8—O1—C7	106.1 (2)	O2—C11—C12	121.3 (3)
C7—N1—N2	103.4 (2)	O2—C11—C10	121.2 (3)
C8—N2—N1	112.4 (2)	C12—C11—C10	117.5 (3)
C8—N2—C9	126.1 (2)	C13—C12—C11	129.7 (3)
N1—N2—C9	121.5 (2)	C13—C12—S2	111.3 (2)
C2—C1—C6	121.1 (3)	C11—C12—S2	119.1 (2)
C2—C1—Cl1	119.1 (3)	C12—C13—C14	110.8 (4)
C6—C1—Cl1	119.8 (3)	C12—C13—H13	124.6
C3—C2—C1	119.8 (3)	C14—C13—H13	124.6
C3—C2—H2	120.1	C15—C14—C13	113.2 (4)
C1—C2—H2	120.1	C15—C14—H14	123.4
C2—C3—C4	119.7 (3)	C13—C14—H14	123.4
C2—C3—H3	120.1	C14—C15—S2	112.6 (3)
C4—C3—H3	120.1	C14—C15—H15	123.7
C5—C4—C3	119.6 (3)	S2—C15—H15	123.7
C5—C4—C7	120.4 (3)	C21—C16—C17	117.7 (3)
C3—C4—C7	119.9 (3)	C21—C16—C9	121.9 (3)
C6—C5—C4	120.4 (3)	C17—C16—C9	120.4 (2)
C6—C5—H5	119.8	C18—C17—C16	121.1 (3)
C4—C5—H5	119.8	C18—C17—H17	119.4
C5—C6—C1	119.4 (3)	C16—C17—H17	119.4
C5—C6—H6	120.3	C19—C18—C17	121.5 (3)
C1—C6—H6	120.3	C19—C18—H18	119.2
N1—C7—O1	113.2 (2)	C17—C18—H18	119.2
N1—C7—C4	128.4 (3)	C18—C19—C20	117.0 (3)
O1—C7—C4	118.4 (2)	C18—C19—C22	122.1 (3)
N2—C8—O1	104.9 (2)	C20—C19—C22	120.9 (3)
N2—C8—S1	131.0 (2)	C21—C20—C19	122.0 (3)
O1—C8—S1	124.1 (2)	C21—C20—H20	119.0
N2—C9—C16	110.8 (2)	C19—C20—H20	119.0
N2—C9—C10	108.9 (2)	C16—C21—C20	120.6 (3)
C16—C9—C10	114.5 (2)	C16—C21—H21	119.7

N2—C9—H9	107.4	C20—C21—H21	119.7
C16—C9—H9	107.4	C19—C22—H22A	109.5
C10—C9—H9	107.4	C19—C22—H22B	109.5
C11—C10—C9	111.5 (2)	H22A—C22—H22B	109.5
C11—C10—H10A	109.3	C19—C22—H22C	109.5
C9—C10—H10A	109.3	H22A—C22—H22C	109.5
C11—C10—H10B	109.3	H22B—C22—H22C	109.5
C9—C10—H10B	109.3		

C7—N1—N2—C8	−1.9 (3)	N2—C9—C10—C11	−161.9 (2)
C7—N1—N2—C9	−179.9 (2)	C16—C9—C10—C11	73.4 (3)
C6—C1—C2—C3	0.9 (5)	C9—C10—C11—O2	20.9 (4)
Cl1—C1—C2—C3	−178.7 (3)	C9—C10—C11—C12	−161.0 (3)
C1—C2—C3—C4	−0.1 (5)	O2—C11—C12—C13	−178.0 (4)
C2—C3—C4—C5	−1.3 (5)	C10—C11—C12—C13	3.9 (5)
C2—C3—C4—C7	177.8 (3)	O2—C11—C12—S2	2.0 (4)
C3—C4—C5—C6	1.8 (4)	C10—C11—C12—S2	−176.1 (2)
C7—C4—C5—C6	−177.3 (3)	C15—S2—C12—C13	−0.6 (3)
C4—C5—C6—C1	−1.0 (4)	C15—S2—C12—C11	179.4 (3)
C2—C1—C6—C5	−0.4 (5)	C11—C12—C13—C14	−179.1 (4)
Cl1—C1—C6—C5	179.2 (2)	S2—C12—C13—C14	0.9 (5)
N2—N1—C7—O1	1.0 (3)	C12—C13—C14—C15	−1.0 (7)
N2—N1—C7—C4	179.4 (3)	C13—C14—C15—S2	0.6 (7)
C8—O1—C7—N1	0.2 (3)	C12—S2—C15—C14	0.0 (4)
C8—O1—C7—C4	−178.5 (2)	N2—C9—C16—C21	−67.6 (3)
C5—C4—C7—N1	−21.6 (5)	C10—C9—C16—C21	56.1 (4)
C3—C4—C7—N1	159.2 (3)	N2—C9—C16—C17	113.2 (3)
C5—C4—C7—O1	156.8 (3)	C10—C9—C16—C17	−123.1 (3)
C3—C4—C7—O1	−22.4 (4)	C21—C16—C17—C18	0.6 (4)
N1—N2—C8—O1	2.0 (3)	C9—C16—C17—C18	179.9 (3)
C9—N2—C8—O1	179.9 (2)	C16—C17—C18—C19	−0.2 (5)
N1—N2—C8—S1	−178.3 (2)	C17—C18—C19—C20	−0.7 (5)
C9—N2—C8—S1	−0.4 (4)	C17—C18—C19—C22	−179.5 (3)
C7—O1—C8—N2	−1.3 (3)	C18—C19—C20—C21	1.1 (5)
C7—O1—C8—S1	179.0 (2)	C22—C19—C20—C21	180.0 (3)
C8—N2—C9—C16	−98.7 (3)	C17—C16—C21—C20	−0.3 (5)
N1—N2—C9—C16	79.0 (3)	C9—C16—C21—C20	−179.5 (3)
C8—N2—C9—C10	134.5 (3)	C19—C20—C21—C16	−0.7 (5)
N1—N2—C9—C10	−47.8 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*3 and *Cg*4 are the centroids of the C1–C6 and C16–C21 rings.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···*Cg*3^{i}	0.93	2.83	3.726 (3)	164
C22—H22*B*···*Cg*4^{ii}	0.96	2.92	3.671 (4)	136

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