

Crystal structure and Hirshfeld surface analysis of 3-(4-methoxyphenyl)-2-[(thiophen-2-yl)carbonyl]-acrylonitrile

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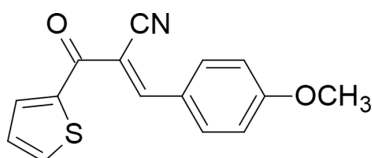
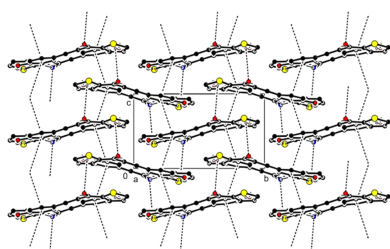
Supporting information: this article has supporting information at journals.iucr.org/e

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In the title compound, C₁₅H₁₁NO₂S, the intramolecular C—H...O hydrogen-bond interaction forms an *S*(6) ring motif. The dihedral angle between the planes of the thiophene and methoxyphenyl rings is 12.26 (15)°. In the crystal, molecular pairs are joined by C—H...N contacts, forming *R*₂²(16) motifs lying parallel to the (001) plane. They are connected by C—O... π and π — π interactions [centroid-to-centroid lengths = 3.9049 (18) and 3.9050 (18) Å], resulting in layers parallel to the (100) plane. These layers are linked by C—H...N interactions. Hirshfeld surface analysis indicates that H...H (35.3%), O...H/H...O (13.5%), C...C (12.5%), N...H/H...N (11.6%), C...H/H...C (11.6%) and S...H/H...S (9.0%) interactions make significant contributions.

1. Chemical context

Knoevenagel condensation reactions play a significant role in carbon–carbon bond formation, providing a versatile strategy for the synthesis of α -functionalized chalcone analogues and other conjugated molecular frameworks (Naghiyev *et al.*, 2023; Mamedov & Khalilov, 2025; Abdullayeva *et al.*, 2026). Depending on the substrates and reaction conditions, these transformations can proceed under relatively mild conditions and afford products in good yields, sometimes with high stereoselectivity (Khalilov *et al.*, 2011; Khalilov *et al.*, 2023; Tüzün *et al.*, 2025). Knoevenagel adducts have also been used as intermediates in the synthesis of compounds investigated in medicinal chemistry and materials research (Naghiyev *et al.*, 2022; Naghiyev *et al.*, 2024; Karimli *et al.*, 2023). Among these chalcone analogues, α,β -unsaturated nitrile derivatives are of particular interest because their structural diversity and reactive functional groups allow further synthetic transformations (Akkurt *et al.*, 2018; Asgarova *et al.*, 2019; Shikhaliyev *et al.*, 2025). Compounds combining a thiophene ring with an α,β -unsaturated carbonyl group and a nitrile group provide substrates for such transformations. In particular, thiophene-2-carbonyl-substituted acrylonitriles have been used in the synthesis of heterocyclic compounds.



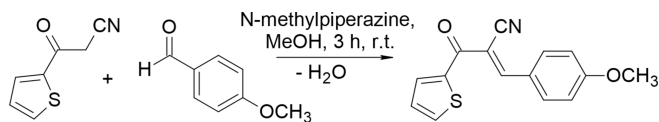


Figure 1
Synthesis of the title compound by Knoevenagel condensation.

In the present study, 3-oxo-3-(thiophen-2-yl)propanenitrile was reacted with 4-methoxybenzaldehyde in methanol at room temperature to afford the title compound (Fig. 1) and we now describe its structure. *N*-Methylpiperazine served as a base, facilitating condensation at the activated methylene group, followed by elimination of water. In this context, we report the crystal structure and Hirshfeld surface analysis of 3-(4-methoxyphenyl)-2-[(thiophen-2-yl)carbonyl]acrylonitrile as part of our ongoing investigations (Askerov *et al.*, 2020; Naghiyev *et al.*, 2021).

2. Structural commentary

The intramolecular C8—H8···O1 hydrogen-bond interaction forms an *S*(6) ring motif in the molecule (Table 1 and Fig. 2; Bernstein *et al.*, 1995). The dihedral angle between the planes of the thiophene ring (S1/C1—C4) and the methoxyphenyl ring (C9—C14) is 12.26 (15)°. The S1—C4—C5—C6, S1—C4—C5—O1, O1—C5—C6—C7, C7—C6—C8—C9 and C6—C8—C9—C14 torsion angles are 4.4 (5), 4.9 (4), −3.1 (5)° and −13.9 (5)°, respectively.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecular pairs are linked by C13—H13···N1 contacts, which form $R_2^2(16)$ motifs lying parallel to the (001) plane (Fig. 3). They are connected by the C—O··· π contact [C5—O1···Cg1^a: C5—O1 = 1.226 (3) Å, O1···Cg1^a = 3.721 (3) Å, C5···Cg1^a = 3.602 (3) Å and C5—O1···Cg1^a = 74.94 (17)°; symmetry code: (a) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; Cg1 is the centroid of the S1/C1—C4 thiophene ring] and weak π — π interactions [Cg2···Cg2^b = 3.9049 (18) Å, slippage = 0.857 Å, Cg2···Cg2^c = 3.9050 (18) Å, slippage = 1.751 Å; symmetry

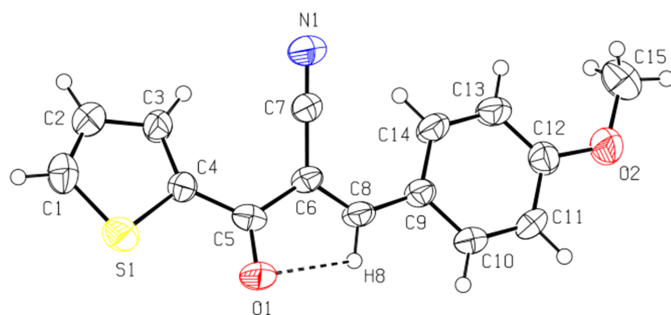


Figure 2
The molecular structure showing the atomic labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular C8—H8···O1 hydrogen bond is shown as a dashed line.

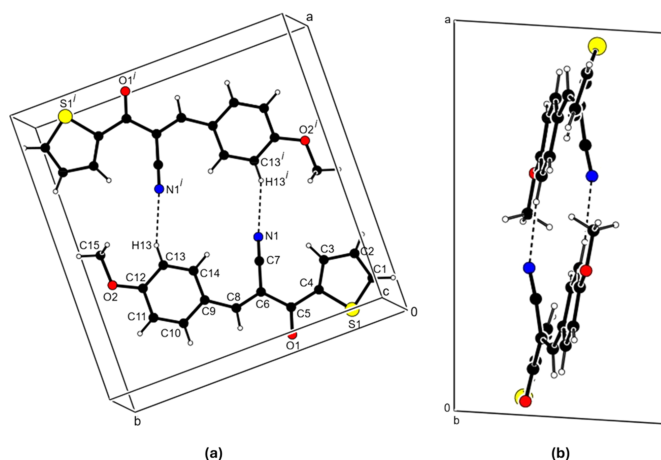


Figure 3
(a) A view of the C—H···N interactions in the unit cell. (b) A view down the *b* axis of the C—H···N interactions (dashed lines) for the situation shown in part (a). The $R_2^2(16)$ graph-set motif formed by a pair of C—H···N interactions. [Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.]

codes: (b) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (c) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; Cg2 is the centroid of the C9—C14 methoxyphenyl ring], producing layers parallel to the (100) plane. These layers are linked by C13—H13···N1 interactions (Fig. 4).

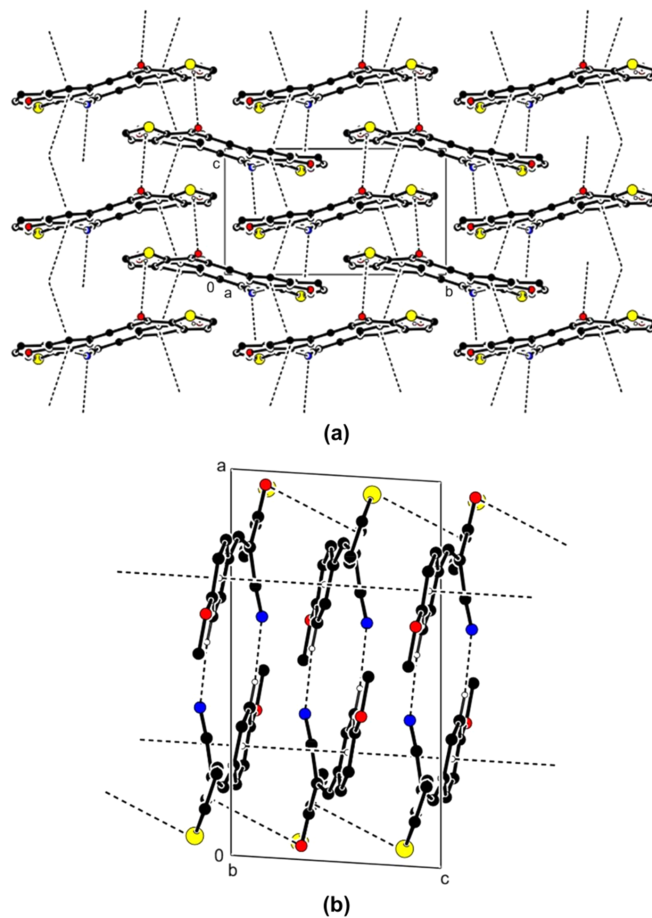


Figure 4
(a) A view of the C—O··· π and π — π interactions (dashed lines) along the *a* axis. (b) A view of the C—H···N, C—O··· π and π — π interactions (dashed lines) along the *b* axis. For clarity, H atoms not involved in hydrogen bonding have been omitted.

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8 $\cdots$ O1	0.93	2.40	2.779 (3)	104
C13—H13 $\cdots$ N1 ⁱ	0.93	2.51	3.394 (4)	158

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

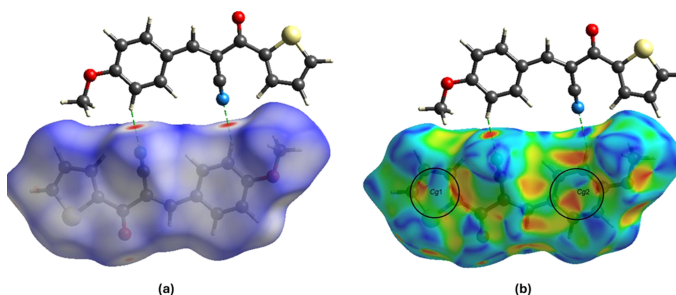
In order to further characterize and quantify the intermolecular interactions in the title compound, a Hirshfeld surface analysis was carried out using *CrystalExplorer21* (Spackman *et al.*, 2021). The Hirshfeld surface mapped over d_{norm} is illustrated in Fig. 5(a). The d_{norm} mappings ranged from -0.20 to $+1.26$ a.u. The shape index [Fig. 5(b)] shows paired red–blue regions typical of π – π stacking, with an additional weak signal in the area of the aromatic ring–O contact.

The fingerprint plots provide quantitative information about the noncovalent interactions in the crystal packing in terms of the percentage contribution of the interatomic contacts. The fingerprint plots (Fig. 6) show that H $\cdots$ H interactions (35.3%) contribute the most to surface contacts. Other notable interactions include O $\cdots$ H/H $\cdots$ O (13.5%), C $\cdots$ C (12.5%), N $\cdots$ H/H $\cdots$ N (11.6%), C $\cdots$ H/H $\cdots$ C (11.6%) and S $\cdots$ H/H $\cdots$ S (9.0%). Less significant interactions include S $\cdots$ O/O $\cdots$ S (1.2%) and O $\cdots$ N/N $\cdots$ O (0.4%).

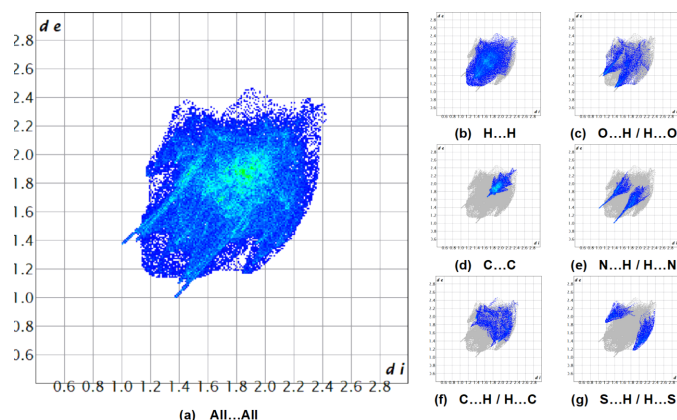
4. Database survey

A search in the Cambridge Structural Database (CSD, Version 6.00, updated April 2025; Groom *et al.*, 2016) for the title compound reveals the five most closely related compounds, viz: (*E*)-2-(2-thienyl)-3-(3,4,5-trimethoxyphenyl)acrylonitrile [CSD refcode PEMBEP (I); Cobo *et al.*, 2006a], (*E*)-3-(4-bromophenyl)-2-(2-thienyl)acrylonitrile [PEMBIT (II); Cobo *et al.*, 2006a], (*E*)-3-phenyl-2-(3-thienyl)acrylonitrile [PEMBOZ (III); Cobo *et al.*, 2006a], (*Z*)-3-(4-methylphenyl)-2-(3-thienyl)acrylonitrile [QERPAF (IV); Cobo *et al.*, 2006b] and (*Z*)-2-phenyl-3-(2,2':5',2''-terthiophen-3'-yl)acrylonitrile [UDUNAJ (V); Wagner *et al.*, 2007].

Compounds (I), (III), (IV) and (V) crystallize in the mononlinic space group $P2_1/c$, whereas (II) crystallizes in the monoclinic space group $P2_1/n$.

**Figure 5**

Hirshfeld surface of the title compound, mapped over (a) d_{norm} and (b) shape index, showing the intermolecular C13—H13 $\cdots$ N1 contacts.

**Figure 6**

The two-dimensional fingerprint plots showing (a) all interactions, and those delineated into (b) H $\cdots$ H, (c) O $\cdots$ H/H $\cdots$ O, (d) C $\cdots$ C, (e) N $\cdots$ H/H $\cdots$ N, (f) C $\cdots$ H/H $\cdots$ C and (g) S $\cdots$ H/H $\cdots$ S interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Compound (I) contains no direction-specific intermolecular interactions. (II) exhibits orientational disorder of the thienyl fragment and the molecules are linked into simple *C*(5) chains by a single C—H $\cdots$ N hydrogen bond. In (III), the molecules are linked into sheets by a combination of one C—H $\cdots$ N hydrogen bond and one C—H $\cdots$ π (arene) hydrogen bond. In (I)–(III), the nitrile components exhibit quite long C—C bonds [1.443 (2)–1.446 (4) Å] and very short C—N bonds [1.143 (4)–1.146 (4) Å]. The remaining bond distances in (I)–(III) show no unusual features. In (IV), the shortest nonbonded intermolecular contacts between potential hydrogen-bond donors and acceptors are all too long to be structurally significant. In crystal structure (V), the van der Waals forces seem to determine the packing. Weak C—H $\cdots$ N and C—H $\cdots$ π interactions also might be of some importance.

While the contributions of the strong interactions are quite consistent, weak interactions vary slightly depending on the molecular conformation and the environment of the molecules.

5. Synthesis and crystallization

A solution of 3-oxo-3-(thiophen-2-yl)propanenitrile (0.5 g, 3.31 mmol) and 4-methoxybenzaldehyde (0.45 g, 3.31 mmol) in methanol (20 ml) was treated with a catalytic amount of *N*-methylpiperazine (1–2 drops). The reaction mixture was stirred vigorously at room temperature for 3 h, and the course of the reaction was monitored by thin-layer chromatography (TLC; Silufol UV-254 plates; hexane–ethyl acetate, 1:4 v/v). The resulting yellow crystals form directly; they were collected by filtration, washed with methanol and dried (m.p. 358 K; yield 91%).

¹H NMR (300 MHz, DMSO-*d*₆, ppm): 3.87 (s, 3H, CH₃O), 7.14–8.15 (*m*, 7H, 4CH_{arom} + 3CH_{thienyl}), 8.29 (s, 1H, CH=). ¹³C NMR (75 MHz, DMSO-*d*₆, ppm): 56.23 (CH₃O), 105.74 (=C_{quat}), 115.40 (2CH_{arom}), 118.14 (CN), 124.85 (C_{thienyl}), 129.45 (CH_{thienyl}), 134.13 (2CH_{arom}), 135.51 (CH_{thienyl}), 136.95

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₁ NO ₂ S
<i>M_r</i>	269.31
Crystal system, space group	Monoclinic, <i>P</i> ₂ /c
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.6250 (19), 13.0153 (18), 7.4161 (9)
β (°)	93.530 (4)
<i>V</i> (Å ³)	1312.6 (3)
<i>Z</i>	4
Radiation type	Mo Kα
μ (mm ⁻¹)	0.24
Crystal size (mm)	0.12 × 0.08 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2012)
<i>T</i> _{min} , <i>T</i> _{max}	0.378, 0.745
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	21480, 2678, 1704
<i>R</i> _{int}	0.095
(sin θ/λ) _{max} (Å ⁻¹)	0.625
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.075, 0.139, 1.11
No. of reflections	2678
No. of parameters	173
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.27, -0.30

Computer programs: APEX2 (Bruker, 2012), SAINT (Bruker, 2012), SHELXT (Sheldrick, 2015a), SHELXL2014 (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2020).

(CH_{thienyl}), 141.54 (C_{arom}), 155.21 (CH=), 164.03 (O—C_{arom}), 180.13 (C=O).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed in calculated positions and were refined as riding atoms with *U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq}(methyl C). The methyl H atoms were allowed to rotate, but not to tip, to best fit the experimental electron density.

Acknowledgements

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References

- Abdullayeva, F. M., Maharramov, A. M., Huseynov, E. Z., Pashayeva, Z. N. & Safarova, A. S. (2026). *New Mater. Compd Appl.* **10**, 138–150.
- Akkurt, M., Duruskari, G. S., Toze, F. A. A., Khalilov, A. N. & Huseynova, A. T. (2018). *Acta Cryst.* **E74**, 1168–1172.
- Asgarova, A. R., Khalilov, A. N., Brito, I., Maharramov, A. M., Shikhaliyev, N. G., Cisterna, J., Cárdenas, A., Gurbanov, A. V., Zubkov, F. I. & Mahmudov, K. T. (2019). *Acta Cryst.* **C75**, 342–347.
- Askerov, R. K., Maharramov, A. M., Khalilov, A. N., Akkurt, M., Akobirshoeva, A. A., Osmanov, V. K. & Borisov, A. V. (2020). *Acta Cryst.* **E76**, 1007–1011.
- Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2012). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cobo, D., Cobo, J., Low, J. N. & Glidewell, C. (2006b). *Acta Cryst.* **E62**, o5179–o5180.
- Cobo, D., Quiroga, J., de la Torre, J. M., Cobo, J., Low, J. N. & Glidewell, C. (2006a). *Acta Cryst.* **C62**, o550–o553.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Karimli, E. G., Khrustalev, V. N., Akkurt, M., Khalilov, A. N., Bhattarai, A., Aleskerova, A. N. & Mamedov, I. G. (2023). *Acta Cryst.* **E79**, 777–781.
- Khalilov, A. N., Abdelhamid, A. A., Gurbanov, A. V. & Ng, S. W. (2011). *Acta Cryst.* **E67**, o1146.
- Khalilov, A. N., Khrustalev, V. N., Aleksandrova, L. V., Akkurt, M., Rzaev, R. M., Bhattarai, A. & Mamedov, I. G. (2023). *Acta Cryst.* **E79**, 436–440.
- Mamedov, I. & Khalilov, A. (2025). *Baghdad Sci. J.* **22**, 2239–2245.
- Naghiyev, F. N., Grishina, M. M., Khrustalev, V. N., Khalilov, A. N., Akkurt, M., Akobirshoeva, A. A. & Mamedov, I. G. (2021). *Acta Cryst.* **E77**, 195–199.
- Naghiyev, F. N., Khrustalev, V. N., Akkurt, M., Asadov, K. A., Bhattarai, A., Khalilov, A. N. & Mamedov, I. G. (2024). *Acta Cryst.* **E80**, 446–451.
- Naghiyev, F. N., Khrustalev, V. N., Akkurt, M., Khalilov, A. N., Bhattarai, A., Kerimli, F. S. & Mamedov, I. G. (2023). *Acta Cryst.* **E79**, 494–498.
- Naghiyev, F. N., Khrustalev, V. N., Dobrokhotova, E. V., Akkurt, M., Khalilov, A. N., Bhattarai, A. & Mamedov, I. G. (2022). *Acta Cryst.* **E78**, 568–573.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Shikhaliyev, N. G., Cisterna, J., Gajar, A. M., Niyazova, A. A., Khalilov, A. N., Khrustalev, V. N., Belay, A. N. & Maharramov, A. M. (2025). *Acta Cryst.* **E81**, 662–666.
- Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
- Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.
- Tüzün, B., Agbektas, T., Naghiyev, F. N., Tas, A., Zontul, C., Ozum, U., Khalilov, A. N., Silig, Y., Çakmak, N. K. & Mamedov, I. G. (2025). *Monatsh. Chem.* **156**, 667–688.
- Wagner, P., Officer, D. L. & Kubicki, M. (2007). *Acta Cryst.* **E63**, o3054–o3055.

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Computing details

3-(4-Methoxyphenyl)-2-[(thiophen-2-yl)carbonyl]prop-2-enenitrile

Crystal data

$C_{15}H_{11}NO_2S$

$M_r = 269.31$

Monoclinic, $P2_1/c$

$a = 13.6250$ (19) Å

$b = 13.0153$ (18) Å

$c = 7.4161$ (9) Å

$\beta = 93.530$ (4)°

$V = 1312.6$ (3) Å³

$Z = 4$

$F(000) = 560$

$D_x = 1.363$ Mg m⁻³

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

Cell parameters from 4702 reflections

$\theta = 3.0\text{--}22.2^\circ$

$\mu = 0.24$ mm⁻¹

$T = 293$ K

Block, yellow

$0.12 \times 0.08 \times 0.07$ mm

Data collection

Bruker APEXII CCD

diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2012)

$T_{\min} = 0.378$, $T_{\max} = 0.745$

21480 measured reflections

2678 independent reflections

1704 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.095$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -16 \rightarrow 17$

$k = -16 \rightarrow 16$

$l = -8 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.075$

$wR(F^2) = 0.139$

$S = 1.11$

2678 reflections

173 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 0.8766P]$

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

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

$\Delta\rho_{\max} = 0.27$ e Å⁻³

$\Delta\rho_{\min} = -0.30$ 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1153 (3)	0.0523 (3)	0.3757 (4)	0.0547 (10)
H1	0.092826	−0.015035	0.364876	0.066*
C2	0.2084 (3)	0.0778 (3)	0.4318 (5)	0.0532 (9)
H2	0.256854	0.029829	0.464225	0.064*
C3	0.2242 (2)	0.1845 (2)	0.4359 (4)	0.0456 (9)
H3	0.284135	0.215146	0.470565	0.055*
C4	0.1405 (2)	0.2382 (2)	0.3825 (4)	0.0362 (7)
C5	0.1196 (2)	0.3491 (3)	0.3706 (4)	0.0398 (8)
C6	0.1994 (2)	0.4266 (2)	0.4097 (4)	0.0387 (8)
C7	0.2993 (2)	0.3988 (2)	0.3836 (5)	0.0485 (9)
C8	0.1746 (2)	0.5218 (2)	0.4635 (4)	0.0401 (8)
H8	0.107219	0.531495	0.469693	0.048*
C9	0.2328 (2)	0.6115 (2)	0.5133 (4)	0.0392 (8)
C10	0.1845 (2)	0.7056 (3)	0.5236 (4)	0.0453 (8)
H10	0.116438	0.707623	0.505124	0.054*
C11	0.2345 (2)	0.7946 (3)	0.5600 (4)	0.0487 (9)
H11	0.200412	0.856348	0.564421	0.058*
C12	0.3361 (2)	0.7934 (3)	0.5904 (4)	0.0439 (8)
C13	0.3847 (2)	0.7009 (3)	0.5890 (4)	0.0497 (9)
H13	0.452436	0.699000	0.613981	0.060*
C14	0.3346 (2)	0.6118 (3)	0.5512 (4)	0.0482 (9)
H14	0.368904	0.549987	0.550763	0.058*
C15	0.4836 (3)	0.8892 (3)	0.6548 (6)	0.0774 (12)
H15A	0.514909	0.862440	0.552324	0.116*
H15B	0.501480	0.848084	0.759237	0.116*
H15C	0.504330	0.958798	0.676470	0.116*
N1	0.3776 (2)	0.3766 (2)	0.3524 (5)	0.0784 (11)
O1	0.03542 (15)	0.37924 (17)	0.3351 (3)	0.0563 (6)
O2	0.37932 (16)	0.88645 (17)	0.6199 (3)	0.0591 (7)
S1	0.04432 (6)	0.15631 (7)	0.32754 (12)	0.0535 (3)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.068 (3)	0.039 (2)	0.057 (2)	−0.0065 (18)	0.0052 (19)	−0.0029 (17)
C2	0.050 (2)	0.046 (2)	0.064 (2)	0.0061 (17)	0.0009 (18)	0.0068 (18)
C3	0.040 (2)	0.036 (2)	0.060 (2)	0.0000 (15)	−0.0060 (16)	0.0078 (16)
C4	0.0377 (17)	0.0354 (19)	0.0354 (18)	0.0000 (15)	0.0020 (13)	−0.0007 (14)
C5	0.0283 (18)	0.052 (2)	0.0393 (19)	0.0012 (16)	0.0020 (14)	0.0007 (16)

C6	0.0305 (18)	0.040 (2)	0.0452 (19)	0.0078 (14)	−0.0014 (14)	0.0049 (15)
C7	0.035 (2)	0.036 (2)	0.074 (3)	0.0019 (16)	0.0008 (17)	−0.0039 (17)
C8	0.0286 (17)	0.044 (2)	0.047 (2)	0.0093 (15)	0.0011 (14)	0.0040 (16)
C9	0.0341 (18)	0.040 (2)	0.0431 (19)	0.0061 (15)	0.0011 (14)	0.0046 (15)
C10	0.0322 (18)	0.045 (2)	0.059 (2)	0.0077 (16)	0.0031 (15)	0.0004 (17)
C11	0.045 (2)	0.035 (2)	0.066 (2)	0.0147 (16)	0.0032 (17)	0.0017 (17)
C12	0.045 (2)	0.041 (2)	0.046 (2)	−0.0035 (17)	0.0040 (16)	−0.0012 (16)
C13	0.0329 (19)	0.050 (2)	0.066 (2)	0.0055 (17)	−0.0048 (16)	−0.0030 (18)
C14	0.038 (2)	0.040 (2)	0.065 (2)	0.0108 (16)	−0.0065 (16)	−0.0013 (17)
C15	0.054 (3)	0.073 (3)	0.105 (3)	−0.019 (2)	0.000 (2)	−0.005 (2)
N1	0.0395 (18)	0.055 (2)	0.141 (3)	0.0077 (16)	0.0098 (19)	−0.006 (2)
O1	0.0294 (13)	0.0551 (15)	0.0832 (17)	0.0061 (11)	−0.0054 (11)	0.0037 (13)
O2	0.0520 (16)	0.0452 (15)	0.0789 (18)	−0.0051 (12)	−0.0061 (13)	−0.0003 (12)
S1	0.0425 (5)	0.0562 (6)	0.0608 (6)	−0.0059 (4)	−0.0039 (4)	−0.0043 (5)

Geometric parameters (Å, °)

C1—C2	1.352 (4)	C9—C10	1.394 (4)
C1—S1	1.689 (4)	C9—C14	1.398 (4)
C1—H1	0.9300	C10—C11	1.361 (4)
C2—C3	1.405 (5)	C10—H10	0.9300
C2—H2	0.9300	C11—C12	1.389 (4)
C3—C4	1.375 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—O2	1.359 (4)
C4—C5	1.473 (4)	C12—C13	1.374 (4)
C4—S1	1.718 (3)	C13—C14	1.367 (4)
C5—O1	1.226 (3)	C13—H13	0.9300
C5—C6	1.498 (4)	C14—H14	0.9300
C6—C8	1.351 (4)	C15—O2	1.428 (4)
C6—C7	1.433 (4)	C15—H15A	0.9600
C7—N1	1.142 (4)	C15—H15B	0.9600
C8—C9	1.447 (4)	C15—H15C	0.9600
C8—H8	0.9300		
C2—C1—S1	112.5 (3)	C14—C9—C8	125.1 (3)
C2—C1—H1	123.8	C11—C10—C9	121.8 (3)
S1—C1—H1	123.8	C11—C10—H10	119.1
C1—C2—C3	112.9 (3)	C9—C10—H10	119.1
C1—C2—H2	123.5	C10—C11—C12	120.2 (3)
C3—C2—H2	123.5	C10—C11—H11	119.9
C4—C3—C2	111.8 (3)	C12—C11—H11	119.9
C4—C3—H3	124.1	O2—C12—C13	125.3 (3)
C2—C3—H3	124.1	O2—C12—C11	115.7 (3)
C3—C4—C5	131.9 (3)	C13—C12—C11	119.0 (3)
C3—C4—S1	111.1 (2)	C14—C13—C12	120.7 (3)
C5—C4—S1	116.9 (2)	C14—C13—H13	119.7
O1—C5—C4	120.1 (3)	C12—C13—H13	119.7
O1—C5—C6	119.0 (3)	C13—C14—C9	121.3 (3)

C4—C5—C6	120.9 (3)	C13—C14—H14	119.3
C8—C6—C7	121.9 (3)	C9—C14—H14	119.3
C8—C6—C5	118.8 (3)	O2—C15—H15A	109.5
C7—C6—C5	119.2 (3)	O2—C15—H15B	109.5
N1—C7—C6	176.1 (4)	H15A—C15—H15B	109.5
C6—C8—C9	132.2 (3)	O2—C15—H15C	109.5
C6—C8—H8	113.9	H15A—C15—H15C	109.5
C9—C8—H8	113.9	H15B—C15—H15C	109.5
C10—C9—C14	116.9 (3)	C12—O2—C15	117.9 (3)
C10—C9—C8	118.0 (3)	C1—S1—C4	91.64 (16)
S1—C1—C2—C3	−0.3 (4)	C14—C9—C10—C11	3.2 (5)
C1—C2—C3—C4	0.3 (4)	C8—C9—C10—C11	−176.4 (3)
C2—C3—C4—C5	177.6 (3)	C9—C10—C11—C12	−0.8 (5)
C2—C3—C4—S1	−0.2 (3)	C10—C11—C12—O2	178.0 (3)
C3—C4—C5—O1	−172.8 (3)	C10—C11—C12—C13	−2.1 (5)
S1—C4—C5—O1	4.9 (4)	O2—C12—C13—C14	−177.5 (3)
C3—C4—C5—C6	4.4 (5)	C11—C12—C13—C14	2.5 (5)
S1—C4—C5—C6	−177.9 (2)	C12—C13—C14—C9	−0.1 (5)
O1—C5—C6—C8	21.7 (4)	C10—C9—C14—C13	−2.7 (5)
C4—C5—C6—C8	−155.6 (3)	C8—C9—C14—C13	176.8 (3)
O1—C5—C6—C7	−156.4 (3)	C13—C12—O2—C15	−0.9 (5)
C4—C5—C6—C7	26.4 (4)	C11—C12—O2—C15	179.0 (3)
C7—C6—C8—C9	−3.1 (5)	C2—C1—S1—C4	0.1 (3)
C5—C6—C8—C9	178.9 (3)	C3—C4—S1—C1	0.1 (2)
C6—C8—C9—C10	165.7 (3)	C5—C4—S1—C1	−178.1 (2)
C6—C8—C9—C14	−13.9 (5)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
C8—H8 $\cdots$ O1	0.93	2.40	2.779 (3)	104
C13—H13 $\cdots$ N1 ⁱ	0.93	2.51	3.394 (4)	158

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