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# 5-[(4,6-Dimethylpyrimidin-2-ylsulfanyl)-methyl]-3-(morpholinomethyl)-1,3,4-oxadiazole-2(3*H*)-thione

**A. Thiruvalluvar,[a]* M. Subramanyam,[a] B. Lingappa[b] and Balakrishna Kalluraya[b]**

[a]PG Research Department of Physics, Rajah Serfoji Government College (Autonomous), Thanjavur 613 005, Tamil Nadu, India, and [b]Department of Studies in Chemistry, Mangalore University, Mangalagangothri 574 199, Karnataka, India
Correspondence e-mail: athiru@vsnl.net

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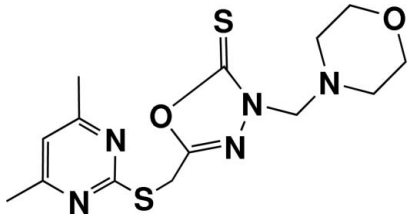
Key indicators: single-crystal X-ray study; $T$ = 160 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.057; $wR$ factor = 0.177; data-to-parameter ratio = 24.7.

In the title compound, $C_{14}H_{19}N_5O_2S_2$, the pyrimidine ring makes a dihedral angle of 82.8 (1)° with the oxadiazole ring. The morpholine ring adopts a chair conformation. There is a short intermolecular contact between the morpholine O atom and the sulfanylmethyl C atom [2.938 (3) Å]. The molecules are linked by C—H···S hydrogen bonds. An intramolecular C—H···N hydrogen bond is also present.

## Related literature

For related literature, see: Wichmann *et al.* (1999); El-Bendary *et al.* (1998); Kirpal (1999); Tsuji & Ishikawa (1994); Mohan *et al.* (1989); Baraldi *et al.* (1996, 2003); Sanjay *et al.* (2006); Thiruvalluvar *et al.* (2007*a*,*b*).



## Experimental

### Crystal data

$C_{14}H_{19}N_5O_2S_2$
$M_r$ = 353.48
Triclinic, $P\overline{1}$
$a$ = 7.1250 (3) Å
$b$ = 10.6735 (3) Å
$c$ = 12.3740 (5) Å
$\alpha$ = 93.607 (2)°
$\beta$ = 90.561 (2)°
$\gamma$ = 107.474 (2)°
$V$ = 895.42 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.31 mm$^{-1}$
$T$ = 160 (1) K
0.28 × 0.23 × 0.20 mm

### Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (Blessing, 1995)
$T_{min}$ = 0.892, $T_{max}$ = 0.964
25642 measured reflections
5188 independent reflections
3963 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.062

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.177
$S$ = 1.06
5188 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.98 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C21—H21$A$···N13 | 0.99 | 2.28 | 2.883 (3) | 118 |
| C21—H21$B$···S5$^{i}$ | 0.99 | 2.84 | 3.632 (2) | 137 |

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

The data collection was carried out by Dr A. Linden of the Institute of Organic Chemistry at the University of Zürich; this help is gratefully acknowledged by AT.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2165).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o3425 [ **doi:10.1107/S1600536807032448** ]

# 5-[(4,6-Dimethylpyrimidin-2-ylsulfanyl)methyl]-3-(morpholinomethyl)-1,3,4-oxadiazole-2(3*H*)-thione

**A. Thiruvalluvar, M. Subramanyam, B. Lingappa and B. Kalluraya**

## Comment

A literature survey shows that large numbers of simple, N-bridged, nitrogen- and sulfur-containing heterocyclic compounds containing the pyrimidine unit have diverse biological activities (Wichmann *et al.*, 1999; El-Bendary *et al.*, 1998; Kirpal, 1999; Tsuji & Ishikawa, 1994). In the light of this significant importance of pyrimidine compounds, and as a continuation of our work on the study of pyrimidine derivatives (Thiruvalluvaret al., 2007*a*,b), an X-ray crystallographic structure determination of the title compound was undertaken and the results are presented here.

In the title compound, Fig.1, the pyrimidine ring makes a dihedral angle of 82.8 (1)° with the oxadiazole ring. The morpholine ring adopts a chair conformation. There is a short intermolecular contact between O21 and C2 [2.938 (3) Å; −*x*, −*y*, −*z* + 1]. The molecules are linked by C—H···S hydrogen bonds (Fig. 2); an intramolecular C—H···N hydrogen bond is also present.

## Experimental

A solution of 5-(4,6-dimethyl-2-thiomethyl pyrimidyl)-1,3,4-oxadiazole-2-thione (2.56 g, 0.01 mol) in absolute ethanol (20 ml) was placed in a round-bottomed flask and treated with formaldehyde (40%, 3.0 ml). Later, morpholine (0.87 g, 0.01 mol) in ethanol (10 ml) was added with stirring and the reaction mixture was stirred overnight. The precipitated yellow solid was collected by filtration, dried and recrystallized from chloroform to give white crystals (1.64 g, 46%).

## Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95, 0.98 and 0.99 Å for C$sp^2$, methyl and methylene, respectively. $U_{iso}$(H) = $xU_{eq}$(C), where $x$ = 1.5 for methyl and 1.2 for all other H atoms. The maximum residual electron-density peak is located 2.79 Å from atom H23B.

## Figures

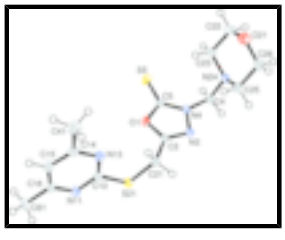

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

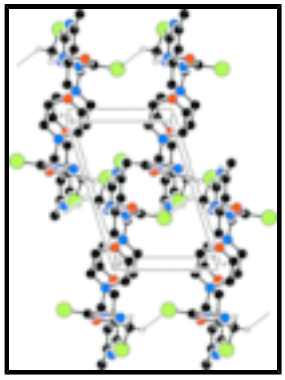

Fig. 2. The packing of the title compound, viewed down the *c* axis. Dashed lines indicate hydrogen bonds.

**5-[(4,6-Dimethylpyrimidin-2-ylsulfanyl)methyl]-3-(morpholinomethyl)-1,3,4- oxadiazole-2(3*H*)-thione**

*Crystal data*

| | |
|---|---|
| $C_{14}H_{19}N_5O_2S_2$ | $Z = 2$ |
| $M_r = 353.48$ | $F_{000} = 372$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.311$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point: 378(1) K |
| $a = 7.1250$ (3) Å | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $b = 10.6735$ (3) Å | Cell parameters from 32939 reflections |
| $c = 12.3740$ (5) Å | $\theta = 2.0$–$30.0°$ |
| $\alpha = 93.607$ (2)° | $\mu = 0.31$ mm$^{-1}$ |
| $\beta = 90.561$ (2)° | $T = 160$ (1) K |
| $\gamma = 107.474$ (2)° | Block, light_brown |
| $V = 895.42$ (6) Å$^3$ | 0.28 × 0.23 × 0.20 mm |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD area-detector diffractometer | 5188 independent reflections |
| Radiation source: Nonius FR590 sealed tube generator | 3963 reflections with $I > 2\sigma(I)$ |
| Monochromator: horizontally mounted graphite crystal | $R_{int} = 0.062$ |
| Detector resolution: 9 pixels mm$^{-1}$ | $\theta_{max} = 30.0°$ |
| $T = 160(1)$ K | $\theta_{min} = 2.0°$ |
| φ and ω scans with κ offsets | $h = -10 \rightarrow 10$ |
| Absorption correction: multi-scan (Blessing, 1995) | $k = -15 \rightarrow 15$ |
| $T_{min} = 0.892$, $T_{max} = 0.964$ | $l = -17 \rightarrow 17$ |
| 25642 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |

| | |
|---|---|
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.057$ | H-atom parameters constrained |
| $wR(F^2) = 0.177$ | $w = 1/[\sigma^2(F_o^2) + (0.0975P)^2 + 0.7899P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.06$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 5188 reflections | $\Delta\rho_{max} = 1.98$ e Å$^{-3}$ |
| 210 parameters | $\Delta\rho_{min} = -0.42$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. Solvent used: Chloroform Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (°.): 1.041 (2) Frames collected: 408 Seconds exposure per frame: 44 Degrees rotation per frame: 2.0 Crystal-Detector distance (mm): 32.0

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2$sigma($F^2$) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S5 | 0.62058 (8) | 0.31119 (6) | 0.52324 (5) | 0.02696 (16) |
| S21 | 0.20019 (9) | 0.59892 (5) | 0.76795 (4) | 0.02255 (15) |
| O1 | 0.3493 (2) | 0.38961 (15) | 0.63170 (13) | 0.0208 (3) |
| O21 | −0.0632 (3) | −0.12209 (17) | 0.34104 (17) | 0.0383 (5) |
| N3 | 0.1046 (3) | 0.36310 (18) | 0.51156 (15) | 0.0197 (4) |
| N4 | 0.2574 (3) | 0.32370 (17) | 0.46596 (14) | 0.0186 (4) |
| N11 | 0.3236 (3) | 0.65029 (19) | 0.96765 (15) | 0.0222 (4) |
| N13 | 0.1632 (3) | 0.42186 (19) | 0.91862 (15) | 0.0229 (4) |
| N24 | 0.1471 (3) | 0.14660 (18) | 0.32052 (15) | 0.0222 (4) |
| C2 | 0.1660 (3) | 0.3999 (2) | 0.60967 (17) | 0.0190 (4) |
| C4 | 0.2486 (3) | 0.2826 (2) | 0.34962 (17) | 0.0216 (4) |
| H4A | 0.1837 | 0.3370 | 0.3103 | 0.026* |
| H4B | 0.3849 | 0.3022 | 0.3241 | 0.026* |
| C5 | 0.4063 (3) | 0.3393 (2) | 0.53748 (18) | 0.0197 (4) |
| C12 | 0.2297 (3) | 0.5477 (2) | 0.89887 (18) | 0.0201 (4) |
| C14 | 0.1957 (3) | 0.3923 (2) | 1.02001 (19) | 0.0249 (5) |
| C15 | 0.2942 (4) | 0.4908 (3) | 1.09725 (19) | 0.0264 (5) |
| H15 | 0.3198 | 0.4700 | 1.1683 | 0.032* |
| C16 | 0.3544 (3) | 0.6198 (2) | 1.06892 (19) | 0.0248 (5) |
| C21 | 0.0579 (3) | 0.4458 (2) | 0.69701 (19) | 0.0240 (5) |

| | | | | |
|---|---|---|---|---|
| H21A | 0.0182 | 0.3772 | 0.7497 | 0.029* |
| H21B | −0.0634 | 0.4576 | 0.6656 | 0.029* |
| C22 | 0.1393 (5) | −0.0825 (3) | 0.3129 (3) | 0.0404 (7) |
| H22A | 0.1482 | −0.0860 | 0.2330 | 0.048* |
| H22B | 0.2040 | −0.1448 | 0.3405 | 0.048* |
| C23 | 0.2460 (4) | 0.0553 (2) | 0.3594 (2) | 0.0291 (5) |
| H23A | 0.2458 | 0.0582 | 0.4395 | 0.035* |
| H23B | 0.3845 | 0.0812 | 0.3367 | 0.035* |
| C25 | −0.0601 (4) | 0.1057 (2) | 0.3506 (2) | 0.0279 (5) |
| H25A | −0.1274 | 0.1662 | 0.3224 | 0.033* |
| H25B | −0.0688 | 0.1093 | 0.4305 | 0.033* |
| C26 | −0.1592 (4) | −0.0334 (2) | 0.3035 (2) | 0.0363 (6) |
| H26A | −0.2986 | −0.0615 | 0.3245 | 0.044* |
| H26B | −0.1564 | −0.0354 | 0.2235 | 0.044* |
| C41 | 0.1210 (5) | 0.2502 (3) | 1.0433 (2) | 0.0370 (6) |
| H41A | −0.0183 | 0.2282 | 1.0612 | 0.056* |
| H41B | 0.1967 | 0.2341 | 1.1046 | 0.056* |
| H41C | 0.1356 | 0.1953 | 0.9794 | 0.056* |
| C61 | 0.4595 (4) | 0.7317 (3) | 1.1477 (2) | 0.0331 (6) |
| H61A | 0.5980 | 0.7349 | 1.1552 | 0.050* |
| H61B | 0.3981 | 0.7189 | 1.2183 | 0.050* |
| H61C | 0.4512 | 0.8146 | 1.1213 | 0.050* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S5 | 0.0179 (3) | 0.0328 (3) | 0.0311 (3) | 0.0095 (2) | −0.0032 (2) | 0.0001 (2) |
| S21 | 0.0281 (3) | 0.0208 (3) | 0.0185 (3) | 0.0072 (2) | −0.0025 (2) | 0.0004 (2) |
| O1 | 0.0184 (7) | 0.0226 (8) | 0.0208 (7) | 0.0057 (6) | −0.0044 (6) | −0.0001 (6) |
| O21 | 0.0448 (12) | 0.0190 (8) | 0.0464 (12) | 0.0026 (8) | −0.0080 (9) | 0.0037 (8) |
| N3 | 0.0181 (9) | 0.0188 (8) | 0.0221 (9) | 0.0058 (7) | −0.0028 (7) | −0.0006 (7) |
| N4 | 0.0172 (8) | 0.0188 (8) | 0.0190 (8) | 0.0049 (7) | −0.0022 (7) | −0.0005 (7) |
| N11 | 0.0217 (9) | 0.0246 (9) | 0.0206 (9) | 0.0079 (7) | −0.0019 (7) | −0.0015 (7) |
| N13 | 0.0237 (9) | 0.0229 (9) | 0.0230 (9) | 0.0079 (8) | 0.0014 (7) | 0.0025 (7) |
| N24 | 0.0278 (10) | 0.0179 (9) | 0.0186 (9) | 0.0040 (7) | −0.0031 (7) | 0.0004 (7) |
| C2 | 0.0171 (9) | 0.0181 (9) | 0.0206 (10) | 0.0036 (8) | −0.0042 (7) | 0.0016 (8) |
| C4 | 0.0261 (11) | 0.0197 (10) | 0.0168 (10) | 0.0034 (8) | −0.0007 (8) | 0.0032 (8) |
| C5 | 0.0189 (10) | 0.0161 (9) | 0.0220 (10) | 0.0020 (7) | −0.0031 (8) | 0.0021 (8) |
| C12 | 0.0172 (10) | 0.0226 (10) | 0.0214 (10) | 0.0079 (8) | 0.0001 (8) | 0.0002 (8) |
| C14 | 0.0248 (11) | 0.0284 (11) | 0.0248 (11) | 0.0122 (9) | 0.0051 (9) | 0.0048 (9) |
| C15 | 0.0274 (12) | 0.0357 (13) | 0.0186 (10) | 0.0131 (10) | 0.0014 (8) | 0.0037 (9) |
| C16 | 0.0221 (11) | 0.0312 (12) | 0.0221 (11) | 0.0103 (9) | −0.0010 (8) | −0.0029 (9) |
| C21 | 0.0202 (10) | 0.0269 (11) | 0.0230 (11) | 0.0052 (9) | −0.0024 (8) | −0.0031 (9) |
| C22 | 0.0482 (17) | 0.0235 (12) | 0.0502 (17) | 0.0136 (12) | −0.0034 (13) | −0.0040 (11) |
| C23 | 0.0299 (12) | 0.0226 (11) | 0.0357 (13) | 0.0094 (9) | −0.0021 (10) | 0.0011 (9) |
| C25 | 0.0254 (12) | 0.0212 (11) | 0.0337 (13) | 0.0024 (9) | −0.0076 (9) | 0.0010 (9) |
| C26 | 0.0359 (14) | 0.0227 (12) | 0.0433 (15) | −0.0009 (10) | −0.0145 (12) | 0.0013 (10) |
| C41 | 0.0491 (17) | 0.0289 (13) | 0.0345 (14) | 0.0125 (12) | 0.0068 (12) | 0.0091 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C61 | 0.0383 (14) | 0.0373 (14) | 0.0218 (12) | 0.0106 (11) | −0.0063 (10) | −0.0071 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S5—C5 | 1.651 (2) | C16—C61 | 1.497 (4) |
| S21—C12 | 1.772 (2) | C22—C23 | 1.512 (4) |
| S21—C21 | 1.810 (2) | C25—C26 | 1.515 (4) |
| O1—C2 | 1.369 (3) | C4—H4A | 0.9900 |
| O1—C5 | 1.369 (3) | C4—H4B | 0.9900 |
| O21—C22 | 1.430 (4) | C15—H15 | 0.9500 |
| O21—C26 | 1.421 (4) | C21—H21A | 0.9900 |
| N3—N4 | 1.392 (3) | C21—H21B | 0.9900 |
| N3—C2 | 1.283 (3) | C22—H22A | 0.9900 |
| N4—C4 | 1.473 (3) | C22—H22B | 0.9900 |
| N4—C5 | 1.339 (3) | C23—H23A | 0.9900 |
| N11—C12 | 1.343 (3) | C23—H23B | 0.9900 |
| N11—C16 | 1.347 (3) | C25—H25A | 0.9900 |
| N13—C12 | 1.323 (3) | C25—H25B | 0.9900 |
| N13—C14 | 1.347 (3) | C26—H26A | 0.9900 |
| N24—C4 | 1.435 (3) | C26—H26B | 0.9900 |
| N24—C23 | 1.464 (3) | C41—H41A | 0.9800 |
| N24—C25 | 1.467 (4) | C41—H41B | 0.9800 |
| C2—C21 | 1.476 (3) | C41—H41C | 0.9800 |
| C14—C15 | 1.389 (4) | C61—H61A | 0.9800 |
| C14—C41 | 1.497 (4) | C61—H61B | 0.9800 |
| C15—C16 | 1.382 (4) | C61—H61C | 0.9800 |
| S5···N3$^{i}$ | 3.331 (2) | C23···C5 | 3.519 (3) |
| S5···C21$^{i}$ | 3.632 (2) | C25···N3 | 3.197 (3) |
| S5···C23 | 3.676 (2) | C26···C61$^{x}$ | 3.547 (4) |
| S5···C2$^{ii}$ | 3.521 (2) | C61···C26$^{xi}$ | 3.547 (4) |
| S5···N3$^{ii}$ | 3.496 (2) | C4···H15$^{ix}$ | 3.0400 |
| S21···O1 | 3.1542 (16) | C4···H41B$^{ix}$ | 3.0400 |
| S5···H21B$^{i}$ | 2.8400 | C5···H23A | 3.0400 |
| S5···H4B | 2.9500 | C14···H61A$^{viii}$ | 3.1000 |
| S5···H22B$^{iii}$ | 3.0400 | C22···H21A$^{v}$ | 3.0500 |
| S21···H4A$^{iv}$ | 3.1700 | C26···H61A$^{x}$ | 3.0500 |
| S21···H4B$^{ii}$ | 3.0800 | H4A···H15$^{ix}$ | 2.3600 |
| S21···H25A$^{iv}$ | 2.9900 | H4A···H25A | 2.4200 |
| O1···S21 | 3.1542 (16) | H4A···S21$^{iv}$ | 3.1700 |
| O1···N4 | 2.155 (2) | H4A···H21B$^{iv}$ | 2.5800 |
| O1···O21$^{v}$ | 3.010 (2) | H4B···S5 | 2.9500 |
| O21···N24 | 2.838 (3) | H4B···H23B | 2.3700 |
| O21···O1$^{v}$ | 3.010 (2) | H4B···S21$^{ii}$ | 3.0800 |
| O21···N3$^{v}$ | 3.190 (3) | H15···C4$^{xii}$ | 3.0400 |
| O21···C2$^{v}$ | 2.938 (3) | H15···H4A$^{xii}$ | 2.3600 |

| | | | |
|---|---|---|---|
| O21···C5$^{v}$ | 3.274 (3) | H15···H41B | 2.4800 |
| N3···S5$^{vi}$ | 3.331 (2) | H15···H61B | 2.5800 |
| N3···O1 | 2.220 (3) | H21A···N13 | 2.2800 |
| N3···N24 | 3.281 (3) | H21A···C22$^{v}$ | 3.0500 |
| N3···C25 | 3.197 (3) | H21B···S5$^{vi}$ | 2.8400 |
| N3···S5$^{ii}$ | 3.496 (2) | H21B···H4A$^{iv}$ | 2.5800 |
| N3···O21$^{v}$ | 3.190 (3) | H22A···H26B | 2.3900 |
| N4···O1 | 2.155 (2) | H22B···S5$^{iii}$ | 3.0400 |
| N24···O21 | 2.838 (3) | H23A···N4 | 2.8100 |
| N24···N3 | 3.281 (3) | H23A···C5 | 3.0400 |
| N3···H25B | 2.7400 | H23A···H25B | 2.4600 |
| N4···H25B | 2.7400 | H23A···H25B$^{v}$ | 2.5300 |
| N4···H23A | 2.8100 | H23B···H4B | 2.3700 |
| N11···H41A$^{vii}$ | 2.8800 | H25A···H4A | 2.4200 |
| N13···H61A$^{viii}$ | 2.8400 | H25A···S21$^{iv}$ | 2.9900 |
| N13···H21A | 2.2800 | H25B···N3 | 2.7400 |
| N24···H41B$^{ix}$ | 2.8800 | H25B···N4 | 2.7400 |
| C2···S5$^{ii}$ | 3.521 (2) | H25B···H23A | 2.4600 |
| C2···O21$^{v}$ | 2.938 (3) | H25B···H23A$^{v}$ | 2.5300 |
| C5···O21$^{v}$ | 3.274 (3) | H26B···H22A | 2.3900 |
| C5···C23 | 3.519 (3) | H41A···N11$^{vii}$ | 2.8800 |
| C5···C5$^{ii}$ | 3.476 (3) | H41B···N24$^{xii}$ | 2.8800 |
| C12···C15$^{viii}$ | 3.538 (4) | H41B···C4$^{xii}$ | 3.0400 |
| C12···C14$^{vii}$ | 3.428 (3) | H41B···H15 | 2.4800 |
| C14···C12$^{vii}$ | 3.428 (3) | H41C···H61A$^{viii}$ | 2.5100 |
| C14···C16$^{viii}$ | 3.436 (3) | H61A···C26$^{xi}$ | 3.0500 |
| C15···C12$^{viii}$ | 3.538 (4) | H61A···N13$^{viii}$ | 2.8400 |
| C16···C14$^{viii}$ | 3.436 (3) | H61A···C14$^{viii}$ | 3.1000 |
| C21···S5$^{vi}$ | 3.632 (2) | H61A···H41C$^{viii}$ | 2.5100 |
| C23···S5 | 3.676 (2) | H61B···H15 | 2.5800 |
| C12—S21—C21 | 101.70 (10) | C14—C15—H15 | 121.00 |
| C2—O1—C5 | 105.80 (17) | C16—C15—H15 | 121.00 |
| C22—O21—C26 | 110.5 (2) | S21—C21—H21A | 109.00 |
| N4—N3—C2 | 103.32 (19) | S21—C21—H21B | 109.00 |
| N3—N4—C4 | 120.00 (18) | C2—C21—H21A | 109.00 |
| N3—N4—C5 | 111.76 (17) | C2—C21—H21B | 109.00 |
| C4—N4—C5 | 128.0 (2) | H21A—C21—H21B | 108.00 |
| C12—N11—C16 | 115.25 (19) | O21—C22—H22A | 109.00 |
| C12—N13—C14 | 116.15 (19) | O21—C22—H22B | 109.00 |
| C4—N24—C23 | 114.03 (19) | C23—C22—H22A | 109.00 |
| C4—N24—C25 | 113.83 (18) | C23—C22—H22B | 109.00 |
| C23—N24—C25 | 110.01 (18) | H22A—C22—H22B | 108.00 |
| O1—C2—N3 | 113.6 (2) | N24—C23—H23A | 110.00 |
| O1—C2—C21 | 119.51 (18) | N24—C23—H23B | 110.00 |

| | | | |
|---|---|---|---|
| N3—C2—C21 | 126.8 (2) | C22—C23—H23A | 110.00 |
| N4—C4—N24 | 115.98 (17) | C22—C23—H23B | 110.00 |
| S5—C5—O1 | 123.87 (16) | H23A—C23—H23B | 108.00 |
| S5—C5—N4 | 130.65 (18) | N24—C25—H25A | 110.00 |
| O1—C5—N4 | 105.47 (18) | N24—C25—H25B | 110.00 |
| S21—C12—N11 | 111.36 (15) | C26—C25—H25A | 110.00 |
| S21—C12—N13 | 120.50 (17) | C26—C25—H25B | 110.00 |
| N11—C12—N13 | 128.1 (2) | H25A—C25—H25B | 108.00 |
| N13—C14—C15 | 120.4 (2) | O21—C26—H26A | 109.00 |
| N13—C14—C41 | 116.6 (2) | O21—C26—H26B | 109.00 |
| C15—C14—C41 | 123.0 (2) | C25—C26—H26A | 109.00 |
| C14—C15—C16 | 118.9 (2) | C25—C26—H26B | 109.00 |
| N11—C16—C15 | 121.1 (2) | H26A—C26—H26B | 108.00 |
| N11—C16—C61 | 116.7 (2) | C14—C41—H41A | 109.00 |
| C15—C16—C61 | 122.1 (2) | C14—C41—H41B | 109.00 |
| S21—C21—C2 | 113.27 (15) | C14—C41—H41C | 109.00 |
| O21—C22—C23 | 111.6 (3) | H41A—C41—H41B | 109.00 |
| N24—C23—C22 | 109.2 (2) | H41A—C41—H41C | 109.00 |
| N24—C25—C26 | 109.3 (2) | H41B—C41—H41C | 110.00 |
| O21—C26—C25 | 111.0 (2) | C16—C61—H61A | 109.00 |
| N4—C4—H4A | 108.00 | C16—C61—H61B | 109.00 |
| N4—C4—H4B | 108.00 | C16—C61—H61C | 109.00 |
| N24—C4—H4A | 108.00 | H61A—C61—H61B | 109.00 |
| N24—C4—H4B | 108.00 | H61A—C61—H61C | 109.00 |
| H4A—C4—H4B | 107.00 | H61B—C61—H61C | 109.00 |
| C21—S21—C12—N11 | −176.28 (17) | C12—N11—C16—C15 | 0.8 (3) |
| C21—S21—C12—N13 | 3.9 (2) | C12—N11—C16—C61 | 179.8 (2) |
| C12—S21—C21—C2 | −113.85 (17) | C14—N13—C12—S21 | 178.84 (17) |
| C5—O1—C2—N3 | −0.9 (2) | C14—N13—C12—N11 | −0.9 (4) |
| C5—O1—C2—C21 | 177.15 (18) | C12—N13—C14—C15 | −0.1 (3) |
| C2—O1—C5—S5 | 179.02 (16) | C12—N13—C14—C41 | 180.0 (2) |
| C2—O1—C5—N4 | 0.4 (2) | C23—N24—C4—N4 | −67.3 (3) |
| C26—O21—C22—C23 | 58.3 (3) | C25—N24—C4—N4 | 60.1 (3) |
| C22—O21—C26—C25 | −58.4 (3) | C4—N24—C23—C22 | −173.3 (2) |
| C2—N3—N4—C4 | −175.71 (18) | C25—N24—C23—C22 | 57.4 (3) |
| C2—N3—N4—C5 | −0.7 (2) | C4—N24—C25—C26 | 172.7 (2) |
| N4—N3—C2—O1 | 1.0 (2) | C23—N24—C25—C26 | −57.9 (3) |
| N4—N3—C2—C21 | −176.9 (2) | O1—C2—C21—S21 | 51.9 (2) |
| N3—N4—C4—N24 | −86.7 (2) | N3—C2—C21—S21 | −130.3 (2) |
| C5—N4—C4—N24 | 99.1 (3) | N13—C14—C15—C16 | 1.4 (4) |
| N3—N4—C5—S5 | −178.33 (17) | C41—C14—C15—C16 | −178.7 (3) |
| N3—N4—C5—O1 | 0.1 (2) | C14—C15—C16—N11 | −1.7 (4) |
| C4—N4—C5—S5 | −3.8 (3) | C14—C15—C16—C61 | 179.4 (2) |
| C4—N4—C5—O1 | 174.69 (18) | O21—C22—C23—N24 | −57.6 (3) |
| C16—N11—C12—S21 | −179.21 (17) | N24—C25—C26—O21 | 58.4 (3) |
| C16—N11—C12—N13 | 0.6 (4) | | |

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*, −*y*+1, −*z*+1; (v) −*x*, −*y*, −*z*+1; (vi) *x*−1, *y*, *z*; (vii) −*x*, −*y*+1, −*z*+2; (viii) −*x*+1, −*y*+1, −*z*+2; (ix) *x*, *y*, *z*−1; (x) *x*−1, *y*−1, *z*−1; (xi) *x*+1, *y*+1, *z*+1; (xii) *x*, *y*, *z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C21—H21A···N13 | 0.99 | 2.28 | 2.883 (3) | 118 |
| C21—H21B···S5$^{vi}$ | 0.99 | 2.84 | 3.632 (2) | 137 |

Symmetry codes: (vi) *x*−1, *y*, *z*.

**Fig. 1**

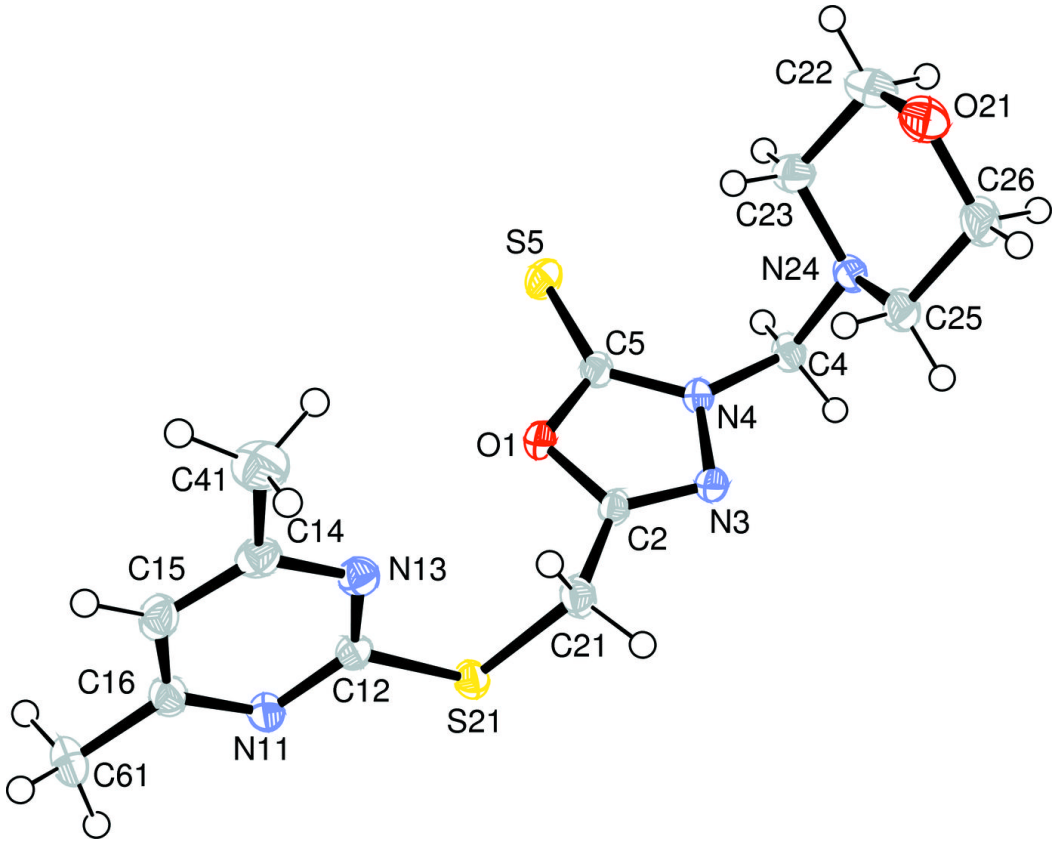
C22
O21
C26
C23
S5
N24
C25
C5
C4
N4
O1
N3
C41
C2
C14
C15
N13
C21
C16
C12
S21
N11
C61

**Fig. 2**