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# *N*-(2,6-Dimethylphenyl)-2-(2-{3-[4-(methylsulfonyl)phenyl]-1,2,4-oxadiazol-5-yl}phenoxy)acetamide

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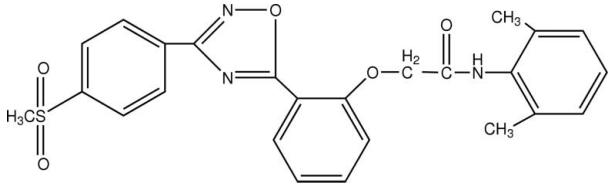
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.075; $wR$ factor = 0.178; data-to-parameter ratio = 16.4.

In the title compound, $C_{25}H_{23}N_3O_5S$, a bifurcated intramolecular N—H···O,N hydrogen bond helps to establish the molecular conformation. The dihedral angles between the oxadiazole ring and its adjacent benzene rings are 24.50 (19) and 12.20 (18)°.

## Related literature

For related literature, see: Romero (2001); Terashita *et al.* (2002).



## Experimental

### *Crystal data*

$C_{25}H_{23}N_3O_5S$
$M_r$ = 477.52
Monoclinic, $C2/c$
$a$ = 28.848 (6) Å
$b$ = 13.648 (3) Å
$c$ = 13.562 (3) Å
$\beta$ = 117.58 (3)°
$V$ = 4733 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 293 (2) K
0.20 × 0.10 × 0.10 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.979, $T_{max}$ = 0.983
4737 measured reflections
4643 independent reflections
3927 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047
3 standard reflections
every 200 reflections
intensity decay: none

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.178
$S$ = 0.97
4643 reflections
283 parameters
146 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$A$···O4 | 0.86 | 2.14 | 2.556 (5) | 109 |
| N3—H3$A$···N2 | 0.86 | 2.43 | 3.288 (5) | 176 |
| C3—H3$B$···O2 | 0.93 | 2.59 | 2.946 (7) | 103 |
| C6—H6$A$···N2 | 0.93 | 2.56 | 2.901 (5) | 102 |
| C14—H14$A$···O2$^{i}$ | 0.93 | 2.54 | 3.429 (7) | 160 |
| C16—H16$A$···O2$^{i}$ | 0.97 | 2.57 | 3.310 (6) | 133 |
| C25—H25$A$···N3 | 0.96 | 2.41 | 2.883 (6) | 110 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2487).

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# supplementary materials

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# *N*-(2,6-Dimethylphenyl)-2-(2-{3-[4-(methylsulfonyl)phenyl]-1,2,4-oxadiazol-5-yl}phenoxy)acetamide

**H.-B. Wang, J. Yin and Z.-T. Xing**

## Comment

1,2,4-Oxadiazole derivatives possess biological properties such as intrinsic analgesic (Terashita *et al.*, 2002) and antipicornaviral (Romero, 2001) effects. As part of out studies in this area, we report here the synthesis and crystal structure of the title compound, (I), (Fig. 1).

The dihedral angles between the N1/O1/C9/N2/C8 ring and its adjacent bezene rings are 24.50 (19) and 12.20 (18)° for the C2 and C10 rings, respectively.

An intramolecular, bifurcated N—H···(N,*O*) hydrogen bond (Table 1) helps to establish the molecular conformation of (I). Some short C—H···O and C—H···N contacts are also present.

## Experimental

2-Chloro-*N*-(2,6-dimethylphenyl)acetamide (10 mmol) was dissolved in acetone (100 ml) and potassium carbonate (15 mmol) was added. Then, 5-(2-hydroxyphenyl)-3-(4-methylsulfonyl)-phenyl-1,2,4-oxadiazole (10 mmol) was added to the reaction. The resulting mixture was refluxed for 12 h. After cooling and filtering, the crude title compound was obtained and purified by recrystalization from ethyl acetate. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

## Refinement

All H atoms were placed geometrically (N—H = 0.86 Å, C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(carrier) or 1.5$U_{eq}$(methyl carrier).

## Figures

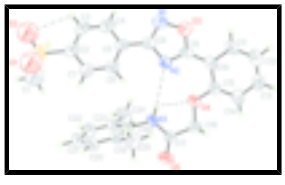


Fig. 1. A view of the molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). Dashed lines indicate the hydrogen bonds.

## *N*-(2,6-Dimethylphenyl)- 2-(2-{3-[4-(methylsulfonyl)phenyl]-1,2,4-oxadiazol-5-yl}phenoxy)acetamide

*Crystal data*

$C_{25}H_{23}N_3O_5S$ $F_{000}$ = 2000

| | |
|---|---|
| $M_r$ = 477.52 | $D_x$ = 1.340 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 25 reflections |
| *a* = 28.848 (6) Å | θ = 9–12º |
| *b* = 13.648 (3) Å | μ = 0.18 mm$^{-1}$ |
| *c* = 13.562 (3) Å | *T* = 293 (2) K |
| β = 117.58 (3)º | Block, colourless |
| *V* = 4733 (2) Å$^3$ | 0.20 × 0.10 × 0.10 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | $R_{int}$ = 0.047 |
| Radiation source: fine-focus sealed tube | $\theta_{max}$ = 26.0º |
| Monochromator: graphite | $\theta_{min}$ = 1.6º |
| *T* = 293(2) K | *h* = −35→31 |
| ω/2θ scans | *k* = 0→16 |
| Absorption correction: ψ scan (North *et al.*, 1968) | *l* = 0→16 |
| $T_{min}$ = 0.979, $T_{max}$ = 0.983 | 3 standard reflections |
| 4737 measured reflections | every 200 reflections |
| 4643 independent reflections | intensity decay: none |
| 3927 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.075 | H-atom parameters constrained |
| $wR(F^2)$ = 0.178 | $w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 0.97 | $(\Delta/\sigma)_{max} < 0.001$ |
| 4643 reflections | $\Delta\rho_{max}$ = 0.34 e Å$^{-3}$ |
| 283 parameters | $\Delta\rho_{min}$ = −0.39 e Å$^{-3}$ |
| 146 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S | 0.14194 (6) | 0.18555 (9) | 0.81078 (14) | 0.0925 (5) |
| O1 | 0.16502 (17) | 0.1933 (3) | 0.9251 (4) | 0.126 |
| O2 | 0.11504 (16) | 0.1004 (3) | 0.7585 (4) | 0.125 |
| O3 | −0.06215 (11) | 0.6306 (2) | 0.5510 (2) | 0.060 |
| O4 | 0.06199 (10) | 0.8113 (2) | 0.6481 (3) | 0.0673 (9) |
| O5 | 0.19856 (11) | 0.8304 (2) | 0.7637 (3) | 0.0934 (13) |
| N1 | −0.04744 (14) | 0.5304 (3) | 0.5690 (3) | 0.0643 (11) |
| N2 | 0.02244 (12) | 0.6304 (2) | 0.6536 (3) | 0.0453 (9) |
| N3 | 0.14383 (11) | 0.7053 (2) | 0.7465 (3) | 0.0481 (9) |
| H3A | 0.1118 | 0.6884 | 0.7242 | 0.058* |
| C1 | 0.1908 (2) | 0.2025 (4) | 0.7674 (5) | 0.108 |
| H1C | 0.2148 | 0.1485 | 0.7927 | 0.163* |
| H1D | 0.2094 | 0.2624 | 0.7983 | 0.163* |
| H1E | 0.1747 | 0.2059 | 0.6877 | 0.163* |
| C2 | 0.10088 (18) | 0.2876 (3) | 0.7563 (4) | 0.0582 (12) |
| C3 | 0.04852 (19) | 0.2760 (3) | 0.6783 (4) | 0.0619 (13) |
| H3B | 0.0351 | 0.2137 | 0.6536 | 0.074* |
| C4 | 0.01671 (17) | 0.3567 (3) | 0.6378 (4) | 0.0615 (12) |
| H4A | −0.0183 | 0.3489 | 0.5867 | 0.074* |
| C5 | 0.03657 (15) | 0.4475 (3) | 0.6726 (3) | 0.0446 (10) |
| C6 | 0.08838 (15) | 0.4603 (3) | 0.7502 (3) | 0.0514 (11) |
| H6A | 0.1015 | 0.5231 | 0.7731 | 0.062* |
| C7 | 0.12050 (17) | 0.3807 (3) | 0.7934 (4) | 0.0640 (13) |
| H7A | 0.1551 | 0.3891 | 0.8469 | 0.077* |
| C8 | 0.00352 (17) | 0.5356 (3) | 0.6299 (3) | 0.0468 (10) |
| C9 | −0.01894 (15) | 0.6851 (3) | 0.6063 (3) | 0.0463 (10) |
| C10 | −0.02598 (14) | 0.7885 (3) | 0.5990 (3) | 0.0460 (10) |
| C11 | −0.07551 (15) | 0.8299 (3) | 0.5674 (4) | 0.0607 (12) |
| H11A | −0.1043 | 0.7892 | 0.5476 | 0.073* |
| C12 | −0.08211 (19) | 0.9311 (4) | 0.5653 (4) | 0.0719 (14) |
| H12A | −0.1153 | 0.9575 | 0.5423 | 0.086* |
| C13 | −0.04122 (19) | 0.9897 (3) | 0.5960 (4) | 0.0657 (13) |
| H13A | −0.0456 | 1.0569 | 0.5992 | 0.079* |
| C14 | 0.00762 (17) | 0.9529 (3) | 0.6232 (3) | 0.0576 (12) |
| H14A | 0.0354 | 0.9958 | 0.6411 | 0.069* |
| C15 | 0.01587 (15) | 0.8543 (3) | 0.6243 (3) | 0.0459 (10) |
| C16 | 0.10881 (14) | 0.8666 (3) | 0.6885 (4) | 0.0538 (11) |
| H16A | 0.1104 | 0.9126 | 0.7446 | 0.065* |
| H16B | 0.1095 | 0.9037 | 0.6281 | 0.065* |
| C17 | 0.15441 (16) | 0.7993 (3) | 0.7373 (4) | 0.0529 (12) |

| | | | | |
|---|---|---|---|---|
| C18 | 0.18426 (14) | 0.6307 (3) | 0.7926 (3) | 0.0416 (9) |
| C19 | 0.20946 (14) | 0.6160 (3) | 0.9060 (3) | 0.0478 (10) |
| C20 | 0.24727 (16) | 0.5436 (3) | 0.9441 (4) | 0.0659 (13) |
| H20A | 0.2655 | 0.5334 | 1.0205 | 0.079* |
| C21 | 0.25960 (16) | 0.4870 (3) | 0.8786 (4) | 0.0641 (13) |
| H21A | 0.2854 | 0.4392 | 0.9087 | 0.077* |
| C22 | 0.23276 (17) | 0.5023 (3) | 0.7657 (4) | 0.0633 (12) |
| H22A | 0.2398 | 0.4620 | 0.7189 | 0.076* |
| C23 | 0.19522 (15) | 0.5760 (3) | 0.7186 (4) | 0.0502 (11) |
| C24 | 0.16793 (17) | 0.5935 (4) | 0.5952 (4) | 0.0819 (16) |
| H24A | 0.1800 | 0.5468 | 0.5593 | 0.123* |
| H24B | 0.1754 | 0.6586 | 0.5799 | 0.123* |
| H24C | 0.1309 | 0.5862 | 0.5676 | 0.123* |
| C25 | 0.19565 (17) | 0.6755 (3) | 0.9839 (4) | 0.0660 (13) |
| H25A | 0.1686 | 0.7216 | 0.9413 | 0.099* |
| H25B | 0.2261 | 0.7102 | 1.0363 | 0.099* |
| H25C | 0.1836 | 0.6323 | 1.0231 | 0.099* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S | 0.1070 (12) | 0.0509 (8) | 0.0930 (12) | 0.0056 (8) | 0.0237 (10) | −0.0028 (8) |
| O1 | 0.126 | 0.126 | 0.126 | 0.000 | 0.059 | 0.000 |
| O2 | 0.125 | 0.125 | 0.125 | 0.000 | 0.058 | 0.000 |
| O3 | 0.060 | 0.060 | 0.060 | 0.000 | 0.028 | 0.000 |
| O4 | 0.0303 (15) | 0.0592 (18) | 0.104 (3) | 0.0045 (14) | 0.0243 (17) | 0.0019 (18) |
| O5 | 0.0352 (18) | 0.081 (2) | 0.139 (3) | −0.0110 (16) | 0.019 (2) | 0.033 (2) |
| N1 | 0.045 (2) | 0.066 (3) | 0.079 (3) | −0.0122 (19) | 0.026 (2) | −0.003 (2) |
| N2 | 0.0366 (19) | 0.051 (2) | 0.047 (2) | 0.0039 (17) | 0.0183 (17) | 0.0049 (17) |
| N3 | 0.0237 (17) | 0.054 (2) | 0.063 (2) | 0.0083 (15) | 0.0174 (17) | 0.0154 (18) |
| C1 | 0.108 | 0.108 | 0.108 | 0.000 | 0.050 | 0.000 |
| C2 | 0.071 (3) | 0.044 (2) | 0.060 (3) | −0.011 (2) | 0.031 (3) | −0.008 (2) |
| C3 | 0.082 (3) | 0.039 (2) | 0.064 (3) | −0.017 (2) | 0.033 (3) | −0.010 (2) |
| C4 | 0.064 (3) | 0.064 (3) | 0.048 (3) | −0.016 (2) | 0.019 (2) | −0.006 (2) |
| C5 | 0.045 (2) | 0.054 (2) | 0.039 (3) | −0.013 (2) | 0.023 (2) | 0.001 (2) |
| C6 | 0.049 (2) | 0.049 (2) | 0.054 (3) | −0.006 (2) | 0.022 (2) | −0.007 (2) |
| C7 | 0.062 (3) | 0.049 (2) | 0.068 (3) | −0.005 (2) | 0.019 (2) | 0.002 (2) |
| C8 | 0.052 (3) | 0.053 (3) | 0.044 (3) | −0.005 (2) | 0.029 (2) | 0.001 (2) |
| C9 | 0.036 (2) | 0.061 (3) | 0.047 (3) | −0.011 (2) | 0.024 (2) | −0.003 (2) |
| C10 | 0.041 (2) | 0.063 (3) | 0.032 (2) | 0.0101 (19) | 0.015 (2) | 0.009 (2) |
| C11 | 0.039 (2) | 0.072 (3) | 0.067 (3) | 0.013 (2) | 0.021 (2) | 0.009 (3) |
| C12 | 0.066 (3) | 0.077 (3) | 0.070 (4) | 0.026 (2) | 0.030 (3) | 0.010 (3) |
| C13 | 0.065 (3) | 0.056 (3) | 0.069 (3) | 0.022 (2) | 0.025 (3) | 0.020 (2) |
| C14 | 0.064 (3) | 0.059 (3) | 0.051 (3) | 0.017 (2) | 0.028 (2) | 0.013 (2) |
| C15 | 0.044 (2) | 0.054 (2) | 0.034 (2) | 0.0106 (19) | 0.013 (2) | 0.003 (2) |
| C16 | 0.043 (3) | 0.056 (3) | 0.054 (3) | −0.010 (2) | 0.016 (2) | 0.009 (2) |
| C17 | 0.043 (3) | 0.042 (2) | 0.056 (3) | −0.009 (2) | 0.007 (2) | 0.014 (2) |
| C18 | 0.032 (2) | 0.043 (2) | 0.046 (3) | −0.0009 (17) | 0.0154 (19) | 0.003 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C19 | 0.039 (2) | 0.057 (2) | 0.044 (3) | 0.0027 (19) | 0.017 (2) | 0.008 (2) |
| C20 | 0.049 (3) | 0.074 (3) | 0.065 (3) | 0.008 (2) | 0.018 (2) | 0.014 (3) |
| C21 | 0.045 (3) | 0.061 (3) | 0.077 (3) | 0.010 (2) | 0.020 (3) | 0.009 (3) |
| C22 | 0.062 (3) | 0.060 (3) | 0.075 (3) | 0.001 (2) | 0.038 (3) | −0.007 (3) |
| C23 | 0.044 (2) | 0.062 (3) | 0.049 (3) | −0.009 (2) | 0.026 (2) | 0.001 (2) |
| C24 | 0.065 (3) | 0.108 (4) | 0.060 (4) | 0.013 (3) | 0.018 (3) | −0.010 (3) |
| C25 | 0.073 (3) | 0.070 (3) | 0.069 (3) | 0.000 (3) | 0.045 (3) | 0.002 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S—O1 | 1.379 (5) | C10—C11 | 1.407 (5) |
| S—O2 | 1.395 (4) | C10—C15 | 1.413 (5) |
| S—C2 | 1.754 (4) | C11—C12 | 1.392 (6) |
| S—C1 | 1.777 (5) | C11—H11A | 0.9300 |
| O3—C9 | 1.343 (4) | C12—C13 | 1.322 (6) |
| O3—N1 | 1.420 (4) | C12—H12A | 0.9300 |
| O4—C15 | 1.349 (4) | C13—C14 | 1.375 (5) |
| O4—C16 | 1.417 (4) | C13—H13A | 0.9300 |
| O5—C17 | 1.228 (4) | C14—C15 | 1.366 (5) |
| N1—C8 | 1.313 (5) | C14—H14A | 0.9300 |
| N2—C9 | 1.298 (4) | C16—C17 | 1.486 (5) |
| N2—C8 | 1.383 (5) | C16—H16A | 0.9700 |
| N3—C17 | 1.337 (4) | C16—H16B | 0.9700 |
| N3—C18 | 1.453 (4) | C18—C19 | 1.378 (5) |
| N3—H3A | 0.8600 | C18—C23 | 1.399 (5) |
| C1—H1C | 0.9600 | C19—C20 | 1.382 (5) |
| C1—H1D | 0.9600 | C19—C25 | 1.524 (5) |
| C1—H1E | 0.9600 | C20—C21 | 1.343 (6) |
| C2—C7 | 1.388 (5) | C20—H20A | 0.9300 |
| C2—C3 | 1.395 (6) | C21—C22 | 1.375 (6) |
| C3—C4 | 1.374 (6) | C21—H21A | 0.9300 |
| C3—H3B | 0.9300 | C22—C23 | 1.398 (5) |
| C4—C5 | 1.356 (5) | C22—H22A | 0.9300 |
| C4—H4A | 0.9300 | C23—C24 | 1.502 (6) |
| C5—C6 | 1.384 (5) | C24—H24A | 0.9600 |
| C5—C8 | 1.476 (5) | C24—H24B | 0.9600 |
| C6—C7 | 1.371 (5) | C24—H24C | 0.9600 |
| C6—H6A | 0.9300 | C25—H25A | 0.9600 |
| C7—H7A | 0.9300 | C25—H25B | 0.9600 |
| C9—C10 | 1.422 (5) | C25—H25C | 0.9600 |
| O1—S—O2 | 120.0 (3) | C13—C12—H12A | 120.0 |
| O1—S—C2 | 107.0 (2) | C11—C12—H12A | 120.0 |
| O2—S—C2 | 109.8 (2) | C12—C13—C14 | 121.2 (4) |
| O1—S—C1 | 108.6 (3) | C12—C13—H13A | 119.4 |
| O2—S—C1 | 106.3 (3) | C14—C13—H13A | 119.4 |
| C2—S—C1 | 104.0 (2) | C15—C14—C13 | 120.9 (4) |
| C9—O3—N1 | 108.2 (3) | C15—C14—H14A | 119.5 |
| C15—O4—C16 | 121.3 (3) | C13—C14—H14A | 119.5 |
| C8—N1—O3 | 102.4 (3) | O4—C15—C14 | 125.3 (4) |

| | | | |
|---|---|---|---|
| C9—N2—C8 | 104.5 (3) | O4—C15—C10 | 114.8 (3) |
| C17—N3—C18 | 122.6 (3) | C14—C15—C10 | 119.9 (4) |
| C17—N3—H3A | 118.7 | O4—C16—C17 | 109.4 (3) |
| C18—N3—H3A | 118.7 | O4—C16—H16A | 109.8 |
| S—C1—H1C | 109.5 | C17—C16—H16A | 109.8 |
| S—C1—H1D | 109.5 | O4—C16—H16B | 109.8 |
| H1C—C1—H1D | 109.5 | C17—C16—H16B | 109.8 |
| S—C1—H1E | 109.5 | H16A—C16—H16B | 108.3 |
| H1C—C1—H1E | 109.5 | O5—C17—N3 | 123.7 (4) |
| H1D—C1—H1E | 109.5 | O5—C17—C16 | 120.1 (3) |
| C7—C2—C3 | 119.7 (4) | N3—C17—C16 | 116.2 (3) |
| C7—C2—S | 119.5 (3) | C19—C18—C23 | 123.0 (4) |
| C3—C2—S | 120.8 (3) | C19—C18—N3 | 119.1 (4) |
| C4—C3—C2 | 120.1 (4) | C23—C18—N3 | 117.9 (4) |
| C4—C3—H3B | 120.0 | C18—C19—C20 | 116.0 (4) |
| C2—C3—H3B | 120.0 | C18—C19—C25 | 121.6 (4) |
| C5—C4—C3 | 119.8 (4) | C20—C19—C25 | 122.4 (4) |
| C5—C4—H4A | 120.1 | C21—C20—C19 | 124.7 (5) |
| C3—C4—H4A | 120.1 | C21—C20—H20A | 117.7 |
| C4—C5—C6 | 120.9 (4) | C19—C20—H20A | 117.7 |
| C4—C5—C8 | 121.1 (4) | C20—C21—C22 | 117.7 (4) |
| C6—C5—C8 | 118.0 (4) | C20—C21—H21A | 121.2 |
| C7—C6—C5 | 120.2 (4) | C22—C21—H21A | 121.2 |
| C7—C6—H6A | 119.9 | C21—C22—C23 | 122.3 (4) |
| C5—C6—H6A | 119.9 | C21—C22—H22A | 118.8 |
| C6—C7—C2 | 119.3 (4) | C23—C22—H22A | 118.8 |
| C6—C7—H7A | 120.3 | C22—C23—C18 | 116.2 (4) |
| C2—C7—H7A | 120.3 | C22—C23—C24 | 121.2 (4) |
| N1—C8—N2 | 113.8 (4) | C18—C23—C24 | 122.6 (4) |
| N1—C8—C5 | 122.3 (4) | C23—C24—H24A | 109.5 |
| N2—C8—C5 | 123.8 (4) | C23—C24—H24B | 109.5 |
| N2—C9—O3 | 111.1 (3) | H24A—C24—H24B | 109.5 |
| N2—C9—C10 | 132.4 (4) | C23—C24—H24C | 109.5 |
| O3—C9—C10 | 116.4 (4) | H24A—C24—H24C | 109.5 |
| C11—C10—C15 | 116.8 (4) | H24B—C24—H24C | 109.5 |
| C11—C10—C9 | 120.8 (4) | C19—C25—H25A | 109.5 |
| C15—C10—C9 | 122.3 (3) | C19—C25—H25B | 109.5 |
| C12—C11—C10 | 121.0 (4) | H25A—C25—H25B | 109.5 |
| C12—C11—H11A | 119.5 | C19—C25—H25C | 109.5 |
| C10—C11—H11A | 119.5 | H25A—C25—H25C | 109.5 |
| C13—C12—C11 | 119.9 (4) | H25B—C25—H25C | 109.5 |
| C9—O3—N1—C8 | −2.3 (4) | C9—C10—C11—C12 | 176.9 (4) |
| O1—S—C2—C7 | 50.9 (4) | C10—C11—C12—C13 | −1.7 (7) |
| O2—S—C2—C7 | −177.3 (4) | C11—C12—C13—C14 | 4.4 (8) |
| C1—S—C2—C7 | −63.9 (4) | C12—C13—C14—C15 | −3.1 (7) |
| O1—S—C2—C3 | −127.6 (4) | C16—O4—C15—C14 | 8.1 (6) |
| O2—S—C2—C3 | 4.2 (5) | C16—O4—C15—C10 | −172.0 (4) |
| C1—S—C2—C3 | 117.6 (4) | C13—C14—C15—O4 | 178.8 (4) |
| C7—C2—C3—C4 | 0.5 (7) | C13—C14—C15—C10 | −1.0 (6) |

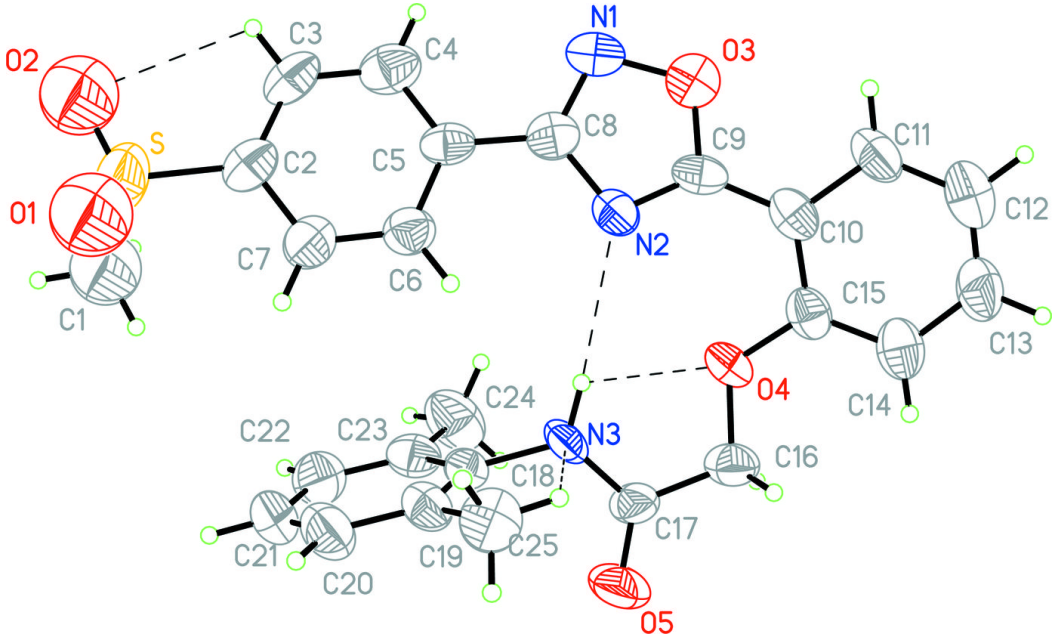
| | | | |
|---|---|---|---|
| S—C2—C3—C4 | 179.0 (4) | C11—C10—C15—O4 | −176.4 (4) |
| C2—C3—C4—C5 | 1.1 (7) | C9—C10—C15—O4 | 4.5 (6) |
| C3—C4—C5—C6 | −1.2 (7) | C11—C10—C15—C14 | 3.5 (6) |
| C3—C4—C5—C8 | 179.4 (4) | C9—C10—C15—C14 | −175.6 (4) |
| C4—C5—C6—C7 | −0.2 (6) | C15—O4—C16—C17 | 163.9 (4) |
| C8—C5—C6—C7 | 179.2 (4) | C18—N3—C17—O5 | 2.2 (7) |
| C5—C6—C7—C2 | 1.7 (7) | C18—N3—C17—C16 | −180.0 (4) |
| C3—C2—C7—C6 | −1.8 (7) | O4—C16—C17—O5 | 170.2 (4) |
| S—C2—C7—C6 | 179.6 (4) | O4—C16—C17—N3 | −7.7 (5) |
| O3—N1—C8—N2 | 0.9 (4) | C17—N3—C18—C19 | 86.6 (5) |
| O3—N1—C8—C5 | 178.2 (3) | C17—N3—C18—C23 | −94.3 (5) |
| C9—N2—C8—N1 | 0.9 (5) | C23—C18—C19—C20 | 0.6 (6) |
| C9—N2—C8—C5 | −176.4 (4) | N3—C18—C19—C20 | 179.7 (3) |
| C4—C5—C8—N1 | 9.5 (6) | C23—C18—C19—C25 | −178.6 (4) |
| C6—C5—C8—N1 | −169.9 (4) | N3—C18—C19—C25 | 0.4 (5) |
| C4—C5—C8—N2 | −173.5 (4) | C18—C19—C20—C21 | −1.6 (6) |
| C6—C5—C8—N2 | 7.1 (6) | C25—C19—C20—C21 | 177.7 (4) |
| C8—N2—C9—O3 | −2.4 (4) | C19—C20—C21—C22 | 0.1 (7) |
| C8—N2—C9—C10 | −179.3 (4) | C20—C21—C22—C23 | 2.5 (7) |
| N1—O3—C9—N2 | 3.1 (4) | C21—C22—C23—C18 | −3.3 (6) |
| N1—O3—C9—C10 | −179.5 (3) | C21—C22—C23—C24 | 177.7 (4) |
| N2—C9—C10—C11 | −163.6 (4) | C19—C18—C23—C22 | 1.7 (6) |
| O3—C9—C10—C11 | 19.6 (6) | N3—C18—C23—C22 | −177.4 (3) |
| N2—C9—C10—C15 | 15.4 (7) | C19—C18—C23—C24 | −179.3 (4) |
| O3—C9—C10—C15 | −161.4 (4) | N3—C18—C23—C24 | 1.6 (6) |
| C15—C10—C11—C12 | −2.2 (6) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3A···O4 | 0.86 | 2.14 | 2.556 (5) | 109 |
| N3—H3A···N2 | 0.86 | 2.43 | 3.288 (5) | 176 |
| C3—H3B···O2 | 0.93 | 2.59 | 2.946 (7) | 103 |
| C6—H6A···N2 | 0.93 | 2.56 | 2.901 (5) | 102 |
| C14—H14A···O2$^{i}$ | 0.93 | 2.54 | 3.429 (7) | 160 |
| C16—H16A···O2$^{i}$ | 0.97 | 2.57 | 3.310 (6) | 133 |
| C25—H25A···N3 | 0.96 | 2.41 | 2.883 (6) | 110 |

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

**Fig. 1**


O2
C3
C4
N1
O3
S
C2
C5
C8
C9
C11
O1
C7
C6
N2
C10
C12
C1
C15
C13
O4
C24
C14
C22
C23
N3
C16
C18
C17
C21
C19
C25
C20
O5