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N-[1-(5-Acetamido-3-acetyl-2-methyl-2,3-dihydro-1,3,4-thiadiazol-2-yl)-2-phenylethyl]acetamide

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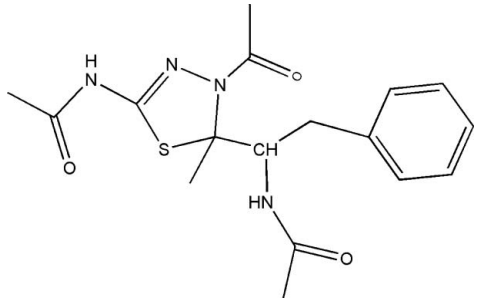
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.142; data-to-parameter ratio = 23.6.

In the title compound, $C_{17}H_{22}N_4O_3S$, the dihedral angle between the planes of the thiadiazole and phenyl rings is 63.47 (7)°. The dihedral angle between the thiadiazole ring and the acetamide side chain is 7.72 (9)°. Molecules related by a 2_1 screw axis along the *a* axis are linked by intermolecular N—H···O hydrogen bonds generating a supramolecular chain.

Related literature

For related literature, see: Allen *et al.* (1987); Bhat *et al.* (1967); Castro *et al.* (1996); Nakagawa *et al.* (1996); Tehranchian *et al.* (2005); Wang *et al.* (1999, 2004).



Experimental

Crystal data

$C_{17}H_{22}N_4O_3S$
M_r = 362.46
Orthorhombic, *Pbca*
a = 18.3623 (9) Å
b = 14.1565 (7) Å
c = 14.1386 (7) Å
V = 3675.3 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 293 (2) K
0.26 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.949, T_{max} = 0.965
81394 measured reflections
5439 independent reflections
3358 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.142
S = 1.08
5439 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O1^{i}	0.87	1.96	2.809 (2)	166

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT-NT* (Bruker, 2004); data reduction: *SAINT-NT* and *XPREP* (Bruker, 2004); 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 set was collected at SAIF (IIT, Chennai), a facility funded by the Department of Science and Technology (New Delhi), India.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GD2020).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, S1–19.
Bhat, A. K., Bharmaria, R. P. & Bellare, R. A. (1967). *Indian J. Chem.* **5**, 1279–1282.
Bruker (2004). *APEX2* (Version 1.22), *SAINT-NT* (Version 6.0), *SADABS* (Version 2004/1) and *XPREP* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Castro, J. L., Ball, R. G., Broughton, H. B., Russell, M. G. N., Rathbone, D., Watt, A. P., Baker, R., Chapman, K. L., Fletcher, A. E., Patel, S., Smith, A. J., Marshall, G. R., Ryecroft, W. & Matassa, V. G. (1996). *J. Med. Chem.* **39**, 842–848.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Nakagawa, Y., Nishimura, K., Izumi, K., Kinoshita, K., Kimura, T., Kurihara, N. & Fujita, T. (1996). *J. Pestic. Sci.* **21**, 195–201.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Tehranchian, S., Akbarzadeh, T., Fazeli, R. M., Jamlifar, H. & Shafiee, A. (2005). *Bioorg. Med. Chem. Lett.* **15**, 1023–1025.
Wang, Y.-G., Cao, L., Yang, J., Ye, W.-F., Zhou, Q.-C. & Lu, B.-X. (1999). *Chem. J. Chin. Univ.* **20**, 1903–1905.
Wang, Y. G., Wang, Z. Y., Zhao, X. Y. & Song, X. J. (2004). *Chin. J. Org. Chem.* **24**, 1606–1609.

supplementary materials

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N-[1-(5-Acetamido-3-acetyl-2-methyl-2,3-dihydro-1,3,4-thiadiazol-2-yl)-2-phenylethyl]acetamide

P. Sakthivel, P. S. Joseph, P. T. Muthiah, K. Sethusankar and S. Thennarasu

Comment

Comment Thiadiazoles and their derivatives represent a group of compounds possessing a wide spectrum of biological activities such as hypoglycemic, antitubercular, antifungal and antibacterial properties (Bhat *et al.*, 1967).

1,3,4-Thiadiazole derivatives are known to display a broad spectrum of pesticidal activity (Nakagawa *et al.*, 1996; Castro & Ball, 1996 Wang *et al.*, 1999, 2004).

Thiadiazole derivatives are known to exhibit high antibacterial activity against Staphylococcus aureus (Tehranchaian *et al.*, 2005).

In the title compound (I), the thiadiazole ring adopts an mild envelop conformation with atom C11 at the flap position. C11 deviates from the mean planes through the other four atoms by 0.085 Å.

The molecular structure of (I) is shown in Fig 1. and selected geometric parameters are listed in Table 1. The bond lengths for C—S, C=N and N—N are within normal ranges (Allen *et al.*, 1987). All the bondlengths and angles in (I) are as expected (Table 1). The dihedral angle between 1,3,4 thiadiazole ring and the phenyl ring is 63.47°. The dihedral angle between thiadiazole ring and the acetamide side chain(N4/C16/O3/C17) is 7.72°.

The molecules related by 2_1 screw along *a* axis (Fig 2)are linked by intermolecular N—H.·O hydrogen bond (Table 1) generating a supramolecular chain.

Experimental

A mixture of powdered thiosemicarbazone (3.0 mmol, acetic hydride(0.5 ml) and pyridine(2.5 ml) was taken in a round bottom flask and heated on a water bath for 3hrs. The reaction mixture was evaporated under reduced pressure and diluted in methanol. The viscous liquid obtained was allowed to stand overnight. The colour less precipitate formed was seperated by filteration and crystalized in methanol.

Refinement

All the hydrogen atoms were geometrically fixed and allowed to ride on their parent atoms with C—H = 0.86 − 0.97 Å, and U_{iso} = 1.5$_{eq}$(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms.

Figures

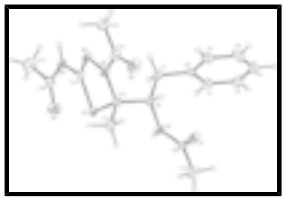

Fig. 1. The molecuar structure and labelling scheme for (I) with displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

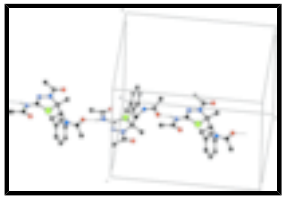

Fig. 2. A packing diagram for (I) is shown. Dashed line indicates intermolecular hydrogen bonding interactions. [Symmetry code: (i) −*x* + 1/2, −*y* + 1/2, −*z* + 1

N-[1-(5-Acetamido-3-acetyl-2-methyl-2,3-dihydro-1,3,4-thiadiazol-2-yl)-2-phenylethyl]acetamide

Crystal data

$C_{17}H_{22}N_4O_3S$	F_{000} = 1536
M_r = 362.46	D_x = 1.310 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 9035 reflections
a = 18.3623 (9) Å	θ = 2.2–26.3º
b = 14.1565 (7) Å	μ = 0.20 mm^{-1}
c = 14.1386 (7) Å	*T* = 293 (2) K
V = 3675.3 (3) Å^3	Block, colourless
Z = 8	0.26 × 0.22 × 0.18 mm

Data collection

Bruker AXS (Kappa Apex2) diffractometer	5439 independent reflections
Radiation source: fine focus sealed tube	3358 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 293(2) K	θ_{max} = 30.2º
ω and φ scan	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2004)	*h* = −25→25
T_{min} = 0.949, T_{max} = 0.965	*k* = −19→19
81394 measured reflections	*l* = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.142$	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 1.6574P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
5439 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
230 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
S1	0.04506 (3)	0.14250 (4)	0.37866 (4)	0.0480 (2)
O1	0.26773 (7)	0.31882 (13)	0.50299 (11)	0.0618 (6)
O2	0.11963 (8)	0.15943 (13)	0.68677 (12)	0.0696 (6)
O3	−0.06481 (10)	0.11352 (16)	0.25369 (12)	0.0888 (8)
N1	0.16783 (7)	0.29087 (11)	0.41582 (11)	0.0401 (5)
N2	0.04313 (8)	0.14086 (11)	0.56343 (11)	0.0422 (5)
N3	−0.02981 (8)	0.13470 (11)	0.53490 (11)	0.0401 (5)
N4	−0.10278 (8)	0.13086 (11)	0.40394 (11)	0.0421 (5)
C1	0.09604 (11)	0.50438 (15)	0.46158 (15)	0.0524 (7)
C2	0.12526 (14)	0.59118 (18)	0.4846 (2)	0.0698 (9)
C3	0.14873 (14)	0.6084 (2)	0.5741 (3)	0.0777 (12)
C4	0.14151 (15)	0.5396 (2)	0.6414 (2)	0.0784 (10)
C5	0.11216 (12)	0.45324 (18)	0.61921 (15)	0.0582 (8)
C6	0.08915 (9)	0.43394 (13)	0.52857 (12)	0.0388 (5)
C7	0.05980 (10)	0.33795 (14)	0.50539 (14)	0.0432 (6)
C8	0.12175 (9)	0.26612 (13)	0.49578 (13)	0.0379 (5)
C9	0.23630 (9)	0.32101 (14)	0.42653 (14)	0.0437 (6)
C10	0.27272 (13)	0.35813 (19)	0.33969 (17)	0.0669 (9)
C11	0.09697 (9)	0.16235 (13)	0.48823 (14)	0.0413 (6)
C12	0.16144 (11)	0.09402 (16)	0.49016 (19)	0.0620 (8)
C13	0.05799 (11)	0.14390 (15)	0.65799 (15)	0.0495 (6)
C14	−0.00481 (13)	0.1274 (2)	0.72238 (15)	0.0648 (9)
C15	−0.03488 (9)	0.13573 (12)	0.44545 (13)	0.0364 (5)
C16	−0.11462 (12)	0.11840 (17)	0.30958 (15)	0.0548 (7)

C17	−0.19294 (14)	0.1094 (2)	0.28282 (19)	0.0813 (10)
H1	0.08074	0.49312	0.39990	0.0629*
H1A	0.14921	0.29688	0.36249	0.0481*
H2	0.12890	0.63805	0.43878	0.0836*
H3	0.16948	0.66629	0.58949	0.0933*
H4	0.15670	0.55149	0.70300	0.0939*
H4A	−0.14116	0.13831	0.43907	0.0506*
H5	0.10777	0.40730	0.66588	0.0698*
H7A	0.02674	0.31781	0.55496	0.0519*
H7B	0.03266	0.34086	0.44660	0.0519*
H8	0.15177	0.27133	0.55285	0.0454*
H10A	0.31957	0.32885	0.33275	0.1004*
H10B	0.24330	0.34413	0.28534	0.1004*
H10C	0.27870	0.42528	0.34516	0.1004*
H12A	0.18898	0.10360	0.54708	0.0929*
H12B	0.14379	0.03021	0.48833	0.0929*
H12C	0.19204	0.10534	0.43629	0.0929*
H14A	0.01262	0.11865	0.78579	0.0971*
H14B	−0.03685	0.18095	0.72041	0.0971*
H14C	−0.03073	0.07196	0.70249	0.0971*
H17A	−0.19782	0.11564	0.21550	0.1219*
H17B	−0.21082	0.04870	0.30220	0.1219*
H17C	−0.22058	0.15813	0.31353	0.1219*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0386 (2)	0.0586 (3)	0.0467 (3)	−0.0125 (2)	0.0111 (2)	−0.0109 (2)
O1	0.0318 (7)	0.0912 (12)	0.0624 (9)	−0.0136 (7)	−0.0069 (6)	0.0129 (8)
O2	0.0470 (8)	0.0966 (13)	0.0652 (10)	−0.0142 (8)	−0.0205 (7)	0.0162 (9)
O3	0.0711 (12)	0.1449 (19)	0.0504 (9)	−0.0258 (12)	0.0057 (9)	−0.0311 (11)
N1	0.0303 (7)	0.0464 (9)	0.0436 (8)	−0.0057 (6)	0.0018 (6)	0.0007 (7)
N2	0.0281 (7)	0.0531 (9)	0.0454 (8)	−0.0080 (6)	−0.0011 (6)	0.0075 (7)
N3	0.0283 (7)	0.0488 (9)	0.0433 (8)	−0.0062 (6)	−0.0009 (6)	0.0066 (7)
N4	0.0320 (7)	0.0535 (10)	0.0409 (8)	−0.0048 (6)	0.0004 (6)	0.0000 (7)
C1	0.0518 (11)	0.0518 (12)	0.0536 (12)	0.0004 (9)	−0.0013 (9)	0.0028 (10)
C2	0.0607 (14)	0.0488 (14)	0.100 (2)	−0.0011 (11)	0.0159 (13)	0.0056 (13)
C3	0.0532 (14)	0.0568 (16)	0.123 (3)	−0.0071 (11)	0.0119 (15)	−0.0369 (17)
C4	0.0715 (16)	0.091 (2)	0.0726 (17)	0.0014 (14)	−0.0091 (13)	−0.0444 (16)
C5	0.0665 (14)	0.0674 (15)	0.0406 (10)	0.0033 (11)	0.0007 (10)	−0.0107 (10)
C6	0.0299 (8)	0.0450 (10)	0.0414 (9)	0.0017 (7)	0.0022 (7)	−0.0062 (8)
C7	0.0293 (8)	0.0481 (11)	0.0523 (11)	−0.0021 (7)	0.0007 (7)	−0.0030 (8)
C8	0.0255 (7)	0.0434 (10)	0.0447 (9)	−0.0043 (7)	0.0017 (7)	0.0002 (8)
C9	0.0323 (9)	0.0447 (11)	0.0540 (11)	−0.0037 (7)	0.0041 (8)	0.0032 (9)
C10	0.0530 (13)	0.0831 (18)	0.0647 (14)	−0.0196 (12)	0.0135 (11)	0.0139 (12)
C11	0.0282 (8)	0.0451 (11)	0.0507 (10)	−0.0038 (7)	0.0041 (7)	0.0027 (8)
C12	0.0401 (11)	0.0489 (13)	0.0969 (18)	0.0046 (9)	0.0076 (11)	0.0088 (12)
C13	0.0444 (10)	0.0548 (12)	0.0492 (11)	−0.0061 (9)	−0.0091 (8)	0.0102 (9)

C14	0.0582 (13)	0.0940 (19)	0.0421 (11)	−0.0131 (12)	−0.0022 (10)	0.0073 (11)
C15	0.0322 (8)	0.0364 (9)	0.0406 (9)	−0.0064 (7)	0.0033 (7)	−0.0010 (7)
C16	0.0531 (12)	0.0622 (14)	0.0490 (11)	−0.0143 (10)	−0.0069 (9)	−0.0075 (10)
C17	0.0591 (14)	0.119 (2)	0.0658 (16)	−0.0205 (15)	−0.0220 (12)	−0.0029 (15)

Geometric parameters (Å, °)

S1—C11	1.841 (2)	C9—C10	1.494 (3)
S1—C15	1.7480 (18)	C11—C12	1.529 (3)
O1—C9	1.226 (2)	C13—C14	1.488 (3)
O2—C13	1.223 (3)	C16—C17	1.493 (3)
O3—C16	1.211 (3)	C1—H1	0.9300
N1—C8	1.455 (2)	C2—H2	0.9300
N1—C9	1.336 (2)	C3—H3	0.9300
N2—N3	1.402 (2)	C4—H4	0.9300
N2—C11	1.483 (2)	C5—H5	0.9300
N2—C13	1.365 (3)	C7—H7A	0.9700
N3—C15	1.268 (2)	C7—H7B	0.9700
N4—C15	1.380 (2)	C8—H8	0.9800
N4—C16	1.363 (3)	C10—H10A	0.9600
N1—H1A	0.8300	C10—H10B	0.9600
N4—H4A	0.8700	C10—H10C	0.9600
C1—C6	1.381 (3)	C12—H12A	0.9600
C1—C2	1.380 (3)	C12—H12B	0.9600
C2—C3	1.359 (5)	C12—H12C	0.9600
C3—C4	1.368 (5)	C14—H14A	0.9600
C4—C5	1.372 (4)	C14—H14B	0.9600
C5—C6	1.377 (3)	C14—H14C	0.9600
C6—C7	1.498 (3)	C17—H17A	0.9600
C7—C8	1.532 (3)	C17—H17B	0.9600
C8—C11	1.542 (3)	C17—H17C	0.9600
S1···O3	2.7130 (19)	C10···H4^{x}	2.6600
S1···N1	3.1257 (15)	C13···H7A	2.9200
S1···N3	2.6042 (16)	C13···H8	2.9000
S1···H1A	2.9100	C13···H12A	2.9300
S1···H7B	2.9800	H1···H7B	2.4200
O1···N4^{i}	2.809 (2)	H1···O3^{xiii}	2.7800
O1···C17^{i}	3.275 (3)	H1···H14A^{xiv}	2.5800
O2···C12	3.029 (3)	H1A···S1	2.9100
O2···C8	3.094 (3)	H1A···H7B	2.5300
O3···S1	2.7130 (19)	H1A···H10B	2.1500
O1···H17C^{i}	2.6200	H1A···O2^{xiv}	2.6200
O1···H4A^{i}	1.9600	H2···H17A^{xiii}	2.5400
O1···H8	2.3400	H3···O1^{xii}	2.7400
O1···H3^{ii}	2.7400	H4···C10^{ix}	2.6600
O2···H8	2.5400	H4···H10A^{ix}	2.5300
O2···H1A^{iii}	2.6200	H4···H10C^{ix}	2.3600

O2···H10B^{iii}	2.6600	H4A···H17C	2.3100
O2···H12A	2.4800	H4A···O1^{v}	1.9600
O3···H1^{iv}	2.7800	H4A···C9^{v}	3.0000
N1···S1	3.1257 (15)	H4A···H12B^{vi}	2.6000
N1···C1	3.360 (3)	H5···H7A	2.5100
N2···S1	2.6127 (17)	H7A···N2	2.5300
N3···S1	2.6042 (16)	H7A···N3	2.8100
N3···C7	3.341 (2)	H7A···C13	2.9200
N4···O1^{v}	2.809 (2)	H7A···H5	2.5100
N1···H12C	2.6800	H7B···S1	2.9800
N2···H7A	2.5300	H7B···H1	2.4200
N3···H14B	2.7100	H7B···H1A	2.5300
N3···H14C	2.5300	H7B···H14A^{xiv}	2.3700
N3···H7A	2.8100	H8···O1	2.3400
N4···H12B^{vi}	2.8400	H8···O2	2.5400
C1···N1	3.360 (3)	H8···C5	2.8400
C1···C6^{vii}	3.514 (3)	H8···C13	2.9000
C2···C7^{vii}	3.546 (3)	H8···H12A	2.4700
C4···C14^{viii}	3.399 (4)	H10A···H4^{x}	2.5300
C4···C10^{ix}	3.527 (4)	H10B···H1A	2.1500
C6···C1^{vii}	3.514 (3)	H10B···O2^{xiv}	2.6600
C6···C9	3.455 (2)	H10C···H4^{x}	2.3600
C7···C13	3.493 (3)	H12A···O2	2.4800
C7···C2^{vii}	3.546 (3)	H12A···C13	2.9300
C7···N3	3.341 (2)	H12A···H8	2.4700
C7···C15	3.455 (3)	H12A···C3^{ii}	3.0100
C8···O2	3.094 (3)	H12B···N4^{vi}	2.8400
C9···C6	3.455 (2)	H12B···H4A^{vi}	2.6000
C10···C4^{x}	3.527 (4)	H12C···N1	2.6800
C12···O2	3.029 (3)	H14A···H1^{iii}	2.5800
C13···C7	3.493 (3)	H14A···H7B^{iii}	2.3700
C14···C4^{xi}	3.399 (4)	H14B···N3	2.7100
C15···C7	3.455 (3)	H14C···N3	2.5300
C17···O1^{v}	3.275 (3)	H14C···C4^{xi}	3.0400
C3···H12A^{xii}	3.0100	H17A···H2^{iv}	2.5400
C4···H14C^{viii}	3.0400	H17B···C4^{v}	3.0900
C4···H17B^{i}	3.0900	H17C···H4A	2.3100
C5···H8	2.8400	H17C···O1^{v}	2.6200
C9···H4A^{i}	3.0000		
C11—S1—C15	89.35 (8)	C6—C1—H1	119.00
C8—N1—C9	122.41 (15)	C1—C2—H2	120.00
N3—N2—C11	116.32 (14)	C3—C2—H2	120.00
N3—N2—C13	118.35 (15)	C2—C3—H3	120.00

C11—N2—C13	124.21 (15)	C4—C3—H3	120.00
N2—N3—C15	110.88 (14)	C3—C4—H4	120.00
C15—N4—C16	124.53 (16)	C5—C4—H4	120.00
C9—N1—H1A	117.00	C4—C5—H5	120.00
C8—N1—H1A	119.00	C6—C5—H5	120.00
C16—N4—H4A	116.00	C6—C7—H7A	109.00
C15—N4—H4A	119.00	C6—C7—H7B	109.00
C2—C1—C6	121.1 (2)	C8—C7—H7A	109.00
C1—C2—C3	120.2 (2)	C8—C7—H7B	109.00
C2—C3—C4	119.3 (3)	H7A—C7—H7B	108.00
C3—C4—C5	120.9 (3)	N1—C8—H8	107.00
C4—C5—C6	120.7 (2)	C7—C8—H8	107.00
C1—C6—C7	122.54 (17)	C11—C8—H8	107.00
C5—C6—C7	119.61 (18)	C9—C10—H10A	109.00
C1—C6—C5	117.84 (19)	C9—C10—H10B	109.00
C6—C7—C8	110.76 (15)	C9—C10—H10C	109.00
N1—C8—C7	109.93 (15)	H10A—C10—H10B	109.00
N1—C8—C11	110.33 (15)	H10A—C10—H10C	109.00
C7—C8—C11	114.81 (14)	H10B—C10—H10C	109.00
O1—C9—C10	121.54 (17)	C11—C12—H12A	109.00
N1—C9—C10	116.13 (17)	C11—C12—H12B	109.00
O1—C9—N1	122.33 (18)	C11—C12—H12C	109.00
N2—C11—C12	111.93 (16)	H12A—C12—H12B	109.00
C8—C11—C12	111.91 (15)	H12A—C12—H12C	109.00
S1—C11—C8	110.89 (13)	H12B—C12—H12C	109.00
S1—C11—C12	108.63 (15)	C13—C14—H14A	109.00
S1—C11—N2	103.11 (11)	C13—C14—H14B	109.00
N2—C11—C8	110.03 (15)	C13—C14—H14C	109.00
O2—C13—N2	121.11 (19)	H14A—C14—H14B	109.00
O2—C13—C14	122.8 (2)	H14A—C14—H14C	109.00
N2—C13—C14	116.07 (17)	H14B—C14—H14C	109.00
S1—C15—N3	118.54 (13)	C16—C17—H17A	109.00
S1—C15—N4	122.13 (14)	C16—C17—H17B	109.00
N3—C15—N4	119.34 (16)	C16—C17—H17C	109.00
O3—C16—C17	123.9 (2)	H17A—C17—H17B	109.00
N4—C16—C17	114.38 (19)	H17A—C17—H17C	109.00
O3—C16—N4	121.7 (2)	H17B—C17—H17C	109.00
C2—C1—H1	119.00		

C15—S1—C11—N2	11.14 (12)	C16—N4—C15—S1	9.0 (3)
C15—S1—C11—C8	−106.59 (13)	C16—N4—C15—N3	−170.58 (19)
C15—S1—C11—C12	130.03 (14)	C15—N4—C16—O3	−2.4 (3)
C11—S1—C15—N3	−7.87 (16)	C15—N4—C16—C17	176.33 (19)
C11—S1—C15—N4	172.58 (15)	C6—C1—C2—C3	0.8 (4)
C9—N1—C8—C7	111.74 (19)	C2—C1—C6—C5	0.2 (3)
C9—N1—C8—C11	−120.66 (18)	C2—C1—C6—C7	−178.1 (2)
C8—N1—C9—O1	9.2 (3)	C1—C2—C3—C4	−1.5 (4)
C8—N1—C9—C10	−170.62 (18)	C2—C3—C4—C5	1.2 (4)
C11—N2—N3—C15	9.4 (2)	C3—C4—C5—C6	−0.1 (4)
C13—N2—N3—C15	177.80 (17)	C4—C5—C6—C1	−0.6 (3)

N3—N2—C11—S1	−13.94 (17)	C4—C5—C6—C7	177.8 (2)
N3—N2—C11—C8	104.40 (17)	C1—C6—C7—C8	101.7 (2)
N3—N2—C11—C12	−130.51 (17)	C5—C6—C7—C8	−76.6 (2)
C13—N2—C11—S1	178.39 (15)	C6—C7—C8—N1	−64.50 (19)
C13—N2—C11—C8	−63.3 (2)	C6—C7—C8—C11	170.43 (15)
C13—N2—C11—C12	61.8 (2)	N1—C8—C11—S1	−59.86 (16)
N3—N2—C13—O2	−172.06 (19)	N1—C8—C11—N2	−173.28 (13)
N3—N2—C13—C14	7.9 (3)	N1—C8—C11—C12	61.6 (2)
C11—N2—C13—O2	−4.6 (3)	C7—C8—C11—S1	65.02 (18)
C11—N2—C13—C14	175.33 (19)	C7—C8—C11—N2	−48.4 (2)
N2—N3—C15—S1	0.9 (2)	C7—C8—C11—C12	−173.52 (17)
N2—N3—C15—N4	−179.59 (15)		

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*+1; (ii) −*x*+1/2, *y*−1/2, *z*; (iii) *x*, −*y*+1/2, *z*+1/2; (iv) −*x*, *y*−1/2, −*z*+1/2; (v) *x*−1/2, −*y*+1/2, −*z*+1; (vi) −*x*, −*y*, −*z*+1; (vii) −*x*, −*y*+1, −*z*+1; (viii) −*x*, *y*+1/2, −*z*+3/2; (ix) −*x*+1/2, −*y*+1, *z*+1/2; (x) −*x*+1/2, −*y*+1, *z*−1/2; (xi) −*x*, *y*−1/2, −*z*+3/2; (xii) −*x*+1/2, *y*+1/2, *z*; (xiii) −*x*, *y*+1/2, −*z*+1/2; (xiv) *x*, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···O1^{v}	0.8700	1.9600	2.809 (2)	166.00

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

Fig. 1

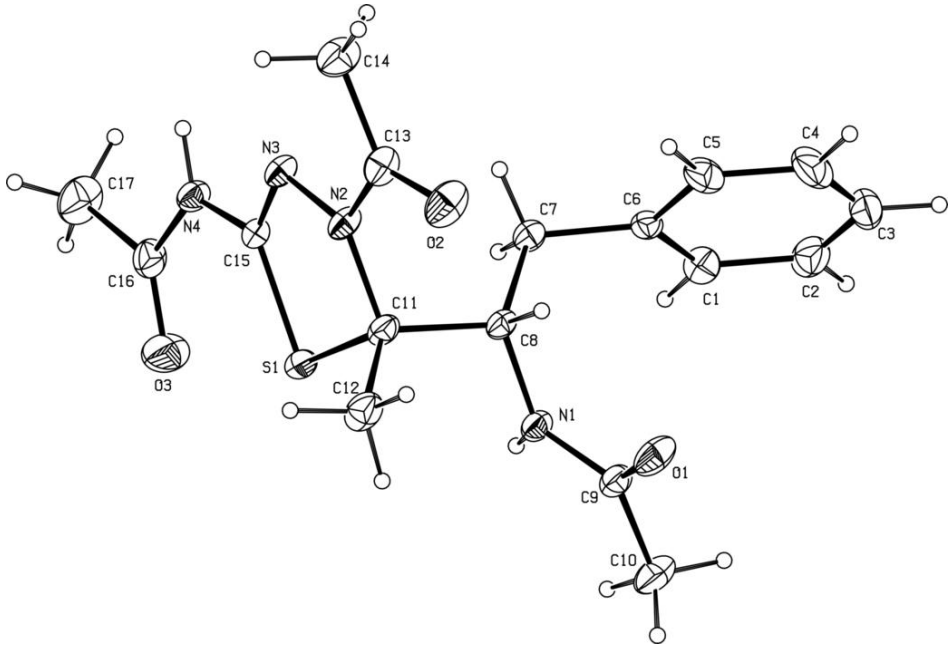
C14
C13
N3
N2
O2
C17
N4
C15
C16
O3
S1
C11
C12
C7
C6
C5
C4
C3
C1
C2
C8
N1
O1
C9
C10

Fig. 2