Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 6-methyl-4-(2-phenyltriazol-4-yl)-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

Fang Xie,[a] He Huang,[b] Gang Liu[a]* and Chen-Jiang Liu[a,c]

[a]Key Laboratory of Oil and Gas Fine Chemicals, Ministry of Education, School of Chemistry and Chemical Engineering, Xinjiang University, Urumqi 830046, People's Republic of China, [b]Xinjiang Uygur Autonomous Region Product Quality Supervision and Inspection Academy, Urumqi 830004, People's Republic of China, and [c]School of Sciences, Xi'an Jiaotong University, Xian 710049, People's Republic of China
Correspondence e-mail: pxylcj@126.com

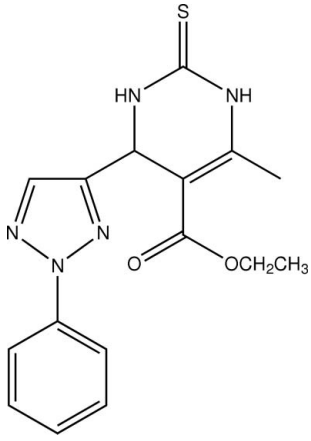
Received 17 May 2007; accepted 25 May 2007

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.124; data-to-parameter ratio = 17.2.

In the crystal structure of the title compound, $C_{16}H_{17}N_5O_2S$, molecules are linked by two N—H···S hydrogen bonds, with N—S distances of 3.3469 (13) and 3.3703 (13) Å and N—H···S angles of 158 and 162°.

Related literature

For related literature, see: Atwal *et al.* (1990); Hua *et al.* (2004); Kappe (1993); Patil *et al.* (1995); Singh & Singh (2006); Tu *et al.* (2004).



Experimental

Crystal data

$C_{16}H_{17}N_5O_2S$
M_r = 343.41
Triclinic, $P\overline{1}$
a = 8.3998 (5) Å
b = 9.4733 (5) Å
c = 11.4989 (8) Å
α = 76.516 (2)°
β = 87.552 (2)°
γ = 68.564 (2)°
V = 827.33 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 153 (2) K
0.65 × 0.56 × 0.48 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.873, T_{max} = 0.904
8180 measured reflections
3754 independent reflections
3399 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.125
S = 1.03
3754 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; 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: *WinGX* (Farrugia, 1999).

The authors gratefully acknowledge support from the National Natural Science Foundation of China (grant No. 20662009), the Programme for New Century Excellent Talents in Universities (grant No. NCET-04-0987) and the Specialized Research Fund for the Doctoral Programme of Higher Education (grant No. 20050755003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2087).

References

Atwal, K. S., Rovnyak, G. C., Kimball, S. D., Floyd, D. M., Moreland, S., Swanson, B. N., Gougoutas, D. Z., Schewartz, J., Smillie, K. M. & Malley, M. F. (1990). *J. Med. Chem.* **33**, 2629–2635.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Hua, G. P., Tu, S. J., Fang, F., Tu, M. S., Shi, D. Q. & Wang, X. S. (2004). *Chin. J. Struct. Chem.* **11**, 1295–1299.
Kappe, C. O. (1993). *Tetrahedron*, **49**, 6937–6963.
Patil, A. D., Kumar, N. V., Kokke, W. C., Bean, M. F., Freyer, A. J., Debrosse, C., Mai, S., Truneh, A., Faulkner, D. J., Carte, B., Breen, A. L., Hertzberg, R. P., Johnson, R. K., Westley, J. W. & Potts, B. C. M. (1995). *J. Org. Chem.* **60**, 1182–1188.
Rigaku (2004). *RAPID-AUTO*. Version 3.0. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Singh, K. & Singh, S. (2006). *Tetrahedron Lett.* **47**, 8143–8146.
Tu, S. J., Fang, F., Hong, J., Zhu, S. L., Li, T. J., Zhang, X. J. & Shi, D. Q. (2004). *Chin. J. Struct. Chem.* pp. 617–619.

  doi:10.1107/S1600536807025639

supplementary materials

Acta Cryst. (2007). E**63**, o3076 [**doi:10.1107/S1600536807025639**]

Ethyl 6-methyl-4-(2-phenyltriazol-4-yl)-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate

F. Xie, H. Huang, G. Liu and C.-J. Liu

Comment

3,4-Dihydropyrimidin-2(1*H*)-ones and their derivatives have attracted considerable interest because of their therapeutic and pharmaceutical properties, such as antiviral, antibacterial, anti-inflammatory and antitumour activities (Kappe, 1993). Their particular structure has been found in natural marine alkaloid Batzelladine A and B which are the first low molecular weight natural products reported in the literature to inhibit the binding of HIV gp-120 to CD4 cells, so disclosing a new field towards the development of AIDS therapy (Patil *et al.*, 1995). Additionally, functionalized dihydropyrimidinones have been used as antihypertensive agents, potent calcium channel blockers, adrenergic and neuropeptide Y (NPY) antagonist (Atwal *et al.*, 1990). The X-ray crystal structure analysis of the title compound, was undertaken in order to study its stereochemistry and crystal packing. 4-(3,4-Methylenedioxylphenyl)-6-methyl-5-ethoxycaronyl-3,4-dihydropyrimidin- 2(H)-one has been reported (Tu *et al.*, 2004). 4-(4-Chlorophenyl)-6-methyl-5-methoxycaronyl-3,4-dihydropyrimidin-2(H)-one has been reported (Hua *et al.*, 2004). *N*-acylated 3,4-dihydropyrimidin-2-ones have been reported (Singh & Singh *et al.*, 2006).

Experimental

A mixture of 2-phenyl-1,2,3-triazolyl-4-formaldehyde (1 mmol), ethyl acetoacetate (1 mmol), thiourea (1.5 mmol) in absolute EtOH was refluxing in the presence of $Sm(ClO_4)_3$ (as catalyst) for 9 h between 343–353 K. The product was isolated by filtration, and dried at room temperature. Yield 76.1% (0.261 g), m.p. 476–478 K. Block-like single-crystal of compound (I) was grown from solution of ethanol by slow evaporation.

Figures

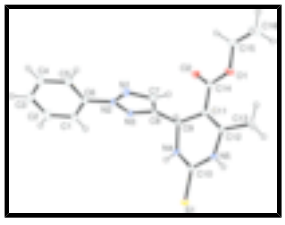


Fig. 1. A view of the molecule structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

Ethyl 6-methyl-4-(2-phenyltriazol-4-yl)-2-thioxo-1,2,3,6- tetrahydropyrimidine-5-carboxylate

Crystal data

$C_{16}H_{17}N_5O_2S$	$Z = 2$
$M_r = 343.41$	$F_{000} = 360$
Triclinic, $P\overline{1}$	$D_x = 1.379$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 476-478 K
$a = 8.3998$ (5) Å	Mo $K\alpha$ radiation

	λ = 0.71073 Å
b = 9.4733 (5) Å	Cell parameters from 7493 reflections
c = 11.4989 (8) Å	θ = 3.1–27.5º
α = 76.516 (2)º	μ = 0.22 mm^{-1}
β = 87.552 (2)º	*T* = 153 (2) K
γ = 68.564 (2)º	Block, colourless
V = 827.33 (9) Å^3	0.65 × 0.56 × 0.48 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer	3754 independent reflections
Radiation source: fine-focus sealed tube	3399 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 153(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −10→10
T_{min} = 0.873, T_{max} = 0.904	*k* = −12→12
8180 measured reflections	*l* = −14→14

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.125	$\Delta\rho_{max}$ = 0.90 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
3754 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997)
218 parameters	Extinction coefficient: 0.038 (5)

Special details

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	0.21949 (5)	0.56030 (4)	0.49008 (4)	0.02980 (15)
O1	0.43152 (15)	−0.21361 (13)	0.71966 (12)	0.0306 (3)
O2	0.68489 (15)	−0.18789 (14)	0.68174 (12)	0.0325 (3)
N1	0.63345 (18)	0.12860 (16)	0.94892 (12)	0.0261 (3)
N2	0.75123 (16)	0.17112 (15)	0.88427 (11)	0.0209 (3)

N3	0.74361 (16)	0.17441 (14)	0.76805 (11)	0.0201 (3)
N4	0.47347 (16)	0.28931 (15)	0.56353 (11)	0.0224 (3)
H4A	0.5403	0.3382	0.5287	0.027*
N5	0.20505 (16)	0.27995 (14)	0.57783 (12)	0.0212 (3)
H5A	0.0935	0.3296	0.5752	0.025*
C1	0.9596 (2)	0.2957 (2)	0.85709 (17)	0.0318 (4)
H1B	0.9323	0.3267	0.7734	0.038*
C2	1.0837 (3)	0.3331 (3)	0.9050 (2)	0.0440 (5)
H2A	1.1433	0.3892	0.8538	0.053*
C3	1.1212 (3)	0.2888 (2)	1.0276 (2)	0.0459 (5)
H3B	1.2067	0.3142	1.0599	0.055*
C4	1.0351 (3)	0.2086 (2)	1.10218 (18)	0.0403 (5)
H4B	1.0600	0.1804	1.1861	0.048*
C5	0.9116 (2)	0.1681 (2)	1.05613 (16)	0.0307 (4)
H5B	0.8528	0.1114	1.1076	0.037*
C6	0.87629 (19)	0.21229 (17)	0.93394 (14)	0.0237 (3)
C7	0.5428 (2)	0.10392 (19)	0.86819 (14)	0.0245 (3)
H7A	0.4476	0.0721	0.8844	0.029*
C8	0.61077 (18)	0.13249 (16)	0.75636 (13)	0.0185 (3)
C9	0.55561 (18)	0.12922 (16)	0.63452 (12)	0.0184 (3)
H9A	0.6604	0.0765	0.5935	0.022*
C10	0.30548 (19)	0.36575 (17)	0.54804 (13)	0.0205 (3)
C11	0.43724 (18)	0.03984 (17)	0.64066 (12)	0.0191 (3)
C12	0.26849 (18)	0.11694 (16)	0.61245 (12)	0.0190 (3)
C13	0.1318 (2)	0.05172 (18)	0.60777 (15)	0.0253 (3)
H13A	0.1816	−0.0624	0.6324	0.030*
H13B	0.0823	0.0834	0.5259	0.030*
H13C	0.0420	0.0914	0.6620	0.030*
C14	0.5302 (2)	−0.13067 (17)	0.68061 (13)	0.0225 (3)
C15	0.5229 (3)	−0.3808 (2)	0.7656 (2)	0.0406 (5)
H15A	0.5880	−0.4273	0.7014	0.049*
H15B	0.6047	−0.3990	0.8319	0.049*
C16	0.3980 (3)	−0.4527 (2)	0.8085 (3)	0.0562 (6)
H16A	0.4576	−0.5650	0.8401	0.067*
H16B	0.3185	−0.4353	0.7421	0.067*
H16C	0.3342	−0.4060	0.8720	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0185 (2)	0.0194 (2)	0.0458 (3)	−0.00878 (15)	−0.00867 (16)	0.00795 (16)
O1	0.0261 (6)	0.0169 (5)	0.0438 (7)	−0.0072 (5)	0.0011 (5)	0.0017 (5)
O2	0.0218 (6)	0.0241 (6)	0.0447 (7)	−0.0040 (5)	−0.0055 (5)	−0.0007 (5)
N1	0.0287 (7)	0.0302 (7)	0.0207 (6)	−0.0148 (6)	0.0005 (5)	−0.0017 (5)
N2	0.0207 (6)	0.0215 (6)	0.0193 (6)	−0.0080 (5)	−0.0032 (5)	−0.0015 (5)
N3	0.0184 (6)	0.0211 (6)	0.0192 (6)	−0.0074 (5)	−0.0029 (4)	−0.0010 (5)
N4	0.0165 (6)	0.0224 (6)	0.0246 (6)	−0.0098 (5)	−0.0050 (5)	0.0070 (5)
N5	0.0135 (5)	0.0181 (6)	0.0294 (6)	−0.0064 (5)	−0.0024 (5)	0.0008 (5)

C1	0.0285 (8)	0.0318 (9)	0.0380 (9)	−0.0139 (7)	−0.0031 (7)	−0.0081 (7)
C2	0.0336 (10)	0.0426 (11)	0.0649 (14)	−0.0210 (9)	−0.0034 (9)	−0.0172 (10)
C3	0.0313 (10)	0.0417 (11)	0.0691 (14)	−0.0083 (8)	−0.0187 (9)	−0.0254 (10)
C4	0.0383 (10)	0.0333 (9)	0.0441 (11)	−0.0007 (8)	−0.0210 (8)	−0.0153 (8)
C5	0.0306 (8)	0.0251 (8)	0.0310 (8)	−0.0026 (7)	−0.0107 (7)	−0.0065 (6)
C6	0.0200 (7)	0.0203 (7)	0.0291 (8)	−0.0035 (6)	−0.0062 (6)	−0.0075 (6)
C7	0.0238 (7)	0.0282 (7)	0.0220 (7)	−0.0134 (6)	−0.0005 (6)	−0.0001 (6)
C8	0.0157 (6)	0.0161 (6)	0.0203 (7)	−0.0047 (5)	−0.0036 (5)	0.0009 (5)
C9	0.0143 (6)	0.0189 (6)	0.0190 (6)	−0.0057 (5)	−0.0033 (5)	0.0010 (5)
C10	0.0181 (7)	0.0214 (7)	0.0200 (6)	−0.0088 (6)	−0.0036 (5)	0.0019 (5)
C11	0.0185 (7)	0.0194 (7)	0.0189 (6)	−0.0080 (6)	−0.0022 (5)	−0.0014 (5)
C12	0.0191 (7)	0.0185 (7)	0.0193 (6)	−0.0085 (5)	−0.0013 (5)	−0.0013 (5)
C13	0.0199 (7)	0.0224 (7)	0.0346 (8)	−0.0112 (6)	−0.0037 (6)	−0.0023 (6)
C14	0.0229 (7)	0.0206 (7)	0.0215 (7)	−0.0063 (6)	−0.0040 (5)	−0.0022 (5)
C15	0.0365 (10)	0.0179 (8)	0.0556 (12)	−0.0037 (7)	0.0026 (8)	0.0033 (7)
C16	0.0514 (13)	0.0256 (10)	0.0841 (18)	−0.0128 (9)	0.0099 (12)	−0.0018 (10)

Geometric parameters (Å, °)

S1—C10	1.6906 (15)	C4—C5	1.392 (2)
O1—C14	1.336 (2)	C4—H4B	0.9500
O1—C15	1.4603 (19)	C5—C6	1.381 (2)
O2—C14	1.2106 (19)	C5—H5B	0.9500
N1—N2	1.3351 (18)	C7—C8	1.393 (2)
N1—C7	1.337 (2)	C7—H7A	0.9500
N2—N3	1.3332 (17)	C8—C9	1.5049 (19)
N2—C6	1.4270 (19)	C9—C11	1.5140 (19)
N3—C8	1.3351 (18)	C9—H9A	1.0000
N4—C10	1.3272 (19)	C11—C12	1.349 (2)
N4—C9	1.4658 (17)	C11—C14	1.481 (2)
N4—H4A	0.8800	C12—C13	1.4975 (19)
N5—C10	1.3551 (19)	C13—H13A	0.9800
N5—C12	1.3989 (18)	C13—H13B	0.9800
N5—H5A	0.8800	C13—H13C	0.9800
C1—C6	1.386 (2)	C15—C16	1.458 (3)
C1—C2	1.388 (2)	C15—H15A	0.9900
C1—H1B	0.9500	C15—H15B	0.9900
C2—C3	1.388 (3)	C16—H16A	0.9800
C2—H2A	0.9500	C16—H16B	0.9800
C3—C4	1.371 (3)	C16—H16C	0.9800
C3—H3B	0.9500		
C14—O1—C15	115.45 (13)	N4—C9—C8	109.47 (12)
N2—N1—C7	103.47 (12)	N4—C9—C11	110.43 (11)
N3—N2—N1	115.25 (12)	C8—C9—C11	112.63 (12)
N3—N2—C6	121.51 (13)	N4—C9—H9A	108.1
N1—N2—C6	123.24 (13)	C8—C9—H9A	108.1
N2—N3—C8	103.71 (12)	C11—C9—H9A	108.1
C10—N4—C9	124.65 (12)	N4—C10—N5	116.91 (13)
C10—N4—H4A	117.7	N4—C10—S1	121.95 (11)

C9—N4—H4A	117.7	N5—C10—S1	121.11 (11)
C10—N5—C12	123.79 (12)	C12—C11—C14	127.96 (13)
C10—N5—H5A	118.1	C12—C11—C9	120.18 (13)
C12—N5—H5A	118.1	C14—C11—C9	111.86 (12)
C6—C1—C2	118.56 (18)	C11—C12—N5	119.08 (13)
C6—C1—H1B	120.7	C11—C12—C13	128.73 (13)
C2—C1—H1B	120.7	N5—C12—C13	112.15 (12)
C3—C2—C1	120.2 (2)	C12—C13—H13A	109.5
C3—C2—H2A	119.9	C12—C13—H13B	109.5
C1—C2—H2A	119.9	H13A—C13—H13B	109.5
C4—C3—C2	120.23 (17)	C12—C13—H13C	109.5
C4—C3—H3B	119.9	H13A—C13—H13C	109.5
C2—C3—H3B	119.9	H13B—C13—H13C	109.5
C3—C4—C5	120.62 (18)	O2—C14—O1	123.33 (14)
C3—C4—H4B	119.7	O2—C14—C11	121.53 (14)
C5—C4—H4B	119.7	O1—C14—C11	115.08 (13)
C6—C5—C4	118.49 (18)	C16—C15—O1	108.53 (16)
C6—C5—H5B	120.8	C16—C15—H15A	110.0
C4—C5—H5B	120.8	O1—C15—H15A	110.0
C5—C6—C1	121.85 (15)	C16—C15—H15B	110.0
C5—C6—N2	119.63 (15)	O1—C15—H15B	110.0
C1—C6—N2	118.51 (14)	H15A—C15—H15B	108.4
N1—C7—C8	108.86 (13)	C15—C16—H16A	109.5
N1—C7—H7A	125.6	C15—C16—H16B	109.5
C8—C7—H7A	125.6	H16A—C16—H16B	109.5
N3—C8—C7	108.71 (13)	C15—C16—H16C	109.5
N3—C8—C9	119.77 (13)	H16A—C16—H16C	109.5
C7—C8—C9	131.48 (13)	H16B—C16—H16C	109.5
C7—N1—N2—N3	−0.48 (17)	C7—C8—C9—N4	105.08 (17)
C7—N1—N2—C6	178.83 (13)	N3—C8—C9—C11	164.70 (13)
N1—N2—N3—C8	0.57 (16)	C7—C8—C9—C11	−18.2 (2)
C6—N2—N3—C8	−178.75 (12)	C9—N4—C10—N5	−14.8 (2)
C6—C1—C2—C3	−0.7 (3)	C9—N4—C10—S1	166.99 (11)
C1—C2—C3—C4	−0.4 (3)	C12—N5—C10—N4	−6.2 (2)
C2—C3—C4—C5	1.2 (3)	C12—N5—C10—S1	172.03 (11)
C3—C4—C5—C6	−0.8 (3)	N4—C9—C11—C12	−16.86 (19)
C4—C5—C6—C1	−0.3 (3)	C8—C9—C11—C12	105.88 (15)
C4—C5—C6—N2	179.47 (14)	N4—C9—C11—C14	163.74 (12)
C2—C1—C6—C5	1.1 (3)	C8—C9—C11—C14	−73.53 (15)
C2—C1—C6—N2	−178.70 (15)	C14—C11—C12—N5	179.19 (13)
N3—N2—C6—C5	−162.42 (14)	C9—C11—C12—N5	−0.1 (2)
N1—N2—C6—C5	18.3 (2)	C14—C11—C12—C13	−3.4 (3)
N3—N2—C6—C1	17.4 (2)	C9—C11—C12—C13	177.27 (14)
N1—N2—C6—C1	−161.88 (15)	C10—N5—C12—C11	13.4 (2)
N2—N1—C7—C8	0.18 (17)	C10—N5—C12—C13	−164.41 (14)
N2—N3—C8—C7	−0.41 (16)	C15—O1—C14—O2	0.4 (2)
N2—N3—C8—C9	177.30 (12)	C15—O1—C14—C11	−176.65 (14)
N1—C7—C8—N3	0.15 (18)	C12—C11—C14—O2	165.89 (16)
N1—C7—C8—C9	−177.20 (15)	C9—C11—C14—O2	−14.8 (2)

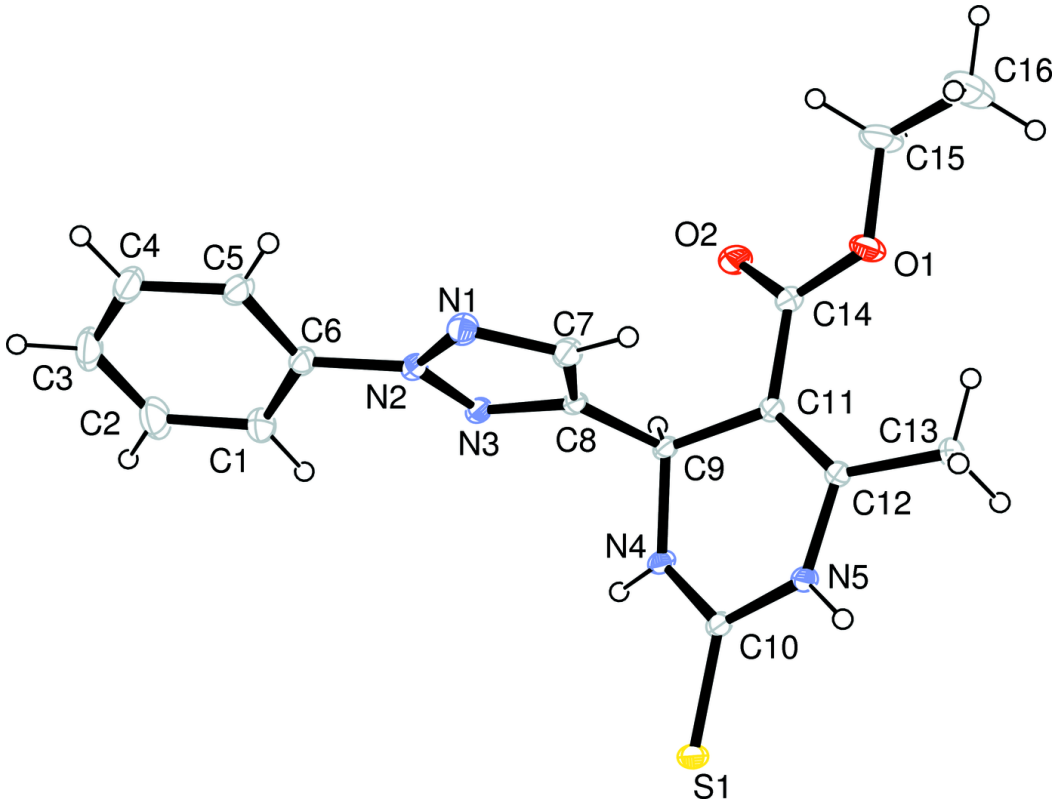
C10—N4—C9—C8	−99.22 (16)	C12—C11—C14—O1	−17.0 (2)
C10—N4—C9—C11	25.3 (2)	C9—C11—C14—O1	162.37 (13)
N3—C8—C9—N4	−72.04 (16)	C14—O1—C15—C16	177.85 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···S1^{i}	0.88	2.52	3.3469 (13)	158
N5—H5A···S1^{ii}	0.88	2.52	3.3703 (13)	162

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

Fig. 1


C16
C15
O2
O1
C4
C5
N1
C6
C7
C14
C3
N2
C11
C13
C2
N3
C8
C9
C1
C12
N4
N5
C10
S1

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 6-methyl-4-(2-phenyltriazol-4-yl)-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate. Corrigendum

Fang Xie,[a] He Huang,[b] Gang Liu[a] and Chen-Jiang Liu[a,c]*

[a]Key Laboratory of Oil and Gas Fine Chemicals, Ministry of Education, School of Chemistry and Chemical Engineering, Xinjiang University, Urumqi 830046, People's Republic of China, [b]Xinjiang Uygur Autonomous Region Product Quality Supervision and Inspection Academy, Urumqi 830004, People's Republic of China, and [c]School of Sciences, Xi'an Jiaotong University, Xian 710049, People's Republic of China
Correspondence e-mail: pxylcj@126.com

Received 10 July 2007; accepted 25 July 2007

In the paper by Xie, Huang, Liu & Liu [*Acta Cryst.* (2006), E**63**, o3076], the incorrect correspondence author is indicated. The correct correspondence author is shown here.

 doi:10.1107/S1600536807036537