Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 5-((1*E*)-1-{(*E*)-2-[1-(4-ethoxycarbonyl-3-methyl-1,2-oxazol-5-yl)ethylidene]hydrazin-1-ylidene}ethyl)-3-methyl-1,2-oxazole-4-carboxylate

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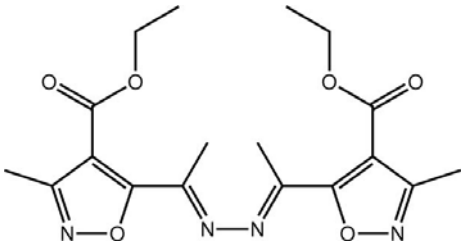
Received 7 August 2011; accepted 8 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.159; data-to-parameter ratio = 16.2.

The complete molecule of the title compound, $C_{18}H_{22}N_4O_6$, is generated by the application of a twofold axis of symmetry. Twists are evident in the molecule, *i.e.* between each —C=N—N group and the adjacent oxazole ring [dihedral angle = 46.08 (12) °] and between the latter and attached ester group [excluding the terminal methyl group; dihedral angle = 24.4 (7) °]. In the crystal, C—H···O and π–π [3.5990 (11) Å] contacts connect molecules into supramolecular arrays in the *ac* plane. These stack along the *b* axis, being connected by weak π–π [3.3903 (11) Å] interactions.

Related literature

For background to the biological activity of hydrazone compounds, see: Faid-Allah *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{22}N_4O_6$
M_r = 390.40
Monoclinic, $P2/n$
a = 9.4509 (5) Å
b = 8.5456 (4) Å
c = 11.9859 (5) Å
β = 104.107 (5)°
V = 938.83 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 K
0.25 × 0.25 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.889, T_{max} = 1.000
4223 measured reflections
2095 independent reflections
1639 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.159
S = 0.87
2095 reflections
129 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9c···O2^{i}	0.98	2.46	3.356 (3)	152

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5078).

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