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ISSN 2414-3146

Ethyl 2-(5-methyl-1,2,4-triazolo[1,5-*a*]pyrimidin-7-yl)pent-4-enoate

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Received 30 August 2018
Accepted 11 September 2018

Edited by S. Parkin, University of Kentucky, USA

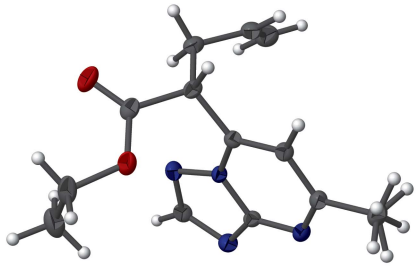
Keywords: crystal structure; triazole; pyrimidine; hydrogen bond; C—H···π(ring) interaction.

CCDC reference: 1866951

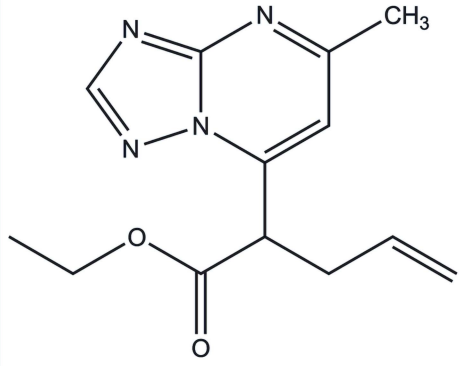
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{13}H_{16}N_4O_2$, the fused triazolopyrimidine ring system is planar. In the crystal, inversion-related C—H···O hydrogen bonds form dimers that are linked into chains extending along the *a*-axis direction by inversion-related C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

Among the various classes of nitrogen-containing heterocyclic compounds, triazolopyrimidine derivatives display a broad spectrum of biological activities, including anti-inflammatory (Ashour *et al.*, 2013), anticancer (Hoffmann *et al.*, 2017) and antibacterial properties (Mabkhot *et al.*, 2016). The present work is a continuation of the investigation of the triazolopyrimidine derivatives published by our team (El Otmani *et al.*, 2002; Lahmidi *et al.*, 2016).

The fused triazolopyrimidine ring system is planar to within 0.011 (1) Å (r.m.s. deviation = 0.001) while the pent-4-enoate unit is nearly orthogonal to this plane as indicated by the C3—C4—C7—H7 torsion angle of −6.5 (9)° (Fig. 1). In the crystal, inversion-related C5—H5···O1 hydrogen bonds form dimers which are connected into chains running along the *a*-axis direction by inversion-related C10—H10*B*···*Cg*1 interactions, where *Cg*1 is the centroid of the C5/N2/C6/N4/N3 ring (Table 1 and Fig. 2).

Synthesis and crystallization

To a solution of ethyl 2-(5-methyl1,2,4-triazolo[1,5-*a*]pyrimidin-7-yl)acetate (1 g, 4.5 mmol) was added potassium hydroxide (0.3 g, 5.4 mmol) in acetone (20 ml). After

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

*Cg*1 is the centroid of the C5/N2/C6/N4/N3 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	1.000 (12)	2.532 (12)	3.4147 (19)	147.1 (9)
C10—H10*B*···*Cg*1^{ii}	0.962 (17)	2.747 (18)	3.657 (3)	143.9 (13)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$.

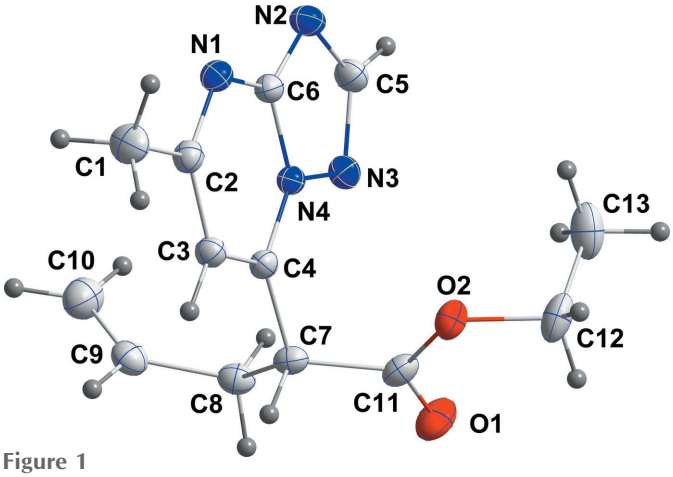


Figure 1
The title molecule with labelling scheme and 50% probability ellipsoids. For the sake of clarity, disorder of methyl group C1 is not shown.

10 min of stirring, allyl bromide (0.94 ml, 10 mmol) was added dropwise. Upon disappearance of the starting material as indicated by TLC, the resulting mixture was evaporated. The crude material was dissolved with EtOAc (50 ml), washed with water and brine, dried over $MgSO_4$ and the solvent was evaporated *in vacuo*. The resulting residue was purified by column chromatography (EtOAc/hexane 2:8). The title compound was recrystallized from ethanol at room temperature giving colourless crystals (yield: 55%; m.p. 350–352 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The methyl group based on C1 is rotationally disordered over two sites in approximately equal amounts.

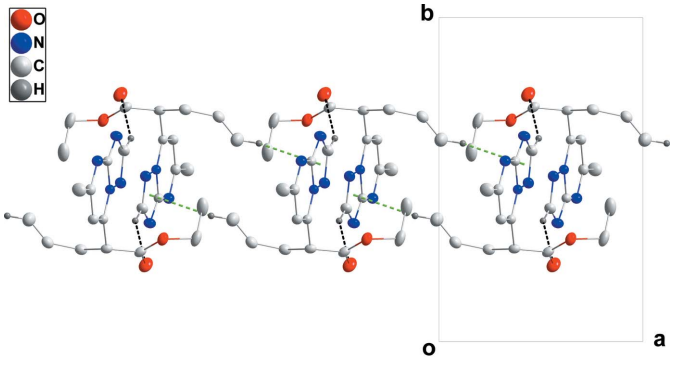


Figure 2
A portion of one chain viewed along the *c*-axis direction. C—H···O hydrogen bonds and C—H···π(ring) interactions are shown, respectively, by black and green dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{16}N_4O_2$
M_r	260.30
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	120
a, *b*, *c* (Å)	9.069 (5), 13.319 (7), 11.851 (7)
β (°)	112.161 (7)
V (Å^3)	1325.8 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.28 × 0.26 × 0.23
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.97, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24464, 3472, 2810
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.683
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.039, 0.115, 1.13
No. of reflections	3472
No. of parameters	225
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.18

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

JTM thanks Tulane University for support of the Tulane Crystallography Laboratory.

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full crystallographic data

IUCrData (2018). **3**, x181280 [https://doi.org/10.1107/S2414314618012804]

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Crystal data

$C_{13}H_{16}N_4O_2$
$M_r = 260.30$
Monoclinic, $P2_1/n$
$a = 9.069$ (5) Å
$b = 13.319$ (7) Å
$c = 11.851$ (7) Å
$\beta = 112.161$ (7)°
$V = 1325.8$ (13) Å^3
$Z = 4$
$F(000) = 552$
$D_x = 1.304$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9961 reflections
$\theta = 2.4$–29.0°
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Block, colourless
0.28 × 0.26 × 0.23 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.97$, $T_{max} = 0.98$
24464 measured reflections
3472 independent reflections
2810 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 29.1°$, $\theta_{min} = 2.4°$
$h = -12 \rightarrow 12$
$k = -17 \rightarrow 18$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.115$
$S = 1.13$
3472 reflections
225 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 0.0365P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.014$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5 deg. in omega, colllected at phi = 0.00, 90.00 and 180.00 deg. and 2 sets of 800 frames, each of width 0.45 deg in phi, collected at omega = -30.00 and 210.00 deg. The scan time was 20 sec/frame.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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. The methyl group based on C1 is rotationally disordered over two sites in approximately equal amounts. The pertinent H-atoms were included as riding contributions with an AFIX 127 instruction.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.56233 (10)	0.23682 (6)	0.58967 (7)	0.0344 (2)	
O2	0.64639 (8)	0.31664 (5)	0.77039 (6)	0.02493 (18)	
N1	0.32526 (10)	0.55771 (6)	0.86016 (8)	0.02209 (19)	
N2	0.41823 (10)	0.63445 (6)	0.71457 (8)	0.0239 (2)	
N3	0.43853 (9)	0.48972 (6)	0.61662 (7)	0.02074 (19)	
N4	0.38663 (9)	0.46935 (5)	0.70826 (7)	0.01672 (18)	
C1	0.23525 (14)	0.46863 (8)	0.99890 (11)	0.0300 (2)	
H1A	0.272897	0.529471	1.047853	0.045*	0.5
H1B	0.277616	0.409356	1.049848	0.045*	0.5
H1C	0.118632	0.466814	0.966951	0.045*	0.5
H1D	0.173199	0.407623	0.995248	0.045*	0.5
H1E	0.168480	0.527738	0.993253	0.045*	0.5
H1F	0.327464	0.470281	1.076151	0.045*	0.5
C2	0.29106 (11)	0.46900 (7)	0.89531 (9)	0.0209 (2)	
C3	0.30429 (11)	0.37708 (7)	0.83846 (9)	0.0196 (2)	
H3	0.2757 (14)	0.3120 (9)	0.8652 (11)	0.027 (3)*	
C4	0.35412 (11)	0.37704 (6)	0.74367 (8)	0.0176 (2)	
C5	0.45486 (12)	0.58899 (7)	0.62636 (9)	0.0231 (2)	
H5	0.4937 (15)	0.6272 (8)	0.5704 (11)	0.025 (3)*	
C6	0.37471 (11)	0.55701 (7)	0.76663 (9)	0.0188 (2)	
C7	0.37022 (12)	0.28654 (7)	0.67375 (9)	0.0199 (2)	
H7	0.3497 (13)	0.2254 (9)	0.7171 (11)	0.023 (3)*	
C8	0.24441 (12)	0.28407 (8)	0.54242 (9)	0.0230 (2)	
H8A	0.2732 (14)	0.3346 (9)	0.4912 (11)	0.025 (3)*	
H8B	0.2499 (14)	0.2163 (9)	0.5127 (11)	0.027 (3)*	
C9	0.08070 (12)	0.30597 (8)	0.53659 (10)	0.0258 (2)	
H9	0.0388 (16)	0.2663 (10)	0.5872 (12)	0.032 (3)*	
C10	−0.01043 (15)	0.37689 (9)	0.46752 (11)	0.0348 (3)	
H10A	0.0325 (18)	0.4190 (11)	0.4135 (14)	0.046 (4)*	
H10B	−0.1163 (18)	0.3876 (10)	0.4648 (14)	0.046 (4)*	
C11	0.53584 (12)	0.27690 (7)	0.67105 (9)	0.0227 (2)	
C12	0.80941 (13)	0.31869 (10)	0.77462 (11)	0.0321 (3)	
H12A	0.8249 (16)	0.2611 (10)	0.7309 (13)	0.035 (3)*	
H12B	0.8722 (16)	0.3147 (9)	0.8617 (13)	0.033 (3)*	
C13	0.84073 (14)	0.41573 (11)	0.72326 (12)	0.0384 (3)	

H13A	0.8213 (18)	0.4730 (11)	0.7691 (15)	0.048 (4)*
H13B	0.9544 (19)	0.4119 (11)	0.7269 (14)	0.048 (4)*
H13C	0.7697 (18)	0.4231 (11)	0.6367 (14)	0.047 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0358 (4)	0.0395 (4)	0.0304 (4)	0.0086 (3)	0.0153 (3)	−0.0084 (3)
O2	0.0220 (4)	0.0319 (4)	0.0213 (4)	0.0054 (3)	0.0086 (3)	0.0003 (3)
N1	0.0237 (4)	0.0214 (4)	0.0231 (4)	−0.0003 (3)	0.0111 (3)	−0.0032 (3)
N2	0.0272 (4)	0.0193 (4)	0.0269 (5)	−0.0022 (3)	0.0123 (4)	0.0002 (3)
N3	0.0231 (4)	0.0225 (4)	0.0194 (4)	−0.0009 (3)	0.0112 (3)	0.0030 (3)
N4	0.0178 (4)	0.0173 (4)	0.0165 (4)	0.0000 (3)	0.0081 (3)	−0.0003 (3)
C1	0.0361 (6)	0.0337 (6)	0.0273 (6)	−0.0027 (5)	0.0201 (5)	−0.0037 (4)
C2	0.0201 (4)	0.0230 (5)	0.0202 (5)	0.0004 (4)	0.0083 (4)	−0.0017 (3)
C3	0.0205 (4)	0.0186 (4)	0.0203 (5)	0.0001 (3)	0.0085 (4)	0.0010 (3)
C4	0.0165 (4)	0.0165 (4)	0.0188 (5)	0.0010 (3)	0.0057 (3)	0.0011 (3)
C5	0.0245 (5)	0.0217 (5)	0.0242 (5)	−0.0022 (4)	0.0104 (4)	0.0022 (4)
C6	0.0181 (4)	0.0167 (4)	0.0206 (5)	0.0005 (3)	0.0062 (4)	−0.0015 (3)
C7	0.0252 (5)	0.0159 (4)	0.0199 (5)	0.0010 (4)	0.0099 (4)	−0.0001 (3)
C8	0.0284 (5)	0.0207 (5)	0.0197 (5)	−0.0022 (4)	0.0089 (4)	−0.0022 (4)
C9	0.0268 (5)	0.0254 (5)	0.0240 (5)	−0.0053 (4)	0.0081 (4)	−0.0045 (4)
C10	0.0317 (6)	0.0358 (6)	0.0316 (6)	0.0027 (5)	0.0060 (5)	−0.0027 (5)
C11	0.0265 (5)	0.0204 (4)	0.0219 (5)	0.0064 (4)	0.0100 (4)	0.0018 (4)
C12	0.0211 (5)	0.0476 (7)	0.0277 (6)	0.0110 (5)	0.0094 (4)	0.0019 (5)
C13	0.0250 (6)	0.0630 (9)	0.0291 (6)	0.0004 (6)	0.0123 (5)	0.0060 (6)

Geometric parameters (Å, º)

O1—C11	1.2032 (13)	C3—H3	0.990 (12)
O2—C11	1.3345 (13)	C4—C7	1.5008 (14)
O2—C12	1.4605 (15)	C5—H5	1.000 (12)
N1—C2	1.3279 (14)	C7—C11	1.5198 (16)
N1—C6	1.3434 (14)	C7—C8	1.5445 (15)
N2—C6	1.3357 (13)	C7—H7	1.017 (12)
N2—C5	1.3535 (14)	C8—C9	1.4889 (16)
N3—C5	1.3306 (15)	C8—H8A	1.005 (12)
N3—N4	1.3638 (12)	C8—H8B	0.977 (12)
N4—C4	1.3667 (13)	C9—C10	1.3172 (17)
N4—C6	1.3820 (13)	C9—H9	0.978 (14)
C1—C2	1.4940 (16)	C10—H10A	1.032 (15)
C1—H1A	0.9800	C10—H10B	0.959 (15)
C1—H1B	0.9800	C12—C13	1.501 (2)
C1—H1C	0.9800	C12—H12A	0.965 (14)
C1—H1D	0.9800	C12—H12B	0.974 (14)
C1—H1E	0.9800	C13—H13A	0.990 (16)
C1—H1F	0.9800	C13—H13B	1.017 (16)
C2—C3	1.4241 (14)	C13—H13C	0.989 (15)

C3—C4	1.3599 (14)		
C11—O2—C12	116.85 (9)	N3—C5—H5	120.3 (7)
C2—N1—C6	116.29 (8)	N2—C5—H5	122.4 (7)
C6—N2—C5	102.29 (9)	N2—C6—N1	128.65 (9)
C5—N3—N4	100.91 (8)	N2—C6—N4	109.18 (9)
N3—N4—C4	127.07 (8)	N1—C6—N4	122.17 (9)
N3—N4—C6	110.26 (8)	C4—C7—C11	112.47 (8)
C4—N4—C6	122.65 (9)	C4—C7—C8	112.63 (8)
C2—C1—H1A	109.5	C11—C7—C8	109.71 (9)
C2—C1—H1B	109.5	C4—C7—H7	106.9 (7)
H1A—C1—H1B	109.5	C11—C7—H7	108.3 (6)
C2—C1—H1C	109.5	C8—C7—H7	106.6 (7)
H1A—C1—H1C	109.5	C9—C8—C7	112.78 (9)
H1B—C1—H1C	109.5	C9—C8—H8A	108.8 (7)
C2—C1—H1D	109.5	C7—C8—H8A	109.5 (7)
H1A—C1—H1D	141.1	C9—C8—H8B	110.5 (7)
H1B—C1—H1D	56.3	C7—C8—H8B	105.3 (7)
H1C—C1—H1D	56.3	H8A—C8—H8B	110.0 (10)
C2—C1—H1E	109.5	C10—C9—C8	123.39 (11)
H1A—C1—H1E	56.3	C10—C9—H9	118.1 (8)
H1B—C1—H1E	141.1	C8—C9—H9	118.5 (8)
H1C—C1—H1E	56.3	C9—C10—H10A	118.7 (8)
H1D—C1—H1E	109.5	C9—C10—H10B	120.9 (9)
C2—C1—H1F	109.5	H10A—C10—H10B	120.4 (12)
H1A—C1—H1F	56.3	O1—C11—O2	124.92 (10)
H1B—C1—H1F	56.3	O1—C11—C7	123.51 (9)
H1C—C1—H1F	141.1	O2—C11—C7	111.56 (8)
H1D—C1—H1F	109.5	O2—C12—C13	110.25 (9)
H1E—C1—H1F	109.5	O2—C12—H12A	108.5 (8)
N1—C2—C3	123.03 (10)	C13—C12—H12A	112.2 (8)
N1—C2—C1	116.90 (9)	O2—C12—H12B	102.4 (8)
C3—C2—C1	120.07 (9)	C13—C12—H12B	110.6 (8)
C4—C3—C2	120.31 (9)	H12A—C12—H12B	112.3 (11)
C4—C3—H3	118.2 (7)	C12—C13—H13A	110.0 (9)
C2—C3—H3	121.5 (7)	C12—C13—H13B	106.5 (8)
C3—C4—N4	115.52 (8)	H13A—C13—H13B	113.7 (12)
C3—C4—C7	126.04 (9)	C12—C13—H13C	110.9 (9)
N4—C4—C7	118.41 (9)	H13A—C13—H13C	108.1 (12)
N3—C5—N2	117.37 (9)	H13B—C13—H13C	107.6 (12)
C5—N3—N4—C4	−177.92 (9)	N3—N4—C6—N2	−0.07 (10)
C5—N3—N4—C6	0.17 (10)	C4—N4—C6—N2	178.12 (8)
C6—N1—C2—C3	−0.25 (14)	N3—N4—C6—N1	179.66 (8)
C6—N1—C2—C1	−179.75 (9)	C4—N4—C6—N1	−2.16 (14)
N1—C2—C3—C4	0.13 (15)	C3—C4—C7—C11	−125.28 (10)
C1—C2—C3—C4	179.61 (9)	N4—C4—C7—C11	57.08 (11)
C2—C3—C4—N4	−0.91 (14)	C3—C4—C7—C8	110.12 (12)

C2—C3—C4—C7	−178.61 (8)	N4—C4—C7—C8	−67.52 (12)
N3—N4—C4—C3	179.76 (8)	C4—C7—C8—C9	−46.69 (12)
C6—N4—C4—C3	1.90 (13)	C11—C7—C8—C9	−172.79 (8)
N3—N4—C4—C7	−2.35 (13)	C7—C8—C9—C10	125.75 (11)
C6—N4—C4—C7	179.78 (8)	C12—O2—C11—O1	5.43 (15)
N4—N3—C5—N2	−0.23 (11)	C12—O2—C11—C7	−175.66 (8)
C6—N2—C5—N3	0.19 (12)	C4—C7—C11—O1	−151.70 (10)
C5—N2—C6—N1	−179.76 (10)	C8—C7—C11—O1	−25.51 (13)
C5—N2—C6—N4	−0.07 (10)	C4—C7—C11—O2	29.37 (11)
C2—N1—C6—N2	−179.11 (9)	C8—C7—C11—O2	155.55 (8)
C2—N1—C6—N4	1.22 (14)	C11—O2—C12—C13	91.48 (12)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C5/N2/C6/N4/N3 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	1.000 (12)	2.532 (12)	3.4147 (19)	147.1 (9)
C10—H10*B*···*Cg*1^{ii}	0.962 (17)	2.747 (18)	3.657 (3)	143.9 (13)

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