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4-[(*Z*)-(4-Ethoxyphenylamino)(phenyl)-methylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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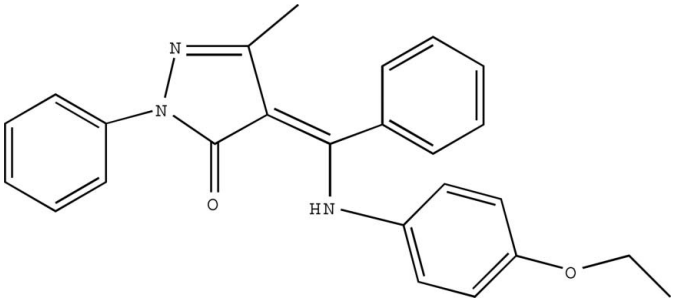
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.211; data-to-parameter ratio = 16.9.

The structure of the title compound, $C_{25}H_{23}N_3O_2$, features a central pyrazole ring; an amine NH unit interacts with the ring CO unit through an intramolecular N—H···O hydrogen bond [N···O = 2.700 (2) Å]

Related literature

For related structures, see: Bao, Lü, Wu, Kang & Ng (2004); Bao, Lü, Wu, & Ng (2004); Jiang *et al.* (2004). For related literature, see: Bao *et al.* (2006).



Experimental

Crystal data

$C_{25}H_{23}N_3O_2$
M_r = 397.46
Triclinic, $P\overline{1}$
a = 6.9269 (9) Å
b = 10.7876 (14) Å
c = 15.531 (2) Å
α = 71.966 (2)°
β = 78.994 (2)°
γ = 81.296 (3)°
V = 1077.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
8649 measured reflections
4588 independent reflections
2518 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.211
S = 0.70
4588 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1	0.86	1.98	2.700 (3)	140

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2438).

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  doi:10.1107/S1600536807026992

supplementary materials

Acta Cryst. (2007). E**63**, o3158 [**doi:10.1107/S1600536807026992**]

4-[(*Z*)-(4-Ethoxyphenylamino)(phenyl)methylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

R. Ma, Y. Chen, Z.-Y. Song, Y.-Q. Bai and F. Bao

Comment

This study is a continuation of our investigations of 4-(*Z*)- [(4-ethoxyphenylamino)(phenyl)methylene]-3-methyl- 1-phenyl-1*H*-pyrazol-5(4*H*)-ones, which are readily synthesized by condensing 4-benzoyl-3-methyl-1- phenyl-5-pyrazolone with a primary amine (Bao, Lü, Wu, Kang & Ng, 2004; Bao, Lü, Wu, & Ng, 2004; Jiang *et al.*, 2004). A characteristic of such pyrazolones is the short intramolecular hydrogen bond between the amino NH unit and the carbonyl C=O unit.

The title compound, (I), (Fig. 1), similarly exists as a monomeric molecule that features an intramolecular N—H···O hydrogen bond (Table 1) despite the presence of possible acceptor atoms in nearby molecules.

Experimental

4-Benzoyl-3-methyl-1-phenyl-5-pyrazolone (1.20 g, 4.3 mmol) and 4-ethoxybenzenamine (0.62 g, 6.5 mmol) were dissolved in ethyl alcohol (20 ml). The solution was heated under reflux for 8 h. The solvent was removed and the pure product obtained upon recrystallization from ethyl alcohol (25 ml) in about 80% yield. Crystals of (I) were grown from ethanol at room temperature. Analysis calculated for $C_{25}H_{23}N_3O_2$: C 75.55, H 5.83, N 10.57%; found: C 75.52, H 5.85, N 10.58%.

Refinement

All H atoms were geometrically placed (C—H = 0.93–0.97 Å, O—H = 0.82 Å, N—H = 0.85–0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O,*N*).

Figures

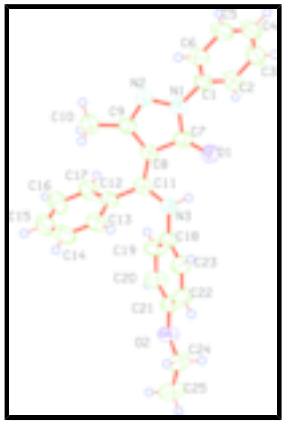


Fig. 1. Vew of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius and the hydrogen bond is indicated by a double-dashed line.

4-[(*Z*)-(4-Ethoxyphenylamino)(phenyl)methylene]-3-methyl-1-phenyl- 1*H*-pyrazol-5(4*H*)-one

Crystal data

$C_{25}H_{23}N_3O_2$	$Z = 2$
$M_r = 397.46$	$F_{000} = 420$
Triclinic, $P\overline{1}$	$D_x = 1.225$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.9269$ (9) Å	Cell parameters from 1701 reflections
$b = 10.7876$ (14) Å	$\theta = 2.8$–23.3º
$c = 15.531$ (2) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 71.966$ (2)º	$T = 293$ (2) K
$\beta = 78.994$ (2)º	Block, yellow
$\gamma = 81.296$ (3)º	0.30 × 0.20 × 0.20 mm
$V = 1077.9$ (2) Å^3	

Data collection

Bruker SMART CCD diffractometer	2518 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.059$
Monochromator: graphite	$\theta_{max} = 27.0$º
$T = 293(2)$ K	$\theta_{min} = 2.0$º
ω scans	$h = -6 \rightarrow 8$
Absorption correction: none	$k = -12 \rightarrow 13$
8649 measured reflections	$l = -19 \rightarrow 19$
4588 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.211$	$w = 1/[\sigma^2(F_o^2) + (0.1794P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.70$	$(\Delta/\sigma)_{max} < 0.001$
4588 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}
271 parameters	$\Delta\rho_{min} = -0.17$ 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 $F^2 > 2\text{sigma}(F^2)$ 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}
O2	0.3867 (2)	0.78662 (17)	0.05284 (11)	0.0580 (5)
N1	1.2631 (3)	1.14403 (18)	0.30935 (12)	0.0503 (5)
O1	1.1023 (2)	1.17814 (16)	0.18320 (10)	0.0597 (5)
N3	0.9036 (3)	0.9699 (2)	0.20785 (13)	0.0552 (5)
H3A	0.9570	1.0391	0.1736	0.066*
N2	1.2852 (3)	1.04592 (18)	0.39146 (12)	0.0517 (5)
C11	0.9511 (3)	0.9213 (2)	0.29198 (15)	0.0461 (5)
C21	0.5236 (3)	0.8295 (2)	0.08632 (14)	0.0483 (5)
C7	1.1391 (3)	1.1128 (2)	0.26106 (14)	0.0479 (5)
C18	0.7734 (3)	0.9196 (2)	0.16823 (15)	0.0499 (6)
C9	1.1726 (3)	0.9562 (2)	0.39721 (14)	0.0468 (5)
C8	1.0718 (3)	0.9901 (2)	0.31896 (14)	0.0450 (5)
C12	0.8815 (3)	0.7945 (2)	0.35031 (15)	0.0466 (5)
C1	1.3747 (3)	1.2522 (2)	0.28323 (15)	0.0495 (6)
C19	0.5790 (4)	0.9105 (3)	0.20650 (17)	0.0622 (7)
H19A	0.5305	0.9350	0.2596	0.075*
C23	0.8423 (4)	0.8833 (3)	0.08965 (15)	0.0612 (7)
H23A	0.9745	0.8891	0.0639	0.073*
C13	0.9534 (4)	0.6814 (2)	0.32642 (18)	0.0598 (6)
H13A	1.0421	0.6854	0.2727	0.072*
C20	0.4556 (4)	0.8647 (3)	0.16570 (17)	0.0620 (7)
H20A	0.3240	0.8575	0.1923	0.074*
C6	1.5599 (4)	1.2363 (3)	0.30841 (17)	0.0605 (7)
H6A	1.6127	1.1539	0.3400	0.073*
C2	1.2973 (4)	1.3750 (2)	0.23493 (17)	0.0613 (7)
H2B	1.1738	1.3858	0.2169	0.074*
C17	0.7493 (4)	0.7871 (2)	0.43025 (16)	0.0596 (6)
H17A	0.7010	0.8625	0.4476	0.072*
C22	0.7190 (4)	0.8383 (3)	0.04823 (15)	0.0601 (7)
H22A	0.7678	0.8142	−0.0050	0.072*
C10	1.1678 (4)	0.8376 (2)	0.47893 (16)	0.0621 (7)
H10A	1.2523	0.8450	0.5191	0.093*
H10B	1.2130	0.7607	0.4592	0.093*

H10C	1.0349	0.8311	0.5109	0.093*
C5	1.6661 (5)	1.3433 (3)	0.28646 (19)	0.0718 (8)
H5A	1.7907	1.3326	0.3034	0.086*
C4	1.5899 (5)	1.4647 (3)	0.24021 (19)	0.0771 (9)
H4A	1.6619	1.5363	0.2264	0.092*
C3	1.4055 (5)	1.4812 (3)	0.21387 (19)	0.0721 (8)
H3B	1.3542	1.5639	0.1819	0.087*
C24	0.4498 (4)	0.7369 (3)	−0.02403 (17)	0.0701 (8)
H24A	0.5562	0.6673	−0.0116	0.084*
H24B	0.4972	0.8059	−0.0776	0.084*
C14	0.8941 (5)	0.5630 (3)	0.3818 (2)	0.0745 (8)
H14A	0.9448	0.4867	0.3661	0.089*
C15	0.7607 (5)	0.5564 (3)	0.4602 (2)	0.0754 (8)
H15A	0.7192	0.4761	0.4970	0.090*
C16	0.6894 (4)	0.6674 (3)	0.48406 (19)	0.0707 (8)
H16A	0.5991	0.6627	0.5374	0.085*
C25	0.2757 (5)	0.6857 (4)	−0.0402 (2)	0.0918 (10)
H25A	0.3131	0.6512	−0.0918	0.138*
H25B	0.1716	0.7554	−0.0525	0.138*
H25C	0.2303	0.6174	0.0132	0.138*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0545 (10)	0.0692 (11)	0.0609 (9)	−0.0116 (8)	−0.0103 (8)	−0.0308 (8)
N1	0.0543 (12)	0.0474 (11)	0.0531 (10)	−0.0130 (9)	−0.0112 (9)	−0.0144 (8)
O1	0.0629 (11)	0.0623 (11)	0.0537 (9)	−0.0193 (8)	−0.0154 (8)	−0.0067 (8)
N3	0.0542 (12)	0.0586 (12)	0.0565 (11)	−0.0221 (10)	−0.0102 (9)	−0.0131 (9)
N2	0.0566 (12)	0.0513 (11)	0.0506 (10)	−0.0098 (9)	−0.0113 (9)	−0.0158 (9)
C11	0.0391 (12)	0.0491 (13)	0.0529 (12)	−0.0018 (10)	−0.0039 (9)	−0.0218 (10)
C21	0.0471 (13)	0.0517 (13)	0.0501 (12)	−0.0086 (10)	−0.0095 (10)	−0.0173 (10)
C7	0.0433 (13)	0.0527 (13)	0.0517 (12)	−0.0068 (10)	−0.0045 (10)	−0.0215 (10)
C18	0.0485 (14)	0.0504 (13)	0.0534 (12)	−0.0111 (11)	−0.0123 (10)	−0.0132 (10)
C9	0.0448 (13)	0.0470 (13)	0.0512 (12)	−0.0050 (10)	−0.0044 (10)	−0.0198 (10)
C8	0.0424 (12)	0.0441 (12)	0.0517 (12)	−0.0063 (10)	−0.0050 (9)	−0.0189 (10)
C12	0.0414 (12)	0.0460 (13)	0.0570 (12)	−0.0050 (10)	−0.0101 (10)	−0.0197 (10)
C1	0.0530 (14)	0.0473 (13)	0.0531 (12)	−0.0128 (11)	−0.0025 (10)	−0.0213 (10)
C19	0.0503 (15)	0.0804 (18)	0.0705 (15)	−0.0101 (13)	−0.0020 (12)	−0.0454 (14)
C23	0.0470 (14)	0.0873 (19)	0.0517 (13)	−0.0215 (13)	−0.0002 (11)	−0.0209 (12)
C13	0.0584 (16)	0.0558 (15)	0.0727 (15)	−0.0070 (12)	−0.0074 (12)	−0.0305 (13)
C20	0.0422 (13)	0.0809 (18)	0.0745 (16)	−0.0096 (12)	0.0002 (11)	−0.0430 (14)
C6	0.0614 (16)	0.0618 (16)	0.0677 (15)	−0.0135 (13)	−0.0154 (12)	−0.0254 (12)
C2	0.0619 (16)	0.0531 (15)	0.0706 (15)	−0.0126 (13)	−0.0072 (12)	−0.0187 (12)
C17	0.0558 (15)	0.0541 (15)	0.0683 (15)	−0.0092 (12)	0.0025 (12)	−0.0221 (12)
C22	0.0552 (15)	0.0810 (18)	0.0462 (12)	−0.0155 (13)	0.0017 (11)	−0.0230 (12)
C10	0.0669 (17)	0.0562 (15)	0.0618 (14)	−0.0110 (13)	−0.0139 (12)	−0.0104 (12)
C5	0.0719 (18)	0.078 (2)	0.0764 (17)	−0.0316 (16)	−0.0116 (14)	−0.0269 (15)
C4	0.093 (2)	0.072 (2)	0.0765 (18)	−0.0439 (17)	−0.0014 (16)	−0.0270 (16)

C3	0.085 (2)	0.0532 (16)	0.0747 (17)	−0.0200 (15)	−0.0042 (15)	−0.0128 (13)
C24	0.0717 (18)	0.093 (2)	0.0563 (14)	−0.0117 (15)	−0.0104 (13)	−0.0342 (14)
C14	0.084 (2)	0.0499 (16)	0.102 (2)	−0.0068 (14)	−0.0240 (18)	−0.0336 (15)
C15	0.075 (2)	0.0558 (17)	0.093 (2)	−0.0218 (15)	−0.0171 (17)	−0.0084 (15)
C16	0.0628 (17)	0.0667 (19)	0.0743 (17)	−0.0174 (14)	0.0019 (13)	−0.0105 (14)
C25	0.088 (2)	0.129 (3)	0.088 (2)	−0.014 (2)	−0.0289 (17)	−0.062 (2)

Geometric parameters (Å, °)

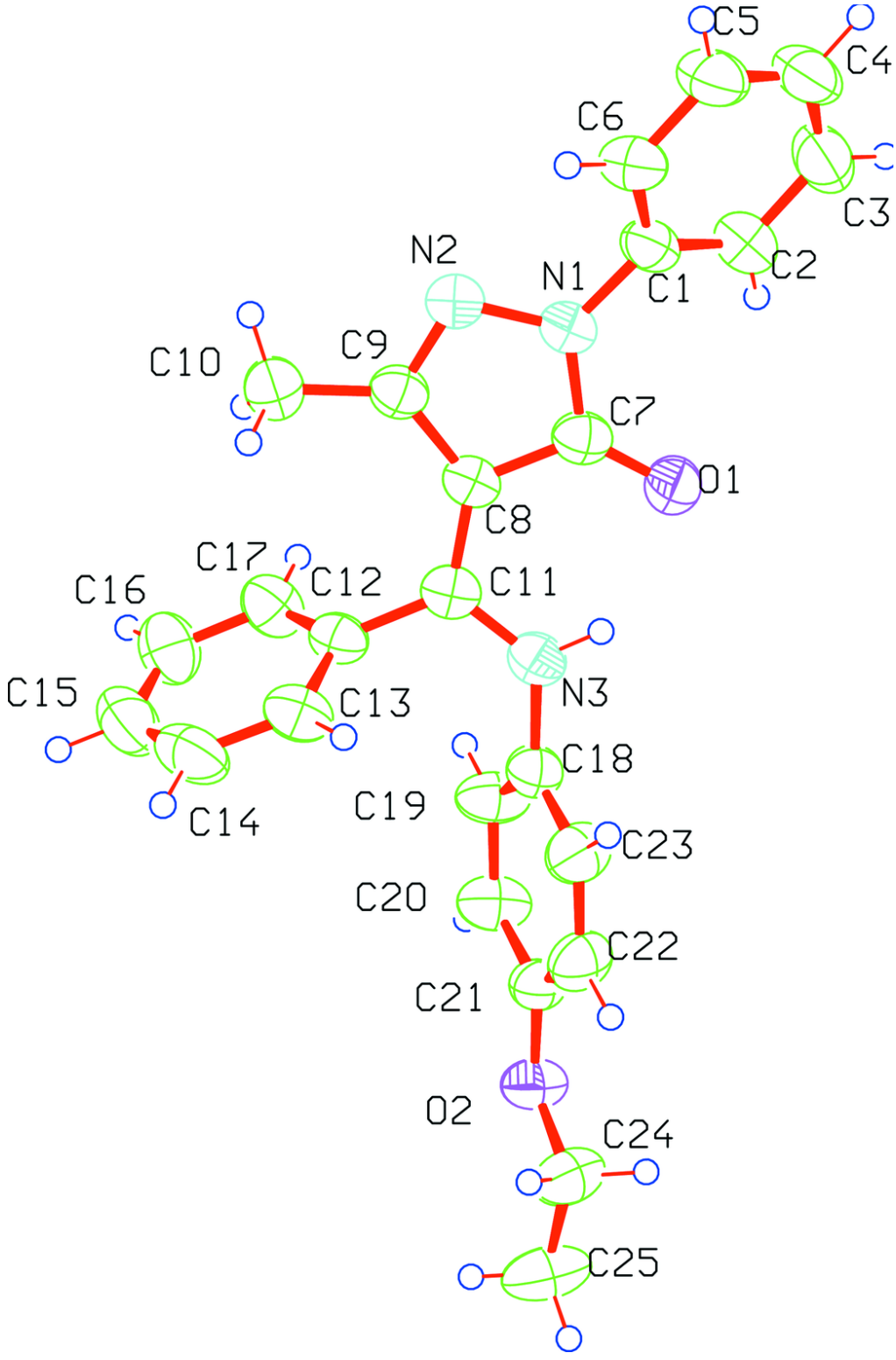
O2—C21	1.361 (3)	C13—H13A	0.9300
O2—C24	1.425 (3)	C20—H20A	0.9300
N1—C7	1.380 (3)	C6—C5	1.381 (4)
N1—N2	1.400 (2)	C6—H6A	0.9300
N1—C1	1.409 (3)	C2—C3	1.384 (4)
O1—C7	1.249 (3)	C2—H2B	0.9300
N3—C11	1.333 (3)	C17—C16	1.378 (3)
N3—C18	1.433 (3)	C17—H17A	0.9300
N3—H3A	0.8600	C22—H22A	0.9300
N2—C9	1.305 (3)	C10—H10A	0.9600
C11—C8	1.392 (3)	C10—H10B	0.9600
C11—C12	1.480 (3)	C10—H10C	0.9600
C21—C22	1.375 (3)	C5—C4	1.364 (4)
C21—C20	1.378 (3)	C5—H5A	0.9300
C7—C8	1.438 (3)	C4—C3	1.384 (4)
C18—C19	1.369 (3)	C4—H4A	0.9300
C18—C23	1.374 (3)	C3—H3B	0.9300
C9—C8	1.439 (3)	C24—C25	1.492 (4)
C9—C10	1.496 (3)	C24—H24A	0.9700
C12—C13	1.378 (3)	C24—H24B	0.9700
C12—C17	1.383 (3)	C14—C15	1.371 (4)
C1—C6	1.382 (3)	C14—H14A	0.9300
C1—C2	1.389 (3)	C15—C16	1.357 (4)
C19—C20	1.380 (3)	C15—H15A	0.9300
C19—H19A	0.9300	C16—H16A	0.9300
C23—C22	1.381 (3)	C25—H25A	0.9600
C23—H23A	0.9300	C25—H25B	0.9600
C13—C14	1.373 (4)	C25—H25C	0.9600
C21—O2—C24	118.67 (19)	C1—C6—H6A	120.1
C7—N1—N2	111.88 (18)	C3—C2—C1	119.4 (3)
C7—N1—C1	128.75 (19)	C3—C2—H2B	120.3
N2—N1—C1	119.18 (18)	C1—C2—H2B	120.3
C11—N3—C18	127.2 (2)	C16—C17—C12	119.6 (2)
C11—N3—H3A	116.4	C16—C17—H17A	120.2
C18—N3—H3A	116.4	C12—C17—H17A	120.2
C9—N2—N1	106.65 (17)	C21—C22—C23	119.4 (2)
N3—C11—C8	118.0 (2)	C21—C22—H22A	120.3
N3—C11—C12	118.73 (19)	C23—C22—H22A	120.3
C8—C11—C12	123.23 (19)	C9—C10—H10A	109.5
O2—C21—C22	125.5 (2)	C9—C10—H10B	109.5

O2—C21—C20	115.4 (2)	H10A—C10—H10B	109.5
C22—C21—C20	119.1 (2)	C9—C10—H10C	109.5
O1—C7—N1	125.8 (2)	H10A—C10—H10C	109.5
O1—C7—C8	129.6 (2)	H10B—C10—H10C	109.5
N1—C7—C8	104.61 (18)	C4—C5—C6	120.6 (3)
C19—C18—C23	119.4 (2)	C4—C5—H5A	119.7
C19—C18—N3	120.7 (2)	C6—C5—H5A	119.7
C23—C18—N3	119.9 (2)	C5—C4—C3	120.1 (3)
N2—C9—C8	111.37 (19)	C5—C4—H4A	120.0
N2—C9—C10	118.4 (2)	C3—C4—H4A	120.0
C8—C9—C10	130.2 (2)	C4—C3—C2	120.1 (3)
C11—C8—C7	122.44 (19)	C4—C3—H3B	119.9
C11—C8—C9	131.8 (2)	C2—C3—H3B	119.9
C7—C8—C9	105.41 (19)	O2—C24—C25	107.2 (2)
C13—C12—C17	119.3 (2)	O2—C24—H24A	110.3
C13—C12—C11	119.8 (2)	C25—C24—H24A	110.3
C17—C12—C11	120.8 (2)	O2—C24—H24B	110.3
C6—C1—C2	120.1 (2)	C25—C24—H24B	110.3
C6—C1—N1	119.5 (2)	H24A—C24—H24B	108.5
C2—C1—N1	120.4 (2)	C15—C14—C13	120.4 (3)
C18—C19—C20	119.5 (2)	C15—C14—H14A	119.8
C18—C19—H19A	120.3	C13—C14—H14A	119.8
C20—C19—H19A	120.3	C16—C15—C14	119.8 (3)
C18—C23—C22	121.3 (2)	C16—C15—H15A	120.1
C18—C23—H23A	119.4	C14—C15—H15A	120.1
C22—C23—H23A	119.4	C15—C16—C17	120.8 (3)
C14—C13—C12	120.0 (2)	C15—C16—H16A	119.6
C14—C13—H13A	120.0	C17—C16—H16A	119.6
C12—C13—H13A	120.0	C24—C25—H25A	109.5
C21—C20—C19	121.3 (2)	C24—C25—H25B	109.5
C21—C20—H20A	119.4	H25A—C25—H25B	109.5
C19—C20—H20A	119.4	C24—C25—H25C	109.5
C5—C6—C1	119.7 (3)	H25A—C25—H25C	109.5
C5—C6—H6A	120.1	H25B—C25—H25C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O1	0.86	1.98	2.700 (3)	140

Fig. 1


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