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6-Amino-3-methyl-1-phenyl-1*H*-pyrazolo[3,4-*b*]-pyrazine-5-carboxamide

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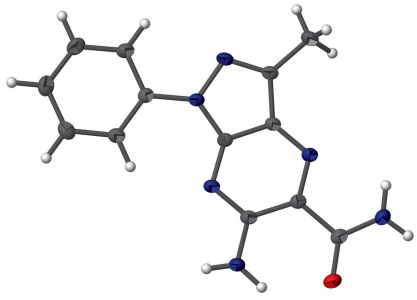
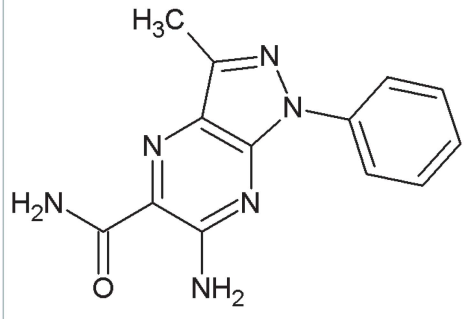
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{13}H_{12}N_6O$, the pyrazolo[3,4-*b*]pyrazine ring system is planar (r.m.s. deviation for the nine fitted atoms = 0.024 Å) and makes a dihedral angle of 5.72 (6)° with the pendent phenyl ring. The molecular conformation is stabilized by intramolecular N—H···O and C—H···N hydrogen bonds, each generating an *S*(6) loop. In the crystal, pairs of molecules are connected into inversion dimers by strong N—H···O hydrogen bonds, forming $R_2^2(8)$ ring motifs. These are linked into sheets parallel to (100) *via* N—H···N hydrogen bonds; π–π interactions between symmetry-related pyrazole and phenyl rings [centroid–centroid distances = 3.4453 (9) Å] within the sheets are also noted.

3D view



Chemical scheme



Structure description

Pyrazole-containing compounds have been shown to exhibit numerous biological activities such as anti-inflammatory (Süküroğlu *et al.*, 2005), antimalarial (Cunico *et al.*, 2006), antitumor (Naito, *et al.*, 2002), antibacterial, antifungal (Akbas *et al.*, 2005; El-Emary, 2006), antiparasitic (El-Kashef *et al.*, 2000; Rathelot *et al.*, 2002) and antiviral (Ding *et al.*, 1994). This led to the structure determination of the title compound (Fig. 1).

The pyrazolo[3,4-*b*]pyrazine ring system of the title compound is essentially planar with puckering parameters $Q(2)$ = 0.0552 (15) Å and $\varphi(2)$ = 251.1 (15)°. It is inclined to the phenyl ring with a dihedral angle of 5.72 (6)°. The bond lengths and bond angles of the title compound are normal and are in agreement with those reported for a similar

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O1	0.93 (2)	1.97 (2)	2.6878 (18)	132.1 (17)
C13—H13···N3	0.95	2.31	2.985 (2)	127
N1—H1A···O1^{i}	0.88	2.07	2.9488 (18)	175
N2—H2A···N2^{ii}	0.86	2.50	3.345 (2)	167

Symmetry codes: (i) $-x+1, -y+3, -z+1$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

compound (Mague *et al.*, 2014). Intramolecular C—H···N and N—H···O hydrogen bonds form $S(6)$ loop systems (Table 1, Fig. 2), stabilizing the molecular conformation.

In the crystal, pairs of molecules are connected into inversion dimers by N—H···O hydrogen bonds, leading to $R_2^2(8)$ ring motifs. These dimers are linked by N—H···N hydrogen bonds, leading to the formation of sheets parallel to the *bc* plane. Further connections within sheets are *via* π–π interactions between symmetry-related pyrazole and phenyl rings [centroid–centroid distances = 3.4453 (9) Å; symmetry operation: $x, 1+y, z$].

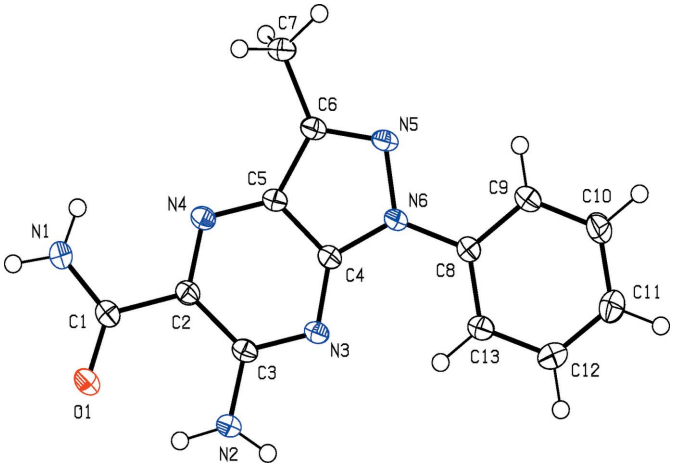


Figure 1
The title compound, with 50% probability displacement ellipsoids.

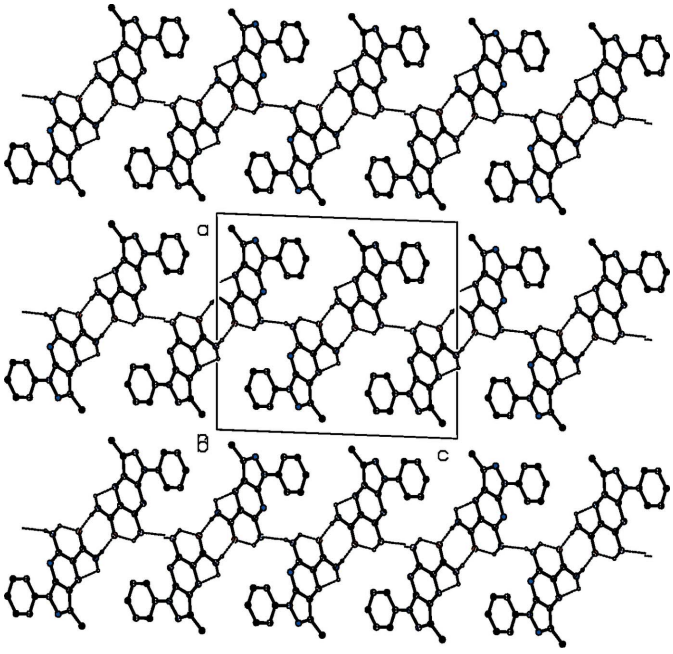


Figure 2
A view down the *b* axis of the unit-cell contents of the title compound. Dashed lines indicate hydrogen bonds.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{12}N_6O$
M_r	268.29
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, b, c (Å)	14.7907 (5), 4.80351 (15), 17.1203 (8)
β (°)	92.067 (4)
V (Å^3)	1215.57 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.83
Crystal size (mm)	0.38 × 0.08 × 0.08
Data collection	
Diffractometer	Rigaku Oxford Diffraction
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.909, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4156, 2307, 2011
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.112, 1.06
No. of reflections	2307
No. of parameters	187
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.27

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Synthesis and crystallization

The title compound was prepared according to our reported method (El-Emary, 2007). Crystals for X-ray diffraction analysis were obtained by slow evaporation of a dimethyl sulfoxide solution of the compound.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161742 [https://doi.org/10.1107/S2414314616017429]

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Crystal data

$C_{13}H_{12}N_6O$
M_r = 268.29
Monoclinic, $P2_1/c$
a = 14.7907 (5) Å
b = 4.80351 (15) Å
c = 17.1203 (8) Å
β = 92.067 (4)°
V = 1215.57 (8) Å^3
Z = 4
$F(000)$ = 560
D_x = 1.466 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 1708 reflections
θ = 3.9–71.0°
μ = 0.83 mm^{-1}
T = 173 K
Needle, yellow
0.38 × 0.08 × 0.08 mm

Data collection

Rigaku Oxford Diffraction diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.909, T_{max} = 1.000
4156 measured reflections
2307 independent reflections
2011 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 71.4°, θ_{min} = 5.2°
h = −13→18
k = −5→3
l = −18→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.06
2307 reflections
187 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.3905P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.49400 (7)	1.2243 (2)	0.57401 (7)	0.0261 (3)
N1	0.61528 (9)	1.3370 (3)	0.50430 (8)	0.0259 (3)
H1A	0.5852	1.4680	0.4785	0.031*
H1B	0.6724	1.3050	0.4945	0.031*
N2	0.51127 (9)	0.8234 (3)	0.68305 (9)	0.0264 (3)
H2A	0.4974	0.6859	0.7128	0.032*
N3	0.64619 (8)	0.5919 (3)	0.69322 (7)	0.0188 (3)
N4	0.71717 (8)	0.9523 (3)	0.57703 (7)	0.0186 (3)
N5	0.88003 (8)	0.4818 (3)	0.66020 (7)	0.0203 (3)
N6	0.80080 (8)	0.4173 (3)	0.69785 (7)	0.0185 (3)
C1	0.57451 (10)	1.1873 (3)	0.55802 (9)	0.0201 (3)
C2	0.63173 (10)	0.9704 (3)	0.59852 (8)	0.0187 (3)
C3	0.59627 (10)	0.7917 (3)	0.65810 (9)	0.0189 (3)
C4	0.73170 (10)	0.5843 (3)	0.67103 (8)	0.0170 (3)
C5	0.76778 (10)	0.7588 (3)	0.61399 (9)	0.0182 (3)
C6	0.86115 (10)	0.6839 (3)	0.61053 (9)	0.0200 (3)
C7	0.93157 (10)	0.8105 (4)	0.56164 (10)	0.0275 (4)
H7A	0.9917	0.7674	0.5844	0.041*
H7B	0.9232	1.0128	0.5598	0.041*
H7C	0.9261	0.7346	0.5085	0.041*
C8	0.80259 (10)	0.2105 (3)	0.75710 (9)	0.0188 (3)
C9	0.88429 (10)	0.0839 (3)	0.77948 (10)	0.0246 (4)
H9	0.9388	0.1388	0.7562	0.030*
C10	0.88520 (11)	−0.1224 (4)	0.83593 (10)	0.0291 (4)
H10	0.9408	−0.2087	0.8512	0.035*
C11	0.80605 (12)	−0.2052 (3)	0.87057 (10)	0.0281 (4)
H11	0.8072	−0.3483	0.9089	0.034*
C12	0.72548 (11)	−0.0761 (3)	0.84836 (9)	0.0257 (4)
H12	0.6710	−0.1311	0.8718	0.031*
C13	0.72332 (10)	0.1325 (3)	0.79237 (9)	0.0223 (3)
H13	0.6678	0.2218	0.7782	0.027*
H2B	0.4722 (14)	0.939 (4)	0.6543 (13)	0.036 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0188 (5)	0.0262 (6)	0.0333 (6)	0.0053 (4)	0.0009 (5)	0.0035 (5)
N1	0.0220 (6)	0.0268 (7)	0.0289 (7)	0.0044 (6)	0.0004 (5)	0.0080 (6)
N2	0.0169 (6)	0.0288 (7)	0.0338 (8)	0.0048 (6)	0.0065 (6)	0.0094 (6)
N3	0.0142 (6)	0.0202 (6)	0.0219 (6)	0.0006 (5)	0.0015 (5)	−0.0010 (5)
N4	0.0156 (6)	0.0200 (6)	0.0201 (6)	−0.0005 (5)	−0.0004 (5)	−0.0020 (5)
N5	0.0135 (6)	0.0255 (7)	0.0221 (6)	0.0001 (5)	0.0024 (5)	−0.0011 (5)
N6	0.0133 (6)	0.0205 (6)	0.0216 (6)	0.0010 (5)	0.0012 (5)	0.0010 (5)
C1	0.0191 (7)	0.0182 (7)	0.0229 (7)	0.0009 (6)	−0.0021 (6)	−0.0029 (6)
C2	0.0171 (7)	0.0182 (7)	0.0208 (7)	0.0000 (6)	−0.0005 (6)	−0.0021 (6)

C3	0.0155 (7)	0.0195 (7)	0.0218 (7)	−0.0002 (5)	0.0004 (6)	−0.0034 (6)
C4	0.0157 (7)	0.0175 (7)	0.0177 (7)	0.0002 (5)	−0.0006 (5)	−0.0027 (5)
C5	0.0151 (7)	0.0195 (7)	0.0201 (7)	−0.0003 (5)	0.0013 (5)	−0.0016 (6)
C6	0.0151 (7)	0.0238 (7)	0.0212 (7)	0.0001 (6)	0.0011 (6)	−0.0012 (6)
C7	0.0177 (7)	0.0356 (9)	0.0295 (8)	0.0003 (6)	0.0049 (6)	0.0057 (7)
C8	0.0185 (7)	0.0183 (7)	0.0195 (7)	0.0008 (6)	−0.0006 (6)	−0.0016 (6)
C9	0.0173 (7)	0.0285 (8)	0.0280 (8)	0.0019 (6)	−0.0007 (6)	0.0017 (7)
C10	0.0236 (8)	0.0312 (8)	0.0319 (9)	0.0038 (7)	−0.0052 (7)	0.0048 (7)
C11	0.0335 (9)	0.0270 (8)	0.0236 (8)	−0.0014 (7)	−0.0025 (7)	0.0039 (7)
C12	0.0262 (8)	0.0277 (8)	0.0235 (8)	−0.0044 (7)	0.0045 (6)	−0.0007 (6)
C13	0.0179 (7)	0.0243 (7)	0.0248 (8)	0.0004 (6)	0.0016 (6)	−0.0004 (6)

Geometric parameters (Å, º)

O1—C1	1.2444 (18)	C4—C5	1.407 (2)
N1—H1A	0.8800	C5—C6	1.430 (2)
N1—H1B	0.8800	C6—C7	1.489 (2)
N1—C1	1.329 (2)	C7—H7A	0.9800
N2—H2A	0.8636	C7—H7B	0.9800
N2—C3	1.3509 (19)	C7—H7C	0.9800
N2—H2B	0.93 (2)	C8—C9	1.394 (2)
N3—C3	1.340 (2)	C8—C13	1.389 (2)
N3—C4	1.3341 (18)	C9—H9	0.9500
N4—C2	1.3316 (19)	C9—C10	1.384 (2)
N4—C5	1.338 (2)	C10—H10	0.9500
N5—N6	1.3927 (16)	C10—C11	1.389 (2)
N5—C6	1.314 (2)	C11—H11	0.9500
N6—C4	1.3656 (19)	C11—C12	1.384 (2)
N6—C8	1.4193 (19)	C12—H12	0.9500
C1—C2	1.497 (2)	C12—C13	1.386 (2)
C2—C3	1.446 (2)	C13—H13	0.9500
H1A—N1—H1B	120.0	N5—C6—C5	110.00 (13)
C1—N1—H1A	120.0	N5—C6—C7	121.93 (13)
C1—N1—H1B	120.0	C5—C6—C7	128.05 (14)
H2A—N2—H2B	127.9	C6—C7—H7A	109.5
C3—N2—H2A	110.1	C6—C7—H7B	109.5
C3—N2—H2B	117.8 (13)	C6—C7—H7C	109.5
C4—N3—C3	113.86 (12)	H7A—C7—H7B	109.5
C2—N4—C5	115.77 (12)	H7A—C7—H7C	109.5
C6—N5—N6	107.54 (12)	H7B—C7—H7C	109.5
N5—N6—C8	119.49 (12)	C9—C8—N6	119.68 (14)
C4—N6—N5	110.22 (12)	C13—C8—N6	120.33 (13)
C4—N6—C8	130.23 (13)	C13—C8—C9	119.98 (14)
O1—C1—N1	122.47 (14)	C8—C9—H9	120.3
O1—C1—C2	121.81 (14)	C10—C9—C8	119.38 (15)
N1—C1—C2	115.72 (13)	C10—C9—H9	120.3
N4—C2—C1	116.34 (13)	C9—C10—H10	119.5

N4—C2—C3	121.88 (13)	C9—C10—C11	121.07 (15)
C3—C2—C1	121.78 (13)	C11—C10—H10	119.5
N2—C3—C2	121.43 (13)	C10—C11—H11	120.5
N3—C3—N2	116.29 (13)	C12—C11—C10	118.98 (15)
N3—C3—C2	122.25 (13)	C12—C11—H11	120.5
N3—C4—N6	128.75 (13)	C11—C12—H12	119.6
N3—C4—C5	124.66 (13)	C11—C12—C13	120.79 (15)
N6—C4—C5	106.58 (13)	C13—C12—H12	119.6
N4—C5—C4	121.50 (13)	C8—C13—H13	120.1
N4—C5—C6	132.81 (14)	C12—C13—C8	119.78 (15)
C4—C5—C6	105.66 (13)	C12—C13—H13	120.1
O1—C1—C2—N4	−179.29 (13)	C2—N4—C5—C4	0.8 (2)
O1—C1—C2—C3	0.3 (2)	C2—N4—C5—C6	−176.75 (15)
N1—C1—C2—N4	0.6 (2)	C3—N3—C4—N6	176.55 (14)
N1—C1—C2—C3	−179.82 (13)	C3—N3—C4—C5	−2.4 (2)
N3—C4—C5—N4	0.4 (2)	C4—N3—C3—N2	−174.80 (13)
N3—C4—C5—C6	178.55 (13)	C4—N3—C3—C2	3.3 (2)
N4—C2—C3—N2	175.69 (14)	C4—N6—C8—C9	−173.91 (14)
N4—C2—C3—N3	−2.3 (2)	C4—N6—C8—C13	6.5 (2)
N4—C5—C6—N5	178.32 (15)	C4—C5—C6—N5	0.45 (17)
N4—C5—C6—C7	0.1 (3)	C4—C5—C6—C7	−177.76 (15)
N5—N6—C4—N3	−178.54 (13)	C5—N4—C2—C1	179.62 (12)
N5—N6—C4—C5	0.58 (16)	C5—N4—C2—C3	0.0 (2)
N5—N6—C8—C9	3.0 (2)	C6—N5—N6—C4	−0.30 (16)
N5—N6—C8—C13	−176.51 (13)	C6—N5—N6—C8	−177.82 (13)
N6—N5—C6—C5	−0.10 (16)	C8—N6—C4—N3	−1.4 (3)
N6—N5—C6—C7	178.24 (13)	C8—N6—C4—C5	177.75 (14)
N6—C4—C5—N4	−178.78 (13)	C8—C9—C10—C11	0.0 (3)
N6—C4—C5—C6	−0.61 (16)	C9—C8—C13—C12	−1.6 (2)
N6—C8—C9—C10	−178.44 (15)	C9—C10—C11—C12	−0.6 (3)
N6—C8—C13—C12	177.92 (14)	C10—C11—C12—C13	0.1 (2)
C1—C2—C3—N2	−3.9 (2)	C11—C12—C13—C8	1.0 (2)
C1—C2—C3—N3	178.17 (13)	C13—C8—C9—C10	1.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O1	0.93 (2)	1.97 (2)	2.6878 (18)	132.1 (17)
C13—H13···N3	0.95	2.31	2.985 (2)	127
N1—H1*A*···O1^{i}	0.88	2.07	2.9488 (18)	175
N2—H2*A*···N2^{ii}	0.86	2.50	3.345 (2)	167

Symmetry codes: (i) −*x*+1, −*y*+3, −*z*+1; (ii) −*x*+1, *y*−1/2, −*z*+3/2.