Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(5-Bromopyrimidin-2-yl)-3-phenyl-1*H*-pyrazole-4-carbaldehyde

A. Thiruvalluvar,[a]* M. Subramanyam,[a] Balakrishna Kalluraya[b] and B. Lingappa[b]

[a]PG Research Department of Physics, Rajah Serfoji Government College (Autonomous), Thanjavur 613 005, Tamil Nadu, India, and [b]Department of Studies in Chemistry, Mangalore University, Mangalagangothri 574 199, Karnataka, India
Correspondence e-mail: athiru@vsnl.net

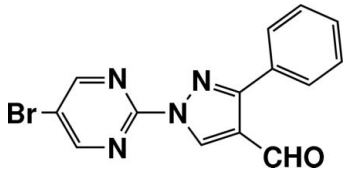
Received 23 June 2007; accepted 27 June 2007

Key indicators: single-crystal X-ray study; T = 160 K; mean σ(C–C) = 0.008 Å; R factor = 0.086; wR factor = 0.238; data-to-parameter ratio = 16.8.

The molecule of the title compound, $C_{14}H_9BrN_4O$, is planar, lying on a mirror plane. The molecules are linked by C—H···N hydrogen bonds; intramolecular C—H···N and C—H···O hydrogen bonds are also present. Furthermore, there is a short intermolecular Br···O contact [2.869 (5) Å].

Related literature

For related literature, see: Wichmann *et al.* (1999); El-Bendary *et al.* (1998); Kirpal (1999); Tsuji & Ishikawa (1994); Mohan *et al.* (1989); Baraldi *et al.* (1996, 2003); Sanjay *et al.*, (2006); Thiruvalluvar *et al.* (2007).



Experimental

Crystal data

$C_{14}H_9BrN_4O$
M_r = 329.15
Monoclinic, $C2/m$
a = 15.1590 (3) Å
b = 6.4761 (2) Å
c = 13.1979 (3) Å
β = 90.584 (2)°
V = 1295.59 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.17 mm^{-1}
T = 160 (1) K
0.25 × 0.25 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.433, T_{max} = 0.628
17133 measured reflections
2049 independent reflections
1780 reflections with $I > 2\sigma(I)$
R_{int} = 0.089

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.238
S = 1.14
2049 reflections
122 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.83 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C32—H32···N2	0.95	2.44	2.774	100
C36—H36···O41	0.95	2.16	3.037	153
C41—H41···N11^{i}	0.95	2.52	3.410	157

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

The data collection was carried out by Dr A. Linden of the Institute of Organic Chemistry at the University of Zürich. This help is gratefully acknowledged by AT.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2161).

References

Baraldi, P. G., Cacciari, B. & Spalluto, G. (1996). *J. Med. Chem.* **39**, 1164–1169.
Baraldi, P. G., Fruttarolo, F., Tabrizi, M. A., Preti, D., Romagnoli, H., El-Kashef, H., Moorman, A., Varani, K., Gessi, S., Merighi, S. & Borea, P. A. (2003). *J. Med. Chem.* **46**, 1229–1233.
Beurskens, P. T., Beurskens, G., de Gelder, R., García-Granda, S., Gould, R. O., Israel, R. & Smits, J. M. M. (1999). *The DIRDIF99 Program System.* Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
El-Bendary, E. R., El-Sherbeny, M. A. & Badri, F. A. (1998). *Bull. Chem. Farm.* **137**, 115–121.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Kirpal, G. (1999). US Patent 5 869 494; *Chem. Abstr.* **130**, 163202.
Mohan, J., Anjaneyulu, G. S. R. & Verma, P. (1989). *Curr. Sci.* **58**, 1028–1031.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. London: Academic Press.
Sanjay, K., Gyanendra, K., Mili, K., Avadhesha, S. & Namita, S. (2006). *Synth. Commun.* **36**, 215–226.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Thiruvalluvar, A., Subramanyam, M., Kalluraya, B. & Lingappa, B. (2007). *Acta Cryst.* E**63**, o2911.
Tsuji, K. & Ishikawa, H. (1994). *Bioorg. Med. Chem. Lett.* **4**, 160–164.
Wichmann, J., Koclzewskis, A. G., Vincent, M. & Woletring, T. (1999). *Bioorg. Med. Chem. Lett.* **9**, 1573–1579.

  doi:10.1107/S1600536807031443

supplementary materials

Acta Cryst. (2007). E**63**, o3362 [**doi:10.1107/S1600536807031443**]

1-(5-Bromopyrimidin-2-yl)-3-phenyl-1*H*-pyrazole-4-carbaldehyde

A. Thiruvalluvar, M. Subramanyam, B. Kalluraya and B. Lingappa

Comment

A literature survey shows that a large number of simple, N-bridged, nitrogen- and sulfur-containing heterocyclic compounds, containing the pyrimidine unit, are associated with diverse biological activities (Wichmann *et al.*, 1999; El-Bendary *et al.*, 1998; Kirpal, 1999; Tsuji & Ishikawa, 1994). Pyrazoles constitute an important class of heterocycles, which display interesting biological properties such as fungicidal, anti-inflammatory, anti-arthritic, antidepressant and antiviral activity. Many pyrazolines also find utility as polymer intermediates in industry (Mohan *et al.*, 1989; Baraldi *et al.*, 1996; Baraldi *et al.*, 2003; Sanjay *et al.*, 2006).

In the title compound, Fig. 1, $C_{14}H_9BrN_4O$, the molecule is planar, lying on a mirror plane (Fig. 3). The molecules are linked by C—H···N hydrogen bonds; intramolecular C—H···N and C—H···O hydrogen bonds are also present. Furthermore, there is a short intermolecular contact between Br1 and $O41^{ii}$ [2.869 (5) Å; symmetry code: (ii) *x*, *y*, *z* − 1]. Recently a similar structure, 3-(4-chlorophenyl)-1- (4,6-dimethylpyrimidin-2-yl)-1*H*-pyrazole-4-carbaldehyde, has been published (Thiruvalluvar *et al.*, 2007); however, it is not planar.

Experimental

To the Vilsmeier-Haack complex (3.22 g), prepared from DMF (20 ml) and $POCl_3$ (3.64 g, 0.021 mol) at 273–278 K was added 1-phenylethanone- (5-bromopyrimidin-2-yl)hydrazone (2.2 g, 0.007 mol). The reaction mixture was stirred at 333–343 K for 4 h, and monitored by TLC. The contents were cooled, poured into ice cold water and neutralized with sodium carbonate. The product that separated was filtered and recrystallized from ethyl acetate to give yellow crystals (1.7 g, 71%).

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95Å and $U_{iso} = 1.2U_{eq}$(C). The maximum residual electron density peak is located 1.53 Å from H35.

Figures

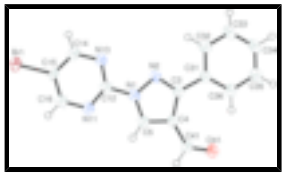


Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

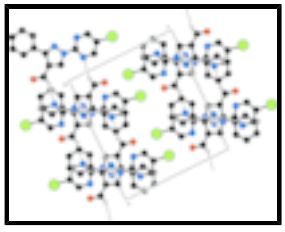


Fig. 2. The packing of the title compound, viewed down the *b* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

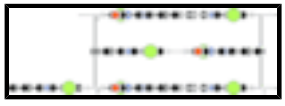


Fig. 3. The packing of the title compound, viewed down the *c* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

1-(5-Bromopyrimidin-2-yl)-3-phenyl-1*H*-pyrazole-4-carbaldehyde

Crystal data

$C_{14}H_9BrN_4O$	F_{000} = 656
M_r = 329.15	D_x = 1.688 Mg m^{-3}
Monoclinic, *C*2/*m*	Melting point: 444(1) K
Hall symbol: -C 2y	Mo *K*α radiation λ = 0.71073 Å
a = 15.1590 (3) Å	Cell parameters from 12482 reflections
b = 6.4761 (2) Å	θ = 2.0–30.0º
c = 13.1979 (3) Å	μ = 3.17 mm^{-1}
β = 90.584 (2)º	*T* = 160 (1) K
V = 1295.59 (6) Å^3	Block, light_brown
Z = 4	0.25 × 0.25 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer	2049 independent reflections
Radiation source: Nonius FR590 sealed tube generator	1780 reflections with $I > 2\sigma(I)$
Monochromator: horizontally mounted graphite crystal	R_{int} = 0.089
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 30.0º
T = 160(1) K	θ_{min} = 2.7º
φ and ω scans with κ offsets	*h* = −21→20
Absorption correction: multi-scan (Blessing, 1995)	*k* = −9→9
T_{min} = 0.433, T_{max} = 0.628	*l* = −18→18
17133 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.086	$w = 1/[\sigma^2(F_o^2) + (0.1474P)^2 + 3.886P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.238$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.14$	$\Delta\rho_{max} = 1.63$ e Å^{-3}
2049 reflections	$\Delta\rho_{min} = -0.83$ e Å^{-3}
122 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.108 (11)
Secondary atom site location: difference Fourier map	

Special details

Experimental. Solvent used: Ethyl Acetate Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (°.): 0.558 (2) Frames collected: 369 Seconds exposure per frame: 60 Degrees rotation per frame: 2.0 Crystal-Detector distance (mm): 30.0

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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}
Br1	0.15553 (4)	0.00000	−0.50849 (4)	0.0521 (3)
O41	0.1309 (3)	0.00000	0.2757 (4)	0.0564 (16)
N1	0.2038 (3)	0.00000	−0.0627 (4)	0.0334 (11)
N2	0.2841 (3)	0.00000	−0.0148 (4)	0.0346 (11)
N11	0.1114 (3)	0.00000	−0.2023 (4)	0.0360 (12)
N13	0.2685 (3)	0.00000	−0.2227 (4)	0.0414 (14)
C3	0.2666 (3)	0.00000	0.0824 (4)	0.0330 (12)
C4	0.1719 (4)	0.00000	0.1001 (4)	0.0360 (14)
C5	0.1368 (4)	0.00000	0.0038 (4)	0.0373 (14)
C12	0.1947 (3)	0.00000	−0.1698 (4)	0.0337 (14)
C14	0.2553 (4)	0.00000	−0.3235 (5)	0.0433 (19)
C15	0.1725 (4)	0.00000	−0.3662 (4)	0.0396 (16)
C16	0.1008 (4)	0.00000	−0.3018 (4)	0.0397 (14)
C31	0.3420 (3)	0.00000	0.1551 (4)	0.0333 (12)
C32	0.4289 (4)	0.00000	0.1154 (5)	0.0407 (16)
C33	0.5010 (4)	0.00000	0.1799 (6)	0.0457 (18)
C34	0.4886 (4)	0.00000	0.2839 (6)	0.050 (2)
C35	0.4060 (4)	0.00000	0.3233 (5)	0.0437 (17)
C36	0.3306 (4)	0.00000	0.2595 (4)	0.0387 (14)
C41	0.1129 (4)	0.00000	0.1855 (4)	0.0437 (18)
H5	0.07575	0.00000	−0.01311	0.0445*

H14	0.30503	0.00000	−0.36665	0.0522*
H16	0.04286	0.00000	−0.32985	0.0476*
H32	0.43727	0.00000	0.04417	0.0487*
H33	0.55897	0.00000	0.15320	0.0550*
H34	0.53843	0.00000	0.32818	0.0597*
H35	0.39894	0.00000	0.39471	0.0525*
H36	0.27306	0.00000	0.28748	0.0465*
H41	0.05171	0.00000	0.16904	0.0521*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0463 (5)	0.0828 (7)	0.0272 (4)	0.0000	−0.0017 (2)	0.0000
O41	0.038 (2)	0.101 (4)	0.030 (2)	0.0000	−0.0030 (16)	0.0000
N1	0.0271 (19)	0.043 (2)	0.030 (2)	0.0000	−0.0009 (15)	0.0000
N2	0.0256 (18)	0.051 (2)	0.027 (2)	0.0000	−0.0044 (15)	0.0000
N11	0.031 (2)	0.050 (2)	0.027 (2)	0.0000	−0.0002 (16)	0.0000
N13	0.028 (2)	0.067 (3)	0.029 (2)	0.0000	−0.0018 (16)	0.0000
C3	0.030 (2)	0.039 (2)	0.030 (2)	0.0000	−0.0008 (17)	0.0000
C4	0.032 (2)	0.051 (3)	0.025 (2)	0.0000	−0.0023 (17)	0.0000
C5	0.028 (2)	0.054 (3)	0.030 (2)	0.0000	−0.0014 (18)	0.0000
C12	0.026 (2)	0.039 (2)	0.036 (3)	0.0000	−0.0010 (18)	0.0000
C14	0.036 (3)	0.064 (4)	0.030 (3)	0.0000	0.005 (2)	0.0000
C15	0.042 (3)	0.060 (3)	0.017 (2)	0.0000	0.0040 (18)	0.0000
C16	0.035 (2)	0.054 (3)	0.030 (2)	0.0000	−0.0027 (19)	0.0000
C31	0.028 (2)	0.041 (2)	0.031 (2)	0.0000	−0.0005 (17)	0.0000
C32	0.030 (2)	0.055 (3)	0.037 (3)	0.0000	0.001 (2)	0.0000
C33	0.031 (2)	0.062 (4)	0.044 (3)	0.0000	−0.009 (2)	0.0000
C34	0.032 (3)	0.067 (4)	0.051 (4)	0.0000	−0.014 (2)	0.0000
C35	0.042 (3)	0.057 (3)	0.032 (3)	0.0000	−0.002 (2)	0.0000
C36	0.037 (2)	0.051 (3)	0.028 (2)	0.0000	−0.0037 (19)	0.0000
C41	0.030 (2)	0.072 (4)	0.029 (3)	0.0000	0.0022 (19)	0.0000

Geometric parameters (Å, °)

Br1—C15	1.893 (5)	C31—C32	1.423 (8)
O41—C41	1.219 (7)	C31—C36	1.390 (7)
N1—N2	1.366 (7)	C32—C33	1.379 (9)
N1—C5	1.349 (8)	C33—C34	1.387 (11)
N1—C12	1.419 (7)	C34—C35	1.361 (9)
N2—C3	1.313 (7)	C35—C36	1.413 (9)
N11—C12	1.330 (7)	C5—H5	0.9500
N11—C16	1.321 (7)	C14—H14	0.9500
N13—C12	1.325 (7)	C16—H16	0.9500
N13—C14	1.343 (8)	C32—H32	0.9500
C3—C4	1.457 (8)	C33—H33	0.9500
C3—C31	1.485 (7)	C34—H34	0.9500
C4—C5	1.373 (8)	C35—H35	0.9500
C4—C41	1.446 (8)	C36—H36	0.9500

C14—C15	1.371 (9)	C41—H41	0.9500
C15—C16	1.387 (8)		
Br1···O41^{i}	2.869 (5)	C31···N11^{x}	3.3709 (19)
Br1···O41^{ii}	2.869 (5)	C31···N11^{vii}	3.3709 (19)
Br1···H36^{i}	3.2400	C31···C12^{x}	3.2916 (12)
Br1···H36^{ii}	3.2400	C31···N11^{viii}	3.3709 (19)
O41···Br1^{iii}	2.869 (5)	C31···C12^{viii}	3.2916 (12)
O41···C36	3.037 (8)	C31···N11^{ix}	3.3709 (19)
O41···Br1^{iv}	2.869 (5)	C31···C12^{ix}	3.2916 (12)
O41···H16^{v}	2.7400	C34···C16^{ix}	3.519 (3)
O41···H16^{vi}	2.7400	C34···C16^{viii}	3.519 (3)
O41···H36	2.1600	C34···C16^{vii}	3.519 (3)
N1···C3^{vii}	3.2797 (11)	C34···C16^{x}	3.519 (3)
N1···C3^{viii}	3.2797 (11)	C35···C15^{ix}	3.498 (3)
N1···C3^{ix}	3.2797 (11)	C35···C16^{x}	3.2520 (8)
N1···C3^{x}	3.2797 (11)	C35···C15^{viii}	3.498 (3)
N2···N13	2.752 (7)	C35···C16^{vii}	3.2520 (8)
N2···C3^{ix}	3.444 (2)	C35···C15^{vii}	3.498 (3)
N2···C3^{vii}	3.444 (2)	C35···C15^{x}	3.498 (3)
N2···C3^{viii}	3.444 (2)	C35···C16^{viii}	3.2520 (8)
N2···C3^{x}	3.444 (2)	C35···C16^{ix}	3.2520 (8)
N11···C31^{x}	3.3709 (19)	C36···C15^{ix}	3.532 (3)
N11···C36^{vii}	3.441 (3)	C36···C14^{x}	3.594 (4)
N11···C41^{v}	3.410 (8)	C36···C16^{viii}	3.445 (3)
N11···C31^{ix}	3.3709 (19)	C36···C15^{viii}	3.532 (3)
N11···C41^{vi}	3.410 (8)	C36···O41	3.037 (8)
N11···C36^{ix}	3.441 (3)	C36···C12^{x}	3.468 (3)
N11···C31^{vii}	3.3709 (19)	C36···C41	3.432 (8)
N11···C31^{viii}	3.3709 (19)	C36···N11^{vii}	3.441 (3)
N11···C36^{viii}	3.441 (3)	C36···N11^{viii}	3.441 (3)
N11···C36^{x}	3.441 (3)	C36···C12^{vii}	3.468 (3)
N13···N2	2.752 (7)	C36···C12^{viii}	3.468 (3)
N2···H32	2.4400	C36···C14^{vii}	3.594 (4)
N11···H41^{vi}	2.5200	C36···C14^{viii}	3.594 (4)
N11···H41^{v}	2.5200	C36···C15^{vii}	3.532 (3)
N11···H5	2.5600	C36···C14^{ix}	3.594 (4)
N13···H33^{xi}	2.7600	C36···C16^{vii}	3.445 (3)
N13···H33^{xii}	2.7600	C36···C12^{ix}	3.468 (3)
C3···N1^{vii}	3.2797 (11)	C36···N11^{ix}	3.441 (3)
C3···N1^{viii}	3.2797 (11)	C36···N11^{x}	3.441 (3)
C3···N2^{vii}	3.444 (2)	C36···C16^{ix}	3.445 (3)

C3···N2^{viii}	3.444 (2)	C36···C16^{x}	3.445 (3)
C3···C12^{vii}	3.485 (3)	C36···C15^{x}	3.532 (3)
C3···C12^{viii}	3.485 (3)	C41···C16^{vi}	3.599 (8)
C3···N1^{ix}	3.2797 (11)	C41···C36	3.432 (8)
C3···N1^{x}	3.2797 (11)	C41···C16^{v}	3.599 (8)
C3···N2^{ix}	3.444 (2)	C41···N11^{v}	3.410 (8)
C3···N2^{x}	3.444 (2)	C41···N11^{vi}	3.410 (8)
C3···C12^{ix}	3.485 (3)	C4···H36	2.9000
C3···C12^{x}	3.485 (3)	C16···H41^{v}	2.9200
C12···C3^{ix}	3.485 (3)	C16···H41^{vi}	2.9200
C12···C3^{vii}	3.485 (3)	C32···H32^{xi}	2.9400
C12···C3^{viii}	3.485 (3)	C32···H32^{xii}	2.9400
C12···C31^{vii}	3.2916 (12)	C41···H36	2.7600
C12···C31^{viii}	3.2916 (12)	C41···H16^{v}	3.0500
C12···C36^{vii}	3.468 (3)	C41···H16^{vi}	3.0500
C12···C36^{viii}	3.468 (3)	H5···N11	2.5600
C12···C31^{x}	3.2916 (12)	H5···H41	2.4400
C12···C3^{x}	3.485 (3)	H5···H5^{v}	2.3300
C12···C31^{ix}	3.2916 (12)	H5···H5^{vi}	2.3300
C12···C36^{ix}	3.468 (3)	H14···H34^{xi}	2.4200
C12···C36^{x}	3.468 (3)	H14···H34^{xii}	2.4200
C14···C36^{ix}	3.594 (4)	H16···O41^{v}	2.7400
C14···C36^{vii}	3.594 (4)	H16···C41^{v}	3.0500
C14···C36^{viii}	3.594 (4)	H16···H41^{v}	2.5700
C14···C36^{x}	3.594 (4)	H16···O41^{vi}	2.7400
C15···C35^{x}	3.498 (3)	H16···C41^{vi}	3.0500
C15···C35^{vii}	3.498 (3)	H16···H41^{vi}	2.5700
C15···C35^{viii}	3.498 (3)	H32···N2	2.4400
C15···C36^{vii}	3.532 (3)	H32···C32^{xi}	2.9400
C15···C36^{viii}	3.532 (3)	H32···H32^{xi}	2.2400
C15···C35^{ix}	3.498 (3)	H32···C32^{xii}	2.9400
C15···C36^{ix}	3.532 (3)	H32···H32^{xii}	2.2400
C15···C36^{x}	3.532 (3)	H33···N13^{xi}	2.7600
C16···C35^{vii}	3.2520 (8)	H33···N13^{xii}	2.7600
C16···C41^{v}	3.599 (8)	H34···H14^{xi}	2.4200
C16···C36^{vii}	3.445 (3)	H34···H14^{xii}	2.4200
C16···C41^{vi}	3.599 (8)	H36···Br1^{iii}	3.2400
C16···C34^{ix}	3.519 (3)	H36···O41	2.1600
C16···C34^{vii}	3.519 (3)	H36···C4	2.9000
C16···C34^{viii}	3.519 (3)	H36···C41	2.7600
C16···C35^{x}	3.2520 (8)	H36···Br1^{iv}	3.2400

C16···C35^{viii}	3.2520 (8)	H41···H5	2.4400
C16···C36^{x}	3.445 (3)	H41···N11^{v}	2.5200
C16···C36^{viii}	3.445 (3)	H41···C16^{v}	2.9200
C16···C34^{x}	3.519 (3)	H41···H16^{v}	2.5700
C16···C35^{ix}	3.2520 (8)	H41···N11^{vi}	2.5200
C16···C36^{ix}	3.445 (3)	H41···C16^{vi}	2.9200
C31···C12^{vii}	3.2916 (12)	H41···H16^{vi}	2.5700
N2—N1—C5	111.9 (5)	C31—C32—C33	120.3 (6)
N2—N1—C12	122.6 (4)	C32—C33—C34	119.8 (6)
C5—N1—C12	125.6 (5)	C33—C34—C35	120.8 (6)
N1—N2—C3	105.3 (4)	C34—C35—C36	121.0 (6)
C12—N11—C16	115.2 (5)	C31—C36—C35	118.9 (5)
C12—N13—C14	113.8 (5)	O41—C41—C4	128.9 (6)
N2—C3—C4	111.5 (4)	N1—C5—H5	126.00
N2—C3—C31	118.0 (4)	C4—C5—H5	126.00
C4—C3—C31	130.5 (5)	N13—C14—H14	119.00
C3—C4—C5	103.0 (5)	C15—C14—H14	119.00
C3—C4—C41	138.0 (5)	N11—C16—H16	119.00
C5—C4—C41	119.0 (5)	C15—C16—H16	119.00
N1—C5—C4	108.4 (5)	C31—C32—H32	120.00
N1—C12—N11	113.8 (4)	C33—C32—H32	120.00
N1—C12—N13	116.8 (4)	C32—C33—H33	120.00
N11—C12—N13	129.4 (5)	C34—C33—H33	120.00
N13—C14—C15	122.3 (6)	C33—C34—H34	120.00
Br1—C15—C14	121.5 (5)	C35—C34—H34	120.00
Br1—C15—C16	120.6 (4)	C34—C35—H35	120.00
C14—C15—C16	117.9 (5)	C36—C35—H35	120.00
N11—C16—C15	121.4 (5)	C31—C36—H36	121.00
C3—C31—C32	118.1 (5)	C35—C36—H36	121.00
C3—C31—C36	122.5 (5)	O41—C41—H41	116.00
C32—C31—C36	119.3 (5)	C4—C41—H41	116.00
C5—N1—N2—C3	0.00 (1)	N2—C3—C31—C32	0.00 (1)
C12—N1—N2—C3	180.00 (1)	N2—C3—C31—C36	−180.00 (1)
N2—N1—C5—C4	0.00 (1)	C4—C3—C31—C32	180.00 (1)
C12—N1—C5—C4	180.00 (1)	C4—C3—C31—C36	0.00 (1)
N2—N1—C12—N11	−180.00 (1)	C3—C4—C5—N1	0.00 (1)
N2—N1—C12—N13	0.00 (1)	C41—C4—C5—N1	180.00 (1)
C5—N1—C12—N11	0.00 (1)	C3—C4—C41—O41	0.00 (1)
C5—N1—C12—N13	180.00 (1)	C5—C4—C41—O41	−180.00 (1)
N1—N2—C3—C4	0.00 (1)	N13—C14—C15—Br1	180.00 (1)
N1—N2—C3—C31	−180.00 (1)	N13—C14—C15—C16	0.00 (1)
C16—N11—C12—N1	−180.00 (1)	Br1—C15—C16—N11	−180.00 (1)
C16—N11—C12—N13	0.00 (1)	C14—C15—C16—N11	0.00 (1)
C12—N11—C16—C15	0.00 (1)	C3—C31—C32—C33	−180.00 (1)
C14—N13—C12—N1	180.00 (1)	C36—C31—C32—C33	0.00 (1)
C14—N13—C12—N11	0.00 (1)	C3—C31—C36—C35	−180.00 (1)
C12—N13—C14—C15	0.00 (1)	C32—C31—C36—C35	0.00 (1)

N2—C3—C4—C5	0.00 (1)	C31—C32—C33—C34	0.00 (1)
N2—C3—C4—C41	−180.00 (1)	C32—C33—C34—C35	0.00 (1)
C31—C3—C4—C5	180.00 (1)	C33—C34—C35—C36	0.00 (1)
C31—C3—C4—C41	0.00 (1)	C34—C35—C36—C31	0.00 (1)

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) *x*, −*y*, *z*−1; (iii) *x*, *y*, *z*+1; (iv) *x*, −*y*, *z*+1; (v) −*x*, *y*, −*z*; (vi) −*x*, −*y*, −*z*; (vii) −*x*+1/2, *y*−1/2, −*z*; (viii) −*x*+1/2, *y*+1/2, −*z*; (ix) −*x*+1/2, −*y*−1/2, −*z*; (x) −*x*+1/2, −*y*+1/2, −*z*; (xi) −*x*+1, *y*, −*z*; (xii) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C32—H32···N2	0.95	2.44	2.774	100
C36—H36···O41	0.95	2.16	3.037	153
C41—H41···N11^{v}	0.95	2.52	3.410	157

Symmetry codes: (v) −*x*, *y*, −*z*.

Fig. 1

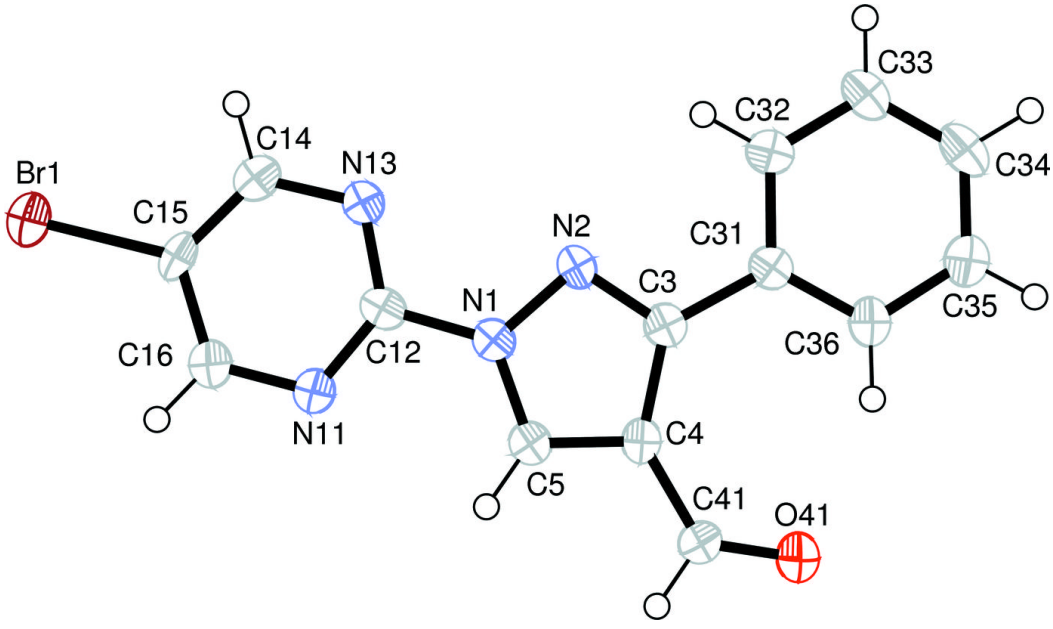

C33
C32
C34
C14
N13
Br1
C15
N2
C31
C3
N1
C35
C36
C16
C12
C4
N11
C5
C41
O41

Fig. 2

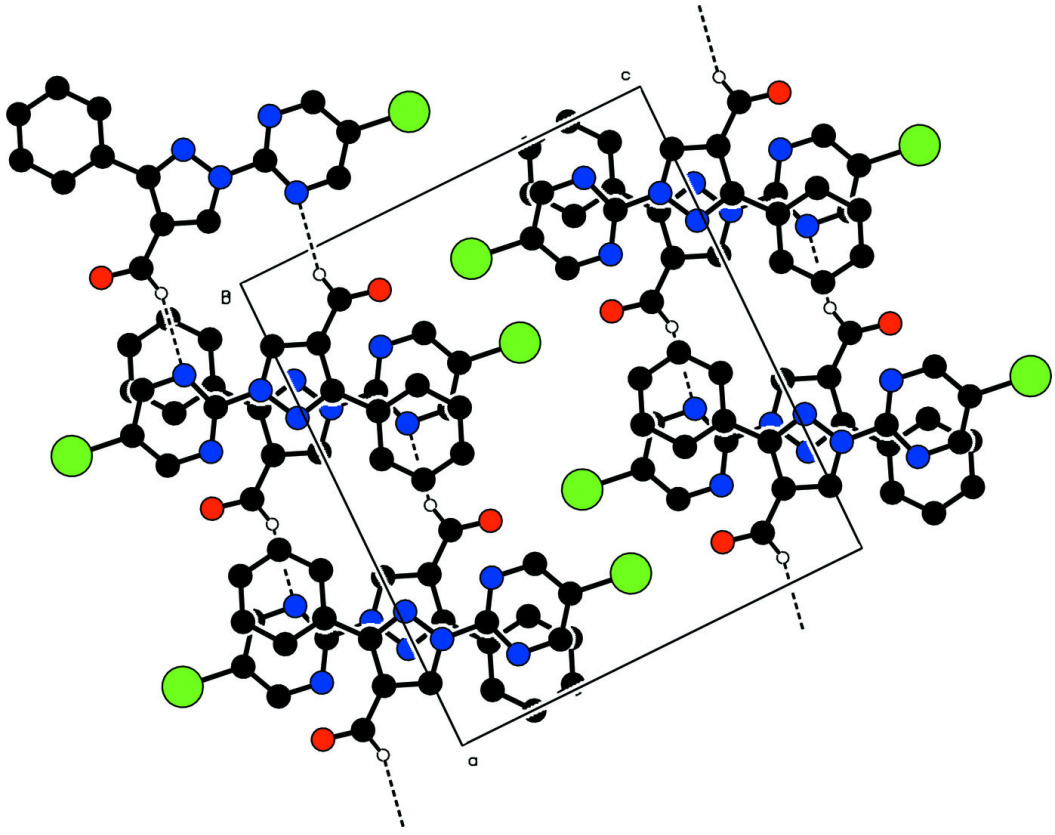


Fig. 3