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Ethyl 5-amino-1-(5-bromopyrimidin-2-yl)-1*H*-pyrazole-4-carboxylate

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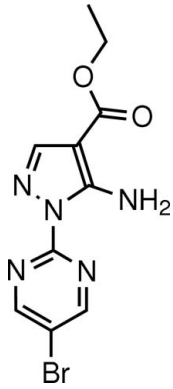
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.077; data-to-parameter ratio = 22.9.

The molecule of the title compound, $C_{10}H_{10}BrN_5O_2$, is planar, except for the amino and carboxylate groups. The molecules are linked by intermolecular C—H···O and N—H···N hydrogen bonds, and by slipped π–π stacking between symmetry-related pyrazole and pyrimidine rings [centroid-to-centroid distance 3.512 (1) Å, interplanar distance 3.391 Å and offset angle 15.1°]. Intramolecular N—H···N and N—H···O hydrogen bonds stabilize the planar conformation.

Related literature

For related crystal structures, see Thiruvalluvar *et al.* (2007*a*,*b*,*c*).



Experimental

Crystal data

$C_{10}H_{10}BrN_5O_2$
M_r = 312.13
Monoclinic, $P2_1/n$
a = 6.3433 (3) Å
b = 28.9030 (8) Å
c = 6.9439 (3) Å
β = 109.821 (5)°
V = 1197.68 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.44 mm^{-1}
T = 200 (2) K
0.52 × 0.39 × 0.14 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.221, T_{max} = 0.633
12255 measured reflections
3933 independent reflections
2361 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.077
S = 1.03
3933 reflections
172 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*A*···O41	0.82 (2)	2.51 (2)	2.980 (2)	118 (2)
N5—H5A···N2^{i}	0.82 (2)	2.32 (3)	3.096 (3)	158.0 (19)
N5—H5*B*···N12	0.89 (2)	2.16 (2)	2.771 (2)	125.0 (17)
C3—H3···O41^{ii}	0.95	2.53	3.096 (2)	118.0

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2257).

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supplementary materials

Acta Cryst. (2007). E**63**, o4535 [**doi:10.1107/S1600536807054554**]

Ethyl 5-amino-1-(5-bromopyrimidin-2-yl)-1*H*-pyrazole-4-carboxylate

M. Subramanyam, B. Lingappa, A. Thiruvalluvar, B. Kalluraya and R. J. Butcher

Comment

Thiruvalluvar *et al.*, (2007*a*,b,c) have reported the crystal structures of pyrimidine derivatives. The title compound, $C_{10}H_{10}BrN_5O_2$, is planar, except the amino and carboxylate group (Fig. 1). The molecules are linked by intermolecular C—H···O and N—H···N hydrogen bonds forming ribbons parallel to the *a* axis (Fig. 2, Table 1). These ribbons are further interconnected through weak slippest π-π stacking between the N1—N2—C3—C4—C5 and the symmetry related (2 − *x*, −*y*, 1 − *z*) N12—C11—N16—C15—C14—C13 rings(centroid-to-centroid distance of 3.512 (1) Å, interplanar distance of 3.391Å and offset angle of 15.1°). Intramolecular N—H···N and N—H···O hydrogen bonds (Table 1) stabilize the planar conformation

Experimental

Ethoxymethylenecyanoacetate (1.7 g, 0.01 mol) was added in small portion to a solution of 2-hydrazino-5-bromo-pyrimidine (1.9.0 g, 0.01 mol) in ethanol (17 ml). The reaction mass was refluxed for 1 h on a water bath, the completion of the reaction was monitored by TLC. The contents were cooled to room temperature and distilled mineral water (17 ml) was added, stirred for 2 h, the solid obtained was filtered, washed with DM water and dried. Recrystallization from ethyl acetate gave the title compound as pinkish crystals, yield (2.0 g, 64%).

Refinement

Amino hydrogen atoms were located from a difference Fourier map and refined isotropically. Remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 to 0.99Å and U_{iso}=1.2–1.5 times U_{eq}(C).

Figures

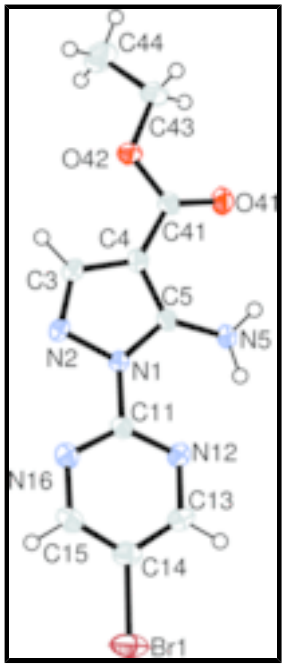

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

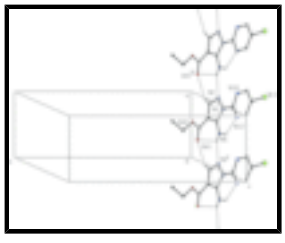

Fig. 2. Partial packing view of the title compound, showing the formation of ribbon through N—H···N and C—H···O hydrogen bonds. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted·[Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$]

Ethyl 5-amino-1-(5-bromopyrimidin-2-yl)-1*H*-pyrazole-4-carboxylate

Crystal data

$C_{10}H_{10}BrN_5O_2$	F_{000} = 624
M_r = 312.13	D_x = 1.731 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 484(1) K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.7107 Å
a = 6.3433 (3) Å	Cell parameters from 4274 reflections
b = 28.9030 (8) Å	θ = 4.7–32.4º
c = 6.9439 (3) Å	μ = 3.44 mm^{-1}
β = 109.821 (5)º	T = 200 (2) K
V = 1197.68 (9) Å^3	Rectangular-plate, colourless
Z = 4	0.52 × 0.39 × 0.14 mm

Data collection

Oxford Diffraction Gemini	3933 independent reflections

diffractometer

Radiation source: Enhance (Mo) X-ray Source

Monochromator: graphite

T = 200(2) K

φ and ω scans

Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)

T_{min} = 0.221, T_{max} = 0.633

12255 measured reflections

2361 reflections with $I > 2\sigma(I)$

R_{int} = 0.030

θ_{max} = 32.4º

θ_{min} = 4.7º

$h = -9 \rightarrow 8$

$k = -42 \rightarrow 41$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.030

$wR(F^2)$ = 0.077

S = 1.03

3933 reflections

172 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = <0.001

$\Delta\rho_{max}$ = 0.37 e Å^{-3}

$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Extinction correction: none

Special details

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 $F^2 > 2$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	1.22590 (4)	−0.15293 (1)	0.84262 (3)	0.0432 (1)
O41	0.4802 (2)	0.14654 (5)	0.5849 (2)	0.0374 (5)
O42	0.7778 (2)	0.19419 (5)	0.6487 (2)	0.0294 (4)
N1	1.0031 (2)	0.04632 (5)	0.7293 (2)	0.0222 (5)
N2	1.1764 (3)	0.07781 (5)	0.7447 (3)	0.0282 (5)
N5	0.6064 (3)	0.04722 (6)	0.6635 (3)	0.0309 (6)
N12	0.8851 (3)	−0.02943 (5)	0.7405 (3)	0.0308 (5)
N16	1.2688 (3)	−0.01193 (6)	0.8024 (3)	0.0338 (5)
C3	1.0773 (3)	0.11816 (7)	0.7149 (3)	0.0263 (6)

C4	0.8460 (3)	0.11555 (7)	0.6794 (3)	0.0233 (5)
C5	0.7997 (3)	0.06879 (6)	0.6884 (3)	0.0213 (5)
C11	1.0544 (3)	−0.00088 (6)	0.7589 (3)	0.0228 (5)
C13	0.9366 (3)	−0.07441 (7)	0.7638 (3)	0.0331 (6)
C14	1.1527 (3)	−0.08978 (7)	0.8098 (3)	0.0290 (6)
C15	1.3162 (4)	−0.05673 (7)	0.8309 (3)	0.0366 (7)
C41	0.6802 (3)	0.15228 (6)	0.6332 (3)	0.0240 (5)
C43	0.6324 (4)	0.23428 (7)	0.6071 (3)	0.0373 (7)
C44	0.7478 (4)	0.27217 (8)	0.5359 (4)	0.0509 (8)
H3	1.15424	0.14647	0.71703	0.0316*
H5A	0.498 (4)	0.0619 (7)	0.668 (3)	0.028 (6)*
H5B	0.603 (3)	0.0169 (8)	0.685 (3)	0.034 (6)*
H13	0.82039	−0.09633	0.74809	0.0397*
H15	1.46789	−0.06636	0.86713	0.0439*
H43A	0.60326	0.24388	0.73262	0.0448*
H43B	0.48727	0.22693	0.50016	0.0448*
H44A	0.77406	0.26244	0.41075	0.0764*
H44B	0.65362	0.29995	0.50771	0.0764*
H44C	0.89149	0.27902	0.64250	0.0764*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0682 (2)	0.0255 (1)	0.0432 (1)	0.0145 (1)	0.0284 (1)	0.0065 (1)
O41	0.0204 (7)	0.0319 (9)	0.0607 (10)	0.0011 (6)	0.0149 (7)	0.0077 (7)
O42	0.0253 (7)	0.0196 (7)	0.0429 (8)	0.0022 (5)	0.0110 (6)	0.0031 (6)
N1	0.0182 (8)	0.0186 (8)	0.0315 (8)	−0.0016 (6)	0.0108 (6)	−0.0030 (6)
N2	0.0215 (8)	0.0208 (8)	0.0443 (9)	−0.0053 (7)	0.0138 (7)	−0.0045 (7)
N5	0.0184 (9)	0.0236 (10)	0.0535 (11)	−0.0001 (7)	0.0160 (8)	0.0010 (8)
N12	0.0238 (8)	0.0218 (9)	0.0472 (10)	−0.0022 (7)	0.0124 (7)	−0.0002 (8)
N16	0.0223 (8)	0.0278 (9)	0.0508 (10)	0.0024 (7)	0.0117 (8)	0.0043 (8)
C3	0.0232 (10)	0.0213 (10)	0.0356 (10)	−0.0053 (7)	0.0115 (8)	−0.0042 (8)
C4	0.0215 (9)	0.0246 (10)	0.0255 (9)	−0.0013 (7)	0.0104 (8)	−0.0001 (8)
C5	0.0190 (9)	0.0237 (9)	0.0230 (9)	0.0003 (7)	0.0095 (7)	−0.0030 (7)
C11	0.0237 (9)	0.0229 (10)	0.0222 (9)	0.0009 (7)	0.0083 (7)	−0.0019 (7)
C13	0.0343 (11)	0.0204 (10)	0.0460 (12)	−0.0034 (8)	0.0154 (10)	−0.0019 (9)
C14	0.0385 (11)	0.0238 (10)	0.0268 (10)	0.0038 (8)	0.0138 (9)	0.0000 (8)
C15	0.0280 (11)	0.0310 (12)	0.0512 (13)	0.0102 (9)	0.0140 (10)	0.0071 (10)
C41	0.0250 (9)	0.0229 (9)	0.0268 (9)	0.0023 (8)	0.0124 (7)	0.0020 (8)
C43	0.0345 (11)	0.0254 (11)	0.0517 (13)	0.0074 (9)	0.0144 (10)	0.0055 (10)
C44	0.0477 (14)	0.0328 (13)	0.0672 (16)	0.0024 (11)	0.0131 (12)	0.0200 (12)

Geometric parameters (Å, °)

Br1—C14	1.878 (2)	C3—C4	1.405 (3)
O41—C41	1.209 (2)	C4—C41	1.452 (3)
O42—C41	1.348 (2)	C4—C5	1.389 (3)
O42—C43	1.448 (3)	C13—C14	1.372 (3)
N1—N2	1.403 (2)	C14—C15	1.381 (3)

N1—C5	1.385 (2)	C43—C44	1.492 (3)
N1—C11	1.401 (2)	C3—H3	0.9500
N2—C3	1.308 (3)	C13—H13	0.9500
N5—C5	1.334 (3)	C15—H15	0.9500
N12—C11	1.326 (3)	C43—H43A	0.9900
N12—C13	1.337 (3)	C43—H43B	0.9900
N16—C11	1.328 (3)	C44—H44A	0.9800
N16—C15	1.329 (3)	C44—H44B	0.9800
N5—H5B	0.89 (2)	C44—H44C	0.9800
N5—H5A	0.82 (2)		
Br1···C4^{i}	3.663 (2)	C11···C11^{ii}	3.424 (3)
Br1···C41^{ii}	3.551 (2)	C13···C3^{ii}	3.530 (3)
Br1···C4^{ii}	3.660 (2)	C13···N2^{ii}	3.358 (3)
Br1···C41^{i}	3.483 (2)	C14···C3^{ii}	3.532 (3)
Br1···H44B^{iii}	3.2300	C14···C5^{i}	3.448 (3)
Br1···H44C^{iv}	3.1000	C14···C4^{ii}	3.480 (3)
O41···N2^{v}	3.216 (2)	C15···C5^{ii}	3.445 (3)
O41···N5	2.980 (2)	C15···N5^{i}	3.387 (3)
O41···C3^{v}	3.096 (2)	C41···Br1^{ii}	3.551 (2)
O42···C44^{vi}	3.410 (3)	C41···Br1^{i}	3.483 (2)
O41···H3^{v}	2.5300	C44···O42^{x}	3.410 (3)
O41···H5A	2.51 (2)	C3···H44B^{vi}	3.0500
O41···H13^{vii}	2.8500	C11···H5B	2.78 (2)
O41···H43B	2.4000	C41···H5A	2.90 (2)
O42···H3	2.6600	C43···H43B^{vi}	3.1000
O42···H44B^{vi}	2.8100	C43···H44C^{x}	3.0900
N2···O41^{viii}	3.216 (2)	C44···H43B^{vi}	3.0600
N2···N5^{viii}	3.096 (3)	H3···O41^{viii}	2.5300
N2···N16	2.659 (2)	H3···O42	2.6600
N2···C13^{ii}	3.358 (3)	H3···H44B^{vi}	2.5500
N5···C15^{i}	3.387 (3)	H5A···O41	2.51 (2)
N5···N12	2.771 (2)	H5A···N2^{v}	2.32 (3)
N5···O41	2.980 (2)	H5A···N16^{v}	2.91 (2)
N5···N2^{v}	3.096 (3)	H5A···C41	2.90 (2)
N5···N16^{v}	3.137 (3)	H5B···N12	2.16 (2)
N12···N5	2.771 (2)	H5B···N16^{v}	2.65 (2)
N16···N2	2.659 (2)	H5B···C11	2.78 (2)
N16···N5^{viii}	3.137 (3)	H13···O41^{vii}	2.8500
N2···H5A^{viii}	2.32 (3)	H15···N2^{ix}	2.8900
N2···H15^{ix}	2.8900	H43B···O41	2.4000
N12···H5B	2.16 (2)	H43B···C43^{x}	3.1000
N16···H5A^{viii}	2.91 (2)	H43B···C44^{x}	3.0600
N16···H5B^{viii}	2.65 (2)	H43B···H44C^{x}	2.3500

C3···O41^{viii}	3.096 (2)	H44B···Br1^{xi}	3.2300
C3···C13^{ii}	3.530 (3)	H44B···O42^{x}	2.8100
C3···C14^{ii}	3.532 (3)	H44B···C3^{x}	3.0500
C4···C14^{ii}	3.480 (3)	H44B···H3^{x}	2.5500
C4···Br1^{ii}	3.660 (2)	H44C···Br1^{xii}	3.1000
C4···Br1^{i}	3.663 (2)	H44C···C43^{vi}	3.0900
C5···C14^{i}	3.448 (3)	H44C···H43B^{vi}	2.3500
C5···C15^{ii}	3.445 (3)		
C41—O42—C43	117.32 (16)	C13—C14—C15	117.13 (19)
N2—N1—C5	111.27 (14)	N16—C15—C14	122.3 (2)
N2—N1—C11	118.90 (14)	O41—C41—O42	123.78 (17)
C5—N1—C11	129.82 (15)	O41—C41—C4	125.07 (17)
N1—N2—C3	104.14 (17)	O42—C41—C4	111.15 (17)
C11—N12—C13	115.91 (19)	O42—C43—C44	107.6 (2)
C11—N16—C15	115.51 (19)	N2—C3—H3	123.00
H5A—N5—H5B	116 (2)	C4—C3—H3	123.00
C5—N5—H5A	120.1 (16)	N12—C13—H13	119.00
C5—N5—H5B	120.8 (13)	C14—C13—H13	119.00
N2—C3—C4	113.41 (19)	N16—C15—H15	119.00
C3—C4—C5	105.58 (18)	C14—C15—H15	119.00
C3—C4—C41	129.40 (18)	O42—C43—H43A	110.00
C5—C4—C41	124.97 (18)	O42—C43—H43B	110.00
N5—C5—C4	130.41 (19)	C44—C43—H43A	110.00
N1—C5—N5	123.99 (16)	C44—C43—H43B	110.00
N1—C5—C4	105.60 (17)	H43A—C43—H43B	108.00
N1—C11—N16	115.87 (16)	C43—C44—H44A	109.00
N1—C11—N12	116.85 (17)	C43—C44—H44B	109.00
N12—C11—N16	127.28 (17)	C43—C44—H44C	109.00
N12—C13—C14	121.81 (19)	H44A—C44—H44B	109.00
Br1—C14—C13	121.97 (15)	H44A—C44—H44C	109.00
Br1—C14—C15	120.90 (16)	H44B—C44—H44C	109.00
C43—O42—C41—O41	0.8 (3)	C15—N16—C11—N1	179.79 (17)
C43—O42—C41—C4	−179.89 (16)	C15—N16—C11—N12	−0.3 (3)
C41—O42—C43—C44	−153.54 (18)	C11—N16—C15—C14	2.2 (3)
N2—N1—C5—C4	−0.5 (2)	N2—C3—C4—C41	−177.5 (2)
C11—N1—C5—N5	−2.1 (3)	N2—C3—C4—C5	−0.1 (2)
C11—N1—C5—C4	178.32 (17)	C3—C4—C5—N5	−179.2 (2)
N2—N1—C11—N12	−179.22 (17)	C3—C4—C41—O41	172.3 (2)
N2—N1—C11—N16	0.8 (2)	C41—C4—C5—N1	177.91 (18)
C5—N1—C11—N12	2.1 (3)	C41—C4—C5—N5	−1.6 (4)
C5—N1—C11—N16	−177.97 (18)	C3—C4—C5—N1	0.3 (2)
C11—N1—N2—C3	−178.50 (16)	C5—C4—C41—O42	176.03 (18)
N2—N1—C5—N5	179.11 (19)	C3—C4—C41—O42	−7.0 (3)
C5—N1—N2—C3	0.4 (2)	C5—C4—C41—O41	−4.7 (3)
N1—N2—C3—C4	−0.2 (2)	N12—C13—C14—Br1	−180.00 (17)
C13—N12—C11—N16	−1.7 (3)	N12—C13—C14—C15	−0.1 (3)
C13—N12—C11—N1	178.25 (17)	Br1—C14—C15—N16	177.87 (16)

C11—N12—C13—C14	1.8 (3)	C13—C14—C15—N16	−2.0 (3)

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2; (ii) −*x*+2, −*y*, −*z*+1; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iv) −*x*+5/2, *y*−1/2, −*z*+3/2; (v) *x*−1, *y*, *z*; (vi) *x*+1/2, −*y*+1/2, *z*+1/2; (vii) −*x*+1, −*y*, −*z*+1; (viii) *x*+1, *y*, *z*; (ix) −*x*+3, −*y*, −*z*+2; (x) *x*−1/2, −*y*+1/2, *z*−1/2; (xi) −*x*+3/2, *y*+1/2, −*z*+3/2; (xii) −*x*+5/2, *y*+1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5A···O41	0.82 (2)	2.51 (2)	2.980 (2)	118 (2)
N5—H5A···N2^{v}	0.82 (2)	2.32 (3)	3.096 (3)	158.0 (19)
N5—H5B···N12	0.89 (2)	2.16 (2)	2.771 (2)	125.0 (17)
C3—H3···O41^{viii}	0.95	2.53	3.096 (2)	118.0

Symmetry codes: (v) *x*−1, *y*, *z*; (viii) *x*+1, *y*, *z*.

Fig. 1

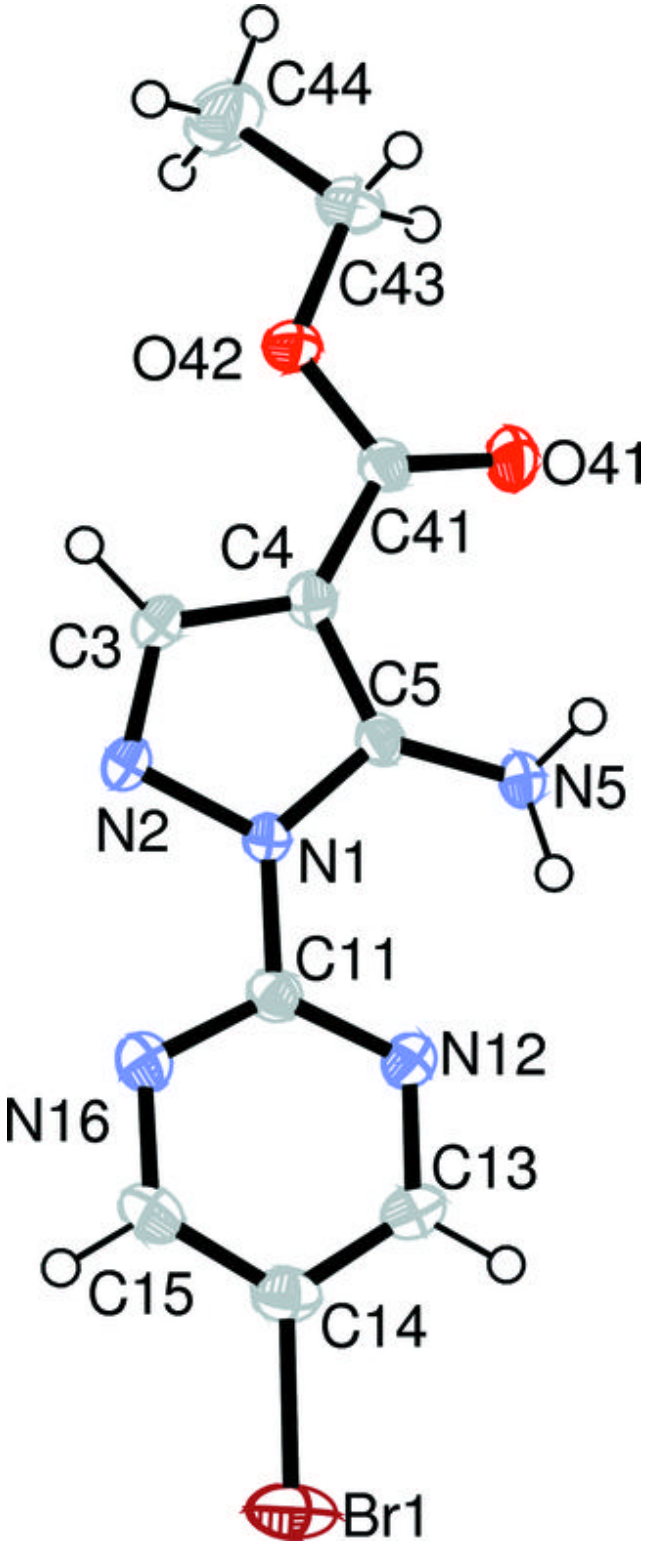

Fig. 2