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1-(Pyridin-4-yl)-3-(2,4,6-trichlorophenyl)benz-[4,5]imidazo[1,2-*d*][1,2,4]triazin-4(3*H*)-one

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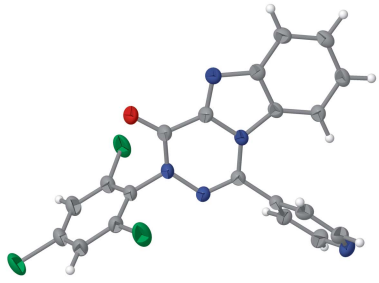
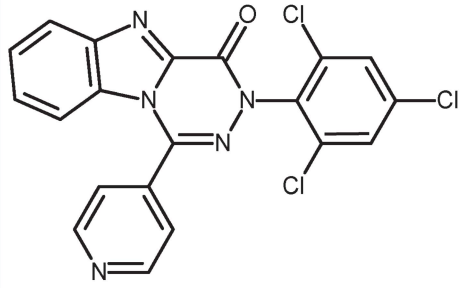
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{20}H_{10}Cl_3N_5O$, the 13-membered ring system makes dihedral angles of 78.64 (9)° with the trichlorophenyl ring and 62.60 (10)° with the pyridine ring. The crystal packing is dominated by π–π interactions between the 13-membered ring systems [centroid–centroid distance = 3.6655 (11)°].

3D view



Chemical scheme



Structure description

Compounds containing a benzimidazole core have been investigated as pharmaceuticals (Karpińka *et al.*, 2011; Singh *et al.*, 2010) and therapeutic agents (Biron, 2006; Pescovitz, 2008), and feature as commercial drugs such as omeprazole (Prilosec), pantoprazole (Protonix), vermox and mibefradil (Karpin'ska *et al.*, 2011). Several benzimidazole based compounds show anti-cancer activity (Thomas *et al.*, 2007), some exhibiting cytotoxic effects against a panel of human cancer cell lines (Refaat, 2010). For example, benzimidazole-4,7-diones exhibit cytotoxicity against colon, breast and lung cell lines (Gellis *et al.*, 2008). The good efficacy of imidazole-based compounds as anti-cancer agents promoted our work to synthesize a masked benzimidazole in a triazine ring as a new scaffold of a potential anti-cancer candidate. The first derivative of this series gave a good crystal and its structure has been published (Abu Thaher *et al.*, 2016).

In the title compound (Fig. 1), the central 13-membered ring is essentially planar with a maximum deviation of 0.133 (2) Å for atom N1 and makes dihedral angles of 78.64 (9)° with the trichlorophenyl ring and 62.60 (10)° with the pyridine ring. In the crystal, two

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{10}Cl_3N_5O$
M_r	442.68
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	193
a, *b*, *c* (Å)	19.5521 (12), 15.1072 (5), 15.5543 (9)
β (°)	126.057 (4)
V (Å^3)	3714.2 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.52
Crystal size (mm)	0.35 × 0.21 × 0.20
Data collection	
Diffractometer	Stoe IPDS 2T
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11381, 4574, 3437
R_{int}	0.022
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.665
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.113, 1.04
No. of reflections	4574
No. of parameters	262
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.89, −0.98

Computer programs: *X-AREA* (Stoe & Cie, 2006), *X-AREA* (Stoe & Cie, 2006), *X-RED32* (Stoe & Cie, 2006), *SIR2004* (Altomare *et al.*, 1995) and *SHELXL2014* (Sheldrick, 2015).

molecules related by a centre of inversion show a π–π interaction. The distance between centroids of the C7–C12 and N1/C5/N6/C7/C12($\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$) rings is 3.6655 (11)°.

Synthesis and crystallization

3.1 mmol of NaH was added slowly to a solution of 3.1 mmol of ethyl-2- benzimidazolcarboxylate in 30 ml dry THF and stirring continued at room temperature for about 20 minutes. To this flask, 3.0 mmol of *N*-(2,4,6-trichlorophenyl)-4-pyridinecarbohydrazonoyl chloride was added slowly portionwise and in parallel 0.5 ml of Et_3N was added drop wise. The reaction was left stirring overnight, monitored by TLC until it had finished. The reaction was filtered and concentrated under vacuum. The solid residue was purified by column chromatography (hexane:ethyl acetate; 2:1, then 1:1). Yield: 20%. Suitable crystals for X-ray analysis were obtained by slow evaporation of a hexane/ethyl acetate solution.

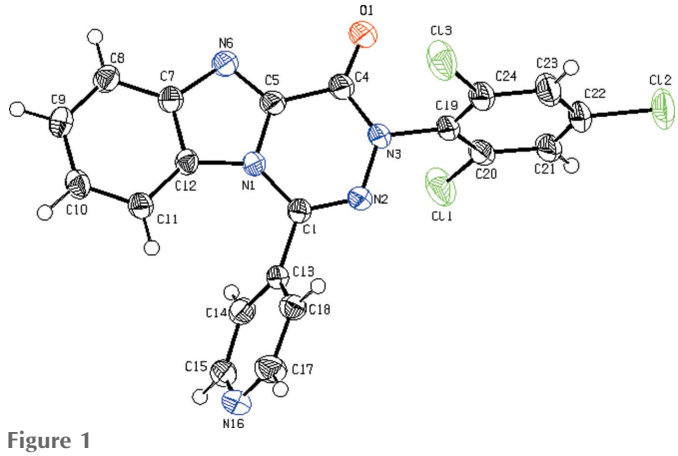


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161529 [https://doi.org/10.1107/S2414314616015297]

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Crystal data

$C_{20}H_{10}Cl_3N_5O$
M_r = 442.68
Monoclinic, $C2/c$
a = 19.5521 (12) Å
b = 15.1072 (5) Å
c = 15.5543 (9) Å
β = 126.057 (4)°
V = 3714.2 (4) Å^3
Z = 8
$F(000)$ = 1792
D_x = 1.583 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 12681 reflections
θ = 2.6–28.3°
μ = 0.52 mm^{-1}
T = 193 K
Plate, colourless
0.35 × 0.21 × 0.20 mm

Data collection

Stoe IPDS 2T diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
11381 measured reflections
4574 independent reflections
3437 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 28.2°, θ_{min} = 2.6°
h = −25→20
k = −20→18
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.113
S = 1.04
4574 reflections
262 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 3.9605P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 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}
Cl1	0.32853 (6)	0.12694 (4)	0.13199 (6)	0.0620 (2)
Cl2	0.43245 (5)	0.39787 (5)	0.01324 (6)	0.0644 (2)
Cl3	0.34201 (5)	0.45705 (4)	0.27335 (5)	0.05540 (18)
O1	0.18165 (10)	0.29896 (13)	0.14004 (12)	0.0496 (4)
N1	0.27697 (10)	0.17190 (11)	0.37941 (11)	0.0276 (3)
N2	0.37972 (10)	0.20832 (11)	0.35279 (12)	0.0300 (3)
N3	0.31780 (11)	0.25749 (12)	0.26496 (12)	0.0336 (4)
C1	0.35845 (11)	0.16738 (12)	0.40623 (13)	0.0272 (4)
C4	0.23280 (13)	0.25910 (15)	0.22150 (14)	0.0359 (4)
C5	0.21233 (12)	0.21304 (14)	0.28666 (14)	0.0316 (4)
N6	0.13953 (10)	0.21308 (12)	0.27260 (12)	0.0346 (4)
C7	0.15680 (12)	0.17234 (13)	0.36360 (14)	0.0303 (4)
C8	0.10192 (12)	0.16098 (14)	0.39282 (15)	0.0336 (4)
H8	0.0442	0.1782	0.3469	0.040*
C9	0.13499 (13)	0.12388 (14)	0.49083 (15)	0.0345 (4)
H9	0.0994	0.1157	0.5131	0.041*
C10	0.21982 (13)	0.09796 (14)	0.55831 (15)	0.0338 (4)
H10	0.2401	0.0722	0.6251	0.041*
C11	0.27507 (12)	0.10858 (13)	0.53118 (14)	0.0305 (4)
H11	0.3327	0.0910	0.5775	0.037*
C12	0.24185 (11)	0.14642 (12)	0.43222 (13)	0.0271 (4)
C13	0.42283 (11)	0.11300 (12)	0.49832 (13)	0.0264 (4)
C14	0.40997 (13)	0.02308 (13)	0.50356 (17)	0.0344 (4)
H14	0.3595	−0.0054	0.4479	0.041*
C15	0.47300 (15)	−0.02355 (15)	0.59233 (19)	0.0429 (5)
H15	0.4647	−0.0851	0.5954	0.051*
N16	0.54470 (12)	0.01269 (14)	0.67379 (15)	0.0459 (5)
C17	0.55553 (14)	0.09801 (16)	0.66609 (16)	0.0415 (5)
H17	0.6064	0.1248	0.7231	0.050*
C18	0.49758 (12)	0.15087 (13)	0.58041 (14)	0.0317 (4)
H18	0.5091	0.2116	0.5783	0.038*
C19	0.34486 (13)	0.29350 (14)	0.20419 (15)	0.0344 (4)
C20	0.35514 (14)	0.23695 (14)	0.14171 (16)	0.0389 (5)
C21	0.38352 (15)	0.26848 (16)	0.08389 (18)	0.0442 (5)
H21	0.3918	0.2295	0.0428	0.053*
C22	0.39927 (15)	0.35738 (17)	0.08770 (18)	0.0441 (5)
C23	0.38711 (16)	0.41627 (16)	0.14555 (17)	0.0440 (5)
H23	0.3971	0.4778	0.1455	0.053*
C24	0.35979 (14)	0.38281 (15)	0.20364 (16)	0.0381 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1095 (6)	0.0359 (3)	0.0802 (4)	0.0179 (3)	0.0779 (5)	0.0153 (3)
Cl2	0.0942 (5)	0.0645 (4)	0.0793 (4)	0.0099 (4)	0.0760 (4)	0.0183 (3)

Cl3	0.0916 (5)	0.0457 (3)	0.0555 (3)	0.0027 (3)	0.0581 (4)	0.0002 (3)
O1	0.0444 (9)	0.0751 (12)	0.0349 (7)	0.0228 (8)	0.0265 (7)	0.0253 (7)
N1	0.0283 (7)	0.0344 (8)	0.0220 (6)	0.0037 (6)	0.0159 (6)	0.0034 (6)
N2	0.0303 (8)	0.0341 (8)	0.0271 (7)	0.0074 (7)	0.0178 (6)	0.0073 (6)
N3	0.0364 (9)	0.0420 (9)	0.0293 (7)	0.0113 (7)	0.0232 (7)	0.0133 (7)
C1	0.0289 (9)	0.0283 (9)	0.0263 (8)	0.0017 (7)	0.0174 (7)	0.0009 (7)
C4	0.0377 (11)	0.0473 (12)	0.0277 (8)	0.0121 (9)	0.0220 (8)	0.0099 (8)
C5	0.0300 (9)	0.0411 (11)	0.0231 (8)	0.0076 (8)	0.0152 (7)	0.0055 (7)
N6	0.0319 (8)	0.0461 (10)	0.0274 (7)	0.0078 (7)	0.0182 (7)	0.0063 (7)
C7	0.0330 (9)	0.0339 (10)	0.0265 (8)	0.0025 (8)	0.0189 (7)	0.0001 (7)
C8	0.0314 (9)	0.0405 (11)	0.0323 (9)	0.0027 (8)	0.0206 (8)	−0.0006 (8)
C9	0.0382 (10)	0.0396 (11)	0.0357 (9)	−0.0021 (9)	0.0272 (9)	−0.0030 (8)
C10	0.0417 (11)	0.0360 (10)	0.0295 (9)	0.0002 (9)	0.0241 (8)	0.0017 (8)
C11	0.0335 (9)	0.0341 (10)	0.0252 (8)	0.0027 (8)	0.0181 (7)	0.0017 (7)
C12	0.0300 (9)	0.0302 (9)	0.0253 (8)	0.0002 (7)	0.0185 (7)	−0.0011 (7)
C13	0.0280 (8)	0.0286 (9)	0.0264 (8)	0.0030 (7)	0.0181 (7)	0.0038 (7)
C14	0.0325 (10)	0.0297 (10)	0.0456 (10)	0.0014 (8)	0.0256 (9)	0.0025 (8)
C15	0.0469 (12)	0.0328 (11)	0.0631 (14)	0.0107 (9)	0.0402 (12)	0.0177 (10)
N16	0.0430 (10)	0.0521 (12)	0.0448 (10)	0.0175 (9)	0.0270 (9)	0.0224 (9)
C17	0.0361 (11)	0.0492 (13)	0.0293 (9)	0.0055 (10)	0.0137 (8)	0.0048 (9)
C18	0.0321 (9)	0.0322 (10)	0.0289 (9)	0.0027 (8)	0.0169 (8)	0.0020 (7)
C19	0.0394 (10)	0.0410 (11)	0.0321 (9)	0.0118 (9)	0.0262 (8)	0.0125 (8)
C20	0.0501 (12)	0.0373 (11)	0.0414 (10)	0.0165 (9)	0.0336 (10)	0.0152 (9)
C21	0.0599 (14)	0.0460 (13)	0.0458 (11)	0.0210 (11)	0.0416 (11)	0.0167 (10)
C22	0.0533 (13)	0.0531 (14)	0.0437 (11)	0.0105 (11)	0.0384 (11)	0.0161 (10)
C23	0.0576 (14)	0.0431 (13)	0.0443 (11)	0.0027 (10)	0.0373 (11)	0.0078 (9)
C24	0.0450 (12)	0.0444 (12)	0.0328 (9)	0.0070 (9)	0.0273 (9)	0.0064 (8)

Geometric parameters (Å, º)

Cl1—C20	1.721 (2)	C10—H10	0.9500
Cl2—C22	1.738 (2)	C11—C12	1.393 (2)
Cl3—C24	1.732 (2)	C11—H11	0.9500
O1—C4	1.215 (2)	C13—C18	1.377 (3)
N1—C5	1.385 (2)	C13—C14	1.393 (3)
N1—C1	1.391 (2)	C14—C15	1.385 (3)
N1—C12	1.400 (2)	C14—H14	0.9500
N2—C1	1.286 (2)	C15—N16	1.334 (3)
N2—N3	1.392 (2)	C15—H15	0.9500
N3—C4	1.377 (3)	N16—C17	1.323 (3)
N3—C19	1.435 (2)	C17—C18	1.386 (3)
C1—C13	1.479 (2)	C17—H17	0.9500
C4—C5	1.466 (3)	C18—H18	0.9500
C5—N6	1.307 (2)	C19—C24	1.382 (3)
N6—C7	1.391 (2)	C19—C20	1.395 (3)
C7—C8	1.400 (3)	C20—C21	1.390 (3)
C7—C12	1.403 (3)	C21—C22	1.371 (3)
C8—C9	1.377 (3)	C21—H21	0.9500

C8—H8	0.9500	C22—C23	1.382 (3)
C9—C10	1.399 (3)	C23—C24	1.388 (3)
C9—H9	0.9500	C23—H23	0.9500
C10—C11	1.381 (3)		

C5—N1—C1	121.08 (15)	C18—C13—C14	118.72 (17)
C5—N1—C12	105.83 (15)	C18—C13—C1	120.06 (17)
C1—N1—C12	132.97 (15)	C14—C13—C1	121.22 (17)
C1—N2—N3	117.77 (16)	C15—C14—C13	117.98 (19)
C4—N3—N2	126.33 (16)	C15—C14—H14	121.0
C4—N3—C19	118.44 (15)	C13—C14—H14	121.0
N2—N3—C19	113.84 (15)	N16—C15—C14	124.0 (2)
N2—C1—N1	122.12 (16)	N16—C15—H15	118.0
N2—C1—C13	118.59 (16)	C14—C15—H15	118.0
N1—C1—C13	119.29 (15)	C17—N16—C15	116.66 (18)
O1—C4—N3	122.37 (18)	N16—C17—C18	124.4 (2)
O1—C4—C5	124.34 (19)	N16—C17—H17	117.8
N3—C4—C5	113.19 (15)	C18—C17—H17	117.8
N6—C5—N1	114.25 (16)	C13—C18—C17	118.23 (19)
N6—C5—C4	126.71 (17)	C13—C18—H18	120.9
N1—C5—C4	118.69 (17)	C17—C18—H18	120.9
C5—N6—C7	103.98 (15)	C24—C19—C20	118.44 (18)
N6—C7—C8	127.68 (18)	C24—C19—N3	122.39 (18)
N6—C7—C12	111.52 (16)	C20—C19—N3	119.16 (19)
C8—C7—C12	120.69 (17)	C21—C20—C19	121.1 (2)
C9—C8—C7	117.32 (18)	C21—C20—Cl1	119.30 (17)
C9—C8—H8	121.3	C19—C20—Cl1	119.51 (16)
C7—C8—H8	121.3	C22—C21—C20	118.2 (2)
C8—C9—C10	121.43 (18)	C22—C21—H21	120.9
C8—C9—H9	119.3	C20—C21—H21	120.9
C10—C9—H9	119.3	C21—C22—C23	122.57 (19)
C11—C10—C9	122.24 (17)	C21—C22—Cl2	118.58 (17)
C11—C10—H10	118.9	C23—C22—Cl2	118.82 (19)
C9—C10—H10	118.9	C22—C23—C24	118.0 (2)
C10—C11—C12	116.45 (17)	C22—C23—H23	121.0
C10—C11—H11	121.8	C24—C23—H23	121.0
C12—C11—H11	121.8	C19—C24—C23	121.6 (2)
C11—C12—N1	133.68 (17)	C19—C24—Cl3	120.51 (15)
C11—C12—C7	121.88 (17)	C23—C24—Cl3	117.90 (18)
N1—C12—C7	104.36 (15)		

C1—N2—N3—C4	−7.9 (3)	C8—C7—C12—C11	0.1 (3)
C1—N2—N3—C19	−174.11 (18)	N6—C7—C12—N1	−0.7 (2)
N3—N2—C1—N1	−0.7 (3)	C8—C7—C12—N1	−177.00 (18)
N3—N2—C1—C13	178.54 (16)	N2—C1—C13—C18	57.3 (2)
C5—N1—C1—N2	7.2 (3)	N1—C1—C13—C18	−123.43 (19)
C12—N1—C1—N2	−168.14 (19)	N2—C1—C13—C14	−121.9 (2)
C5—N1—C1—C13	−172.08 (17)	N1—C1—C13—C14	57.3 (2)

C12—N1—C1—C13	12.6 (3)	C18—C13—C14—C15	0.8 (3)
N2—N3—C4—O1	−174.6 (2)	C1—C13—C14—C15	−179.91 (17)
C19—N3—C4—O1	−9.0 (3)	C13—C14—C15—N16	1.0 (3)
N2—N3—C4—C5	8.9 (3)	C14—C15—N16—C17	−1.7 (3)
C19—N3—C4—C5	174.55 (18)	C15—N16—C17—C18	0.5 (3)
C1—N1—C5—N6	−179.24 (17)	C14—C13—C18—C17	−1.9 (3)
C12—N1—C5—N6	−2.8 (2)	C1—C13—C18—C17	178.83 (17)
C1—N1—C5—C4	−5.5 (3)	N16—C17—C18—C13	1.3 (3)
C12—N1—C5—C4	170.92 (17)	C4—N3—C19—C24	84.0 (3)
O1—C4—C5—N6	−5.5 (4)	N2—N3—C19—C24	−108.6 (2)
N3—C4—C5—N6	170.9 (2)	C4—N3—C19—C20	−94.8 (2)
O1—C4—C5—N1	−178.4 (2)	N2—N3—C19—C20	72.6 (2)
N3—C4—C5—N1	−2.0 (3)	C24—C19—C20—C21	3.0 (3)
N1—C5—N6—C7	2.3 (2)	N3—C19—C20—C21	−178.17 (19)
C4—C5—N6—C7	−170.8 (2)	C24—C19—C20—Cl1	−174.58 (16)
C5—N6—C7—C8	175.1 (2)	N3—C19—C20—Cl1	4.3 (3)
C5—N6—C7—C12	−1.0 (2)	C19—C20—C21—C22	−1.6 (3)
N6—C7—C8—C9	−175.5 (2)	Cl1—C20—C21—C22	175.98 (18)
C12—C7—C8—C9	0.2 (3)	C20—C21—C22—C23	−0.7 (4)
C7—C8—C9—C10	−0.4 (3)	C20—C21—C22—Cl2	−178.54 (18)
C8—C9—C10—C11	0.5 (3)	C21—C22—C23—C24	1.6 (4)
C9—C10—C11—C12	−0.2 (3)	Cl2—C22—C23—C24	179.36 (18)
C10—C11—C12—N1	176.0 (2)	C20—C19—C24—C23	−2.1 (3)
C10—C11—C12—C7	0.0 (3)	N3—C19—C24—C23	179.1 (2)
C5—N1—C12—C11	−174.6 (2)	C20—C19—C24—Cl3	176.14 (16)
C1—N1—C12—C11	1.2 (4)	N3—C19—C24—Cl3	−2.7 (3)
C5—N1—C12—C7	1.9 (2)	C22—C23—C24—C19	−0.1 (3)
C1—N1—C12—C7	177.75 (19)	C22—C23—C24—Cl3	−178.39 (18)
N6—C7—C12—C11	176.42 (18)		