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4-[5-(4-Fluorophenyl)-1,2-oxazol-4-yl]pyridine

Pierre Koch,^{a*} Dieter Schollmeyer^b and Stefan Laufer^c

^aUniversität Regensburg, Universitätsstrasse 31, 93053 Regensburg, Germany, ^bUniversity Mainz, Department of Chemistry, Duesbergweg 10-14, 55099 Mainz, Germany, and ^cEberhard Karls Universität Tübingen, Department of Pharmaceutical/Medicinal Chemistry, Auf der Morgenstelle 8, 72076 Tübingen, Germany. *Correspondence e-mail: pierre.koch@ur.de

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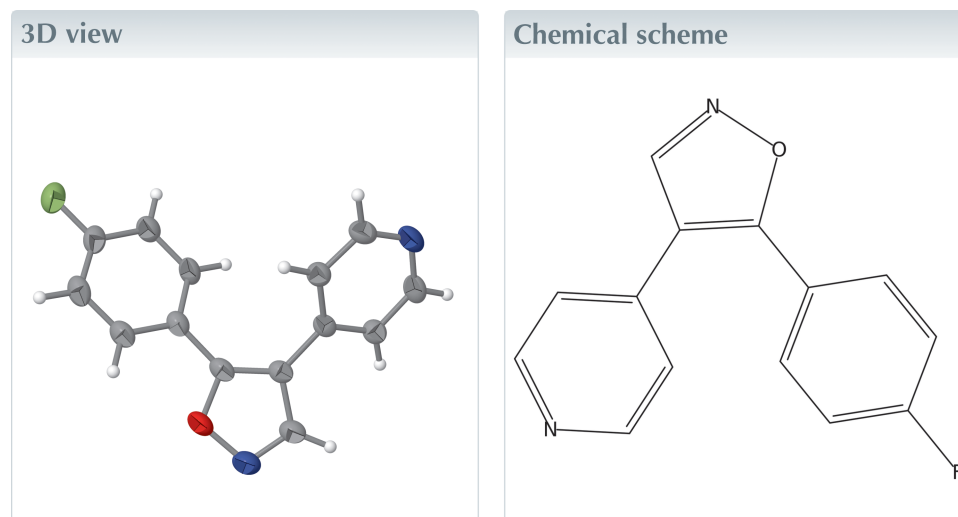
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Keywords: crystal structure; pyridine; isooxazole; MAP kinase inhibitor.

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

The title compound, C₁₄H₉FN₂O, crystallizes in the monoclinic space group *P*2₁/*c*. The dihedral angles between the central isoxazole ring and the 4-fluorophenyl and pyridine rings are 32.64 (5) and 32.70 (7)°, respectively.



Structure description

The title compound, C₁₄H₉FN₂O (Fig. 1), was synthesized to extend our study on the role of the hydrogen-bonding heteroatom-Lys53 interaction between pyridinyl-substituted five-membered heterocyclic ring inhibitors and the p38 α mitogen-activated protein (MAP) kinase (Abu Thaher *et al.*, 2009). The isoxazole ring (O1, C2–C4, N5) makes dihedral angles of 32.64 (5) and 32.70 (7)° with the 4-fluorophenyl ring (C6–C11) and the pyridine ring (C12–C14, N15, C16, C17), respectively. The 4-fluorophenyl ring makes a dihedral angle of 46.37 (6)° with the pyridine ring. In the extended structure, C–H...N bonds link the molecules into *C*(6) chains running along the *c*-axis direction (Table 1, Fig. 2).

Synthesis and crystallization

The title compound was synthesized according to the protocol reported by Laufer *et al.* (2006). 500 mg of 3-(dimethylamino)-1-(4-fluorophenyl)-2-(pyridin-4-yl)prop-2-en-1-one were dissolved in methanol (8 ml) and water (4 ml). 106 mg of sodium carbonate and 123 mg hydroxylamine hydrochloride were added. The pH was adjusted to 5 by dropwise addition of acetic acid. The reaction mixture was heated to reflux temperature for 2.5 h. After cooling to room temperature, the pH was set to 7 by addition of ammonia. Ice was added to the mixture and the title compound slowly crystallized as a colorless solid (290 mg).

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C7–H7···N5 ⁱ	0.95	2.44	3.2772 (19)	148

Symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

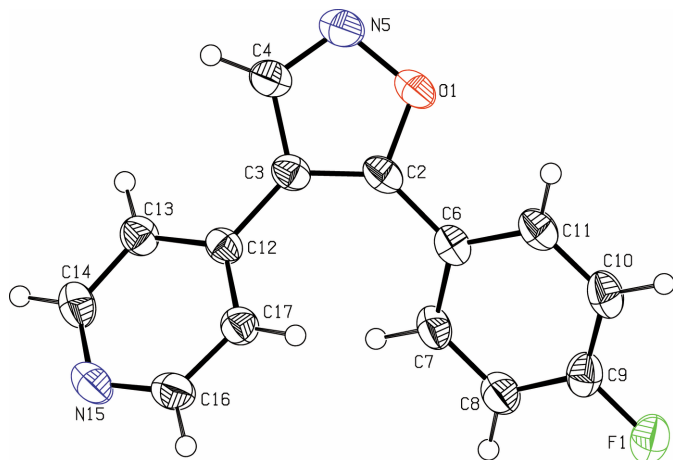


Figure 1
View of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

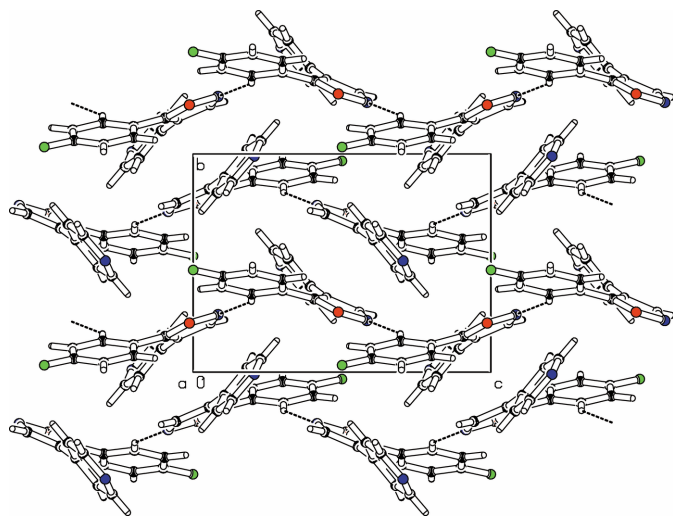


Figure 2
Part of the packing diagram. View along *a*-axis direction. Hydrogen bonds are drawn with dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₄ H ₉ FN ₂ O
<i>M_r</i>	240.23
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	193
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.0938 (9), 8.6289 (3), 13.1513 (12)
β (°)	116.342 (4)
<i>V</i> (Å ³)	1128.21 (15)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	0.86
Crystal size (mm)	0.25 × 0.25 × 0.20
Data collection	
Diffractometer	Enraf–Nonius CAD-4
Absorption correction	–
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	2139, 2139, 1997
<i>R</i> _{int}	0
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.610
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.042, 0.124, 1.07
No. of reflections	2139
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.28, –0.28

Computer programs: *Enraf–Nonius Software* (Enraf–Nonius, 1989), *CORINC* (Dräger & Gattow 1971), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2019/3* (Sheldrick, 2015b) and *PLATON* (Spek, 2009).

Refinement

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

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full crystallographic data

IUCrData (2025). **10**, x250987 [https://doi.org/10.1107/S2414314625009873]

4-[5-(4-Fluorophenyl)-1,2-oxazol-4-yl]pyridine

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4-[5-(4-Fluorophenyl)-1,2-oxazol-4-yl]pyridine

Crystal data

$C_{14}H_9FN_2O$

$M_r = 240.23$

Monoclinic, $P2_1/c$

$a = 11.0938$ (9) Å

$b = 8.6289$ (3) Å

$c = 13.1513$ (12) Å

$\beta = 116.342$ (4)°

$V = 1128.21$ (15) Å³

$Z = 4$

$F(000) = 496$

$D_x = 1.414$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 25 reflections

$\theta = 65$ – 69°

$\mu = 0.86$ mm⁻¹

$T = 193$ K

Block, colourless

$0.25 \times 0.25 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4

diffractometer

Radiation source: rotating anode

Graphite monochromator

$\omega/2\theta$ scans

2139 measured reflections

2139 independent reflections

1997 reflections with $I > 2\sigma(I)$

$R_{int} = 0$

$\theta_{max} = 70.1^\circ$, $\theta_{min} = 4.5^\circ$

$h = -13 \rightarrow 12$

$k = 0 \rightarrow 10$

$l = 0 \rightarrow 16$

3 standard reflections every 60 min

intensity decay: 1%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.124$

$S = 1.07$

2139 reflections

164 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 0.3458P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.28$ e Å⁻³

$\Delta\rho_{min} = -0.28$ e Å⁻³

Extinction correction: SHELXL-2019/3

(Sheldrick, 2015b),

$Fc^* = kFc[1 + 0.001x Fc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0086 (11)

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.

Refinement. Hydrogen atoms were placed at calculated positions and were refined in the riding-model approximation with C–H = 0.95 Å, and with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.13611 (9)	0.46819 (11)	0.00038 (8)	0.0473 (3)
O1	0.55369 (11)	0.27510 (14)	0.48748 (9)	0.0424 (3)
C2	0.58461 (15)	0.33567 (17)	0.40706 (12)	0.0335 (3)
C3	0.72080 (14)	0.33966 (16)	0.44657 (12)	0.0310 (3)
C4	0.76924 (16)	0.27421 (18)	0.55716 (13)	0.0372 (4)
H4	0.862023	0.259844	0.606378	0.045*
N5	0.67381 (14)	0.23630 (18)	0.58372 (11)	0.0452 (4)
C6	0.46742 (14)	0.37489 (17)	0.29991 (12)	0.0332 (3)
C7	0.47353 (14)	0.35792 (18)	0.19678 (13)	0.0372 (4)
H7	0.554463	0.323746	0.195893	0.045*
C8	0.36212 (15)	0.39071 (19)	0.09582 (13)	0.0396 (4)
H8	0.365560	0.380371	0.025244	0.047*
C9	0.24600 (14)	0.43875 (17)	0.10017 (14)	0.0373 (4)
C10	0.23548 (15)	0.45675 (18)	0.19966 (15)	0.0401 (4)
H10	0.153807	0.490165	0.199504	0.048*
C11	0.34809 (15)	0.42451 (18)	0.30042 (13)	0.0376 (4)
H11	0.343831	0.436385	0.370570	0.045*
C12	0.80557 (14)	0.39405 (16)	0.39348 (11)	0.0294 (3)
C13	0.92774 (14)	0.32139 (17)	0.41942 (13)	0.0344 (3)
H13	0.956804	0.237041	0.471192	0.041*
C14	1.00631 (15)	0.37309 (19)	0.36917 (14)	0.0400 (4)
H14	1.089593	0.322108	0.388691	0.048*
N15	0.97329 (13)	0.48966 (17)	0.29514 (11)	0.0420 (4)
C16	0.85625 (17)	0.55986 (19)	0.27201 (13)	0.0407 (4)
H16	0.829864	0.643649	0.219731	0.049*
C17	0.77120 (15)	0.51901 (17)	0.31884 (12)	0.0339 (3)
H17	0.690549	0.575274	0.300406	0.041*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0339 (5)	0.0487 (6)	0.0518 (6)	−0.0011 (4)	0.0122 (4)	0.0010 (4)
O1	0.0423 (6)	0.0510 (7)	0.0450 (6)	−0.0004 (5)	0.0296 (5)	0.0066 (5)
C2	0.0396 (8)	0.0324 (7)	0.0380 (8)	0.0001 (6)	0.0258 (7)	−0.0007 (6)
C3	0.0367 (7)	0.0277 (7)	0.0339 (7)	0.0019 (5)	0.0205 (6)	0.0004 (5)
C4	0.0433 (8)	0.0372 (8)	0.0369 (8)	0.0021 (6)	0.0230 (7)	0.0033 (6)
N5	0.0493 (8)	0.0521 (8)	0.0418 (8)	0.0038 (6)	0.0271 (7)	0.0093 (6)
C6	0.0327 (7)	0.0324 (7)	0.0400 (8)	−0.0020 (5)	0.0210 (6)	−0.0021 (6)
C7	0.0304 (7)	0.0441 (8)	0.0426 (8)	−0.0011 (6)	0.0212 (7)	−0.0054 (7)
C8	0.0371 (8)	0.0459 (9)	0.0402 (8)	−0.0047 (7)	0.0212 (7)	−0.0049 (7)
C9	0.0296 (7)	0.0339 (8)	0.0451 (8)	−0.0030 (6)	0.0135 (6)	−0.0008 (6)
C10	0.0339 (8)	0.0362 (8)	0.0574 (10)	0.0032 (6)	0.0266 (7)	−0.0001 (7)

C11	0.0395 (8)	0.0375 (8)	0.0454 (9)	0.0010 (6)	0.0276 (7)	-0.0014 (6)
C12	0.0327 (7)	0.0294 (7)	0.0298 (7)	-0.0036 (5)	0.0171 (6)	-0.0045 (5)
C13	0.0360 (7)	0.0322 (7)	0.0386 (8)	0.0018 (6)	0.0197 (6)	0.0000 (6)
C14	0.0346 (8)	0.0439 (9)	0.0472 (9)	-0.0005 (6)	0.0233 (7)	-0.0063 (7)
N15	0.0429 (7)	0.0493 (8)	0.0433 (7)	-0.0090 (6)	0.0278 (6)	-0.0052 (6)
C16	0.0461 (9)	0.0422 (8)	0.0376 (8)	-0.0048 (7)	0.0221 (7)	0.0038 (6)
C17	0.0341 (7)	0.0341 (7)	0.0354 (7)	0.0015 (6)	0.0173 (6)	0.0015 (6)

Geometric parameters (Å, °)

F1—C9	1.3614 (17)	C9—C10	1.373 (2)
O1—C2	1.3533 (17)	C10—C11	1.387 (2)
O1—N5	1.4118 (17)	C10—H10	0.9500
C2—C3	1.363 (2)	C11—H11	0.9500
C2—C6	1.471 (2)	C12—C13	1.391 (2)
C3—C4	1.425 (2)	C12—C17	1.393 (2)
C3—C12	1.4748 (18)	C13—C14	1.381 (2)
C4—N5	1.295 (2)	C13—H13	0.9500
C4—H4	0.9500	C14—N15	1.333 (2)
C6—C11	1.394 (2)	C14—H14	0.9500
C6—C7	1.395 (2)	N15—C16	1.340 (2)
C7—C8	1.384 (2)	C16—C17	1.382 (2)
C7—H7	0.9500	C16—H16	0.9500
C8—C9	1.378 (2)	C17—H17	0.9500
C8—H8	0.9500		
C2—O1—N5	109.06 (11)	C9—C10—C11	117.79 (14)
O1—C2—C3	109.53 (13)	C9—C10—H10	121.1
O1—C2—C6	114.50 (12)	C11—C10—H10	121.1
C3—C2—C6	135.92 (13)	C10—C11—C6	120.76 (14)
C2—C3—C4	103.39 (12)	C10—C11—H11	119.6
C2—C3—C12	131.26 (13)	C6—C11—H11	119.6
C4—C3—C12	125.35 (13)	C13—C12—C17	117.00 (13)
N5—C4—C3	113.09 (14)	C13—C12—C3	119.80 (13)
N5—C4—H4	123.5	C17—C12—C3	123.19 (13)
C3—C4—H4	123.5	C14—C13—C12	119.35 (14)
C4—N5—O1	104.93 (12)	C14—C13—H13	120.3
C11—C6—C7	119.52 (14)	C12—C13—H13	120.3
C11—C6—C2	120.23 (13)	N15—C14—C13	124.47 (14)
C7—C6—C2	120.22 (13)	N15—C14—H14	117.8
C8—C7—C6	120.21 (14)	C13—C14—H14	117.8
C8—C7—H7	119.9	C14—N15—C16	115.57 (13)
C6—C7—H7	119.9	N15—C16—C17	124.62 (15)
C9—C8—C7	118.36 (14)	N15—C16—H16	117.7
C9—C8—H8	120.8	C17—C16—H16	117.7
C7—C8—H8	120.8	C16—C17—C12	118.96 (14)
F1—C9—C10	118.64 (13)	C16—C17—H17	120.5
F1—C9—C8	118.01 (14)	C12—C17—H17	120.5

C10—C9—C8	123.35 (15)		
N5—O1—C2—C3	-0.45 (17)	C7—C8—C9—C10	0.5 (2)
N5—O1—C2—C6	177.46 (12)	F1—C9—C10—C11	179.28 (13)
O1—C2—C3—C4	0.79 (16)	C8—C9—C10—C11	0.0 (2)
C6—C2—C3—C4	-176.47 (16)	C9—C10—C11—C6	-0.3 (2)
O1—C2—C3—C12	-179.98 (14)	C7—C6—C11—C10	0.2 (2)
C6—C2—C3—C12	2.8 (3)	C2—C6—C11—C10	-177.78 (14)
C2—C3—C4—N5	-0.93 (18)	C2—C3—C12—C13	-147.29 (16)
C12—C3—C4—N5	179.79 (14)	C4—C3—C12—C13	31.8 (2)
C3—C4—N5—O1	0.66 (18)	C2—C3—C12—C17	34.1 (2)
C2—O1—N5—C4	-0.13 (17)	C4—C3—C12—C17	-146.80 (15)
O1—C2—C6—C11	32.3 (2)	C17—C12—C13—C14	-1.4 (2)
C3—C2—C6—C11	-150.50 (17)	C3—C12—C13—C14	179.94 (13)
O1—C2—C6—C7	-145.61 (14)	C12—C13—C14—N15	-0.5 (2)
C3—C2—C6—C7	31.6 (3)	C13—C14—N15—C16	1.3 (2)
C11—C6—C7—C8	0.3 (2)	C14—N15—C16—C17	-0.2 (2)
C2—C6—C7—C8	178.20 (14)	N15—C16—C17—C12	-1.7 (2)
C6—C7—C8—C9	-0.6 (2)	C13—C12—C17—C16	2.4 (2)
C7—C8—C9—F1	-178.88 (13)	C3—C12—C17—C16	-179.02 (13)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C7—H7 \cdots N5 ⁱ	0.95	2.44	3.2772 (19)	148

Symmetry code: (i) *x*, -*y*+1/2, *z*-1/2.