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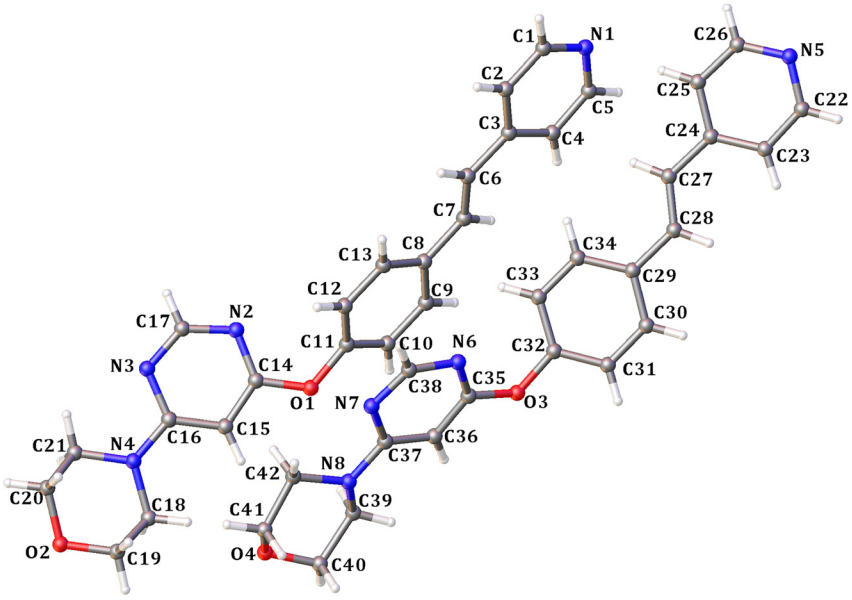
Crystal structure of (*E*)-4-(6-(4-(2-(pyridin-4-yl) vinyl)phenoxy)pyrimidin-4-yl)morpholine, $C_{21}H_{20}N_4O_2$



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Abstract

$C_{21}H_{20}N_4O_2$, triclinic, $P\bar{1}$ (no. 2), a = 5.874(3) Å, b = 16.526(7) Å, c = 20.147(8) Å, α = 67.140(5)°, β = 83.287(6)°, γ = 86.910(6)°, V = 1789.7(14) Å^3, Z = 4, $R_{gt}(F)$ = 0.0614, w$R_{ref}(F^2)$ = 0.1675, T = 296 K.

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The asymmetric unit of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.18 × 0.16 × 0.14 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.2°, 98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9263, 6352, 0.050
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2989
$N(param)_{refined}$:	487
Programs:	Bruker [1], SHELX [2, 3]

Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of (*E*)-4-(2-(pyridin-4-yl)vinyl)phenol (197 mg, 1 mmol) and 4,6-dichloropyrimidine (205 mg, 1 mmol) was suspended in DMF (5 ml), then copper powder (6.4 mg, 0.1 mmol) and cesium carbonate (815 mg, 2.5 mmol) were added. The reaction mixture was held at 110 °C under nitrogen for 6 h and then diluted with ethyl

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5299 (4)	0.62884 (16)	0.30751 (11)	0.0577 (7)
O2	1.0063 (4)	0.64440 (17)	−0.05117 (11)	0.0653 (7)
O3	0.0291 (4)	0.85345 (16)	0.41130 (11)	0.0560 (7)
O4	0.4165 (4)	0.79593 (18)	0.07116 (12)	0.0639 (7)
N1	0.5381 (6)	0.6460 (2)	0.83867 (15)	0.0627 (9)
N2	0.8961 (5)	0.56661 (18)	0.31338 (13)	0.0500 (7)
N3	1.0908 (4)	0.55214 (18)	0.20679 (14)	0.0469 (7)
N4	0.9242 (4)	0.59575 (18)	0.10022 (13)	0.0475 (7)
N5	0.0921 (8)	0.9195 (2)	0.92154 (17)	0.0829 (11)
N6	0.3983 (5)	0.90779 (18)	0.36990 (14)	0.0493 (7)
N7	0.5769 (5)	0.90094 (19)	0.25852 (14)	0.0499 (7)
N8	0.3838 (4)	0.85246 (17)	0.18781 (13)	0.0444 (7)
C1	0.7242 (7)	0.6753 (2)	0.79246 (19)	0.0614 (10)
H1	0.845922	0.693583	0.808712	0.074*
C2	0.7491 (6)	0.6803 (2)	0.72236 (17)	0.0529 (9)
H2	0.883826	0.702357	0.692853	0.063*
C3	0.5771 (6)	0.6532 (2)	0.69539 (16)	0.0429 (8)
C4	0.3817 (6)	0.6221 (2)	0.74314 (17)	0.0526 (9)
H4	0.258953	0.602480	0.728277	0.063*
C5	0.3690 (6)	0.6201 (2)	0.81203 (18)	0.0607 (10)
H5	0.234769	0.599600	0.842341	0.073*
C6	0.6064 (6)	0.6565 (2)	0.62072 (16)	0.0486 (9)
H6	0.740367	0.681911	0.592455	0.058*
C7	0.4625 (6)	0.6273 (2)	0.58992 (16)	0.0478 (9)
H7	0.329677	0.601653	0.618782	0.057*
C8	0.4853 (6)	0.6302 (2)	0.51631 (16)	0.0439 (8)
C9	0.3167 (6)	0.5944 (2)	0.49335 (17)	0.0541 (10)
H9	0.186883	0.570678	0.524956	0.065*
C10	0.3368 (6)	0.5931 (2)	0.42456 (17)	0.0549 (10)
H10	0.222363	0.567991	0.410732	0.066*
C11	0.5238 (6)	0.6284 (2)	0.37732 (16)	0.0466 (9)
C12	0.6907 (6)	0.6679 (2)	0.39679 (17)	0.0547 (10)
H12	0.816655	0.693599	0.364019	0.066*
C13	0.6691 (6)	0.6691 (2)	0.46550 (17)	0.0545 (10)
H13	0.780851	0.696784	0.478084	0.065*
C14	0.7183 (6)	0.6018 (2)	0.27506 (16)	0.0447 (8)
C15	0.7092 (5)	0.6116 (2)	0.20517 (15)	0.0434 (8)
H15	0.579583	0.634376	0.181411	0.052*
C16	0.9034 (5)	0.5860 (2)	0.17059 (16)	0.0405 (8)
C17	1.0709 (6)	0.5442 (2)	0.27502 (17)	0.0493 (9)
H17	1.197056	0.519446	0.300015	0.059*
C18	0.7348 (5)	0.6230 (2)	0.05496 (15)	0.0528 (10)
H18A	0.619510	0.653879	0.074943	0.063*
H18B	0.664353	0.571627	0.054180	0.063*
C19	0.8224 (6)	0.6818 (3)	−0.02057 (17)	0.0600 (10)
H19A	0.697878	0.695368	−0.050990	0.072*
H19B	0.872330	0.736505	−0.020025	0.072*
C20	1.1932 (6)	0.6233 (3)	−0.00672 (17)	0.0635 (11)
H20A	1.247410	0.676542	−0.004640	0.076*
H20B	1.318893	0.597930	−0.028235	0.076*
C21	1.1200 (6)	0.5599 (2)	0.06813 (17)	0.0545 (10)
H21A	1.077780	0.504715	0.066611	0.065*
H21B	1.246191	0.548514	0.097682	0.065*
C22	−0.0776 (8)	0.9434 (3)	0.8785 (2)	0.0799 (13)
H22	−0.204368	0.972142	0.891800	0.096*
C23	−0.0767 (7)	0.9285 (2)	0.81633 (18)	0.0634 (11)
H23	−0.199303	0.947950	0.788544	0.076*
C24	0.1047 (6)	0.8846 (2)	0.79436 (17)	0.0496 (9)
C25	0.2794 (7)	0.8582 (2)	0.83933 (18)	0.0644 (11)
H25	0.406764	0.828357	0.827838	0.077*
C26	0.2642 (8)	0.8760 (3)	0.9004 (2)	0.0762 (12)
H26	0.383350	0.856288	0.929661	0.091*
C27	0.1235 (6)	0.8684 (2)	0.72777 (17)	0.0562 (10)
H27	0.249662	0.835502	0.719988	0.067*
C28	−0.0204 (6)	0.8956 (2)	0.67702 (17)	0.0514 (9)
H28	−0.149375	0.926434	0.686060	0.062*
C29	−0.0008 (6)	0.8830 (2)	0.60926 (16)	0.0443 (8)
C30	−0.1779 (6)	0.9112 (2)	0.56425 (17)	0.0509 (9)
H30	−0.308912	0.936674	0.578915	0.061*
C31	−0.1624 (6)	0.9021 (2)	0.49902 (17)	0.0516 (9)
H31	−0.281980	0.921612	0.469955	0.062*
C32	0.0286 (6)	0.8644 (2)	0.47657 (16)	0.0454 (9)
C33	0.2054 (6)	0.8333 (2)	0.52050 (17)	0.0528 (9)
H33	0.333924	0.806485	0.505977	0.063*
C34	0.1878 (6)	0.8427 (2)	0.58560 (17)	0.0512 (9)
H34	0.305996	0.821501	0.615011	0.061*
C35	0.2167 (6)	0.8697 (2)	0.36136 (16)	0.0428 (8)
C36	0.1984 (6)	0.8480 (2)	0.30351 (16)	0.0467 (9)
H36	0.066137	0.822365	0.299623	0.056*
C37	0.3830 (5)	0.8654 (2)	0.25067 (16)	0.0417 (8)
C38	0.5680 (6)	0.9195 (2)	0.31673 (18)	0.0550 (10)
H38	0.699830	0.944670	0.321572	0.066*
C39	0.2086 (6)	0.7952 (2)	0.18246 (16)	0.0534 (9)
H39A	0.060153	0.808887	0.202404	0.064*
H39B	0.245130	0.734340	0.210680	0.064*
C40	0.1974 (6)	0.8072 (3)	0.10508 (17)	0.0602 (10)
H40A	0.091910	0.764916	0.103507	0.072*
H40B	0.138941	0.865535	0.078556	0.072*
C41	0.5633 (6)	0.8630 (3)	0.06904 (17)	0.0621 (11)
H41A	0.495182	0.920083	0.043990	0.075*
H41B	0.709438	0.859647	0.042244	0.075*
C42	0.6018 (6)	0.8537 (2)	0.14389 (16)	0.0514 (9)
H42A	0.686069	0.799735	0.166924	0.062*
H42B	0.693383	0.902329	0.141000	0.062*

acetate (30 ml). The organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by chromatography (petroleum ether: ethyl acetate = 6:1, *v*/*v*) on silica gel to give (*E*)-4-chloro-6-(4-(2-(pyridin-4-yl)vinyl)phenoxy)pyrimidine as a yellow solid. A mixture of (*E*)-4-chloro-6-(4-(2-(pyridin-4-yl)vinyl)phenoxy)pyrimidine (307 mg, 1 mmol) and morpholine (87 mg, 1 mmol) in DMF (5 ml) was heated in a microwave reactor at 130 °C and 100 W for 30 min. The reaction mixture was diluted with ethyl acetate (30 ml). The organic layer was washed with brine, dried over anhydrous Na_2SO_4, filtered and

concentrated. The residue was purified by chromatography (petroleum ether: ethyl acetate = 10:1, *v*/*v*) on silica gel to give the title compound as a white solid [4].

Experimental details

All hydrogen atoms were placed in the calculated positions and constrained to ride on their parent atoms.

Comment

Nitrogen containing heterocycles especially pyrimidines form an important class of heterocyclic compounds [5, 6]. Heterocycles containing pyrimidine ring exist as the basic structures of many natural botanicals and bioactive compounds, and are widely found in herbal medicines with therapeutic effects on diabetes [7–9].

There are two crystallographically independent molecules in the asymmetric unit (see the figure). The bond lengths and angles are in the expected ranges [10].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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