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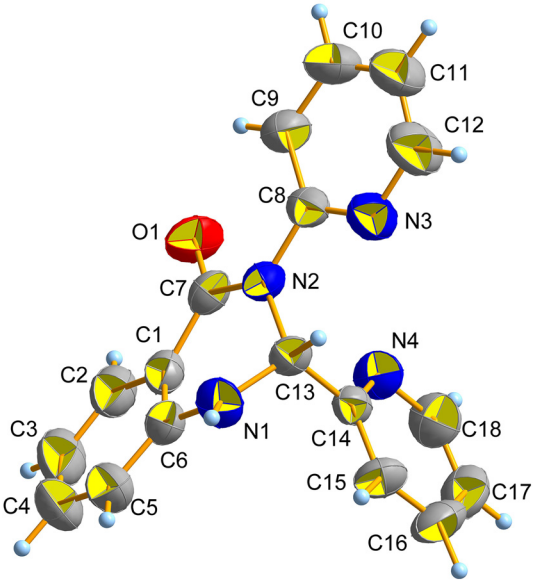
The crystal structure of 2,3-di(pyridin-2-yl)-2,3-dihydroquinazolin-4(1*H*)-one, $C_{18}H_{14}N_4O$



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Abstract

$C_{18}H_{14}N_4O$, orthorhombic, *Pbca* (no. 61), a = 7.963(3) Å, b = 12.629(5) Å, c = 30.116(11) Å, V = 3,028.3(19) Å^3, Z = 8, $R_{gt}(F)$ = 0.0475, w$R_{ref}(F^2)$ = 0.1444, T = 296(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colorless, block
Size:	0.50 × 0.43 × 0.36 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:	25.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	25,773, 2,670, 0.030
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} >2 $\sigma(I_{obs})$, 2184
$N(param)_{refined}$:	208
Programs:	Bruker[1], SHELX[2,3]

1 Source of material

2-Amino-*N*-(pyridin-2-yl)benzamide (213.24 mg, 1 mmol) and pyridine-2-carboxaldehyde (107.11 mg, 1 mmol) were dissolved in ethanol (10 mL) and the mixture was refluxed for 4 h. The reaction mixture was concentrated in vacuum, and the title compound was isolated through a silica gel column chromatography (PE: EtOAc = 3:1) as a white solid (120.64 mg, 40 % yield). Single crystals of the product can be obtained by recrystallization in ethanol through slow evaporation within 3 days.

2 Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The U_{iso} values of all hydrogen atoms were set to 1.2U_{eq} (C).

3 Comment

2,3-Dihydroquinazolin-4(1*H*)-ones are components of many bioactive molecules with broad-spectrum pharmacological properties, such as anti-malaria, anti-cancer, anti-microbial, anti-hypertension, anti-oxidation, anti-inflammatory and so on.[4–8]

The crystal structure reveals that the title molecule is non-planar. Plane I (C1–C6) forms a dihedral angle of 35.443(8)° with plane II (C8–N3), and 86.885(7)° with plane III (C14–N4). The dihedral angle between plane II and plane III is 89.799(9). The C(13) atom is sp^3 hybridized and R-type chiral carbon. The bond lengths of O(1)–C(7) and C(1)–C(7) are 1.226(2) Å and 1.484(3) Å. The sp^3 C(13)–N(1), C(13)–N(2) bond lengths are

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1223 (2)	0.78869 (15)	0.30912 (6)	0.0543 (5)
C2	0.0655 (3)	0.71410 (19)	0.27878 (8)	0.0733 (6)
H2	0.0368	0.6466	0.2885	0.088*
C3	0.0515 (4)	0.7390 (3)	0.23482 (9)	0.0985 (9)
H3	0.0108	0.6894	0.2147	0.118*
C4	0.0981 (4)	0.8386 (3)	0.22044 (9)	0.1065 (11)
H4	0.0926	0.8546	0.1903	0.128*
C5	0.1525 (3)	0.9146 (2)	0.24983 (9)	0.0840 (7)
H5	0.1842	0.9812	0.2397	0.101*
C6	0.1598 (2)	0.89094 (17)	0.29489 (7)	0.0585 (5)
C7	0.1639 (2)	0.75471 (14)	0.35500 (7)	0.0513 (5)
C8	0.2610 (2)	0.81737 (15)	0.42827 (6)	0.0516 (5)
C9	0.3257 (3)	0.72266 (19)	0.44397 (8)	0.0741 (6)
H9	0.3312	0.6632	0.4258	0.089*
C10	0.3818 (4)	0.7191 (2)	0.48725 (9)	0.0882 (8)
H10	0.4251	0.6564	0.4987	0.106*
C11	0.3740 (4)	0.8065 (3)	0.51299 (9)	0.0927 (8)
H11	0.4122	0.8052	0.5422	0.111*
C12	0.3094 (4)	0.8955 (2)	0.49527 (9)	0.0939 (9)
H12	0.3049	0.9557	0.5130	0.113*
C13	0.1542 (2)	0.94176 (13)	0.37130 (6)	0.0458 (4)
H13	0.2131	0.9915	0.3909	0.055*
C14	−0.0339 (2)	0.95845 (13)	0.37785 (5)	0.0457 (4)
C15	−0.1002 (3)	1.05442 (15)	0.36609 (7)	0.0644 (5)
H15	−0.0333	1.1069	0.3535	0.077*
C16	−0.2692 (3)	1.0711 (2)	0.37341 (9)	0.0815 (7)
H16	−0.3178	1.1356	0.3660	0.098*
C17	−0.3647 (3)	0.9927 (2)	0.39158 (8)	0.0800 (7)
H17	−0.4791	1.0026	0.3963	0.096*
C18	−0.2906 (3)	0.9009 (2)	0.40257 (8)	0.0783 (7)
H18	−0.3563	0.8481	0.4153	0.094*
N1	0.2079 (2)	0.96241 (13)	0.32681 (6)	0.0626 (5)
H1	0.2675	1.0171	0.3204	0.075*
N2	0.20569 (19)	0.83406 (11)	0.38396 (5)	0.0477 (4)
N3	0.2513 (3)	0.90276 (14)	0.45360 (6)	0.0722 (5)
N4	−0.1254 (2)	0.88098 (14)	0.39609 (6)	0.0650 (5)
O1	0.1694 (2)	0.66070 (10)	0.36501 (5)	0.0731 (5)

1.430(2) Å, 1.471(2) Å, which are longer than the sp^2 C(7)–N(2), C(8)–N(2), C(6)–N(1), C(14)–N(4), C(18)–N(4), C(8)–N(3), C(12)–N(3) bond lengths of 1.369(2) Å, 1.421(2) Å, 1.373(3) Å, 1.337(2) Å, 1.354(3) Å, 1.323(3) Å, 1.341(3) Å, respectively. The bond angles of O(1)–C(7)–C(1), O(1)–C(7)–N(2), C(1)–C(7)–N(2), C(6)–N(1)–C(13), C(8)–N(3)–C(12), C(14)–N(4)–C(18), N(2)–C(13)–N(1), N(1)–C(13)–C(14) and N(2)–C(13)–C(14) are 121.13(17)°, 122.92(18)°, 115.82(16)°, 116.92(16)°, 117.6(2)°, 116.91(19)°, 109.16(14)°, 112.91(15)° and 111.59(14)°, respectively. Geometric parameters are all in the expected ranges.[6,9]

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References

1. Bruker. APEX3, SAINT–Plus, XPREP; Bruker AXS Inc.: Madison, Wisconsin, USA, 2016.
2. Sheldrick, G. M. SHELXT – Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallogr.* **2015**, *A71*, 3–8.
3. Sheldrick, G. M. Crystal Structure Refinement with S*HELXL*. *Acta Crystallogr.* **2015**, *C71*, 3–8.
4. Shi, D.; Li, Z.; Shi, C.; Zhuang, Q.; Zhang, Y. 3-(4-Bromo-phenyl)-2,2-Di-Methyl-2,3-Di-Hydro-Quinazolin-4(1*H*)-One. *Acta Crystallogr.* **2004**, *E60*, 1992–1994.
5. Shi, D.; Wang, J.; Rong, L.; Wang, X.; Hu, H. 2,2-Di-Methyl-3-(4-Methyl-Phenyl)-1,2-Di-Hydro-Quinazolin-4(3*H*)-One. *Acta Crystallogr.* **2003**, *E59*, 1689–1690.
6. Lu, Z. S.; Wang, X. S.; Zhu, G. Z.; Li, X. L.; Niu, D. Z. Crystal Structure of 2,3-Dihydro-2-Phenyl-3-[(*E*)-(1- Phyenylethylidene)amino]-4(1*H*)-Quinazolinone, $C_{22}H_{19}N_3O$. *Z. Kristallogr. N. Cryst. Struct.* **2012**, *227*, 499–500.
7. Jain, S. C.; Bharadvaja, A.; Kumar, R.; Agarwal, D.; Errington, W. 3-[4-(3,4-Dimethylphenyl)-1,3-Thiazol-2-yl]-2-(2-hydroxyphenyl)-1,2,3,4-Tetrahydroquinazolin-4-One. *Acta Crystallogr.* **2000**, *C56*, 592–593.
8. Memarian, H. R.; Ebrahimi, S.; Rudbari, H. A.; Sabzyan, H.; Nardo, V. M. Inter- and Intramolecular Interactions in 2,3-Dihydroquinazolin-4(1*H*)-Ones: Molecular Structure and Conformational Analysis. *J. Iran. Chem. Soc.* **2016**, *13*, 1395–1404.
9. Baykova, S. O.; Geyl K. K.; Baykov S. V.; Boyarskiy V. P. Synthesis of 3-(Pyridin-2-yl)Quinazolin-2,4(1*H*,3*H*)-Diones Via Annulation of Anthranilic Esters with *N*-Pyridyl Ureas. *Int. J. Mol. Sci.* **2023**, *24*, 7633.