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Crystal structure of 3-(2-diethylaminoethyl)-2,3-dihydro-2-thioxoquinazolin-4(1*H*)-one, $C_{14}H_{19}N_3OS$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.20 × 0.15 × 0.10 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.23 mm ⁻¹
Diffractometer, scan mode:	SMART CCD, φ and ω
$\theta_{\max}$, completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6954, 2417, 0.020
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2174
$N(\text{param})_{\text{refined}}$:	173
Programs:	Bruker [1], SHELX [2]

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Abstract

$C_{14}H_{19}N_3OS$, monoclinic, $P2_1/c$ (no. 14), $a = 7.641(3)$ Å, $b = 24.184(8)$ Å, $c = 7.947(3)$ Å, $\beta = 111.196(5)^\circ$, $V = 1369.2(8)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0322$, $wR_{\text{ref}}(F^2) = 0.0968$, $T = 296(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was synthesized according to the literature method [5]. The crystal suitable for single X-ray diffraction was obtained by recrystallization from acetonitrile solution at room temperature.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.80389(19)	0.02664(6)	0.77881(19)	0.0280(3)
C2	0.76221(19)	0.00197(6)	0.60203(19)	0.0274(3)
C3	0.6974(2)	−0.05185(6)	0.5679(2)	0.0345(4)
H3A	0.680545	−0.072740	0.659097	0.041*
C4	0.6581(2)	−0.07445(7)	0.4001(2)	0.0409(4)
H4A	0.616016	−0.110766	0.377677	0.049*
C5	0.6811(2)	−0.04297(7)	0.2640(2)	0.0403(4)
H5A	0.653190	−0.058312	0.149988	0.048*
C6	0.7442(2)	0.01019(6)	0.2948(2)	0.0348(4)
H6A	0.758676	0.031052	0.202339	0.042*
C7	0.78668(19)	0.03284(6)	0.46527(19)	0.0274(3)
C8	0.9059(2)	0.11008(6)	0.66449(19)	0.0309(3)
C9	0.9367(2)	0.10386(6)	0.98200(18)	0.0297(3)
H9A	1.044512	0.127754	1.002820	0.036*
H9B	0.972994	0.074579	1.071443	0.036*
C10	0.7778(2)	0.13681(6)	1.00258(18)	0.0286(3)
H10A	0.745651	0.166876	0.915937	0.034*
H10B	0.668404	0.113169	0.975062	0.034*
C11	0.9934(2)	0.19450(7)	1.2393(2)	0.0393(4)
H11A	1.098266	0.171505	1.241779	0.047*
H11B	1.018418	0.206969	1.361875	0.047*
C12	0.9894(3)	0.24477(8)	1.1246(3)	0.0598(6)
H12A	1.106816	0.264043	1.173545	0.090*
H12B	0.969437	0.233276	1.003392	0.090*
H12C	0.889299	0.268870	1.123925	0.090*
C13	0.6656(2)	0.19201(7)	1.1943(2)	0.0404(4)
H13A	0.631753	0.219730	1.099760	0.048*
H13B	0.705705	0.211250	1.309170	0.048*
C14	0.4953(3)	0.15855(9)	1.1759(4)	0.0671(6)
H14A	0.398271	0.182457	1.183817	0.101*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H14B	0.452100	0.140092	1.061236	0.101*
H14C	0.526153	0.131601	1.270934	0.101*
O1	0.77666(16)	0.00389(4)	0.90308(14)	0.0381(3)
N1	0.85353(18)	0.08593(5)	0.50197(16)	0.0314(3)
H1A	0.862412	0.105078	0.414214	0.038*
N2	0.88059(16)	0.07973(5)	0.80085(15)	0.0277(3)
N3	0.82404(17)	0.15968(5)	1.18435(16)	0.0287(3)
S1	0.99591(7)	0.17323(2)	0.69561(6)	0.04860(19)

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with constrained isotropic displacement parameters.

Comment

Quinazoline derivatives have attracted much attention due to their wide variety of pharmacological activities [3–5]. Our previous work report the structures of several 2,3-dihydro-2-thioxoquinazolin-4(1*H*)-ones [6–8]. As part of our continuous work, the structure of the title compound 3-(2-diethylaminoethyl)-2,3-dihydro-2-thioxoquinazolin-4(1*H*)-one is presented in this contribution.

In the title structure (*cf.* the figure) the bond lengths are comparable with those found in our previous work [6–8], and others [9, 10]. In the crystal, classical intermolecular

N—H···N hydrogen bonds link the molecules into one dimensional chain along *c* axis.

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