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Crystal structure of methyl 2-methyl-4-(3-methoxyphenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate, $C_{19}H_{21}NO_4$

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Abstract

$C_{19}H_{21}NO_4$, monoclinic, $C2/c$ (no. 15), $a = 17.349(5)$ Å, $b = 7.354(2)$ Å, $c = 25.757(7)$ Å, $\beta = 97.637(5)^\circ$, $V = 3257.1(16)$ Å³, $Z = 8$, $R_{gt}(F) = 0.0444$, $wR_{ref}(F^2) = 0.1141$, $T = 296(2)$ K.

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The 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.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	$0.29 \times 0.21 \times 0.18$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	25.0° , 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7966, 2826, 0.038
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1900
$N(\text{param})_{\text{refined}}$:	218
Programs:	OLEX2 [1], SHELX [2], Bruker [3]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.07774(10)	0.7931(2)	0.46712(6)	0.0391(4)
H1	0.087324	0.901129	0.479047	0.047*
O1	0.18249(11)	0.0444(2)	0.29375(6)	0.0657(5)
O2	−0.04951(9)	0.4084(2)	0.33962(5)	0.0572(5)
O3	−0.06651(11)	0.7004(2)	0.32210(6)	0.0761(6)
O4	0.12282(9)	0.17061(17)	0.48917(5)	0.0478(4)
C1	0.11903(19)	−0.0762(3)	0.29398(10)	0.0742(8)
H1A	0.126778	−0.180920	0.273022	0.111*
H1B	0.115410	−0.113802	0.329272	0.111*
H1C	0.071828	−0.015838	0.279813	0.111*
C2	0.18162(14)	0.2019(3)	0.32165(7)	0.0440(6)
C3	0.12708(12)	0.2415(3)	0.35456(7)	0.0384(5)
H3	0.088294	0.157432	0.358683	0.046*
C4	0.12956(12)	0.4049(3)	0.38147(6)	0.0336(5)
C5	0.18748(13)	0.5273(3)	0.37482(8)	0.0465(6)
H5	0.189956	0.637810	0.392508	0.056*
C6	0.24173(14)	0.4869(3)	0.34214(9)	0.0565(6)
H6	0.280625	0.570529	0.337918	0.068*
C7	0.23904(14)	0.3250(4)	0.31578(8)	0.0536(6)
H7	0.276126	0.298677	0.293917	0.064*
C8	0.06953(11)	0.4483(2)	0.41766(6)	0.0324(5)
H8	0.035490	0.342185	0.418314	0.039*
C9	0.01943(12)	0.6091(2)	0.39781(6)	0.0330(5)
C10	−0.03583(13)	0.5835(3)	0.35019(8)	0.0432(5)
C11	−0.10141(17)	0.3681(4)	0.29265(9)	0.0805(9)
H11A	−0.107094	0.238777	0.288878	0.121*
H11B	−0.151279	0.421961	0.294865	0.121*
H11C	−0.080466	0.416813	0.262898	0.121*
C12	0.02589(11)	0.7715(3)	0.42161(7)	0.0352(5)
C13	−0.02040(13)	0.9386(3)	0.40650(8)	0.0458(6)
H13A	−0.003459	1.035082	0.430427	0.069*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H13B	−0.013044	0.973916	0.371616	0.069*
H13C	−0.074494	0.914326	0.407733	0.069*
C14	0.11406(12)	0.6500(2)	0.49364(7)	0.0338(5)
C15	0.10855(11)	0.4815(2)	0.47304(7)	0.0324(5)
C16	0.13686(12)	0.3273(3)	0.50428(7)	0.0348(5)
C17	0.18360(13)	0.3605(3)	0.55689(7)	0.0412(5)
H17A	0.225414	0.272197	0.562293	0.049*
H17B	0.150472	0.341671	0.583928	0.049*
C18	0.21792(13)	0.5492(3)	0.56270(8)	0.0466(6)
H18A	0.239698	0.569231	0.598919	0.056*
H18B	0.259648	0.559981	0.541286	0.056*
C19	0.15692(13)	0.6917(3)	0.54631(7)	0.0422(5)
H19A	0.120516	0.696713	0.571780	0.051*
H19B	0.181601	0.809804	0.545483	0.051*

Source of material

A mixture of 1,3-cyclohexanedione (10 mmol), 3-methoxybenzaldehyde (10 mmol), 3-amino-2-butenic acid methyl ester (10 mmol) in ethanol (100 mL) was refluxed for 2–3 h and then cooled to room temperature. After filtering the precipitates, they were sequentially washed with ice-cooled water and ethanol and then dried under a vacuum.

Experimental details

H atoms bonded to C and N atoms were positioned geometrically and refined using a riding model, with C–H = 0.93–0.98 Å and N–H = 0.86 Å with $U_{iso}(H) = 1.2$ times $U_{eq}(C)$ and 1.2 times $U_{eq}(N)$.

Comment

The progress achieved in the synthesis of heterocyclic compounds with biological potential is due to improvement of the

methodological study of tested substances. It is known that many polyhydroquinoline derivatives have biological activity, with their antibacterial, antimycobacterial, anti cancer and cardiotoxic action being notable [4–6].

In the crystal structure of the title compound (Figure), the six-membered ring containing nitrogen atom is nearly planar and the adjacent annulated ring adopts a flattened chair conformation. The bond distances and angles of the title compound are all in their normal scopes and they are similar with those of a previously reported compound [7]. As there are many structures reported that are very similar to the title compound it doesn't matter to try to list all of them.

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