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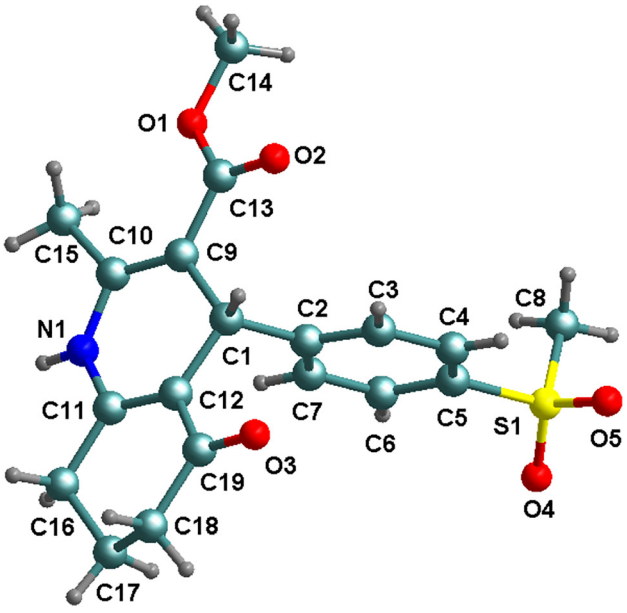
# The crystal structure of methyl 4-(4-(methylsulfonyl)phenyl)-2-methyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate, $C_{19}H_{21}NO_5S$

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**Abstract**

$C_{19}H_{21}NO_5S$, triclinic, $P\bar{1}$ (no. 2), $a$ = 8.428(2) Å, $b$ = 10.638(3) Å, $c$ = 11.177(3) Å, $\alpha$ = 63.125(4)°, $\beta$ = 77.819(4)°, $\gamma$ = 79.845(4)°, $V$ = 869.9(4) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0472, $wR_{ref}(F^2)$ = 0.1379, $T$ = 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.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colorless block |
| Size: | 0.26 × 0.21 × 0.17 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.22 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 25.2°, 99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 4,474, 3,098, 0.030 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2,490 |
| $N(param)_{refined}$: | 238 |
| Programs: | Bruker,[1] Olex2,[2] SHELX[3,4] |

## 1 Source of materials

All reagents were commercial and used directly without any purification. The targeted compound was synthesized via a concise one-pot method. A mixture containing 1 mmol 1,3-cyclohexanedione, 1 mmol methyl 3-aminocrotonate, and 1 mmol 4-methylsulphonyl benzaldehyde was thoroughly combined in a 50 mL solution of anhydrous ethanol. The mixture was heated to a temperature of 333 K and maintained at this level for 6 h. Upon completion of the reaction, the mixture was allowed to cool to room temperature, at which point the resulting precipitate was collected. The precipitate was recrystallized in 95 % ethanol, yielding 58.4 % (based on 4-methylsulphonyl benzaldehyde). The colorless block crystals were isolated.

## 2 Experimental details

The structure was solved by Direct Methods with the SHELXTL-2018 program. All H-atoms from C and atoms were positioned with idealized geometry and refined isotropically ($U_{iso}$(H) = 1.2 $U_{eq}$(C) or $U_{eq}$(N)) using a riding model.

## 3 Comment

To date, the single-crystal structures of 4-phenyl-2-methyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate[5]

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5943 (3) | 0.3812 (2) | 0.2334 (2) | 0.0349 (5) |
| H1 | 0.492167 | 0.433531 | 0.252907 | 0.042* |
| C2 | 0.6903 (3) | 0.3345 (2) | 0.3491 (2) | 0.0336 (5) |
| C3 | 0.6277 (3) | 0.3638 (3) | 0.4591 (2) | 0.0406 (5) |
| H3 | 0.524623 | 0.412030 | 0.462298 | 0.049* |
| C4 | 0.7142 (3) | 0.3232 (3) | 0.5644 (2) | 0.0421 (6) |
| H4 | 0.670848 | 0.343842 | 0.637869 | 0.051* |
| C5 | 0.8661 (3) | 0.2514 (2) | 0.5587 (2) | 0.0358 (5) |
| C6 | 0.9305 (3) | 0.2179 (3) | 0.4514 (2) | 0.0412 (5) |
| H6 | 1.032602 | 0.167977 | 0.449204 | 0.049* |
| C7 | 0.8413 (3) | 0.2594 (3) | 0.3482 (2) | 0.0400 (5) |
| H7 | 0.883629 | 0.236440 | 0.275926 | 0.048* |
| C8 | 1.1271 (3) | 0.3195 (3) | 0.6247 (3) | 0.0536 (7) |
| H8A | 1.198781 | 0.294517 | 0.690007 | 0.080* |
| H8B | 1.074803 | 0.413113 | 0.604913 | 0.080* |
| H8C | 1.188825 | 0.317072 | 0.543038 | 0.080* |
| C9 | 0.6863 (3) | 0.4797 (2) | 0.0996 (2) | 0.0360 (5) |
| C10 | 0.7498 (3) | 0.4367 (3) | 0.0009 (2) | 0.0389 (5) |
| C11 | 0.6251 (3) | 0.2185 (2) | 0.1245 (2) | 0.0377 (5) |
| C12 | 0.5522 (2) | 0.2549 (2) | 0.2244 (2) | 0.0351 (5) |
| C13 | 0.6988 (3) | 0.6171 (3) | 0.0925 (2) | 0.0431 (6) |
| C14 | 0.8341 (4) | 0.8255 (3) | −0.0166 (3) | 0.0639 (8) |
| H14A | 0.906654 | 0.874566 | −0.097903 | 0.096* |
| H14B | 0.881599 | 0.808213 | 0.060987 | 0.096* |
| H14C | 0.732024 | 0.882371 | −0.016722 | 0.096* |
| C15 | 0.8463 (3) | 0.5190 (3) | −0.1336 (2) | 0.0516 (6) |
| H15A | 0.953059 | 0.525964 | −0.121040 | 0.077* |
| H15B | 0.792093 | 0.612155 | −0.175583 | 0.077* |
| H15C | 0.855636 | 0.471622 | −0.190667 | 0.077* |
| C16 | 0.6005 (3) | 0.0867 (3) | 0.1183 (3) | 0.0484 (6) |
| H16A | 0.704216 | 0.046578 | 0.087225 | 0.058* |
| H16B | 0.527591 | 0.109238 | 0.053425 | 0.058* |
| C17 | 0.5299 (4) | −0.0209 (3) | 0.2551 (3) | 0.0586 (7) |
| H17A | 0.493847 | −0.096129 | 0.243887 | 0.070* |
| H17B | 0.614104 | −0.062287 | 0.312848 | 0.070* |
| C18 | 0.3902 (3) | 0.0428 (3) | 0.3220 (3) | 0.0560 (7) |
| H18A | 0.358331 | −0.027069 | 0.413737 | 0.067* |
| H18B | 0.298355 | 0.067100 | 0.273390 | 0.067* |
| C19 | 0.4274 (3) | 0.1728 (3) | 0.3274 (2) | 0.0408 (5) |
| N1 | 0.7275 (2) | 0.3049 (2) | 0.01943 (19) | 0.0425 (5) |
| H1A | 0.781076 | 0.274881 | −0.038597 | 0.051* |
| O1 | 0.8074 (2) | 0.6945 (2) | −0.01074 (19) | 0.0596 (5) |
| O2 | 0.6245 (2) | 0.6584 (2) | 0.1738 (2) | 0.0631 (5) |
| O3 | 0.3511 (2) | 0.2105 (2) | 0.41209 (18) | 0.0578 (5) |
| O4 | 1.0599 (2) | 0.0617 (2) | 0.71842 (19) | 0.0590 (5) |
| O5 | 0.8746 (2) | 0.2186 (2) | 0.80022 (18) | 0.0638 (6) |
| S1 | 0.97971 (7) | 0.19934 (7) | 0.69068 (5) | 0.0433 (2) |

and some 4-(mono- or multi-substituted-phenyl)-2-methyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate have been reported elsewhere, such as methyl 2-methyl-4-(4-nitrophenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate,[6] methyl 4-(3-bromo-4- fluorophenyl)-2-methyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline- 3-carboxylate,[7] ethyl 2-methyl-5-oxo-4-(2,3,4-trimethoxyphenyl)-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate,[8] etc.[9–17]

As shown in the figure, the asymmetric unit is made of a one molecule of the title compound, methyl 4-(4-(methylsulfonyl)phenyl)-2-methyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate. Notably, the phenyl group is coplanar and the S atom is in tetrahedral configuration. Neighbouring ketone ring adopts a flattened chair conformation. Intermolecularly, an infinitely supramolecular chain facilitated by a network of hydrogen bonds involving the N1···H1A···O5 interaction is found. All bond lengths and angles within this structure align closely with those reported for analogous compounds.[5–17]

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

**Author contribution:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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