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1-Cyclopropyl-6-fluoro-7-(4-formylpiperazin-1-yl)-4-oxo-1,4-dihydroquinoline-3-carboxylic acid. Corrigendum

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.140
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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The crystal structure of the title compound, $C_{18}H_{18}FN_3O_4$, was published [Li *et al.* (2005). *Acta Cryst.* E**61**, o2235–o2236] with an error in the chemical formula and without location of the carboxyl H atom. This has now been corrected. The missing H atom was located and refined. This H atom is involved in an intramolecular O—H···O hydrogen bond with the carbonyl O atom.

Experimental

Crystal data

$C_{18}H_{18}FN_3O_4$
M_r = 359.35
Triclinic, $P\overline{1}$
a = 8.414 (2) Å
b = 9.513 (2) Å
c = 10.497 (2) Å
α = 102.57 (3)°
β = 96.58 (3)°
γ = 97.08 (3)°
V = 805.1 (3) Å^3
Z = 2
D_x = 1.482 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–13°
μ = 0.11 mm^{-1}
T = 293 (2) K
Block, yellow
0.48 × 0.21 × 0.19 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*XCAD4*; Harms & Wocadlo, 1995)
T_{min} = 0.947, T_{max} = 0.979
3379 measured reflections
3154 independent reflections
1822 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.0°
$h = 0 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.140
S = 1.01
3154 reflections
238 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.035P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.90 (1)	1.69 (2)	2.514 (3)	151 (3)

References

Harms, K. & Wocadlo, S. (1995) *XCAD4*. University of Marburg, Germany.
Li, X.-W., Zhi, F., Shen, J.-H. & Hu, Y.-Q. (2005). *Acta Cryst.* E**61**, o2235–o2236.