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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.

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Acta Cryst. (2005). E**61**, e3 [https://doi.org/10.1107/S1600536805024426]

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$M_r = 359.35$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.414$ (2) Å
$b = 9.513$ (2) Å
$c = 10.497$ (2) Å
$\alpha = 102.57$ (3)°
$\beta = 96.58$ (3)°
$\gamma = 97.08$ (3)°
$V = 805.1$ (3) Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.482$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–13°
$\mu = 0.11$ mm^{-1}
$T = 293$ K
Block, yellow
0.48 × 0.21 × 0.19 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ 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 $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
$h = 0 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$
3 standard reflections every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.140$
$S = 1.01$
3154 reflections
238 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
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}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.52063 (18)	0.74819 (15)	−0.07309 (14)	0.0470 (4)
O1	0.7511 (3)	1.3189 (2)	0.4184 (2)	0.0826 (8)
O2	0.0708 (2)	0.32798 (18)	−0.24166 (17)	0.0451 (5)
O3	−0.1250 (3)	0.1022 (2)	−0.25234 (19)	0.0545 (5)
O4	−0.1734 (2)	0.0351 (2)	−0.06989 (19)	0.0544 (5)
N1	0.7420 (3)	1.0744 (2)	0.36587 (19)	0.0403 (5)
N2	0.5558 (2)	0.8162 (2)	0.20153 (19)	0.0362 (5)
N3	0.1515 (2)	0.38818 (19)	0.16083 (18)	0.0316 (5)
C1	0.7561 (4)	1.2033 (3)	0.4492 (3)	0.0548 (8)
H1A	0.7711	1.2056	0.5389	0.066*
C2	0.7396 (3)	0.9372 (3)	0.4054 (2)	0.0435 (7)
H2B	0.7486	0.9556	0.5008	0.052*
H2C	0.8322	0.8929	0.3790	0.052*
C3	0.5846 (3)	0.8319 (3)	0.3435 (2)	0.0440 (7)
H3A	0.5932	0.7375	0.3623	0.053*
H3B	0.4937	0.8678	0.3822	0.053*
C4	0.5543 (3)	0.9592 (3)	0.1686 (3)	0.0491 (7)
H4A	0.4662	1.0040	0.2039	0.059*
H4B	0.5366	0.9459	0.0735	0.059*
C5	0.7127 (3)	1.0574 (3)	0.2252 (2)	0.0458 (7)
H5A	0.8001	1.0157	0.1856	0.055*
H5B	0.7093	1.1519	0.2051	0.055*
C6	0.4412 (3)	0.6999 (2)	0.1267 (2)	0.0329 (6)
C7	0.4207 (3)	0.6684 (2)	−0.0128 (2)	0.0341 (6)
C8	0.3098 (3)	0.5589 (2)	−0.0912 (2)	0.0342 (6)
H8A	0.2966	0.5468	−0.1823	0.041*
C9	0.2149 (3)	0.4638 (2)	−0.0344 (2)	0.0318 (6)
C10	0.0981 (3)	0.3454 (2)	−0.1176 (2)	0.0335 (6)
C11	0.0169 (3)	0.2494 (2)	−0.0500 (2)	0.0343 (6)
C12	−0.1022 (3)	0.1194 (3)	−0.1222 (3)	0.0391 (6)
C13	0.0465 (3)	0.2758 (2)	0.0842 (2)	0.0340 (6)
H13A	−0.0094	0.2120	0.1251	0.041*
C14	0.2387 (3)	0.4863 (2)	0.1032 (2)	0.0298 (5)
C15	0.3470 (3)	0.6054 (2)	0.1819 (2)	0.0328 (6)
H15A	0.3561	0.6216	0.2732	0.039*

C16	0.1684 (3)	0.4125 (3)	0.3041 (2)	0.0364 (6)
H16A	0.1203	0.4948	0.3491	0.044*
C17	0.1618 (4)	0.2866 (3)	0.3656 (3)	0.0519 (8)
H17A	0.1490	0.1901	0.3079	0.062*
H17B	0.1088	0.2922	0.4435	0.062*
C18	0.3182 (3)	0.3848 (3)	0.3778 (3)	0.0487 (7)
H18A	0.3599	0.4500	0.4631	0.058*
H18B	0.4001	0.3479	0.3274	0.058*
H3	−0.066 (3)	0.174 (3)	−0.277 (3)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0499 (10)	0.0444 (9)	0.0495 (9)	−0.0030 (7)	0.0129 (7)	0.0197 (7)
O1	0.110 (2)	0.0391 (12)	0.0880 (18)	0.0120 (13)	0.0026 (15)	−0.0020 (11)
O2	0.0506 (12)	0.0433 (10)	0.0369 (10)	0.0042 (9)	−0.0016 (9)	0.0053 (8)
O3	0.0563 (13)	0.0474 (12)	0.0469 (12)	−0.0068 (10)	−0.0070 (10)	−0.0012 (9)
O4	0.0480 (12)	0.0434 (11)	0.0616 (13)	−0.0125 (9)	−0.0044 (10)	0.0075 (10)
N1	0.0481 (14)	0.0320 (11)	0.0355 (12)	−0.0028 (10)	0.0015 (10)	0.0041 (9)
N2	0.0397 (13)	0.0290 (10)	0.0375 (12)	−0.0045 (9)	−0.0032 (9)	0.0128 (9)
N3	0.0324 (12)	0.0250 (10)	0.0346 (11)	−0.0003 (8)	0.0035 (9)	0.0046 (8)
C1	0.0558 (19)	0.0458 (17)	0.0520 (18)	−0.0011 (14)	0.0053 (15)	−0.0054 (14)
C2	0.0512 (17)	0.0388 (14)	0.0351 (14)	−0.0024 (13)	−0.0029 (12)	0.0074 (11)
C3	0.0490 (17)	0.0368 (14)	0.0435 (16)	−0.0042 (12)	0.0013 (13)	0.0127 (11)
C4	0.0552 (18)	0.0328 (14)	0.0544 (17)	−0.0023 (13)	−0.0128 (14)	0.0157 (12)
C5	0.0565 (18)	0.0326 (14)	0.0466 (16)	−0.0039 (13)	0.0041 (13)	0.0135 (12)
C6	0.0328 (14)	0.0262 (12)	0.0392 (14)	0.0052 (10)	0.0005 (11)	0.0085 (10)
C7	0.0351 (14)	0.0297 (12)	0.0403 (14)	0.0046 (11)	0.0058 (11)	0.0144 (11)
C8	0.0423 (15)	0.0316 (12)	0.0296 (13)	0.0092 (11)	0.0043 (11)	0.0074 (10)
C9	0.0334 (14)	0.0258 (12)	0.0359 (13)	0.0069 (10)	0.0030 (11)	0.0064 (10)
C10	0.0322 (14)	0.0293 (12)	0.0380 (15)	0.0095 (10)	0.0022 (11)	0.0049 (10)
C11	0.0296 (13)	0.0286 (12)	0.0412 (15)	0.0056 (10)	0.0005 (11)	0.0023 (11)
C12	0.0335 (15)	0.0319 (13)	0.0469 (16)	0.0051 (11)	−0.0017 (12)	0.0024 (11)
C13	0.0312 (14)	0.0258 (12)	0.0435 (15)	−0.0003 (10)	0.0040 (11)	0.0082 (10)
C14	0.0308 (13)	0.0233 (11)	0.0354 (13)	0.0056 (10)	0.0061 (10)	0.0057 (9)
C15	0.0370 (14)	0.0275 (12)	0.0330 (13)	0.0036 (10)	0.0039 (11)	0.0065 (10)
C16	0.0401 (15)	0.0322 (13)	0.0346 (13)	−0.0007 (11)	0.0058 (11)	0.0064 (10)
C17	0.0624 (19)	0.0425 (15)	0.0472 (16)	−0.0100 (14)	−0.0013 (14)	0.0176 (13)
C18	0.0450 (17)	0.0559 (17)	0.0414 (15)	0.0025 (14)	−0.0017 (13)	0.0102 (13)

Geometric parameters (Å, º)

F1—C7	1.363 (3)	C5—H5A	0.97
O1—C1	1.216 (3)	C5—H5B	0.97
O2—C10	1.267 (3)	C6—C15	1.388 (3)
O3—C12	1.328 (3)	C6—C7	1.415 (3)
O3—H3	0.900 (10)	C7—C8	1.359 (3)
O4—C12	1.206 (3)	C8—C9	1.406 (3)

N1—C1	1.326 (3)	C8—H8A	0.93
N1—C5	1.439 (3)	C9—C14	1.400 (3)
N1—C2	1.452 (3)	C9—C10	1.449 (3)
N2—C6	1.398 (3)	C10—C11	1.429 (3)
N2—C3	1.454 (3)	C11—C13	1.363 (3)
N2—C4	1.475 (3)	C11—C12	1.490 (3)
N3—C13	1.341 (3)	C13—H13A	0.93
N3—C14	1.398 (3)	C14—C15	1.401 (3)
N3—C16	1.459 (3)	C15—H15A	0.93
C1—H1A	0.93	C16—C17	1.477 (3)
C2—C3	1.525 (3)	C16—C18	1.485 (4)
C2—H2B	0.97	C16—H16A	0.98
C2—H2C	0.97	C17—C18	1.492 (4)
C3—H3A	0.97	C17—H17A	0.97
C3—H3B	0.97	C17—H17B	0.97
C4—C5	1.508 (4)	C18—H18A	0.97
C4—H4A	0.97	C18—H18B	0.97
C4—H4B	0.97		

C12—O3—H3	112 (2)	C7—C8—C9	119.9 (2)
C1—N1—C5	122.0 (2)	C7—C8—H8A	120.1
C1—N1—C2	124.3 (2)	C9—C8—H8A	120.1
C5—N1—C2	113.53 (19)	C14—C9—C8	118.1 (2)
C6—N2—C3	117.8 (2)	C14—C9—C10	121.8 (2)
C6—N2—C4	117.43 (19)	C8—C9—C10	120.2 (2)
C3—N2—C4	111.2 (2)	O2—C10—C11	122.5 (2)
C13—N3—C14	119.8 (2)	O2—C10—C9	122.2 (2)
C13—N3—C16	120.2 (2)	C11—C10—C9	115.4 (2)
C14—N3—C16	119.98 (18)	C13—C11—C10	120.2 (2)
O1—C1—N1	125.5 (3)	C13—C11—C12	118.1 (2)
O1—C1—H1A	117.2	C10—C11—C12	121.7 (2)
N1—C1—H1A	117.2	O4—C12—O3	121.4 (2)
N1—C2—C3	111.7 (2)	O4—C12—C11	124.3 (2)
N1—C2—H2B	109.3	O3—C12—C11	114.3 (2)
C3—C2—H2B	109.3	N3—C13—C11	124.1 (2)
N1—C2—H2C	109.3	N3—C13—H13A	118.0
C3—C2—H2C	109.3	C11—C13—H13A	118.0
H2B—C2—H2C	107.9	N3—C14—C9	118.8 (2)
N2—C3—C2	111.0 (2)	N3—C14—C15	120.5 (2)
N2—C3—H3A	109.4	C9—C14—C15	120.7 (2)
C2—C3—H3A	109.4	C6—C15—C14	121.6 (2)
N2—C3—H3B	109.4	C6—C15—H15A	119.2
C2—C3—H3B	109.4	C14—C15—H15A	119.2
H3A—C3—H3B	108.0	N3—C16—C17	119.7 (2)
N2—C4—C5	110.4 (2)	N3—C16—C18	119.6 (2)
N2—C4—H4A	109.6	C17—C16—C18	60.49 (18)
C5—C4—H4A	109.6	N3—C16—H16A	115.4
N2—C4—H4B	109.6	C17—C16—H16A	115.4

C5—C4—H4B	109.6	C18—C16—H16A	115.4
H4A—C4—H4B	108.1	C16—C17—C18	60.02 (17)
N1—C5—C4	109.9 (2)	C16—C17—H17A	117.8
N1—C5—H5A	109.7	C18—C17—H17A	117.8
C4—C5—H5A	109.7	C16—C17—H17B	117.8
N1—C5—H5B	109.7	C18—C17—H17B	117.8
C4—C5—H5B	109.7	H17A—C17—H17B	114.9
H5A—C5—H5B	108.2	C16—C18—C17	59.49 (17)
C15—C6—N2	123.4 (2)	C16—C18—H18A	117.8
C15—C6—C7	116.0 (2)	C17—C18—H18A	117.8
N2—C6—C7	120.6 (2)	C16—C18—H18B	117.8
C8—C7—F1	117.5 (2)	C17—C18—H18B	117.8
C8—C7—C6	123.6 (2)	H18A—C18—H18B	115.0
F1—C7—C6	118.9 (2)		

Hydrogen-bond geometry (Å, º)

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)