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2-(2-Thienyl)-4,5-dihydro-1*H*-imidazole. Corrigendum

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Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.027; wR factor = 0.080; data-to-parameter ratio = 32.3.

Consideration of a previous unrecognized twinning of the original investigated crystal of the title compound [Kia *et al.* (2009). *Acta Cryst.* E**65**, o301] led to improved reliability factors and to a slightly higher precision for all geometric parameters. The crystal under investigation was twinned by pseudo-merohedry with [100, 0$\bar{1}$0, 00$\bar{1}$] as the twin matrix and a refined twin domain fraction of 0.9610 (5):0.0390 (5). The results of the new crystal structure refinement are given here.

Experimental

Crystal data

$C_7H_8N_2S$
M_r = 152.21
Monoclinic, $P2_1/c$
a = 6.1321 (2) Å
b = 11.5663 (3) Å
c = 10.0098 (3) Å
β = 90.154 (1)°
V = 709.95 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 100 K
0.54 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.825, T_{max} = 0.922
28316 measured reflections
3100 independent reflections
3040 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.080
S = 1.15
3100 reflections
96 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.857 (16)	2.130 (16)	2.9803 (10)	171.5 (16)
C3—H3A···N2^{i}	0.95	2.59	3.4815 (11)	156

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2233).

References

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc. Madison, Wisconsin, USA.
Kia, R., Fun, H.-K. & Kargar, H. (2009). *Acta Cryst.* E**65**, o301.
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