Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Butyl-4-chloro-1-(4-nitrobenzyl)-1*H*-imidazole-5-carboxaldehyde

Santhosh L. Gaonkar,[a] Hemmige S. Yathirajan,[a] Basavegowda Nagaraj,[a] Rajenahally S. Narasegowda[a] and Daniel E. Lynch[b]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, and [b]School of Science and the Environment, Coventry University, Coventry CV1 5FB, England

Correspondence e-mail: apx106@coventry.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.057
wR factor = 0.139
Data-to-parameter ratio = 14.4

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

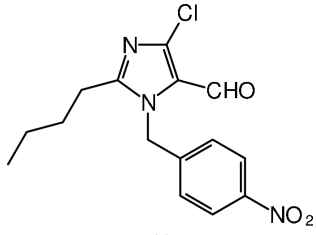
© 2004 International Union of Crystallography
Printed in Great Britain – all rights reserved

Received 25 November 2004
Accepted 26 November 2004
Online 30 November 2004

The asymmetric unit of the title compound, $C_{15}H_{16}ClN_3O_3$, comprises two molecules that are each twisted about the benzyl C atom. The second and fourth C atoms of the butyl chain of one molecule are disordered (0.75:0.25 and 0.5:0.5, respectively). The dihedral angles between the imidazole and benzene rings are 76.46 (9) and 76.3 (1)°.

Comment

Imidazole derivatives are reported to be biologically active molecules, and both imidazoles and benzimidazoles are components of larger molecules used in pharmaceuticals, agrochemicals, dyestuffs and high-temperature polymer products (Rasmussen, 1999; Ambalvanan *et al.*, 2003). With this in mind, the title compound, (I), was prepared in a series of syntheses to produce new imidazole derivatives. The Cambridge Structural Database (Version of April 2004; Allen, 2002) reveals that there are currently 42 known structures containing a 3-benzylimidazole moiety, but not yet the title compound.



(I)

The asymmetric unit of (I) comprises two molecules, *A* and *B*, that are each twisted about the benzyl C atom (Fig. 1). The butyl chain of molecule *B* is disordered, with the second and fourth C atoms in the chain occupying two sites each. The second C atom is unequally disordered, with occupancies of 0.75:0.25 for C22*B* and C22*C*, respectively, whereas the fourth C atom is equally disordered across two sites (C24*B* and C24*C*). In early refinements, the third C atom (C23*B*) was split (similar to C22*B*/*C*), but this proved not to be a viable option, with the lesser refining unsatisfactorily. Stable refinement was achieved with C23*B* being treated as a whole atom, even though it displays larger displacement ellipsoids compared with neighbouring atoms. The dihedral angles between the imidazole and benzene rings are 76.46 (9) and 76.3 (1)° for molecules *A* and *B*, respectively.

Experimental

The title compound was prepared by stirring an equimolar mixture of 2-butyl-5-chloro-3*H*-imidazole-4-carboxaldehyde, 4-nitrobenzyl-

bromide and K_2CO_3 in dimethylformamide at room temperature for 6 h. The product was filtered and recrystallized from ethanol to yield colourless plates.

Crystal data

$C_{15}H_{16}ClN_3O_3$
M_r = 321.76
Triclinic, $P\overline{1}$
a = 8.3007 (5) Å
b = 12.2295 (6) Å
c = 16.5605 (10) Å
α = 103.420 (4)°
β = 95.561 (3)°
γ = 106.758 (3)°
V = 1541.35 (15) Å^3
Z = 4
D_x = 1.387 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6811 reflections
θ = 2.9–27.5°
μ = 0.26 mm^{-1}
T = 120 (2) K
Plate, colourless
0.36 × 0.30 × 0.04 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997*b*)
T_{min} = 0.911, T_{max} = 0.990
30 632 measured reflections
6038 independent reflections
3622 reflections with $I > 2\sigma(I)$
R_{int} = 0.098
θ_{max} = 26.0°
$h = -10 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.139
S = 1.04
6038 reflections
418 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

All H atoms were included in the refinement at calculated positions in the riding-model approximation, with C—H distances of 0.95 (aromatic H atoms and CHO H atoms), 0.98 (CH_3 H atoms) and 0.99 Å (CH_2 H atoms). The isotropic displacement parameters were set equal to 1.25U_{eq} of the carrier atom. A high R_{int} was the result of weak high-angle data.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *PLATON*97 (Spek, 2003); software used to prepare material for publication: *SHELXL*97.

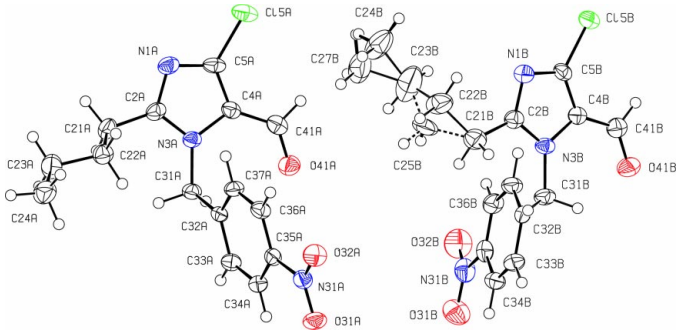


Figure 1
The molecular configurations and atom-numbering schemes for the two independent molecules, *A* and *B*, of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

The authors thank the EPSRC National Crystallography Service (Southampton, England) and acknowledge the use of the EPSRC's Chemical Database Service at Daresbury.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Ambalvanan, P., Palani, K., Ponnuswamy, M. N., Thirumuruhan, R. A., Yathirajan, H. S., Prabhuswamy, B., Raju, C. R., Nagaraja, P. & Mohana, K. N. (2003). *Mol. Cryst. Liq. Cryst.* **393**, 75–82.
Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Rasmussen, P. G. (1999). *J. Chem. Educ.* **76**, 1345.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.