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1-(2-Methyl-2,3-dihydroindol-1-ylmethyl)-1*H*-benzotriazole

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.006 Å
R factor = 0.060
wR factor = 0.146
Data-to-parameter ratio = 8.5

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

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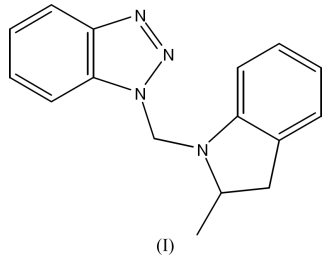
There are no short inter- or intramolecular contacts in the structure of the title compound, $C_{16}H_{16}N_4$, which contains two molecules in the asymmetric unit.

Comment

The title compound, (I), was prepared as a precursor in the synthesis of new pyrrolo–quinoline derivatives, target compounds with potential biological and pharmacological activity (Abonia *et al.*, 2001).



(I)

There are two molecules in the asymmetric unit and these are of opposite hand; nevertheless, a search for possible additional symmetry using the *ADDSYM* routine of *PLATON* (Spek, 2001) indicated that no additional symmetry was present. In addition repeated attempts to solve the structure in the possible centrosymmetric space groups were consistently unsuccessful.

There are no short inter- or intramolecular contacts in the structure.

Examination of the structure with *PLATON* (Spek, 2001) showed that there were no solvent-accessible voids in the crystal lattice.

Experimental

A mixture of 2-methyl-2,3-dihydro-1*H*-indoline (8.4 mmol), benzotriazole (8.4 mmol) and formaldehyde (37% *w*/*w* solution, 12.6 mmol) in 10 ml of ethyl ether, was stirred at room temperature for 30 min. and the resulting precipitate was filtered and recrystallized from ethanol. White crystals (suitable for X-ray diffraction), 86% yield; m.p. 343 K. Analysis calculated for $C_{16}H_{16}N_4$ (264.12): C, 72.70; H, 6.10; N, 21.20%; found: C, 72.73; H, 6.08; N, 21.17%.

Crystal data

$C_{16}H_{16}N_4$
M_r = 264.33
Monoclinic, $P2_1$
a = 7.5660 (3) Å
b = 17.7842 (8) Å
c = 10.2284 (4) Å
β = 104.689 (3)°
V = 1331.30 (10) Å^3
Z = 4
D_x = 1.319 Mg m^{-3}
Mo Kα radiation
Cell parameters from 3086 reflections
θ = 3.0–27.5°
μ = 0.08 mm^{-1}
T = 120 (1) K
Block, colourless
0.15 × 0.10 × 0.03 mm

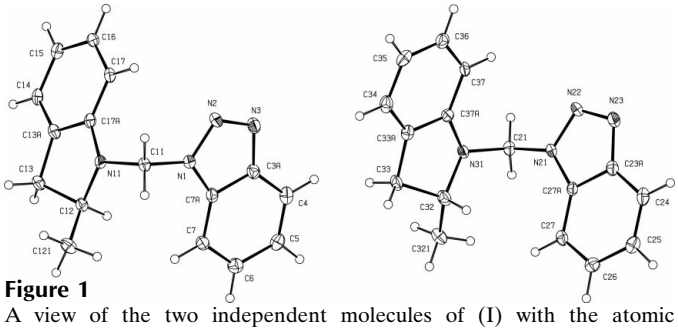


Figure 1
A view of the two independent molecules of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Data collection

Kappa–CCD diffractometer	3086 independent reflections
φ scans, and ω scans with κ offsets	2083 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)	$R_{int} = 0.074$
	$\theta_{max} = 27.5^\circ$
$T_{min} = 0.988$, $T_{max} = 0.998$	$h = -9 \rightarrow 9$
10 746 measured reflections	$k = -20 \rightarrow 23$
	$l = -11 \rightarrow 13$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.0773P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.146$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.98$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
3086 reflections	$\Delta\rho_{min} = -0.37$ e Å^{-3}
363 parameters	

H atoms were treated as riding atoms with C—H = 0.90–0.98 Å, N—H = 0.90 Å and O—H = 0.82 Å. The absolute configuration was not determined. Friedel pairs were merged.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976) and *PLATON* (Spek, 2001); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, using a Nonius KappaCCD diffractometer. The authors thank the staff for all their help and advice. JNL thanks NCR Self Service Dundee for grants which have provided computing facilities for this work.

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