Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Morpholinoaniline

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Key indicators

Single-crystal X-ray study
T = 90 K
Mean σ(C–C) = 0.002 Å
R factor = 0.047
wR factor = 0.132
Data-to-parameter ratio = 17.9

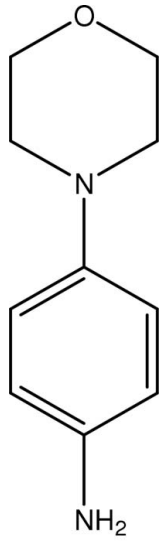
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 September 2006
Accepted 30 September 2006

The asymmetric unit of the title compound, $C_{10}H_{14}N_2O$, contains two molecules having similar conformation. The molecules are connected *via* N—H···O hydrogen bonds, forming a three-dimensional network in the crystal structure.

Comment

The title compound, (I), used as a starting material to synthesize reversine (Chen *et al.*, 2004), was partially recovered as single crystals in an attempt to purify the target molecule by recrystallization. Although it is commercially available, its structure, as far as we know, has not been reported. The asymmetric unit of (I) (Fig. 1) contains two molecules which have similar conformation. As expected, the morphiline rings take a chair form. The molecules are connected *via* N—H···O hydrogen bonds (Table 1), forming a three-dimensional network in the crystal structure.



(I)

Experimental

2-Fluoro-6-cyclohexylaminopurine (235 mg, 0.5 mmol) was dissolved in ethanol (1 ml), followed by addition of 4-morpholinoaniline (178 mg, 1.0 mmol). The mixture was heated to 348 K in a sealed tube with vigorous stirring for 24 h. The solvent was then removed under reduced pressure and the residue was dissolved in EtOAc by heating. Crystals of (I), which is one of the starting materials (4-morpholinoaniline), were obtained as orange–brown blocks the next day. Crystals of the target molecule (reversine) were not obtained.

Crystal data

$C_{10}H_{14}N_2O$
$M_r = 178.23$
Triclinic, $P\overline{1}$
$a = 9.7252$ (2) Å
$b = 10.4534$ (2) Å
$c = 10.6002$ (3) Å
$\alpha = 100.4721$ (9)°
$\beta = 97.0821$ (9)°
$\gamma = 117.4777$ (10)°
$V = 913.25$ (4) Å^3
$Z = 4$
$D_x = 1.296$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 90.0$ (2) K
Block, orange–brown
0.25 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: none
8318 measured reflections
4199 independent reflections
2903 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.132$
$S = 1.04$
4199 reflections
235 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2 + 0.0298P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ 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
N1A—H1NA···N1B^{i}	0.99	2.30	3.2728 (17)	168
N1A—H2NA···O1A^{ii}	1.01	2.27	3.2197 (15)	157
N1B—H1NB···O1B^{ii}	0.98	2.11	3.0513 (15)	160
N1B—H2NB···O1A^{ii}	1.01	2.14	3.1461 (16)	174

Symmetry codes: (i) $-x+2, -y, -z+2$; (ii) $x, y, z+1$.

N-bound H atoms were located in difference Fourier maps and their coordinates were fixed with $U_{iso}(H) = 1.5U_{eq}(N)$. Other H atoms were positioned geometrically and treated as riding with C—H = 0.95–0.99 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*–SMN (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97* and local procedures.

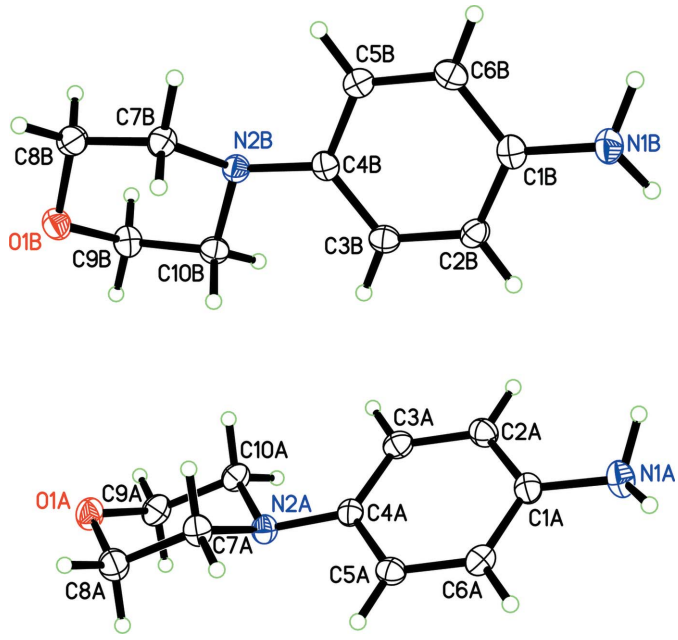


Figure 1
The asymmetric unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

SL thanks Dr Arthur Cammers for providing support and laboratory facilities.

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