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9-(Cyclohexylmethyl)-6-(dimethylamino)-9*H*-purine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.057
wR factor = 0.124
Data-to-parameter ratio = 15.2

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

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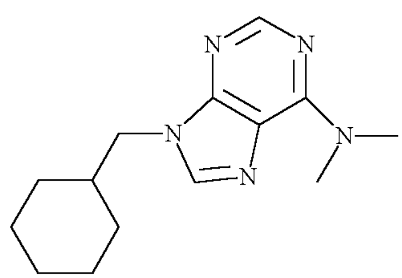
The purine fragment of the title compound, $C_{14}H_{21}N_5$, is planar and the dimethylamino group is almost coplanar with it. The cyclohexyl fragment (in a chair conformation) is disordered between two positions. C—H···N hydrogen bonds determine the crystal packing.

Comment

The title compound, (I), was synthesized as part of a series of potential anticonvulsants. Its activity against maximum electroshock-induced seizures was evaluated as moderate. An effective dose, ED_{50}, is 25 mg kg^{-1} for an ip admission in rats (Kelley *et al.*, 1988). The compound was also tested for an activity against apomorphine-induced aggresive behavior (Kelley *et al.*, 1997), but the results were negative.



(I)

Fig. 1 shows a perspective view of the molecule. The purine fragment is almost perfectly planar; the maximum deviation from the least-squares plane through the nine ring atoms is 0.025 (3) Å. The dihedral angle between this plane and the dimethylamino plane is small [3.2 (3)°] and indicates significant conjugation. The bond lengths and angles pattern is quite typical, including the large value of the N1—C2—N3 angle [129.9 (2)°; for 244 similar fragments in CSD (Allen & Kennard, 1993), the mean value is 129 (1)°].

The cyclohexyl fragment is disordered, and the site-occupation factors for two alternative positions (hereinafter referred to as *A* and *B*) are 0.841 (3) and 0.159 (3). In both positions, the cyclohexane ring adopts a chair conformation. This conformation is close to an ideal one for molecule *A*; the largest value of the asymmetry parameter (Duax & Norton, 1975) is 1.10°. View of the disordered fragments is shown in Fig. 2; the dihedral angle between least-squares planes of the 'seats' of both chairs is 64.3 (5)°.

The molecules are connected into infinite chains along the [010] direction by C—H···N hydrogen bonds. This interaction determines the crystal packing, and therefore can not be treated as an artifact. The linearity of this bond as well as short H···N and C···N distances allows us to classify this hydrogen

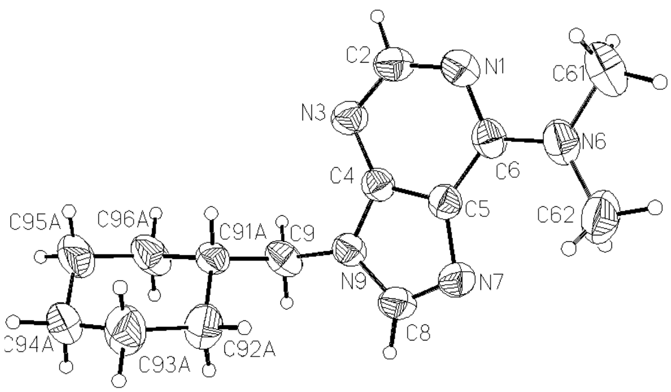


Figure 1
A perspective view of the molecule with the numbering scheme (Siemens, 1989). Displacement ellipsoids are drawn at the 33% probability level and H atoms are depicted as spheres of arbitrary radii. Only the molecule of higher occupancy is shown.

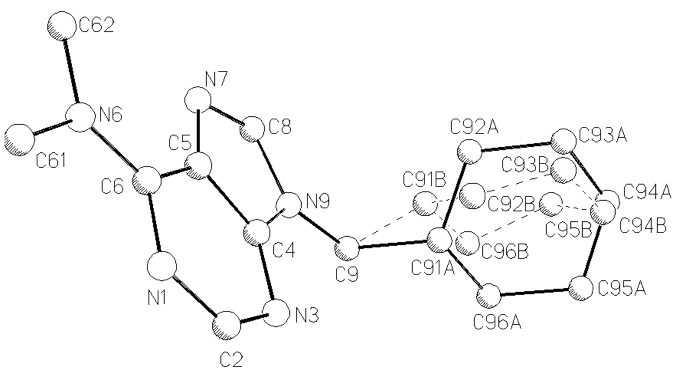


Figure 2
A comparison of disordered cyclohexyl fragments (Siemens, 1989). The bonds in the less occupied part are shown as dashed lines. H atoms have been omitted for clarity.

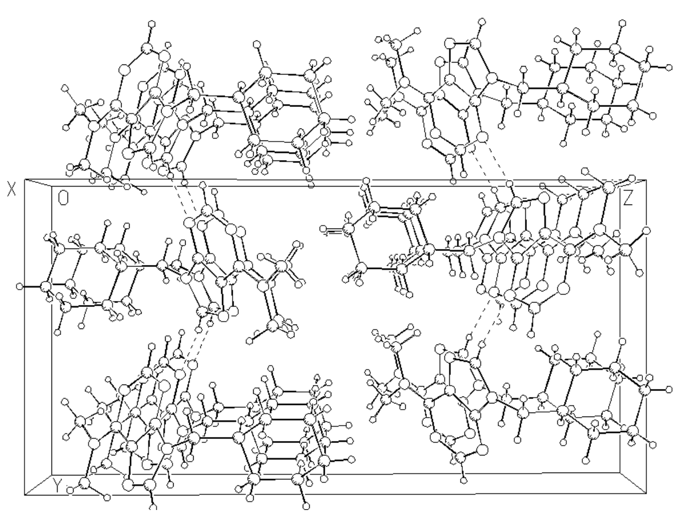


Figure 3
The crystal-packing scheme (Siemens, 1989). Hydrogen bonds are drawn as dashed lines and the view is approximately along the [001] direction.

bond as a relatively strong one (*cf*. Taylor & Kennard, 1982; Reddy *et al*., 1993; Kubicki, Borowiak, Suwiński & Wagner, 2001). Also, the results of charge–density studies of 1-phenyl-4-nitroimidazole suggest that the C—H···N hydrogen bond of similar geometry has topological features comparable with well defined C—H···O hydrogen bonds (Kubicki, Borowiak, Dutkiewicz *et al*., 2001).

There are three potential hydrogen-bond acceptors (N1, N3 and N7), but the in-plane access to N1 and N7 is partially hindered by the C61 and C62 methyl groups. In the crystal structure, there are alternate hydrophobic (dimethylamine and cyclohexylmethyl) and hydrophilic (purine) layers (Fig. 3).

Experimental

Colorless crystals of (I) were grown from ethanol by slow evaporation.

Crystal data

$C_{14}H_{21}N_5$	$D_x = 1.178$ Mg m^{-3}
$M_r = 259.36$	Cu $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
$a = 5.7702$ (5) Å	$\theta = 11$–$37°$
$b = 11.321$ (1) Å	$\mu = 0.59$ mm^{-1}
$c = 22.390$ (1) Å	$T = 293$ (2) K
$\beta = 91.47$ (1)°	Block, colorless
$V = 1462.1$ (2) Å^3	$0.25 \times 0.20 \times 0.10$ mm
$Z = 4$	

Data collection

CAD-4F four-circle diffractometer	$h = 0 \rightarrow 7$
$\omega/2\theta$ scans	$k = -14 \rightarrow 14$
6589 measured reflections	$l = -28 \rightarrow 28$
2992 independent reflections	2 standard reflections
2162 reflections with $I > 2\sigma(I)$	frequency: 33 min
$R_{int} = 0.043$	intensity decay: 3%
$\theta_{max} = 74.8°$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 0.5P]$
$R[F^2 > 2\sigma(F^2)] = 0.057$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.124$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
2992 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
197 parameters	Extinction correction: *SHELXL*97
H-atom parameters constrained	Extinction coefficient: 0.0173 (10)

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.326 (2)	C5—N7	1.394 (2)
N1—C6	1.351 (2)	C5—C6	1.416 (3)
C2—N3	1.323 (2)	C6—N6	1.348 (2)
N3—C4	1.345 (2)	N7—C8	1.300 (3)
C4—N9	1.370 (2)	C8—N9	1.359 (2)
C4—C5	1.382 (2)	N9—C9	1.458 (2)
C2—N1—C6	118.7 (2)	N7—C5—C6	134.1 (2)
N3—C2—N1	129.9 (2)	N6—C6—N1	117.3 (2)
C2—N3—C4	110.3 (2)	N6—C6—C5	125.1 (2)
N3—C4—N9	126.3 (2)	N1—C6—C5	117.6 (2)
N3—C4—C5	127.4 (2)	C8—N7—C5	104.0 (2)
N9—C4—C5	106.3 (2)	N7—C8—N9	114.4 (2)
C4—C5—N7	109.7 (2)	C8—N9—C4	105.6 (2)
C4—C5—C6	116.1 (2)		
C8—N9—C9—C91*B*	67.3 (6)	N9—C9—C91*A*—C92*A*	−66.4 (3)
C4—N9—C9—C91*B*	−112.0 (6)	N9—C9—C91*A*—C96*A*	170.6 (2)
C8—N9—C9—C91*A*	99.4 (2)	N9—C9—C91*B*—C92*B*	65 (1)
C4—N9—C9—C91*A*	−79.9 (2)	C91*A*—C9—C91*B*—C92*B*	−42.0 (8)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N3^{i}	0.93	2.45	3.369 (3)	171

Symmetry codes: (i) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$.

The sum of site-occupancy factors for the disordered fragment was constrained to unity. The C atoms in the less occupied cyclohexane ring were refined isotropically and the U_{iso} value of C94 was fixed; bond lengths and angles in this fragment were constrained to typical values.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *ENPROC* (Rettig, 1978); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *Stereochemical Workstation* (Siemens, 1989).

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