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N,*N*′-Bis(3,5-dimethyl-1*H*-pyrazol-1-ylmethyl)piperazine

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.100
Data-to-parameter ratio = 15.3

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

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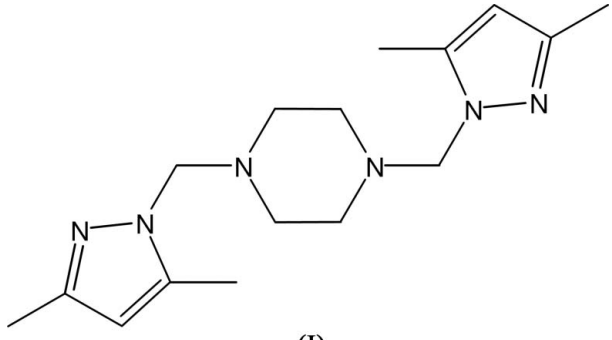
The molecule of the title compound, $C_{16}H_{26}N_6$, is located on a crystallographic centre of inversion; as a result, there is just one half-molecule in the asymmetric unit. The piperazine ring adopts an ideal chair conformation. The substituents at the piperazine N atoms are in equatorial positions.

Comment

A perspective view of the the title compound, (I), is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27 plus one update; *MOGUL* Version 1.1; Allen, 2002). The piperazine ring adopts an ideal chair conformation. The sum of the bond angles at the piperazine N atoms (328.48°) clearly shows the pyramidal geometry. The dimethylpyrazolylmethyl residues are attached to the piperazine N atoms in equatorial positions. There are no significant C—H···N or C—H···π contacts. The molecules in the crystal structure are held together by van der Waals interactions only.



(I)

Experimental

The title compound was prepared according to the procedure described by Ratilainen *et al.* (1999).

Crystal data

$C_{16}H_{26}N_6$
M_r = 302.43
Orthorhombic, *Pbca*
a = 9.6944 (9) Å
b = 12.1761 (11) Å
c = 13.7141 (12) Å
V = 1618.8 (3) Å^3
Z = 4
D_x = 1.241 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 14373 reflections
θ = 3.6–25.7°
μ = 0.08 mm^{-1}
T = 173 (2) K
Block, colourless
0.28 × 0.26 × 0.23 mm

Data collection

Stoe IPDS-II two-circle diffractometer	1319 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.044$
ω scans	$\theta_{max} = 25.8^\circ$
Absorption correction: none	$h = -11 \rightarrow 11$
16864 measured reflections	$k = -14 \rightarrow 14$
1560 independent reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.1979P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.035$	
$wR(F^2) = 0.100$	
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
1560 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
102 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N11—C13^{i}	1.4563 (17)	N11—C12	1.4601 (16)
C11—N11—C13^{i}	113.99 (10)	C13^{i}—N11—C12	110.19 (10)
C11—N11—C12	114.30 (10)		
C13^{i}—N11—C12—C13	58.69 (15)	C12^{i}—C13^{i}—N11—C12	−58.89 (14)
N11—C12—C13—N11^{i}	−58.61 (15)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

H atoms were located in a difference electron-density map, but they were positioned geometrically and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C)] using a riding model, with C—H = 0.95–0.99 Å. The methyl groups were allowed to rotate but not to tip.

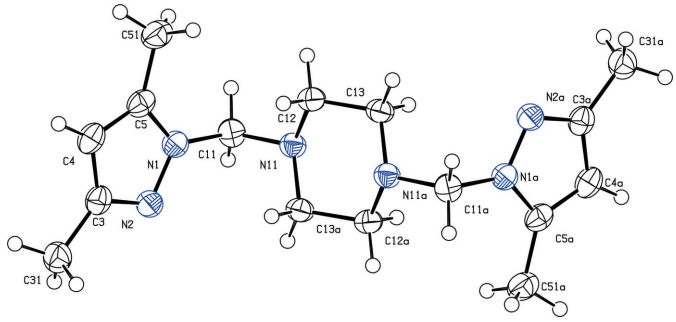


Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are drawn at the 50% probability level. Atoms labelled with the suffix a were generated by the symmetry code $(1 - x, 1 - y, 1 - z)$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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