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6-Chloro-2-methylthio-4-[(2-phenylethyl)amino]-pyrimidine

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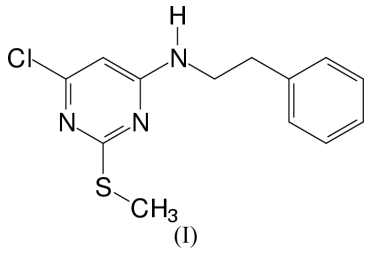
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.123
Data-to-parameter ratio = 18.6

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

The structure of the title compound, $C_{26}H_{28}Cl_2N_6S_2$, comprises two independent molecules that separately associate *via* N—H···N hydrogen-bonding interactions to like molecules. The dihedral angles between the two rings in each case are 25.79 (12) and 10.72 (12)°.



(I)

Experimental

Crystals obtained from Spa Contract Synthesis.

Crystal data

$C_{26}H_{28}Cl_2N_6S_2$
M_r = 559.56
Monoclinic, $P2_1/c$
a = 20.038 (4) Å
b = 11.358 (2) Å
c = 12.043 (2) Å
β = 92.03 (3)°
V = 2739.3 (10) Å^3
Z = 4
D_x = 1.357 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11927 reflections
θ = 2.9–27.5°
μ = 0.42 mm^{-1}
T = 150 (2) K
Block, colourless
0.20 × 0.18 × 0.10 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.921, T_{max} = 0.960
23 836 measured reflections
6216 independent reflections
4274 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 27.5°
$h = -25 \rightarrow 26$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.123
S = 1.00
6216 reflections
335 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.5559P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N41A—H4A···N1A^{i}	0.87 (3)	2.14 (3)	3.005 (3)	171 (2)
N41B—H4B···N1B^{ii}	0.82 (2)	2.24 (3)	3.022 (2)	161 (2)

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

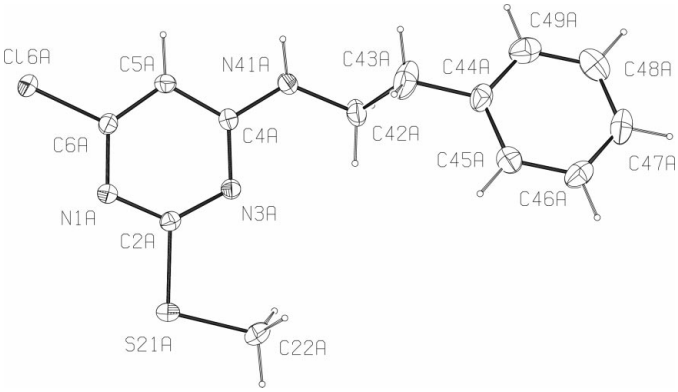


Figure 1
The molecular configuration and atom-numbering scheme for molecule *A*, showing 30% probability ellipsoids.

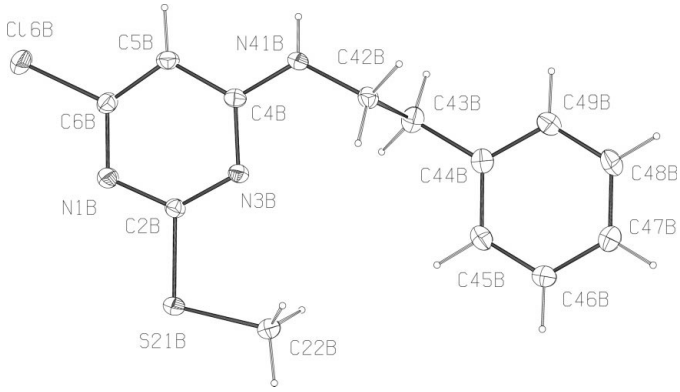


Figure 2
The molecular configuration and atom-numbering scheme for molecule *B*, showing 30% probability ellipsoids.

All H atoms were included in the refinement at calculated positions as riding models, with C—H set to 0.95 (Ar–H), 0.98 (CH_3) and 0.99 Å (CH_2), except for the amine H atoms which were located on difference syntheses and for which both positional and displacement parameters were refined.

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

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