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2-Amino-6-chloro-4-(1-phenylethylamino)pyrimidine

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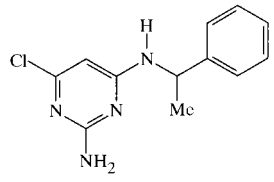
The structure of the title compound, $C_{12}H_{13}ClN_4$, (I), comprises a racemic mixture of chiral molecules associated by N—H···N hydrogen-bonding interactions. The dihedral angle between the two rings is 77.90 (6)°.



(I)

Experimental

Crystals of (I) were obtained from Spa Contract Synthesis.

Crystal data

$C_{12}H_{13}ClN_4$
M_r = 248.71
Tetragonal, $I4_1/a$
a = 17.4851 (7) Å
c = 16.2878 (9) Å
V = 4979.6 (4) Å^3
Z = 16
D_x = 1.327 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10256 reflections
θ = 2.91–27.48°
μ = 0.290 mm^{-1}
T = 150 (2) K
Block, yellow
0.15 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.958, T_{max} = 0.972
15 828 measured reflections
2828 independent reflections
1893 reflections with $I > 2\sigma(I)$
R_{int} = 0.137
θ_{max} = 27.43°
$h = -22 \rightarrow 22$
$k = -19 \rightarrow 19$
$l = -17 \rightarrow 21$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.134
S = 1.012
2828 reflections
156 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.1078P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0014 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···N3^{i}	0.88	2.23	3.098 (2)	169
N21—H22···N1^{ii}	0.88	2.17	3.043 (2)	172

Symmetry codes: (i) $\frac{3}{4} - y, x - \frac{1}{4}, \frac{3}{4} - z$; (ii) $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z$.

All H atoms were included in the refinement at calculated positions as riding, with the C—H distance set to either 0.98 (for CH_3) or 0.95 Å (for aryl H) and the N—H distance set to 0.88 Å.

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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