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2-Amino-4-chloro-6-(4-carbamoylpiperidin-1-yl)-pyrimidine hemihydrate

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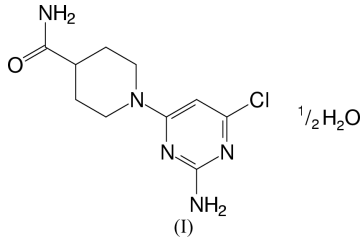
The structure of the title compound, $C_{10}H_{15}ClN_5O\cdot0.5H_2O$, comprises non-planar molecules that associate *via* N—H···N and N—H···O interactions to form a three-dimensional hydrogen-bonded array. The water molecule resides on a twofold axis and is also involved in the hydrogen-bonding network.

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from a dimethylformamide/water (1:25) solution.



(I)

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.116
Data-to-parameter ratio = 14.6

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

Crystal data

$C_{10}H_{15}ClN_5O\cdot0.5H_2O$
M_r = 264.72
Monoclinic, $C2/c$
a = 15.559 (3) Å
b = 9.3139 (19) Å
c = 16.493 (3) Å
β = 102.08 (3)°
V = 2337.2 (8) Å^3
Z = 8
D_x = 1.505 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5223 reflections
θ = 2.9–27.5°
μ = 0.325 mm^{-1}
T = 150 (2) K
Block, colourless
0.26 × 0.14 × 0.14 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.920, T_{max} = 0.956
10 159 measured reflections
2672 independent reflections
2113 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.5°
$h = -20 \rightarrow 19$
$k = -12 \rightarrow 12$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.116
S = 1.02
2672 reflections
183 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0659P)^2 + 0.5619P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

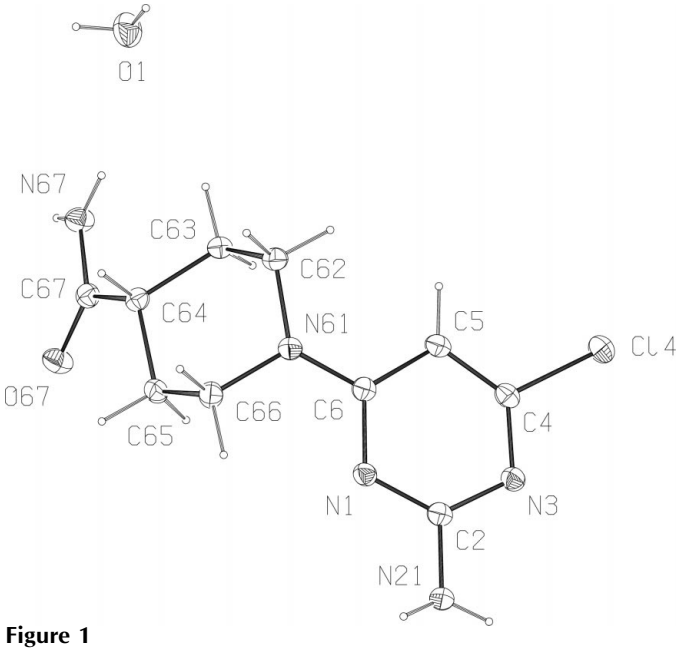


Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 30% probability displacement ellipsoids.

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

D—H···A	D—H	H···A	D···A	D—H···A
N21—H21···O67^{i}	0.79 (2)	2.35 (2)	3.049 (2)	148 (2)
N21—H22···O67^{ii}	0.83 (2)	2.25 (2)	3.069 (2)	170.6 (19)
N67—H671···O1W^{iii}	0.862 (18)	2.481 (19)	3.320 (2)	164.6 (16)
N67—H672···N3^{iv}	0.85 (2)	2.15 (2)	2.972 (2)	163.7 (18)
O1W—H1W···N1^{v}	0.82 (2)	2.32 (2)	3.1171 (19)	164 (2)

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

All H atoms were included in the refinement at calculated positions as riding models with C—H set to 0.95 (Ar-H) and 0.99 Å (CH_2), except for the H atoms involved in the hydrogen-bonding associations, 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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