# Pyrimidine-2-carboxamide

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In the crystal strucuture of the title compound, $C_5H_5N_3O$, which was obtained upon recrystallization of 2-cyano-pyrimidine from aqueous sodium hydroxide, the amide group is twisted with respect to the aromatic ring by 24.9 (1)°. $\pi$–$\pi$ stacking is observed between partially overlapped rings at a face-to-face separation of 3.439 (6) Å. The structure features a centrosymmetric pair of intermolecular N—H⋯O hydrogen bonds. Another N—H⋯O hydrogen bond between adjacent molecules links them into a helical chain motif.

## Related literature

For general background, see: Cheng *et al.* (2000); Xu & Xu (2004); Zhang *et al.* (2008). For a similar structure, see: Zhang *et al.* (2007).
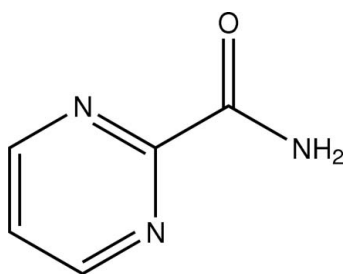
## Experimental

### Crystal data

| | |
|---|---|
| $C_5H_5N_3O$ | Monoclinic, $P2_1/c$ |
| $M_r$ = 123.12 | $a$ = 7.9241 (7) Å |
| $b$ = 7.3059 (7) Å | Mo $K\alpha$ radiation |
| $c$ = 9.8223 (9) Å | $\mu$ = 0.11 mm$^{-1}$ |
| $\beta$ = 103.512 (6)° | $T$ = 291 (2) K |
| $V$ = 552.90 (9) Å$^3$ | 0.34 × 0.26 × 0.20 mm |
| $Z$ = 4 | |

### Data collection

| | |
|---|---|
| Rigaku R-AXIS RAPID IP diffractometer | 1365 independent reflections |
| Absorption correction: none | 1202 reflections with $I > 2\sigma(I)$ |
| 7501 measured reflections | $R_{int}$ = 0.020 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.038 | 82 parameters |
| $wR(F^2)$ = 0.107 | H-atom parameters constrained |
| $S$ = 1.01 | $\Delta\rho_{max}$ = 0.25 e Å$^{-3}$ |
| 1365 reflections | $\Delta\rho_{min}$ = −0.19 e Å$^{-3}$ |

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N3—H1$A$⋯O1$^i$ | 0.94 | 2.06 | 2.994 (1) | 172 |
| N3—H1$B$⋯O1$^{ii}$ | 0.96 | 2.04 | 2.986 (2) | 167 |

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

## References

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# supporting information

## Pyrimidine-2-carboxamide

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### S1. Comment

In order to study the nature of $\pi$–$\pi$ stacking, a series of metal complexes incorporating substituted benzoate ligand have been prepared in our laboratory (Cheng *et al.*, 2000; Xu & Xu, 2004). As a continuing work, metal complexes with pyrimidine-2-carboxylate ligand have recently been prepared (Zhang *et al.*, 2007). In the process of preparing pyrimidine-2-carboxylic acid from cyanopyrimidine, the title compound has been obtained.

The molecular structure of the title complex is shown in Fig. 1. The bond distances and angles are normal. The amide group is twisted with respect to the benzene ring by a dihedral angel of 24.92 (12)°. The amino group links with carbonyl groups of adjacent molecules *via* O—H···O hydrogen bonding (Table 1). $\pi$–$\pi$ stacking is observed between parallel, partially overlapped N1-pyrimidine and $N^i$-pyrimidine rings (Fig. 1) [symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*], face-to-face separation being 3.439 (6) Å; similar to the situation found in the pyrimidine-2-carboxylate complex of copper(II) (Zhang *et al.*, 2007).

### S2. Experimental

2-Cyanopyrimidine (1.0 g, 9.5 mmol) was dissolved in 10 ml water, then a NaOH solution (0.1 *M*) was dropped to the solution until to pH = 12. Single crystals of the title compound were obtained from the solution after one week.

### S3. Refinement

Amino H atoms were located in a difference Fourier map and refined as riding in as-found relative positions with $U_{iso}(H)$ = $1.5U_{eq}(N)$. Other H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode with $U_{iso}(H)$ = $1.2U_{eq}(C)$.
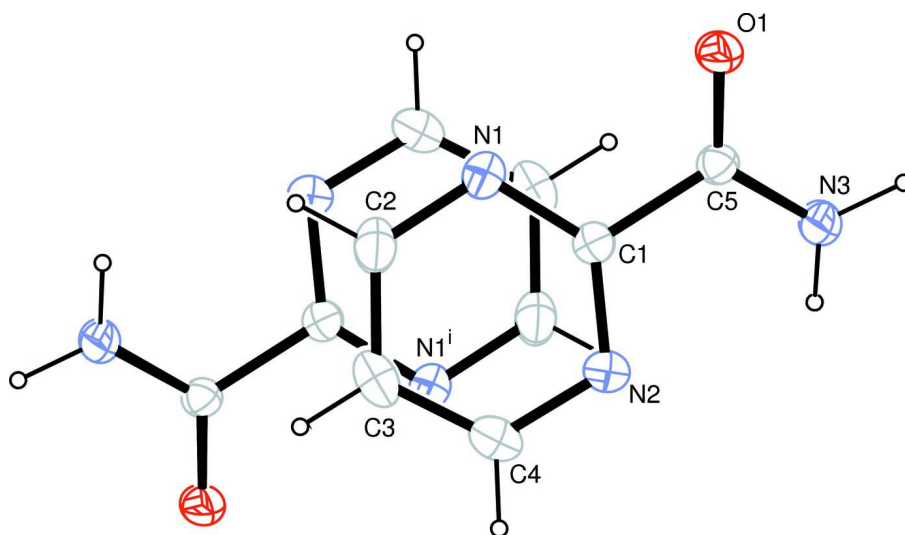
**Figure 1**

The molecular structure of the title compound with 30% probability displacement (arbitrary spheres for H atoms) [symmetry codes: (i) 1 - $x$, 1 - $y$, 1 - $z$].

**pyrimidine-2-carboxamide**

*Crystal data*

| | |
|---|---|
| $C_5H_5N_3O$ | $F(000) = 256$ |
| $M_r = 123.12$ | $D_x = 1.479$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 2086 reflections |
| $a = 7.9241$ (7) Å | $\theta = 3.0–25.5°$ |
| $b = 7.3059$ (7) Å | $\mu = 0.11$ mm$^{-1}$ |
| $c = 9.8223$ (9) Å | $T = 291$ K |
| $\beta = 103.512$ (6)° | Prism, yellow |
| $V = 552.90$ (9) Å$^3$ | $0.34 \times 0.26 \times 0.20$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID IP diffractometer | 1202 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{int} = 0.020$ |
| Graphite monochromator | $\theta_{max} = 28.3°$, $\theta_{min} = 2.6°$ |
| $\omega$ scans | $h = -10 \rightarrow 10$ |
| 7501 measured reflections | $k = -9 \rightarrow 9$ |
| 1365 independent reflections | $l = -12 \rightarrow 13$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | Secondary atom site location: difference Fourier map |
| $wR(F^2) = 0.107$ | |
| $S = 1.02$ | Hydrogen site location: inferred from neighbouring sites |
| 1365 reflections | |
| 82 parameters | H-atom parameters constrained |
| 0 restraints | |

$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.1258P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.25$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

|  | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.35320 (14) | 0.45375 (15) | 0.64547 (11) | 0.0431 (3) |
| N2 | 0.18202 (13) | 0.54314 (14) | 0.42171 (10) | 0.0383 (3) |
| O1 | 0.13605 (12) | 0.15236 (12) | 0.61860 (8) | 0.0431 (3) |
| N3 | 0.07527 (15) | 0.18634 (15) | 0.38330 (10) | 0.0435 (3) |
| H1A | 0.0949 | 0.2477 | 0.3043 | 0.065* |
| H1B | 0.0039 | 0.0783 | 0.3675 | 0.065* |
| C1 | 0.23238 (14) | 0.42647 (15) | 0.52761 (11) | 0.0315 (2) |
| C2 | 0.43153 (18) | 0.6167 (2) | 0.65658 (14) | 0.0495 (3) |
| H2 | 0.5193 | 0.6412 | 0.7355 | 0.059* |
| C3 | 0.38709 (19) | 0.74967 (19) | 0.55555 (15) | 0.0502 (3) |
| H3 | 0.4405 | 0.8638 | 0.5659 | 0.060* |
| C4 | 0.26039 (18) | 0.70681 (18) | 0.43855 (14) | 0.0462 (3) |
| H4 | 0.2279 | 0.7944 | 0.3686 | 0.055* |
| C5 | 0.14304 (14) | 0.24129 (15) | 0.51331 (11) | 0.0325 (3) |

*Atomic displacement parameters (Å$^2$)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0446 (6) | 0.0418 (6) | 0.0383 (5) | −0.0037 (4) | 0.0002 (4) | −0.0014 (4) |
| N2 | 0.0417 (5) | 0.0350 (5) | 0.0375 (5) | 0.0003 (4) | 0.0080 (4) | 0.0046 (4) |
| O1 | 0.0602 (6) | 0.0366 (5) | 0.0316 (4) | −0.0065 (4) | 0.0087 (4) | 0.0025 (3) |
| N3 | 0.0593 (7) | 0.0389 (6) | 0.0304 (5) | −0.0120 (5) | 0.0065 (4) | −0.0018 (4) |
| C1 | 0.0325 (5) | 0.0315 (5) | 0.0311 (5) | 0.0019 (4) | 0.0085 (4) | −0.0016 (4) |
| C2 | 0.0478 (7) | 0.0501 (8) | 0.0473 (7) | −0.0108 (6) | 0.0046 (5) | −0.0103 (6) |
| C3 | 0.0530 (8) | 0.0377 (7) | 0.0628 (9) | −0.0123 (5) | 0.0194 (6) | −0.0072 (6) |
| C4 | 0.0506 (7) | 0.0367 (6) | 0.0538 (7) | 0.0001 (5) | 0.0175 (6) | 0.0084 (5) |
| C5 | 0.0362 (5) | 0.0304 (5) | 0.0302 (5) | 0.0018 (4) | 0.0067 (4) | −0.0001 (4) |

*Geometric parameters (Å, º)*

| N1—C1 | 1.3336 (14) | N3—H1B | 0.9622 |
|---|---|---|---|
| N1—C2 | 1.3355 (18) | C1—C5 | 1.5182 (15) |

| N2—C1 | 1.3319 (14) | C2—C3 | 1.374 (2) |
|---|---|---|---|
| N2—C4 | 1.3397 (17) | C2—H2 | 0.9300 |
| O1—C5 | 1.2335 (13) | C3—C4 | 1.374 (2) |
| N3—C5 | 1.3265 (14) | C3—H3 | 0.9300 |
| N3—H1A | 0.9406 | C4—H4 | 0.9300 |
| | | | |
| C1—N1—C2 | 115.46 (11) | C3—C2—H2 | 118.8 |
| C1—N2—C4 | 115.41 (10) | C2—C3—C4 | 117.18 (12) |
| C5—N3—H1A | 122.9 | C2—C3—H3 | 121.4 |
| C5—N3—H1B | 119.6 | C4—C3—H3 | 121.4 |
| H1A—N3—H1B | 117.5 | N2—C4—C3 | 122.26 (12) |
| N2—C1—N1 | 127.28 (11) | N2—C4—H4 | 118.9 |
| N2—C1—C5 | 116.74 (9) | C3—C4—H4 | 118.9 |
| N1—C1—C5 | 115.99 (10) | O1—C5—N3 | 124.08 (11) |
| N1—C2—C3 | 122.37 (12) | O1—C5—C1 | 120.20 (9) |
| N1—C2—H2 | 118.8 | N3—C5—C1 | 115.72 (9) |

*Hydrogen-bond geometry (Å, º)*

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| N3—H1$A$⋯O1[i] | 0.94 | 2.06 | 2.994 (1) | 172 |
| N3—H1$B$⋯O1[ii] | 0.96 | 2.04 | 2.986 (2) | 167 |

Symmetry codes: (i) $x$, $-y+1/2$, $z-1/2$; (ii) $-x$, $-y$, $-z+1$.