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# *tert*-Butyl 6-amino-3,4-dihydro-2*H*-1,4-benzoxazine-4-carboxylate

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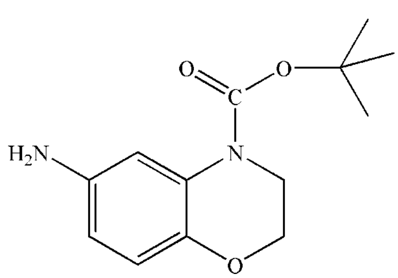
Key indicators: single-crystal X-ray study; $T$ = 103 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.047; $wR$ factor = 0.106; data-to-parameter ratio = 21.9.

The title molecule, $C_{13}H_{18}N_2O_3$, contains a benzene ring fused to an oxazine ring and one *tert*-butoxycarbonyl group bound to the N atom of the oxazine ring. A weak intramolecular C—H···O interaction occurs. In the crystal, intermolecular N—H···O and C—H···O hydrogen bonds stack the molecules down the $b$ axis. Weak C—H···N contacts connect the stacks, generating a three-dimensional network.

## Related literature

For the pharmacological properties of phenylmorpholine derivatives, see: Albanese *et al.* (2003); La *et al.* (2008); McCormick *et al.* (2008). For related structures, see: Chen *et al.* (2003); Olmstead *et al.* (2003); Vergeer *et al.* (1999).




## Experimental

*Crystal data*

$C_{13}H_{18}N_2O_3$
$M_r$ = 250.29
Monoclinic, $P2_1/n$
$a$ = 9.439 (4) Å
$b$ = 7.941 (3) Å
$c$ = 17.598 (7) Å
$\beta$ = 97.235 (6)°
$V$ = 1308.6 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 103 K
0.37 × 0.27 × 0.21 mm

*Data collection*

Rigaku AFC10/Saturn724+ diffractometer
13574 measured reflections
3816 independent reflections
3118 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.106
$S$ = 1.00
3816 reflections
174 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$B$···O3$^{i}$ | 0.885 (17) | 2.088 (17) | 2.9581 (19) | 167.4 (16) |
| C2—H2···O3 | 0.95 | 2.23 | 2.7981 (18) | 117 |
| C7—H7$A$···O1$^{ii}$ | 0.99 | 2.55 | 3.364 (2) | 139 |
| C13—H13$B$···N2 | 0.98 | 2.61 | 3.586 (2) | 172 |

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

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5053).

## References

Albanese, D., Landini, D., Lupi, V. & Penso, M. (2003). *Ind. Eng. Chem. Res.* **42**, 680–686.
Chen, Y., Zhang, L. & Chen, Z. (2003). *Acta Cryst.* E**59**, m429–m430.
La, D. S., Belzile, J., Bready, J. V., Coxon, A., DeMelfi, T., Doerr, N., Estrada, J., Flynn, J. C., Flynn, S. R., Graceffa, R. F., Harriman, S. P., Larrow, J. F., Long, A. M., Martin, M. W., Morrison, M. J., Patel, V. F., Roveto, P. M., Wang, L., Weiss, M. N., Whittington, D. A., Teffera, Y., Zhao, Z., Polverino, A. J. & Harmange, J.-C. (2008). *J. Med. Chem.* **51**, 1695–1705.
McCormick, K. D., Boyce, C. W. & Shih, N.-Y. (2008). PCT/US2008/001776.
Olmstead, M. M., Troeltzsch, C. & Patten, T. E. (2003). *Acta Cryst.* E**59**, m502–m503.
Rigaku (2008). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Vergeer, P., Kooijman, H., Schreurs, A. M. M., Kroon, J. & Grech, E. (1999). *Acta Cryst.* C**55**, 1822–1824.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o3269 [ doi:10.1107/S160053681004777X ]

## *tert*-Butyl 6-amino-3,4-dihydro-2*H*-1,4-benzoxazine-4-carboxylate

**X.-B. Gu, M.-J. Jiang, G.-M. Cai and Y.-Y. Zhou**

### Comment

The title compound, (I), is an important phenylmorpholine derivative. Phenylmorpholine compounds are used as α2 C adrenergic receptor agonists. (McCormick *et al.*, 2008). Numerous phenylmorpholine derivatives possess various other pharmacological properties. (Albanese, *et al.*, 2003; La, *et al.*, 2008).

We report here the crystal structure of the title compound. (Fig. 1). The title molecule of (I) contains a benzene ring fused to an oxazine ring and one *tert*-butoxycarbonyl bound to the N atom. The N1—C1 bond distance is 1.4230 (14)Å and agrees with literature values (Vergeer, *et al.*, 1999; Chen, *et al.*, 2003; Olmstead, *et al.*, 2003). The six-membered heterocyclic ring adopts a half-chair conformation with atoms C7 and C8 lying out of the plane through the remaining four atoms by 0.3264 (14) and -0.4174 (13) Å, respectively.

In the crystal structure intermolecular N2—H2B···O3 and C7—H7···O1 hydrogen bonds stack the molecules down the *b* axis. Weak C13—H13B···N2 contacts connect the stacks generating a three-dimensional network, Table 1.

### Experimental

The title compound was crystallized from a mixed solvent composed of dichloromethane and hexane (1:1); colorless block-shaped crystals were obtained after several days.

### Refinement

Positional parameters of all the H atoms bonded to C atoms were calculated geometrically and were allowed to ride on the C atoms to which they were bonded, with C—H distances of 0.95Å (CH), 0.98Å ($CH_3$) or 0.99Å ($CH_2$), and with Uiso(H) =1.2 or 1.5 (methyl) Ueq of the parent atoms. The H-atoms bound to N were found in a difference map and allowed to refine freely.

### Figures

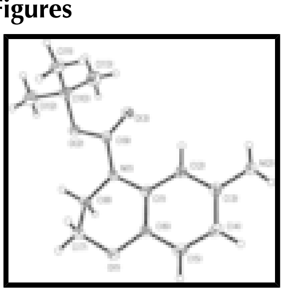

Fig. 1. A view of the title compound with the atomic numbering scheme with displacement ellipsoids drawn at the 50% probability level.

### *tert*-Butyl 6-amino-3,4-dihydro-2*H*-1,4-benzoxazine-4-carboxylate

*Crystal data*

| | |
|---|---|
| $C_{13}H_{18}N_2O_3$ | $F(000) = 536$ |
| $M_r = 250.29$ | $D_x = 1.270$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 3844 reflections |
| $a = 9.439$ (4) Å | $\theta = 3.6$–$30.0°$ |
| $b = 7.941$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $c = 17.598$ (7) Å | $T = 103$ K |
| $\beta = 97.235$ (6)° | Block, colorless |
| $V = 1308.6$ (8) Å$^3$ | 0.37 × 0.27 × 0.21 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Rigaku AFC10/Saturn724+ diffractometer | 3118 reflections with $I > 2\sigma(I)$ |
| Radiation source: Rotating Anode | $R_{int} = 0.035$ |
| graphite | $\theta_{max} = 30.0°$, $\theta_{min} = 2.3°$ |
| Detector resolution: 28.5714 pixels mm$^{-1}$ | $h = -13 \rightarrow 13$ |
| φ and ω scans | $k = -11 \rightarrow 11$ |
| 13574 measured reflections | $l = -22 \rightarrow 24$ |
| 3816 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.047$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.106$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.00$ | $w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.506P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 3816 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 174 parameters | $\Delta\rho_{max} = 0.41$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.19$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.29075 (9) | 0.23440 (12) | 0.77441 (5) | 0.0238 (2) |
| O2 | 0.27308 (9) | 0.60469 (11) | 0.55727 (5) | 0.01769 (18) |
| O3 | 0.47393 (9) | 0.70065 (11) | 0.62807 (5) | 0.01852 (19) |
| N1 | 0.36964 (10) | 0.45345 (12) | 0.65823 (6) | 0.0148 (2) |
| N2 | 0.84770 (11) | 0.48161 (15) | 0.80355 (7) | 0.0226 (2) |
| C1 | 0.46953 (11) | 0.41260 (14) | 0.72306 (6) | 0.0138 (2) |
| C2 | 0.61108 (12) | 0.46877 (14) | 0.73224 (6) | 0.0153 (2) |
| H2 | 0.6415 | 0.5440 | 0.6956 | 0.018* |
| C3 | 0.70861 (12) | 0.41698 (15) | 0.79396 (7) | 0.0166 (2) |
| C4 | 0.66399 (13) | 0.30549 (15) | 0.84764 (7) | 0.0191 (2) |
| H4 | 0.7294 | 0.2684 | 0.8898 | 0.023* |
| C5 | 0.52391 (13) | 0.24943 (15) | 0.83905 (7) | 0.0200 (2) |
| H5 | 0.4941 | 0.1738 | 0.8757 | 0.024* |
| C6 | 0.42614 (12) | 0.30153 (15) | 0.77789 (7) | 0.0172 (2) |
| C7 | 0.18660 (13) | 0.31174 (17) | 0.71949 (8) | 0.0243 (3) |
| H7A | 0.1574 | 0.4212 | 0.7395 | 0.029* |
| H7B | 0.1010 | 0.2389 | 0.7105 | 0.029* |
| C8 | 0.24682 (13) | 0.33916 (16) | 0.64505 (7) | 0.0220 (3) |
| H8A | 0.2771 | 0.2301 | 0.6251 | 0.026* |
| H8B | 0.1728 | 0.3884 | 0.6066 | 0.026* |
| C9 | 0.37957 (11) | 0.59648 (14) | 0.61556 (6) | 0.0140 (2) |
| C10 | 0.27444 (13) | 0.74056 (16) | 0.49941 (7) | 0.0195 (2) |
| C11 | 0.25934 (15) | 0.91226 (17) | 0.53576 (8) | 0.0268 (3) |
| H11A | 0.1790 | 0.9102 | 0.5660 | 0.040* |
| H11B | 0.2419 | 0.9978 | 0.4955 | 0.040* |
| H11C | 0.3474 | 0.9395 | 0.5692 | 0.040* |
| C12 | 0.14095 (16) | 0.7002 (2) | 0.44419 (8) | 0.0338 (3) |
| H12A | 0.1490 | 0.5864 | 0.4236 | 0.051* |
| H12B | 0.1314 | 0.7817 | 0.4020 | 0.051* |
| H12C | 0.0567 | 0.7065 | 0.4714 | 0.051* |
| C13 | 0.40675 (16) | 0.7250 (2) | 0.45926 (8) | 0.0305 (3) |
| H13A | 0.4910 | 0.7576 | 0.4946 | 0.046* |
| H13B | 0.3977 | 0.7992 | 0.4144 | 0.046* |
| H13C | 0.4171 | 0.6082 | 0.4429 | 0.046* |
| H2A | 0.8731 (17) | 0.538 (2) | 0.7639 (10) | 0.030 (4)* |
| H2B | 0.9124 (19) | 0.408 (2) | 0.8234 (10) | 0.039 (5)* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0165 (4) | 0.0260 (5) | 0.0295 (5) | −0.0026 (3) | 0.0048 (3) | 0.0108 (4) |
| O2 | 0.0174 (4) | 0.0176 (4) | 0.0170 (4) | −0.0026 (3) | −0.0021 (3) | 0.0026 (3) |
| O3 | 0.0171 (4) | 0.0165 (4) | 0.0210 (4) | −0.0041 (3) | −0.0015 (3) | 0.0022 (3) |
| N1 | 0.0124 (4) | 0.0144 (5) | 0.0174 (5) | −0.0023 (3) | 0.0006 (3) | 0.0006 (4) |
| N2 | 0.0170 (5) | 0.0221 (6) | 0.0268 (6) | −0.0006 (4) | −0.0040 (4) | 0.0055 (5) |
| C1 | 0.0147 (5) | 0.0122 (5) | 0.0146 (5) | 0.0021 (4) | 0.0023 (4) | −0.0006 (4) |
| C2 | 0.0159 (5) | 0.0137 (5) | 0.0164 (5) | 0.0012 (4) | 0.0029 (4) | 0.0006 (4) |
| C3 | 0.0164 (5) | 0.0145 (5) | 0.0184 (5) | 0.0022 (4) | 0.0007 (4) | −0.0026 (4) |
| C4 | 0.0220 (6) | 0.0182 (6) | 0.0167 (5) | 0.0054 (4) | 0.0002 (4) | 0.0012 (4) |
| C5 | 0.0243 (6) | 0.0180 (6) | 0.0185 (6) | 0.0027 (5) | 0.0057 (4) | 0.0045 (5) |
| C6 | 0.0161 (5) | 0.0162 (5) | 0.0201 (5) | 0.0009 (4) | 0.0057 (4) | 0.0012 (4) |
| C7 | 0.0151 (5) | 0.0241 (7) | 0.0337 (7) | −0.0021 (5) | 0.0025 (5) | 0.0094 (5) |
| C8 | 0.0191 (6) | 0.0200 (6) | 0.0257 (6) | −0.0085 (5) | −0.0015 (5) | 0.0034 (5) |
| C9 | 0.0136 (5) | 0.0147 (5) | 0.0138 (5) | 0.0014 (4) | 0.0022 (4) | −0.0015 (4) |
| C10 | 0.0216 (6) | 0.0199 (6) | 0.0160 (5) | −0.0003 (5) | −0.0017 (4) | 0.0041 (4) |
| C11 | 0.0323 (7) | 0.0191 (6) | 0.0280 (7) | 0.0036 (5) | −0.0006 (5) | 0.0032 (5) |
| C12 | 0.0350 (8) | 0.0345 (8) | 0.0274 (7) | −0.0065 (6) | −0.0143 (6) | 0.0071 (6) |
| C13 | 0.0328 (7) | 0.0392 (8) | 0.0209 (6) | 0.0035 (6) | 0.0090 (5) | 0.0066 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C6 | 1.3789 (15) | C5—H5 | 0.9500 |
| O1—C7 | 1.4278 (15) | C7—C8 | 1.5081 (19) |
| O2—C9 | 1.3443 (13) | C7—H7A | 0.9900 |
| O2—C10 | 1.4848 (15) | C7—H7B | 0.9900 |
| O3—C9 | 1.2152 (14) | C8—H8A | 0.9900 |
| N1—C9 | 1.3713 (15) | C8—H8B | 0.9900 |
| N1—C1 | 1.4230 (14) | C10—C13 | 1.5154 (19) |
| N1—C8 | 1.4675 (15) | C10—C11 | 1.5204 (19) |
| N2—C3 | 1.3999 (16) | C10—C12 | 1.5253 (17) |
| N2—H2A | 0.887 (17) | C11—H11A | 0.9800 |
| N2—H2B | 0.884 (19) | C11—H11B | 0.9800 |
| C1—C2 | 1.3985 (16) | C11—H11C | 0.9800 |
| C1—C6 | 1.4058 (16) | C12—H12A | 0.9800 |
| C2—C3 | 1.3945 (16) | C12—H12B | 0.9800 |
| C2—H2 | 0.9500 | C12—H12C | 0.9800 |
| C3—C4 | 1.3977 (17) | C13—H13A | 0.9800 |
| C4—C5 | 1.3853 (18) | C13—H13B | 0.9800 |
| C4—H4 | 0.9500 | C13—H13C | 0.9800 |
| C5—C6 | 1.3896 (17) | | |
| C6—O1—C7 | 114.78 (10) | N1—C8—H8A | 109.8 |
| C9—O2—C10 | 119.23 (9) | C7—C8—H8A | 109.8 |
| C9—N1—C1 | 122.94 (9) | N1—C8—H8B | 109.8 |
| C9—N1—C8 | 122.19 (10) | C7—C8—H8B | 109.8 |

| | | | |
|---|---|---|---|
| C1—N1—C8 | 114.60 (9) | H8A—C8—H8B | 108.3 |
| C3—N2—H2A | 115.6 (10) | O3—C9—O2 | 124.46 (10) |
| C3—N2—H2B | 113.3 (12) | O3—C9—N1 | 124.31 (10) |
| H2A—N2—H2B | 113.7 (16) | O2—C9—N1 | 111.22 (9) |
| C2—C1—C6 | 118.52 (10) | O2—C10—C13 | 109.84 (10) |
| C2—C1—N1 | 123.15 (10) | O2—C10—C11 | 110.72 (10) |
| C6—C1—N1 | 118.19 (10) | C13—C10—C11 | 113.31 (12) |
| C3—C2—C1 | 121.55 (11) | O2—C10—C12 | 101.90 (10) |
| C3—C2—H2 | 119.2 | C13—C10—C12 | 110.43 (12) |
| C1—C2—H2 | 119.2 | C11—C10—C12 | 110.06 (11) |
| C2—C3—C4 | 119.19 (11) | C10—C11—H11A | 109.5 |
| C2—C3—N2 | 120.19 (11) | C10—C11—H11B | 109.5 |
| C4—C3—N2 | 120.57 (11) | H11A—C11—H11B | 109.5 |
| C5—C4—C3 | 119.64 (11) | C10—C11—H11C | 109.5 |
| C5—C4—H4 | 120.2 | H11A—C11—H11C | 109.5 |
| C3—C4—H4 | 120.2 | H11B—C11—H11C | 109.5 |
| C4—C5—C6 | 121.37 (11) | C10—C12—H12A | 109.5 |
| C4—C5—H5 | 119.3 | C10—C12—H12B | 109.5 |
| C6—C5—H5 | 119.3 | H12A—C12—H12B | 109.5 |
| O1—C6—C5 | 116.15 (11) | C10—C12—H12C | 109.5 |
| O1—C6—C1 | 124.09 (10) | H12A—C12—H12C | 109.5 |
| C5—C6—C1 | 119.73 (11) | H12B—C12—H12C | 109.5 |
| O1—C7—C8 | 110.33 (10) | C10—C13—H13A | 109.5 |
| O1—C7—H7A | 109.6 | C10—C13—H13B | 109.5 |
| C8—C7—H7A | 109.6 | H13A—C13—H13B | 109.5 |
| O1—C7—H7B | 109.6 | C10—C13—H13C | 109.5 |
| C8—C7—H7B | 109.6 | H13A—C13—H13C | 109.5 |
| H7A—C7—H7B | 108.1 | H13B—C13—H13C | 109.5 |
| N1—C8—C7 | 109.19 (10) | | |

| | | | |
|---|---|---|---|
| C9—N1—C1—C2 | −26.57 (17) | N1—C1—C6—O1 | −2.62 (17) |
| C8—N1—C1—C2 | 159.29 (11) | C2—C1—C6—C5 | −0.48 (17) |
| C9—N1—C1—C6 | 157.74 (11) | N1—C1—C6—C5 | 175.41 (11) |
| C8—N1—C1—C6 | −16.40 (15) | C6—O1—C7—C8 | 44.10 (15) |
| C6—C1—C2—C3 | 0.09 (17) | C9—N1—C8—C7 | −126.86 (12) |
| N1—C1—C2—C3 | −175.59 (10) | C1—N1—C8—C7 | 47.33 (14) |
| C1—C2—C3—C4 | 0.40 (17) | O1—C7—C8—N1 | −61.83 (14) |
| C1—C2—C3—N2 | −176.97 (11) | C10—O2—C9—O3 | 5.54 (17) |
| C2—C3—C4—C5 | −0.49 (17) | C10—O2—C9—N1 | −173.22 (9) |
| N2—C3—C4—C5 | 176.87 (11) | C1—N1—C9—O3 | 0.71 (17) |
| C3—C4—C5—C6 | 0.10 (18) | C8—N1—C9—O3 | 174.42 (11) |
| C7—O1—C6—C5 | 169.42 (11) | C1—N1—C9—O2 | 179.48 (10) |
| C7—O1—C6—C1 | −12.48 (17) | C8—N1—C9—O2 | −6.81 (15) |
| C4—C5—C6—O1 | 178.58 (11) | C9—O2—C10—C13 | 61.25 (14) |
| C4—C5—C6—C1 | 0.40 (18) | C9—O2—C10—C11 | −64.64 (14) |
| C2—C1—C6—O1 | −178.52 (11) | C9—O2—C10—C12 | 178.33 (11) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| N2—H2B···O3[i] | 0.885 (17) | 2.088 (17) | 2.9581 (19) | 167.4 (16) |
| C2—H2···O3 | 0.95 | 2.23 | 2.7981 (18) | 117 |
| C7—H7A···O1[ii] | 0.99 | 2.55 | 3.364 (2) | 139 |
| C13—H13B···N2[iii] | 0.98 | 2.61 | 3.586 (2) | 172 |

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iii) .

**Fig. 1**