

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

3-(1,3-Dioxolan-2-yl)-2-hydrazino-7-methylquinoline

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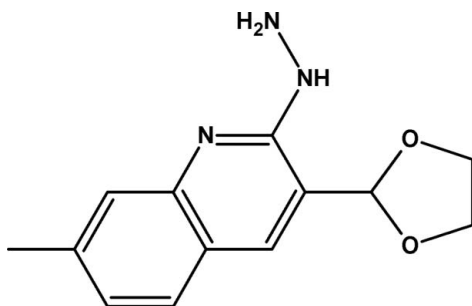
Received 18 December 2008; accepted 24 January 2009

 Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.044; wR factor = 0.129; data-to-parameter ratio = 12.9.

In the title molecule, $\text{C}_{13}\text{H}_{15}\text{N}_3\text{O}_2$, the dihedral angle between the mean plane of the 1,3-dioxolane group and the 2-hydrazino-7-methylisoquinoline unit is $85.21(5)^\circ$. The conformation of the molecule is influenced by bifurcated $\text{N}-\text{H}\cdots(\text{O},\text{O})$ and $\text{N}-\text{H}\cdots\text{N}$ intramolecular hydrogen bonds. In the crystal structure, molecules are linked *via* intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming extended chains along [001].

Related literature

For general background to hydrazine compounds, see: Broadhurst *et al.* (2001); Behrens (1999); Broadhurst (1991); Chao *et al.* (1999); Kametani (1968). For related crystal structures, see: Yang *et al.* (2008); Choudhury & Guru Row (2006); Choudhury *et al.* (2002); Hathwar *et al.* (2008); Cho *et al.* (2002); Manivel *et al.* (2009), and references therein. For bond-length data, see: Allen *et al.*, 1987)



Experimental

Crystal data

 $\text{C}_{13}\text{H}_{15}\text{N}_3\text{O}_2$
 $M_r = 245.28$
 Monoclinic, $P2_1/c$
 $a = 13.1909(17)$ Å
 $b = 10.1165(13)$ Å
 $c = 9.7805(13)$ Å

 $\beta = 109.956(2)^\circ$
 $V = 1226.8(3)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation

 $\mu = 0.09$ mm⁻¹
 $T = 290(2)$ K
 $0.30 \times 0.21 \times 0.14$ mm

Data collection

 Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.942$, $T_{\max} = 0.987$
 8929 measured reflections
 2279 independent reflections
 1699 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.129$
 $S = 1.06$
 2279 reflections
 176 parameters

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.19$ e Å⁻³
 $\Delta\rho_{\min} = -0.14$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N2}-\text{H2N}\cdots\text{O1}$ | 0.843 (19) | 2.372 (18) | 2.9329 (17) | 124.5 (15) |
| $\text{N2}-\text{H2N}\cdots\text{O2}$ | 0.843 (19) | 2.653 (18) | 3.0968 (19) | 114.3 (14) |
| $\text{N3}-\text{H3NA}\cdots\text{N1}$ | 0.94 (2) | 2.35 (2) | 2.691 (2) | 100.9 (15) |
| $\text{N3}-\text{H3NB}\cdots\text{O2}^i$ | 0.92 (2) | 2.44 (2) | 3.207 (2) | 141.2 (19) |

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

We thank the Department of Science and Technology, India, for use of the CCD facility setup under the IRHPA-DST program at IISc. We thank Professor T. N. Guru Row, IISc, Bangalore, for useful crystallographic discussions. FNK thanks the DST for Fast Track Proposal funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2748).

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supporting information

Acta Cryst. (2009). E65, o407–o408 [doi:10.1107/S1600536809003031]

3-(1,3-Dioxolan-2-yl)-2-hydrazino-7-methylquinoline

R. Subashini, Venkatesha R. Hathwar, P. Nithya, K. Prabakaran and F. Nawaz Khan

S1. Comment

The title compound (I), belongs to the quinoline class. Quinolines and quinolinones are an integral part of many naturally occurring fused heterocycles and find application in synthetic and pharmaceutical chemistry (Kametani, 1968). Isoquinolinones and isoquinolineamines have been reported as cancer chemotherapeutic agents (Behrens, 1999) whereas quinolyl and isoquinolyl derivatives have been reported as insecticidal compounds (Broadhurst, 1991). 3-substituted isoquinolines have potent use in medicine (Chao *et al.*, 1999) and in general, hydrazine derivatives can be used as medicaments (Broadhurst *et al.*, 2001; Choudhury, *et al.*, 2002; Choudhury & Guru Row, 2006; Yang, *et al.*, 2008). Due to the importance of quinoline derivatives (Cho *et al.*, 2002) and in continuous of our research on quinolines and isoquinoline derivatives (Hathwar *et al.*, 2008; Manivel *et al.*, 2009) we present here crystal structure of the title compound.

In (I) the dihedral angle between 1,3-dioxolane moiety and 2 hydrazino-7-methyl isoquinoline unit is 85.21 (5)°. All bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The conformation of the molecule is influenced by N—H···O and N—H···N intramolecular hydrogen bonds whereas the crystal structure is stabilized by intermolecular N—H···O hydrogen bonds forming extended chains along [001].

S2. Experimental

A solution of 2-chloro (3-(1,3-dioxolan-2-yl)-7-methylquinoline in ethanol was treated with hydrazine hydrate and stirred at 323 K for 3hr. The product was filtered. The solid was washed with water and diethyl ether and dried under vacuum. Single crystals were obtained by recrystallization of (I) from DMSO.

S3. Refinement

All H atoms positioned geometrically and refined using a riding model with bond lengths C—H = 0.93 Å (for aromatic), 0.97 Å (for methylene) and 0.96 Å (for methyl). The $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all other carbon bound H atoms. H atoms bonded to N atoms were located in difference Fourier maps and refined isotropically.

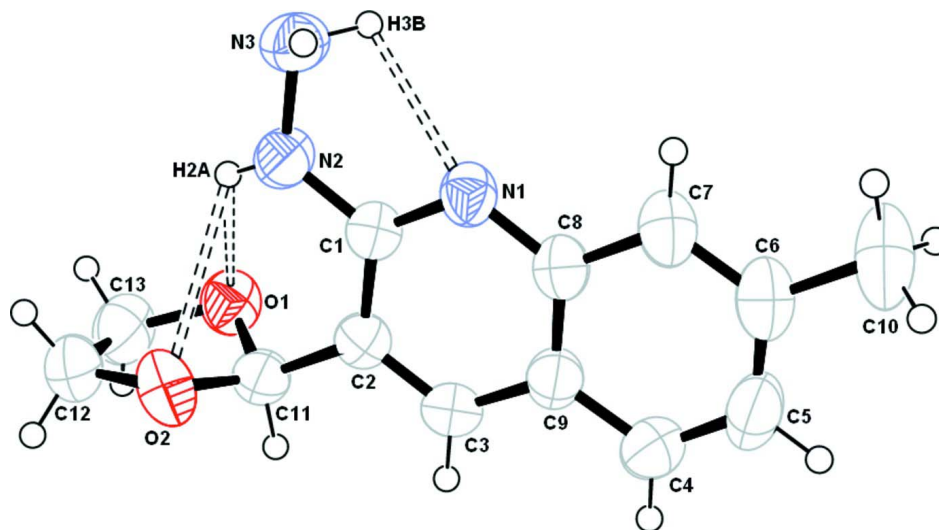


Figure 1

The molecular structure of (I) with 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

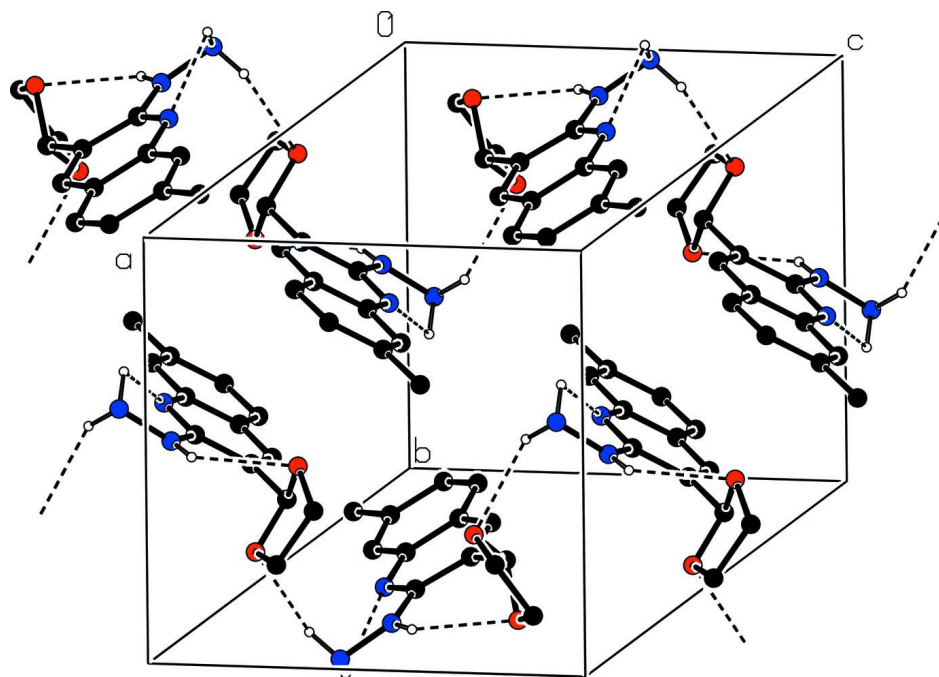


Figure 2

Part of the crystal structure of (I) showing hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

3-(1,3-Dioxolan-2-yl)-2-hydrazino-7-methylquinoline

Crystal data

$C_{13}H_{15}N_3O_2$

$M_r = 245.28$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 13.1909\ (17)\ \text{\AA}$

$b = 10.1165\ (13)\ \text{\AA}$

$c = 9.7805\ (13)\ \text{\AA}$

$\beta = 109.956\ (2)^\circ$

$V = 1226.8 (3) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 520$
 $D_x = 1.328 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 948 reflections

$\theta = 1.8\text{--}24.6^\circ$
 $\mu = 0.09 \text{ mm}^{-1}$
 $T = 290 \text{ K}$
 Block, brown
 $0.30 \times 0.21 \times 0.14 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.942$, $T_{\max} = 0.987$

8929 measured reflections
 2279 independent reflections
 1699 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 $\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 1.6^\circ$
 $h = -15 \rightarrow 15$
 $k = -10 \rightarrow 12$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.129$
 $S = 1.06$
 2279 reflections
 176 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.072P)^2 + 0.1104P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.19 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.14 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| O1 | 0.10652 (9) | 0.42297 (12) | -0.28334 (11) | 0.0621 (4) |
| O2 | 0.09919 (10) | 0.22186 (13) | -0.18872 (12) | 0.0701 (4) |
| N1 | 0.32415 (10) | 0.45872 (13) | 0.15262 (13) | 0.0524 (4) |
| N2 | 0.14264 (11) | 0.45599 (16) | 0.02767 (15) | 0.0597 (4) |
| N3 | 0.12501 (13) | 0.53613 (19) | 0.13548 (18) | 0.0664 (4) |
| C1 | 0.24495 (12) | 0.42351 (15) | 0.03448 (15) | 0.0464 (4) |
| C2 | 0.26133 (12) | 0.35152 (15) | -0.08326 (15) | 0.0480 (4) |
| C3 | 0.36404 (13) | 0.31857 (15) | -0.06896 (17) | 0.0550 (4) |
| H3A | 0.3772 | 0.2726 | -0.1435 | 0.066* |
| C4 | 0.56033 (15) | 0.32091 (18) | 0.0793 (2) | 0.0688 (5) |

| | | | | |
|------|---------------|--------------|---------------|------------|
| H4A | 0.5778 | 0.2750 | 0.0080 | 0.083* |
| C5 | 0.64009 (14) | 0.35734 (19) | 0.2051 (2) | 0.0732 (6) |
| H5A | 0.7111 | 0.3344 | 0.2186 | 0.088* |
| C6 | 0.61719 (14) | 0.4286 (2) | 0.3145 (2) | 0.0662 (5) |
| C7 | 0.51244 (13) | 0.46184 (19) | 0.29207 (17) | 0.0615 (5) |
| H7A | 0.4966 | 0.5107 | 0.3628 | 0.074* |
| C8 | 0.42773 (12) | 0.42464 (15) | 0.16556 (16) | 0.0496 (4) |
| C9 | 0.45173 (12) | 0.35270 (15) | 0.05728 (17) | 0.0533 (4) |
| C10 | 0.70689 (16) | 0.4661 (3) | 0.4525 (2) | 0.0949 (8) |
| H10A | 0.6767 | 0.4936 | 0.5244 | 0.142* |
| H10B | 0.7481 | 0.5372 | 0.4329 | 0.142* |
| H10C | 0.7530 | 0.3911 | 0.4882 | 0.142* |
| C11 | 0.17109 (13) | 0.31376 (16) | -0.21833 (17) | 0.0540 (4) |
| H11A | 0.2010 | 0.2745 | -0.2879 | 0.065* |
| C12 | -0.00343 (14) | 0.2421 (2) | -0.2979 (2) | 0.0782 (6) |
| H12A | -0.0588 | 0.2540 | -0.2544 | 0.094* |
| H12B | -0.0228 | 0.1675 | -0.3640 | 0.094* |
| C13 | 0.00918 (15) | 0.3653 (2) | -0.37670 (19) | 0.0764 (6) |
| H13A | 0.0146 | 0.3440 | -0.4706 | 0.092* |
| H13B | -0.0513 | 0.4247 | -0.3910 | 0.092* |
| H2N | 0.0904 (15) | 0.4447 (17) | -0.050 (2) | 0.064 (5)* |
| H3NB | 0.1453 (18) | 0.484 (2) | 0.218 (2) | 0.095 (7)* |
| H3NA | 0.1821 (17) | 0.597 (2) | 0.158 (2) | 0.078 (6)* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| O1 | 0.0577 (7) | 0.0724 (8) | 0.0494 (6) | 0.0026 (6) | 0.0095 (5) | 0.0034 (5) |
| O2 | 0.0667 (8) | 0.0722 (8) | 0.0642 (7) | -0.0201 (6) | 0.0130 (6) | -0.0040 (6) |
| N1 | 0.0475 (8) | 0.0647 (9) | 0.0438 (7) | -0.0047 (6) | 0.0141 (6) | -0.0015 (6) |
| N2 | 0.0476 (8) | 0.0838 (11) | 0.0443 (7) | 0.0051 (7) | 0.0114 (6) | -0.0113 (7) |
| N3 | 0.0626 (10) | 0.0782 (11) | 0.0586 (9) | 0.0087 (9) | 0.0211 (7) | -0.0131 (9) |
| C1 | 0.0467 (8) | 0.0495 (9) | 0.0426 (8) | 0.0001 (7) | 0.0145 (7) | 0.0037 (6) |
| C2 | 0.0497 (9) | 0.0465 (8) | 0.0470 (8) | 0.0006 (7) | 0.0153 (7) | 0.0012 (6) |
| C3 | 0.0580 (10) | 0.0492 (9) | 0.0589 (9) | 0.0019 (7) | 0.0214 (8) | -0.0077 (7) |
| C4 | 0.0566 (10) | 0.0607 (11) | 0.0890 (13) | 0.0055 (8) | 0.0245 (9) | -0.0053 (10) |
| C5 | 0.0424 (9) | 0.0707 (12) | 0.0974 (14) | 0.0022 (8) | 0.0122 (9) | 0.0105 (11) |
| C6 | 0.0518 (10) | 0.0774 (13) | 0.0628 (11) | -0.0136 (9) | 0.0108 (8) | 0.0122 (9) |
| C7 | 0.0526 (10) | 0.0785 (12) | 0.0512 (9) | -0.0134 (8) | 0.0148 (8) | 0.0024 (8) |
| C8 | 0.0480 (9) | 0.0526 (9) | 0.0470 (8) | -0.0057 (7) | 0.0147 (7) | 0.0065 (7) |
| C9 | 0.0474 (9) | 0.0470 (9) | 0.0629 (10) | 0.0001 (7) | 0.0156 (7) | 0.0035 (7) |
| C10 | 0.0550 (11) | 0.138 (2) | 0.0771 (13) | -0.0265 (12) | 0.0040 (10) | 0.0078 (13) |
| C11 | 0.0531 (9) | 0.0597 (10) | 0.0492 (9) | -0.0007 (7) | 0.0175 (7) | -0.0083 (7) |
| C12 | 0.0554 (11) | 0.0901 (15) | 0.0852 (13) | -0.0112 (10) | 0.0188 (10) | -0.0274 (12) |
| C13 | 0.0565 (11) | 0.1135 (17) | 0.0500 (9) | 0.0012 (11) | 0.0065 (8) | -0.0119 (11) |

Geometric parameters (Å, °)

| | | | |
|--------------|-------------|---------------|-------------|
| O1—C11 | 1.4074 (19) | C4—H4A | 0.9300 |
| O1—C13 | 1.422 (2) | C5—C6 | 1.406 (3) |
| O2—C12 | 1.424 (2) | C5—H5A | 0.9300 |
| O2—C11 | 1.427 (2) | C6—C7 | 1.365 (3) |
| N1—C1 | 1.3151 (18) | C6—C10 | 1.509 (2) |
| N1—C8 | 1.372 (2) | C7—C8 | 1.406 (2) |
| N2—C1 | 1.3683 (19) | C7—H7A | 0.9300 |
| N2—N3 | 1.411 (2) | C8—C9 | 1.407 (2) |
| N2—H2N | 0.843 (19) | C10—H10A | 0.9600 |
| N3—H3NB | 0.92 (2) | C10—H10B | 0.9600 |
| N3—H3NA | 0.94 (2) | C10—H10C | 0.9600 |
| C1—C2 | 1.440 (2) | C11—H11A | 0.9800 |
| C2—C3 | 1.355 (2) | C12—C13 | 1.504 (3) |
| C2—C11 | 1.495 (2) | C12—H12A | 0.9700 |
| C3—C9 | 1.417 (2) | C12—H12B | 0.9700 |
| C3—H3A | 0.9300 | C13—H13A | 0.9700 |
| C4—C5 | 1.368 (3) | C13—H13B | 0.9700 |
| C4—C9 | 1.411 (2) | | |
| C11—O1—C13 | 104.05 (14) | N1—C8—C7 | 118.75 (15) |
| C12—O2—C11 | 106.35 (14) | N1—C8—C9 | 122.22 (14) |
| C1—N1—C8 | 118.70 (13) | C7—C8—C9 | 119.03 (15) |
| C1—N2—N3 | 120.87 (13) | C8—C9—C4 | 118.70 (15) |
| C1—N2—H2N | 120.1 (12) | C8—C9—C3 | 117.09 (14) |
| N3—N2—H2N | 117.4 (12) | C4—C9—C3 | 124.20 (16) |
| N2—N3—H3NB | 104.8 (14) | C6—C10—H10A | 109.5 |
| N2—N3—H3NA | 102.9 (12) | C6—C10—H10B | 109.5 |
| H3NB—N3—H3NA | 101.6 (18) | H10A—C10—H10B | 109.5 |
| N1—C1—N2 | 116.89 (14) | C6—C10—H10C | 109.5 |
| N1—C1—C2 | 123.28 (14) | H10A—C10—H10C | 109.5 |
| N2—C1—C2 | 119.82 (13) | H10B—C10—H10C | 109.5 |
| C3—C2—C1 | 117.35 (13) | O1—C11—O2 | 105.16 (13) |
| C3—C2—C11 | 119.66 (14) | O1—C11—C2 | 112.04 (13) |
| C1—C2—C11 | 122.99 (13) | O2—C11—C2 | 111.79 (13) |
| C2—C3—C9 | 121.34 (15) | O1—C11—H11A | 109.2 |
| C2—C3—H3A | 119.3 | O2—C11—H11A | 109.2 |
| C9—C3—H3A | 119.3 | C2—C11—H11A | 109.2 |
| C5—C4—C9 | 120.33 (18) | O2—C12—C13 | 105.10 (14) |
| C5—C4—H4A | 119.8 | O2—C12—H12A | 110.7 |
| C9—C4—H4A | 119.8 | C13—C12—H12A | 110.7 |
| C4—C5—C6 | 121.55 (17) | O2—C12—H12B | 110.7 |
| C4—C5—H5A | 119.2 | C13—C12—H12B | 110.7 |
| C6—C5—H5A | 119.2 | H12A—C12—H12B | 108.8 |
| C7—C6—C5 | 118.21 (16) | O1—C13—C12 | 104.14 (14) |
| C7—C6—C10 | 121.57 (19) | O1—C13—H13A | 110.9 |
| C5—C6—C10 | 120.22 (17) | C12—C13—H13A | 110.9 |

| | | | |
|-----------|-------------|---------------|-------|
| C6—C7—C8 | 122.15 (17) | O1—C13—H13B | 110.9 |
| C6—C7—H7A | 118.9 | C12—C13—H13B | 110.9 |
| C8—C7—H7A | 118.9 | H13A—C13—H13B | 108.9 |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N2—H2N \cdots O1 | 0.843 (19) | 2.372 (18) | 2.9329 (17) | 124.5 (15) |
| N2—H2N \cdots O2 | 0.843 (19) | 2.653 (18) | 3.0968 (19) | 114.3 (14) |
| N3—H3NA \cdots N1 | 0.94 (2) | 2.35 (2) | 2.691 (2) | 100.9 (15) |
| N3—H3NB \cdots O2 ⁱ | 0.92 (2) | 2.44 (2) | 3.207 (2) | 141.2 (19) |

Symmetry code: (i) *x*, $-y+1/2$, *z*+1/2.