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Crystal structure of *N*-(3-oxobutanoyl)-L-homoserine lactone

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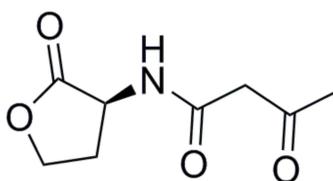
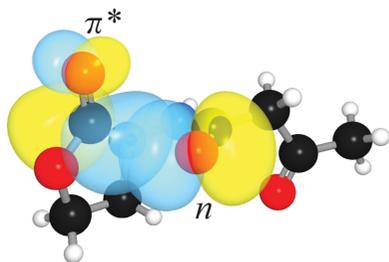
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The structure and absolute configuration of the title compound, C₈H₁₁NO₄, which is a known quorum-sensing modulator, have been determined. The molecule exhibits signs of an intramolecular attractive carbonyl–carbonyl $n \rightarrow \pi^*$ interaction between the amide and lactone ester groups, specifically – a short contact of 2.709 (2) Å between the amide oxygen atom and ester carbon atom, approach of the amide oxygen atom to the ester carbonyl group along the Bürgi–Dunitz trajectory, at 99.1 (1)°, and pyramidalization of the ester carbonyl group by 1.1 (1)°. Moreover, a similar $n \rightarrow \pi^*$ interaction is observed for the amide carbonyl group approached by the ketone oxygen donor. These interactions apparently affect the conformation of the uncomplexed molecule, which adopts a different shape when bound to protein receptors. In the crystal, the molecules form translational chains along the *a* axis via N–H···O hydrogen bonds.

1. Chemical context

N-Acyl homoserine lactones (AHLs) mediate quorum sensing in Gram-negative bacteria (Miller & Bassler, 2001; Waters & Bassler, 2005). We have previously shown that AHLs engage in $n \rightarrow \pi^*$ interactions between the acyl and lactone ester carbonyl groups (Newberry & Raines, 2014). These interactions cause attraction through donation of oxygen lone pair (*n*) electron density into the π^* antibonding orbital of an acceptor carbonyl group (Hinderaker & Raines, 2003). This interaction is observed in the free molecule but not in structures of these compounds bound to their protein receptors, implicating these interactions in the potency of AHLs and their analogs. Background to carbonyl–carbonyl interactions is given by Bretscher *et al.* (2001), DeRider *et al.* (2002), Hinderaker & Raines (2003), and Bartlett *et al.* (2010). Our previous studies were restricted to AHLs with simple acyl appendages, but natural AHLs are also often oxidized at the 3-position to yield β -keto acyl groups, such as that reported here.



2. Structural commentary and NBO analysis

This is, to our knowledge, the first report of the structure of a free 3-oxo AHL (Fig. 1). Individual molecules pack in linear arrays thanks to intermolecular hydrogen bonds between

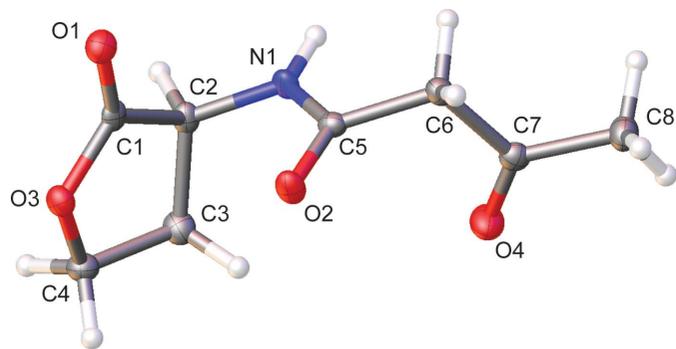


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

amide groups (Fig. 2). The molecule crystallizes as the keto tautomer, consistent with other β -keto amides (Allen, 2002). Like unoxidized AHLs, it displays the hallmark features of an attractive $n \rightarrow \pi^*$ interaction between the amide and ester carbonyl groups (Fig. 3). Specifically, the donor oxygen atom makes a sub-van der Waals contact of 2.709 (2) Å with the acceptor carbonyl group, with an angle of approach of 99.1 (1)°, characteristic of the Bürgi–Dunitz trajectory for nucleophilic addition (Bürgi *et al.*, 1973, 1974). This geometry enables electron donation that, in turn, causes a characteristic pyramidalization of the acceptor carbonyl group. We observe that the carbonyl carbon atom rises 0.016 (1) Å out of the plane of its substituents, creating a distortion angle θ (see Fig. 3) of 1.1 (1)°. This signature has been used to diagnose the presence of these interactions in many molecules (Choudhary

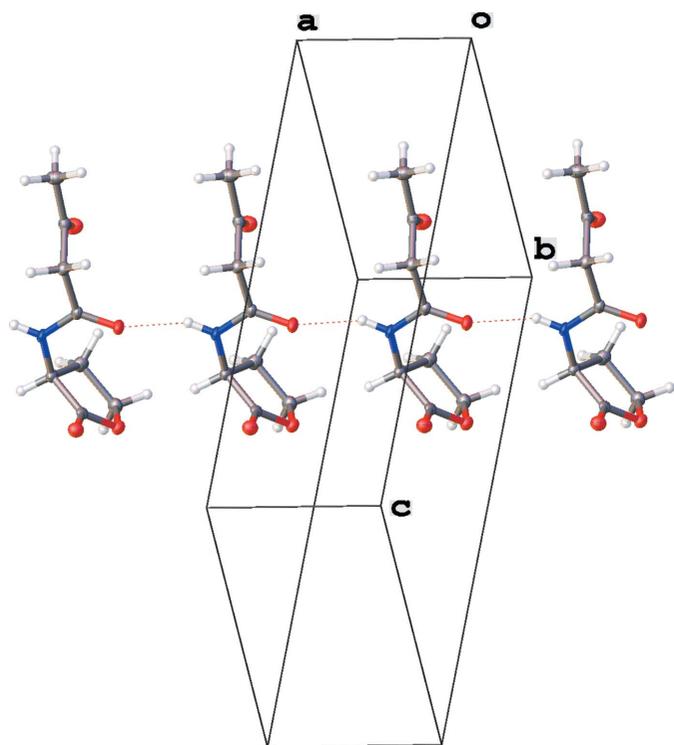


Figure 2
Packing of the title compound.

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

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---------------------|----------|--------------|--------------|----------------|
| $N1-H1 \cdots O2^i$ | 0.83 (2) | 2.05 (2) | 2.7973 (19) | 149 (2) |

Symmetry code: (i) $x + 1, y, z$.

et al., 2009, 2014; Choudhary & Raines, 2011; Newberry *et al.*, 2013), including polymers (Newberry & Raines, 2013) and proteins (Newberry *et al.*, 2014). Consistent with these observations, natural bond orbital (NBO) analysis (Reed *et al.*, 1988; Glendening *et al.*, 2012) of the crystal structure at the B3LYP/6-311+G(2d,p) level of theory predicts the release of 2.67 kcal mol⁻¹ of energy due to the $n \rightarrow \pi^*$ interaction, indicating a significant contribution of this interaction to the conformation of this molecule (Fig. 4).

Interestingly, a short contact is also observed between the ketone oxygen and amide carbonyl groups. In this case, the donor oxygen atom makes a 2.746 (2) Å contact at 107.5 (1)° to the amide carbonyl group. This contact causes the amide carbonyl group to distort 0.008 (1) Å out of plane, corre-

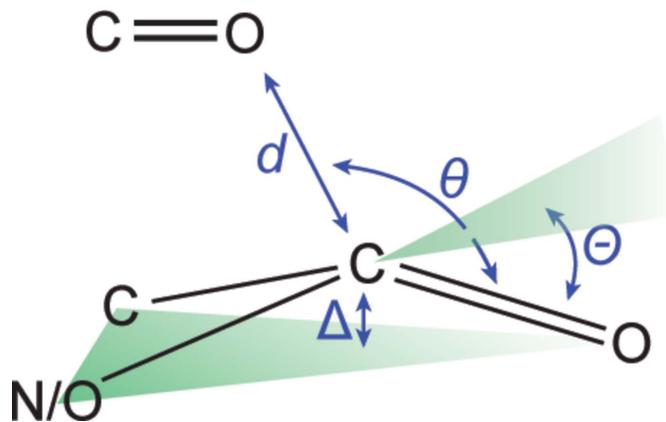


Figure 3
Structural parameters describing an $n \rightarrow \pi^*$ interaction

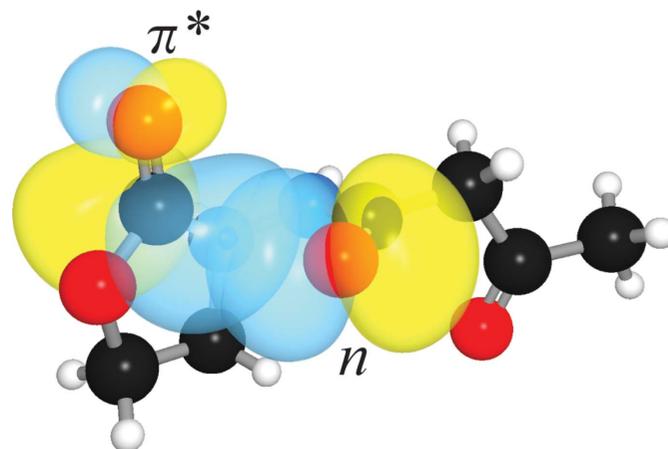


Figure 4
Overlap of amide lone pair (n) and ester π^* orbitals.

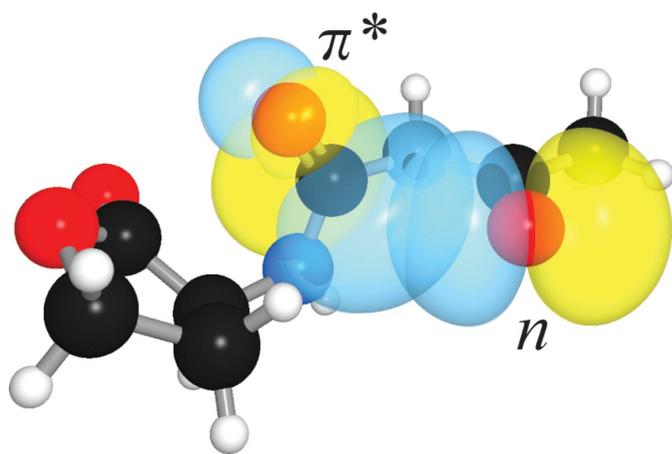


Figure 5
Overlap of ketone lone pair (n) and amide π^* orbitals.

sponding to a distortion angle Θ of $0.59(6)^\circ$. The pyramidalization of the amide carbonyl group indicates a weaker $n \rightarrow \pi^*$ interaction from the ketone to the amide than from the amide to the ester, as would be expected for the enclosing of a four-membered ring relative to the enclosing of a five-membered ring, respectively. Indeed, NBO analysis predicts release of $1.42 \text{ kcal mol}^{-1}$ of energy due to the $n \rightarrow \pi^*$ interaction between the ketone and amide (Fig. 5), which is nevertheless a significant contribution that likely biases the conformation of this molecule.

Based on the specific geometric parameters measured in this crystal structure, we conclude that the structure of unbound oxo-AHLs are influenced by $n \rightarrow \pi^*$ interactions, similarly to simple AHLs. Moreover, an additional $n \rightarrow \pi^*$ interaction specific to oxo-AHLs might bias their conformation further and thus affect their binding to protein receptors.

3. Supramolecular features

In the crystal, the molecules form translational chains along the a axis *via* $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds (Table 1 and Fig. 2).

4. Synthesis and crystallization

The title compound was prepared as reported previously (Eberhard & Schineller, 2000). A small amount of solid product was dissolved in hexanes with a minimal amount of dichloromethane. Slow evaporation afforded high-quality crystals after 4 days.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Except for hydrogen-bond donors and terminal methyl groups, all H atoms were placed in idealized locations and refined as riding with appropriate thermal displacement coefficients $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times $U_{\text{eq}}(\text{bearing atom})$.

Table 2
Experimental details.

| | |
|--|--|
| Crystal data | |
| Chemical formula | $\text{C}_8\text{H}_{11}\text{NO}_4$ |
| M_r | 185.18 |
| Crystal system, space group | Orthorhombic, $P2_12_12_1$ |
| Temperature (K) | 100 |
| a, b, c (Å) | 5.0215 (4), 9.8852 (10), 17.7668 (14) |
| V (Å ³) | 881.91 (14) |
| Z | 4 |
| Radiation type | Cu $K\alpha$ |
| μ (mm ⁻¹) | 0.96 |
| Crystal size (mm) | $0.23 \times 0.13 \times 0.04$ |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (SADABS; Bruker, 2014/5) |
| $T_{\text{min}}, T_{\text{max}}$ | 0.785, 0.841 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 11955, 1755, 1702 |
| R_{int} | 0.028 |
| $(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹) | 0.621 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$ | 0.026, 0.067, 1.04 |
| No. of reflections | 1755 |
| No. of parameters | 134 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³) | 0.22, -0.15 |
| Absolute structure | Flack x determined using 657 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013). |
| Absolute structure parameter | -0.01 (8) |

Computer programs: APEX2 (Bruker, 2012), SAINT (Bruker, 2013), SHELXS (Sheldrick, 2008), SHELXL (Sheldrick, 2015) and OLEX2 (Dolomanov *et al.*, 2009).

Acknowledgements

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Crystal structure of *N*-(3-oxobutanoyl)-*L*-homoserine lactone

R.W. Newberry and R.T. Raines

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

N-(3-Oxobutanoyl)-*L*-homoserine lactone

Crystal data

$C_8H_{11}NO_4$

$M_r = 185.18$

Orthorhombic, $P2_12_12_1$

$a = 5.0215$ (4) Å

$b = 9.8852$ (10) Å

$c = 17.7668$ (14) Å

$V = 881.91$ (14) Å³

$Z = 4$

$F(000) = 392$

$D_x = 1.395$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 6262 reflections

$\theta = 5.0$ – 73.3°

$\mu = 0.96$ mm⁻¹

$T = 100$ K

Block, colourless

$0.23 \times 0.13 \times 0.04$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2014/5)

$T_{\min} = 0.785$, $T_{\max} = 0.841$

11955 measured reflections

1755 independent reflections

1702 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 73.3^\circ$, $\theta_{\min} = 5.0^\circ$

$h = -6 \rightarrow 6$

$k = -12 \rightarrow 11$

$l = -22 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.067$

$S = 1.04$

1755 reflections

134 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 0.2168P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.22$ e Å⁻³

$\Delta\rho_{\min} = -0.15$ e Å⁻³

Absolute structure: Flack x determined using

657 quotients $[(I^-)-(I)]/[(I^+)+(I)]$ (Parsons *et al.*,
2013).

Absolute structure parameter: -0.01 (8)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|--------------|----------------------------------|
| O1 | 0.1639 (3) | 0.52850 (12) | 0.55760 (7) | 0.0190 (3) |
| O2 | −0.0589 (2) | 0.37968 (12) | 0.41512 (7) | 0.0189 (3) |
| N1 | 0.3857 (3) | 0.39964 (14) | 0.42086 (8) | 0.0156 (3) |
| O3 | 0.0157 (2) | 0.68079 (12) | 0.47556 (7) | 0.0164 (3) |
| O4 | 0.2366 (3) | 0.25259 (13) | 0.26283 (7) | 0.0253 (3) |
| C4 | 0.0901 (4) | 0.73341 (18) | 0.40163 (10) | 0.0189 (4) |
| H4A | 0.1855 | 0.8206 | 0.4069 | 0.023* |
| H4B | −0.0703 | 0.7480 | 0.3703 | 0.023* |
| C7 | 0.2289 (3) | 0.15843 (17) | 0.30622 (9) | 0.0166 (3) |
| C1 | 0.1762 (3) | 0.57897 (16) | 0.49600 (9) | 0.0141 (3) |
| C8 | 0.2475 (5) | 0.01346 (18) | 0.28126 (11) | 0.0230 (4) |
| C5 | 0.1638 (3) | 0.32746 (17) | 0.41024 (9) | 0.0142 (3) |
| C6 | 0.2005 (3) | 0.17999 (16) | 0.39064 (9) | 0.0161 (3) |
| H6A | 0.0454 | 0.1279 | 0.4092 | 0.019* |
| H6B | 0.3615 | 0.1451 | 0.4163 | 0.019* |
| C2 | 0.3719 (3) | 0.54444 (16) | 0.43286 (10) | 0.0158 (3) |
| H2 | 0.5528 | 0.5780 | 0.4472 | 0.019* |
| C3 | 0.2703 (4) | 0.62767 (17) | 0.36590 (10) | 0.0200 (4) |
| H3A | 0.4199 | 0.6710 | 0.3387 | 0.024* |
| H3B | 0.1696 | 0.5701 | 0.3303 | 0.024* |
| H1 | 0.534 (5) | 0.363 (2) | 0.4159 (12) | 0.018 (5)* |
| H8A | 0.389 (5) | −0.031 (3) | 0.3095 (14) | 0.030 (6)* |
| H8B | 0.073 (6) | −0.032 (3) | 0.2945 (15) | 0.044 (8)* |
| H8C | 0.272 (6) | 0.006 (3) | 0.2277 (15) | 0.034 (6)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|------------|------------|-------------|-------------|-------------|
| O1 | 0.0201 (6) | 0.0182 (6) | 0.0187 (6) | −0.0031 (5) | 0.0022 (5) | 0.0006 (5) |
| O2 | 0.0105 (5) | 0.0182 (6) | 0.0279 (6) | 0.0009 (5) | 0.0000 (5) | −0.0035 (5) |
| N1 | 0.0093 (6) | 0.0163 (7) | 0.0213 (7) | 0.0032 (6) | 0.0009 (5) | −0.0034 (6) |
| O3 | 0.0141 (5) | 0.0160 (6) | 0.0192 (6) | 0.0013 (5) | 0.0027 (5) | −0.0007 (5) |
| O4 | 0.0359 (8) | 0.0200 (6) | 0.0201 (6) | 0.0004 (6) | 0.0007 (6) | 0.0030 (5) |
| C4 | 0.0192 (8) | 0.0199 (8) | 0.0176 (8) | 0.0009 (7) | −0.0012 (7) | 0.0018 (7) |
| C7 | 0.0131 (7) | 0.0182 (8) | 0.0185 (8) | −0.0006 (7) | −0.0008 (6) | 0.0003 (6) |
| C1 | 0.0107 (7) | 0.0125 (7) | 0.0191 (8) | −0.0046 (6) | 0.0004 (6) | −0.0033 (6) |
| C8 | 0.0316 (10) | 0.0185 (8) | 0.0190 (8) | 0.0005 (8) | −0.0004 (8) | −0.0024 (7) |
| C5 | 0.0125 (7) | 0.0170 (7) | 0.0132 (7) | 0.0016 (7) | 0.0000 (6) | 0.0009 (6) |
| C6 | 0.0158 (8) | 0.0145 (7) | 0.0180 (8) | 0.0011 (7) | −0.0001 (6) | 0.0005 (6) |

| | | | | | | |
|----|------------|------------|------------|-------------|------------|-------------|
| C2 | 0.0121 (7) | 0.0155 (8) | 0.0196 (8) | -0.0013 (6) | 0.0021 (6) | -0.0028 (6) |
| C3 | 0.0205 (8) | 0.0202 (8) | 0.0193 (8) | -0.0001 (8) | 0.0037 (7) | 0.0012 (6) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|------------|------------|
| O1—C1 | 1.204 (2) | C2—C3 | 1.534 (2) |
| O2—C5 | 1.235 (2) | C2—H2 | 1.000 |
| N1—C5 | 1.337 (2) | C3—H3a | 0.990 |
| N1—C2 | 1.449 (2) | C3—H3b | 0.990 |
| O3—C4 | 1.461 (2) | C4—H4a | 0.990 |
| O3—C1 | 1.340 (2) | C4—H4b | 0.990 |
| O4—C7 | 1.209 (2) | N1—H1 | 0.83 (2) |
| C4—C3 | 1.521 (2) | C6—H6a | 0.990 |
| C7—C8 | 1.503 (2) | C6—H6b | 0.990 |
| C7—C6 | 1.522 (2) | C8—H8a | 0.98 (3) |
| C1—C2 | 1.530 (2) | C8—H8b | 1.01 (3) |
| C5—C6 | 1.510 (2) | C8—H8c | 0.96 (3) |
| C5—N1—C2 | 120.55 (14) | C4—C3—H3a | 111.0 |
| C1—O3—C4 | 110.93 (13) | C4—C3—H3b | 111.0 |
| O3—C4—C3 | 106.42 (13) | H3a—C3—H3b | 109.0 |
| O4—C7—C8 | 122.95 (15) | C3—C4—H4a | 110.4 |
| O4—C7—C6 | 121.57 (15) | C3—C4—H4b | 110.4 |
| C8—C7—C6 | 115.48 (14) | O3—C4—H4a | 110.4 |
| O1—C1—O3 | 121.79 (15) | O3—C4—H4b | 110.4 |
| O1—C1—C2 | 127.35 (15) | H4a—C4—H4b | 108.6 |
| O3—C1—C2 | 110.82 (14) | C2—N1—H1 | 119.2 (15) |
| O2—C5—N1 | 121.47 (15) | C5—N1—H1 | 119.9 (15) |
| O2—C5—C6 | 122.02 (15) | C5—C6—H6a | 109.2 |
| N1—C5—C6 | 116.50 (14) | C5—C6—H6b | 109.2 |
| C5—C6—C7 | 111.96 (13) | C7—C6—H6a | 109.2 |
| N1—C2—C1 | 111.04 (13) | C7—C6—H6b | 109.2 |
| N1—C2—C3 | 115.58 (15) | H6a—C6—H6b | 107.9 |
| C1—C2—C3 | 103.61 (14) | C7—C8—H8a | 108.9 (17) |
| C4—C3—C2 | 104.05 (14) | C7—C8—H8b | 107.5 (17) |
| C1—C2—H2 | 108.8 | C7—C8—H8c | 111.9 (18) |
| N1—C2—H2 | 108.8 | H8a—C8—H8b | 108 (2) |
| C3—C2—H2 | 108.8 | H8b—C8—H8c | 108 (2) |
| C2—C3—H3a | 111.0 | H8c—C8—H8a | 112 (2) |
| C2—C3—H3b | 111.0 | | |

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> |
|--------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N1—H1 \cdots O2 ⁱ | 0.83 (2) | 2.05 (2) | 2.7973 (19) | 149 (2) |

Symmetry code: (i) $x+1, y, z$.