

# A monoclinic modification of (4Z)-1-benzyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one

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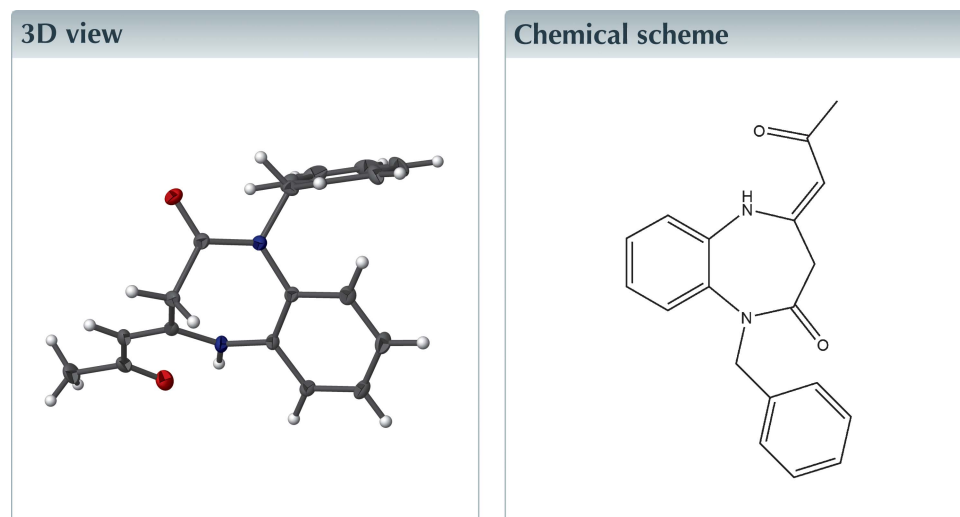
Keywords: crystal structure; benzodiazepine; hydrogen bond;  $\pi$ -stacking.

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Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

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In the title molecule, C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>, the orientation of the oxopropylidene substituent is largely determined by an intramolecular N—H...O hydrogen bond. In the crystal, C—H...O hydrogen bonds form zigzag chains, which are elaborated into sheets lying parallel to (10 $\bar{1}$ ) by complementary C—H... $\pi$  interactions. Comparisons to the structure of the triclinic modification are made.



## Structure description

Benzodiazepine derivatives are widely used as anticonvulsants, antidepressives, sedatives and analgesics (Schultz *et al.*, 1982; Olkkola *et al.*, 2008). In addition, they are used as medicinal agents in the treatment of central nervous system (CNS) disturbances (Stefancich *et al.*, 1992). They also exhibit antitumor and antineoplastic activities (Werner *et al.*, 1990). As part of our ongoing studies in this area (Sebhaoui *et al.*, 2016, 2017) we now describe the synthesis and crystal structure of a monoclinic modification of the title compound to complement the known triclinic polymorph (Samba *et al.*, 2016).

The dihedral angle between the mean planes of the C1–C6 and C11–C16 rings is 79.02 (5)°. A puckering analysis of the seven-membered ring gave the parameters  $Q(2) = 0.866$  (1) Å,  $Q(3) = 0.230$  (1) Å,  $\varphi(2) = 210.27$  (7)° and  $\varphi(3) = 311.2$  (2)°. The orientation of the oxopropylidene substituent is largely determined by the intramolecular N2—H2A...O2 hydrogen bond (Table 1 and Fig. 1). In the crystal, C5—H5...O1<sup>i</sup> and C10—H10A...O1<sup>i</sup> hydrogen bonds form zigzag chains aligned with the  $a/2 + c/2$  diagonal of the  $ac$  face (Table 1 and Fig. 2). The chains have the benzyl substituents all protruding from

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the C11–C16 benzene ring.

D–H...A	D–H	H...A	D...A	D–H...A
N2–H2A...O2	0.927 (16)	1.921 (15)	2.6613 (11)	135.4 (12)
C5–H5...O1 <sup>i</sup>	0.943 (15)	2.350 (15)	3.2823 (12)	170.0 (13)
C10–H10A...O1 <sup>i</sup>	1.005 (14)	2.571 (14)	3.5518 (12)	165.2 (11)
C2–H2...Cg2 <sup>ii</sup>	0.973 (14)	2.81 (2)	3.625 (1)	142 (1)

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

the same side and are joined into sheets lying parallel to (10 $\bar{1}$ ) by complementary C2–H2... $\pi$ (Cg2)<sup>iii</sup> interactions (Table 1 and Figs. 2 and 3).

While the various conformational parameters of the title compound are quite similar to those of the two independent molecules in the triclinic modification (Samba *et al.*, 2016; CSD refcode AWUXUN) [*e.g.*  $Q(2) = 0.872(1) \text{ \AA}$ ,  $Q(3) = 0.208(1) \text{ \AA}$ ,  $\varphi(2) = 206.93(3)^\circ$  and  $\varphi(3) = 303.3(4)^\circ$  for mol-

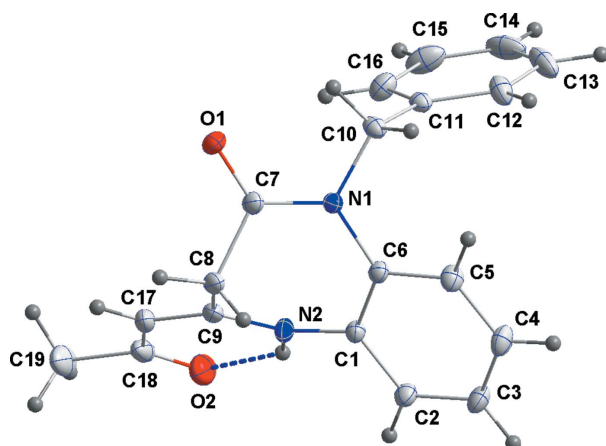


Figure 1

The title molecule with the labelling scheme and 50% probability ellipsoids. The intramolecular N–H...O hydrogen bond is shown as a dashed line.

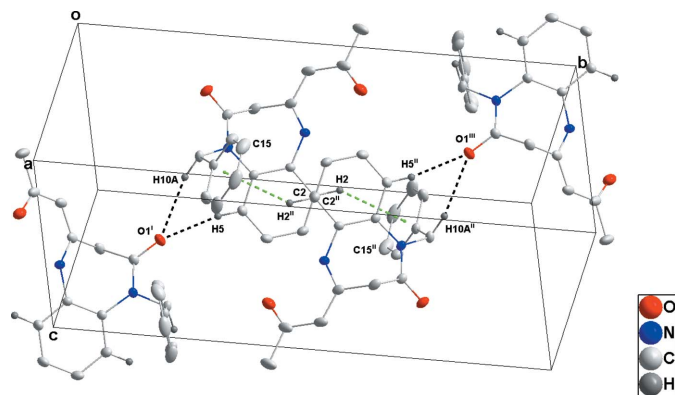


Figure 2

Details of the intermolecular C–H...O hydrogen bonding (black dashed lines) and the C–H... $\pi$ (ring) interactions (green dashed lines). [Symmetry codes: (i)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ .]

Table 2

Experimental details.

Crystal data	
Chemical formula	C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
$M_r$	306.35
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
$a, b, c$ (Å)	8.9229 (5), 18.8922 (10), 9.7147 (5)
$\beta$ (°)	104.879 (1)
$V$ (Å <sup>3</sup> )	1582.73 (15)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	0.08
Crystal size (mm)	0.43 × 0.34 × 0.33
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2016)
$T_{\min}, T_{\max}$	0.90, 0.97
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	30264, 4290, 3840
$R_{\text{int}}$	0.027
( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.687
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.043, 0.120, 1.03
No. of reflections	4290
No. of parameters	269
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.45, -0.28

Computer programs: APEX3 (Bruker, 2016), SAINT (Bruker, 2016), SHELXT (Sheldrick, 2015a), SHELXL2016 (Sheldrick, 2015b), DIAMOND (Brandenburg & Putz, 2012), SHELXTL (Sheldrick, 2008).

ecule 1, while for molecule 2, the corresponding values are 0.814 (1) Å, 0.199 (1) Å, 207.66 (9)° and 313.3 (4)°, respectively), the crystal packing is distinctly different. In the triclinic form, complementary C–H...O hydrogen bonds between centrosymmetrically related pairs of molecule 2 form weak dimers with each member of the pair making a weak C–H...O hydrogen bond to a molecule 1. These entities then pack in rows extending parallel to the  $c$ -axis direction.

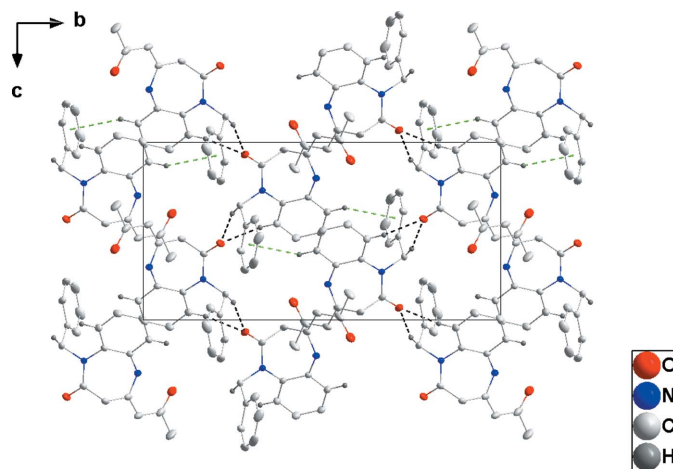


Figure 3

Packing viewed along the  $a$ -axis direction with intermolecular interactions depicted as in Fig. 2.

## Synthesis and crystallization

(4Z)-4-(2-Oxopropylidene)-1,5-benzodiazepin-2-one (0.01 mol) and potassium carbonate  $K_2CO_3$  (0.02 mol) were dissolved in DMF, then benzylbromide (0.02 mol) and tetrabutylammonium bromide as a phase-transfer catalyst (0.001 mol) were added. The reaction mixture was stirred at room temperature for 48 h. The residue obtained, after evaporation of solvent, was chromatographed on a silica gel column using a hexane/ethyl acetate 9:1 mixture as eluent. The solid obtained was crystallized from dichloromethane solution to afford as colourless blocks. The triclinic modification was crystallized from ethanol solution (Samba *et al.*, 2016).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

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## full crystallographic data

*IUCrData* (2018). 3, x180326 [https://doi.org/10.1107/S2414314618003267]

## A monoclinic modification of (4*Z*)-1-benzyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepin-2-one

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(4*Z*)-1-Benzyl-4-(2-oxopropylidene)-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepin-2-one

### Crystal data

C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>

*M<sub>r</sub>* = 306.35

Monoclinic, *P*2<sub>1</sub>/*n*

*a* = 8.9229 (5) Å

*b* = 18.8922 (10) Å

*c* = 9.7147 (5) Å

β = 104.879 (1)°

*V* = 1582.73 (15) Å<sup>3</sup>

*Z* = 4

*F*(000) = 648

*D<sub>x</sub>* = 1.286 Mg m<sup>-3</sup>

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 9497 reflections

θ = 2.8–29.2°

μ = 0.08 mm<sup>-1</sup>

*T* = 100 K

Block, colourless

0.43 × 0.34 × 0.33 mm

### Data collection

Bruker SMART APEX CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.3333 pixels mm<sup>-1</sup>

φ and ω scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2016)

*T<sub>min</sub>* = 0.90, *T<sub>max</sub>* = 0.97

30264 measured reflections

4290 independent reflections

3840 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.027

θ<sub>max</sub> = 29.2°, θ<sub>min</sub> = 2.2°

*h* = -12→12

*k* = -25→25

*l* = -13→13

### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.043

*wR*(*F*<sup>2</sup>) = 0.120

*S* = 1.03

4290 reflections

269 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent  
and constrained refinement

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0723*P*)<sup>2</sup> + 0.4643*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = 0.001

Δρ<sub>max</sub> = 0.45 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.28 e Å<sup>-3</sup>

*Special details*

**Experimental.** The diffraction data were obtained from 3 sets of 400 frames, each of width  $0.5^\circ$  in  $\omega$ , collected at  $\varphi = 0.00, 90.00$  and  $180.00^\circ$  and 2 sets of 800 frames, each of width  $0.45^\circ$  in  $\varphi$ , collected at  $\omega = -30.00$  and  $210.00^\circ$ . The scan time was 15 sec/frame.

**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  $F^2 > 2\sigma(F^2)$  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.

Independent refinement of the hydrogens attached to C19 led to an unsatisfactory geometry so they were placed in calculated positions and included as riding contributions.

Independent refinement of the H atoms attached to C19 led to an unsatisfactory geometry so they were placed in calculated positions and included as riding contributions.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.32106 (9)	0.28428 (4)	0.06813 (8)	0.02234 (17)
O2	0.18336 (10)	0.57963 (4)	0.09910 (9)	0.02928 (19)
N1	0.47383 (10)	0.33296 (4)	0.27077 (8)	0.01491 (17)
N2	0.40185 (10)	0.48362 (4)	0.20128 (9)	0.01720 (17)
H2A	0.3522 (18)	0.5254 (8)	0.2131 (15)	0.029 (4)*
C1	0.53064 (11)	0.46141 (5)	0.30978 (9)	0.01433 (18)
C2	0.62092 (12)	0.51468 (5)	0.39148 (10)	0.01812 (19)
H2	0.5929 (16)	0.5639 (8)	0.3687 (15)	0.024 (3)*
C3	0.74494 (12)	0.49803 (5)	0.50523 (11)	0.0212 (2)
H3	0.8050 (17)	0.5351 (8)	0.5616 (15)	0.028 (4)*
C4	0.78186 (12)	0.42744 (6)	0.53783 (11)	0.0220 (2)
H4	0.8681 (18)	0.4154 (8)	0.6179 (16)	0.031 (4)*
C5	0.69518 (12)	0.37418 (5)	0.45648 (11)	0.0189 (2)
H5	0.7218 (17)	0.3265 (8)	0.4788 (16)	0.027 (3)*
C6	0.56769 (10)	0.38998 (5)	0.34242 (9)	0.01408 (18)
C7	0.40872 (11)	0.33147 (5)	0.12711 (10)	0.01607 (19)
C8	0.44886 (12)	0.39302 (5)	0.04263 (10)	0.0187 (2)
H8A	0.5607 (16)	0.4023 (7)	0.0738 (15)	0.025 (3)*
H8B	0.4211 (16)	0.3796 (7)	-0.0595 (15)	0.023 (3)*
C9	0.36035 (11)	0.45702 (5)	0.06729 (10)	0.0178 (2)
C10	0.45330 (12)	0.27023 (5)	0.35546 (10)	0.01635 (19)
H10A	0.5572 (16)	0.2486 (8)	0.4007 (14)	0.021 (3)*
H10B	0.3908 (17)	0.2358 (8)	0.2861 (15)	0.025 (3)*
C11	0.37144 (11)	0.28643 (5)	0.46926 (10)	0.01497 (18)
C12	0.44441 (14)	0.27264 (5)	0.61138 (11)	0.0233 (2)
H12	0.5538 (18)	0.2535 (8)	0.6382 (16)	0.034 (4)*
C13	0.36628 (18)	0.28330 (6)	0.71659 (12)	0.0318 (3)
H13	0.417 (2)	0.2742 (10)	0.8183 (19)	0.048 (5)*
C14	0.21624 (17)	0.30856 (6)	0.68034 (14)	0.0338 (3)

H14	0.163 (2)	0.3172 (10)	0.752 (2)	0.058 (6)*
C15	0.14262 (14)	0.32281 (7)	0.53895 (15)	0.0318 (3)
H15	0.041 (2)	0.3410 (10)	0.513 (2)	0.053 (5)*
C16	0.22028 (12)	0.31183 (6)	0.43331 (12)	0.0224 (2)
H16	0.1684 (18)	0.3224 (8)	0.3322 (17)	0.033 (4)*
C17	0.24371 (13)	0.48605 (6)	-0.03786 (11)	0.0229 (2)
H17	0.2218 (18)	0.4641 (8)	-0.1292 (17)	0.031 (4)*
C18	0.15993 (13)	0.54845 (6)	-0.01710 (12)	0.0257 (2)
C19	0.04049 (15)	0.57702 (7)	-0.14480 (14)	0.0367 (3)
H19A	-0.021533	0.613573	-0.113690	0.055*
H19B	-0.027467	0.538449	-0.191022	0.055*
H19C	0.093060	0.597542	-0.212431	0.055*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0274 (4)	0.0206 (3)	0.0178 (4)	-0.0092 (3)	0.0035 (3)	-0.0039 (3)
O2	0.0279 (4)	0.0269 (4)	0.0280 (4)	0.0030 (3)	-0.0019 (3)	0.0056 (3)
N1	0.0192 (4)	0.0135 (3)	0.0120 (4)	-0.0021 (3)	0.0041 (3)	-0.0009 (3)
N2	0.0186 (4)	0.0168 (4)	0.0135 (4)	0.0007 (3)	-0.0009 (3)	0.0003 (3)
C1	0.0148 (4)	0.0155 (4)	0.0119 (4)	0.0002 (3)	0.0019 (3)	-0.0002 (3)
C2	0.0204 (4)	0.0155 (4)	0.0169 (4)	-0.0010 (3)	0.0018 (4)	-0.0021 (3)
C3	0.0202 (5)	0.0211 (5)	0.0190 (5)	-0.0016 (4)	-0.0011 (4)	-0.0056 (4)
C4	0.0185 (4)	0.0242 (5)	0.0191 (5)	0.0042 (4)	-0.0026 (4)	-0.0027 (4)
C5	0.0193 (4)	0.0172 (4)	0.0185 (4)	0.0040 (3)	0.0017 (4)	-0.0006 (3)
C6	0.0154 (4)	0.0142 (4)	0.0126 (4)	-0.0005 (3)	0.0036 (3)	-0.0019 (3)
C7	0.0184 (4)	0.0170 (4)	0.0136 (4)	-0.0026 (3)	0.0056 (3)	-0.0022 (3)
C8	0.0250 (5)	0.0197 (4)	0.0122 (4)	-0.0071 (4)	0.0061 (3)	-0.0011 (3)
C9	0.0203 (4)	0.0187 (4)	0.0133 (4)	-0.0072 (3)	0.0026 (3)	0.0021 (3)
C10	0.0228 (5)	0.0120 (4)	0.0153 (4)	0.0012 (3)	0.0069 (3)	0.0004 (3)
C11	0.0195 (4)	0.0114 (4)	0.0147 (4)	-0.0012 (3)	0.0058 (3)	-0.0001 (3)
C12	0.0347 (6)	0.0191 (4)	0.0160 (5)	0.0062 (4)	0.0063 (4)	0.0025 (3)
C13	0.0605 (8)	0.0210 (5)	0.0184 (5)	0.0015 (5)	0.0183 (5)	0.0023 (4)
C14	0.0510 (7)	0.0248 (5)	0.0378 (7)	-0.0117 (5)	0.0338 (6)	-0.0077 (5)
C15	0.0218 (5)	0.0322 (6)	0.0462 (7)	-0.0062 (4)	0.0172 (5)	-0.0133 (5)
C16	0.0184 (5)	0.0241 (5)	0.0237 (5)	-0.0015 (4)	0.0035 (4)	-0.0055 (4)
C17	0.0247 (5)	0.0254 (5)	0.0150 (5)	-0.0083 (4)	-0.0016 (4)	0.0052 (4)
C18	0.0217 (5)	0.0256 (5)	0.0245 (5)	-0.0069 (4)	-0.0038 (4)	0.0113 (4)
C19	0.0321 (6)	0.0351 (6)	0.0327 (6)	-0.0030 (5)	-0.0102 (5)	0.0163 (5)

*Geometric parameters (Å, °)*

O1—C7	1.2267 (12)	C9—C17	1.3716 (14)
O2—C18	1.2425 (15)	C10—C11	1.5047 (13)
N1—C7	1.3674 (12)	C10—H10A	1.005 (14)
N1—C6	1.4309 (11)	C10—H10B	0.997 (14)
N1—C10	1.4806 (12)	C11—C16	1.3891 (14)
N2—C9	1.3552 (12)	C11—C12	1.3915 (14)

N2—C1	1.4091 (12)	C12—C13	1.3918 (16)
N2—H2A	0.927 (16)	C12—H12	1.010 (16)
C1—C2	1.4012 (13)	C13—C14	1.379 (2)
C1—C6	1.4061 (12)	C13—H13	0.990 (18)
C2—C3	1.3844 (14)	C14—C15	1.388 (2)
C2—H2	0.973 (14)	C14—H14	0.95 (2)
C3—C4	1.3907 (14)	C15—C16	1.3934 (16)
C3—H3	0.963 (15)	C15—H15	0.941 (19)
C4—C5	1.3861 (14)	C16—H16	0.993 (16)
C4—H4	0.971 (15)	C17—C18	1.4376 (17)
C5—C6	1.4013 (13)	C17—H17	0.954 (16)
C5—H5	0.943 (15)	C18—C19	1.5123 (15)
C7—C8	1.5182 (13)	C19—H19A	0.9800
C8—C9	1.4968 (14)	C19—H19B	0.9800
C8—H8A	0.981 (14)	C19—H19C	0.9800
C8—H8B	0.992 (14)		
C7—N1—C6	123.66 (8)	N1—C10—C11	113.46 (7)
C7—N1—C10	118.03 (8)	N1—C10—H10A	109.7 (8)
C6—N1—C10	118.22 (7)	C11—C10—H10A	109.2 (8)
C9—N2—C1	125.27 (9)	N1—C10—H10B	105.9 (8)
C9—N2—H2A	114.4 (9)	C11—C10—H10B	109.7 (8)
C1—N2—H2A	119.0 (9)	H10A—C10—H10B	108.8 (11)
C2—C1—C6	119.60 (8)	C16—C11—C12	119.40 (9)
C2—C1—N2	116.73 (8)	C16—C11—C10	120.58 (9)
C6—C1—N2	123.63 (8)	C12—C11—C10	119.94 (9)
C3—C2—C1	120.96 (9)	C11—C12—C13	120.43 (11)
C3—C2—H2	120.3 (8)	C11—C12—H12	119.8 (9)
C1—C2—H2	118.7 (8)	C13—C12—H12	119.7 (8)
C2—C3—C4	119.59 (9)	C14—C13—C12	119.94 (11)
C2—C3—H3	120.2 (9)	C14—C13—H13	118.5 (11)
C4—C3—H3	120.2 (9)	C12—C13—H13	121.5 (11)
C5—C4—C3	120.10 (9)	C13—C14—C15	120.09 (11)
C5—C4—H4	119.8 (9)	C13—C14—H14	120.5 (12)
C3—C4—H4	120.1 (9)	C15—C14—H14	119.4 (12)
C4—C5—C6	121.13 (9)	C14—C15—C16	120.09 (11)
C4—C5—H5	119.5 (9)	C14—C15—H15	120.8 (12)
C6—C5—H5	119.4 (9)	C16—C15—H15	119.1 (12)
C5—C6—C1	118.62 (8)	C11—C16—C15	120.04 (11)
C5—C6—N1	118.63 (8)	C11—C16—H16	119.6 (9)
C1—C6—N1	122.59 (8)	C15—C16—H16	120.3 (9)
O1—C7—N1	122.99 (9)	C9—C17—C18	123.08 (10)
O1—C7—C8	120.99 (9)	C9—C17—H17	117.0 (9)
N1—C7—C8	116.02 (8)	C18—C17—H17	119.8 (9)
C9—C8—C7	108.95 (8)	O2—C18—C17	122.95 (10)
C9—C8—H8A	110.0 (8)	O2—C18—C19	119.66 (11)
C7—C8—H8A	109.4 (8)	C17—C18—C19	117.38 (11)
C9—C8—H8B	111.1 (8)	C18—C19—H19A	109.5

C7—C8—H8B	108.2 (8)	C18—C19—H19B	109.5
H8A—C8—H8B	109.1 (12)	H19A—C19—H19B	109.5
N2—C9—C17	122.35 (10)	C18—C19—H19C	109.5
N2—C9—C8	115.34 (8)	H19A—C19—H19C	109.5
C17—C9—C8	122.31 (9)	H19B—C19—H19C	109.5
C9—N2—C1—C2	136.19 (10)	N1—C7—C8—C9	-75.07 (11)
C9—N2—C1—C6	-46.44 (14)	C1—N2—C9—C17	-172.77 (9)
C6—C1—C2—C3	-0.89 (15)	C1—N2—C9—C8	8.21 (13)
N2—C1—C2—C3	176.59 (9)	C7—C8—C9—N2	67.29 (11)
C1—C2—C3—C4	0.87 (16)	C7—C8—C9—C17	-111.73 (10)
C2—C3—C4—C5	0.22 (16)	C7—N1—C10—C11	-120.24 (9)
C3—C4—C5—C6	-1.29 (16)	C6—N1—C10—C11	63.16 (11)
C4—C5—C6—C1	1.25 (15)	N1—C10—C11—C16	62.23 (12)
C4—C5—C6—N1	-174.18 (9)	N1—C10—C11—C12	-121.00 (10)
C2—C1—C6—C5	-0.16 (14)	C16—C11—C12—C13	0.79 (15)
N2—C1—C6—C5	-177.46 (9)	C10—C11—C12—C13	-176.02 (9)
C2—C1—C6—N1	175.07 (8)	C11—C12—C13—C14	-0.83 (17)
N2—C1—C6—N1	-2.22 (14)	C12—C13—C14—C15	0.53 (18)
C7—N1—C6—C5	-142.94 (10)	C13—C14—C15—C16	-0.19 (18)
C10—N1—C6—C5	33.45 (12)	C12—C11—C16—C15	-0.45 (15)
C7—N1—C6—C1	41.82 (13)	C10—C11—C16—C15	176.34 (9)
C10—N1—C6—C1	-141.79 (9)	C14—C15—C16—C11	0.15 (17)
C6—N1—C7—O1	-175.57 (9)	N2—C9—C17—C18	2.56 (16)
C10—N1—C7—O1	8.03 (14)	C8—C9—C17—C18	-178.49 (9)
C6—N1—C7—C8	3.42 (13)	C9—C17—C18—O2	-2.38 (17)
C10—N1—C7—C8	-172.98 (8)	C9—C17—C18—C19	176.56 (10)
O1—C7—C8—C9	103.94 (10)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg2 is the centroid of the C11–C16 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A $\cdots$ O2	0.927 (16)	1.921 (15)	2.6613 (11)	135.4 (12)
C5—H5 $\cdots$ O1 <sup>i</sup>	0.943 (15)	2.350 (15)	3.2823 (12)	170.0 (13)
C10—H10A $\cdots$ O1 <sup>i</sup>	1.005 (14)	2.571 (14)	3.5518 (12)	165.2 (11)
C2—H2 $\cdots$ Cg2 <sup>ii</sup>	0.973 (14)	2.81 (2)	3.625 (1)	142 (1)

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