IUCrData

ISSN 2414-3146

(4*Z*)-4-(2-Oxopropylidene)-1,3-bis(prop-2-en-1-yl)-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepin-2-one

Jihad Sebhaoui,[a]* Youness El Bakri,[a] Ibtissam Rayni,[a] Khadija El Bourakadi,[a] El Mokhtar Essassi[a] and Joel T. Mague[b]

[a]Laboratoire de Chimie Organique Hétérocyclique, URAC 21, Pôle de Compétence Pharmacochimie, Av Ibn Battouta, BP 1014, Faculté des Sciences, Mohammed V University, Rabat, Morocco, and [b]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: sebhaoui.jihad@gmail.com

Received 27 March 2017
Accepted 29 March 2017

Edited by J. Simpson, University of Otago, New Zealand

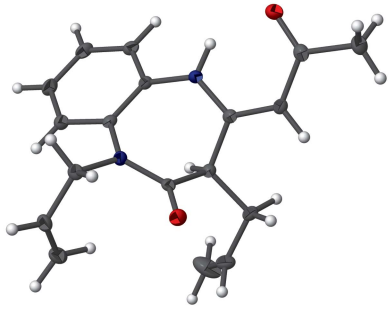
Keywords: crystal structure; hydrogen bond; diazepine; crystal structure.

CCDC reference: 1541017

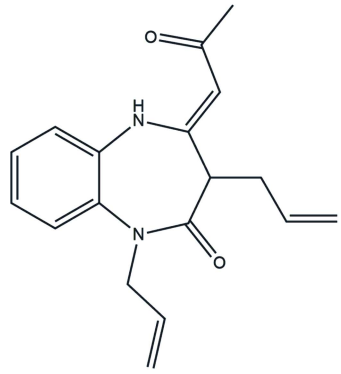
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{20}N_2O_2$, the diazepin-2-one ring adopts a tub conformation. The conformation of the acetyl group is partially determined by an intramolecular N—H···O hydrogen bond. In the crystal, pairwise C—H···O hydrogen bonds form inversion dimers.

3D view



Chemical scheme



Structure description

1,5-Benzodiazepine derivatives have attracted much attention as they exhibit pronounced anxiolytic, sedative, hypnotic and anticonvulsant activities with low toxicity (Landquist *et al.*, 1984; Hamor *et al.*, 1984; Ben-Cherif *et al.*, 2010). They are also used as an intermediates for the synthesis of new heterocyclic systems (Ahabchane *et al.*, 2001; Minnih *et al.*, 2014). In a continuation of our work on the synthesis and structure of 1,5-benzodiazepine derivatives (Sebhaoui *et al.*, 2016), we report here the preparation and crystal structure of the title compound.

The seven-membered ring adopts a tub conformation. Puckering analysis of the conformation gave the parameters $Q(2)$ = 0.891 (1) Å, $Q(3)$ = 0.295 (1) Å, $\varphi(2)$ = 204.93 (7)° and $\varphi(3)$ = 311.0 (2)° with a total puckering amplitude of 0.928 (1) Å. The orientation of the acetyl substituent is determined in part by the intramolecular N1—H1···O2 hydrogen bond (Table 1 and Fig. 1).

In the crystal, molecules form inversion dimers through complementary C10—H10···O1^{i} hydrogen bonds (Table 1 and Fig. 2).

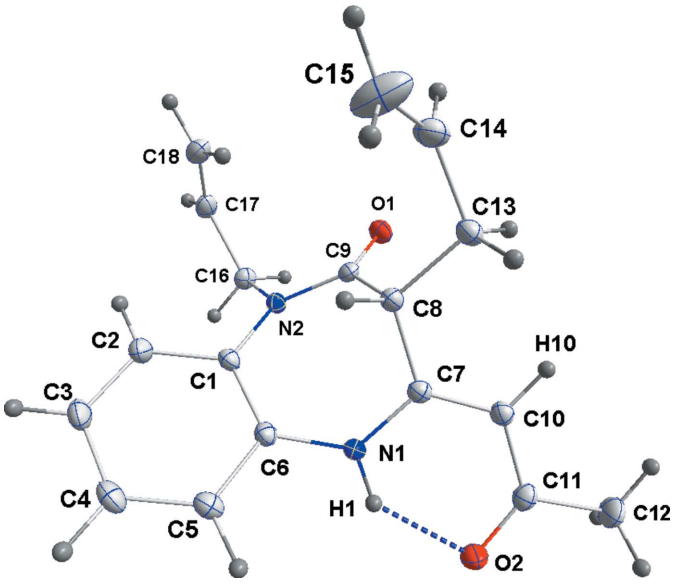


Figure 1
The title molecule with the labeling scheme and 50% probability ellipsoids. The intramolecular hydrogen bond is shown as a dashed line.

Synthesis and crystallization

To a solution of (4*Z*)-4-(-2-oxopropylidene)-1,5-benzodiazepin-2-one (0.01 mol) in 60 ml of *N*,*N*-dimethylformamide were added K_2CO_3 (0.02 mol), allyl bromide (0.02 mol) and tetra *n*-butylammonium bromide (TBAB) (0.001 mol). The reaction mixture was stirred at room temperature for 48 h. The solution was filtered and the solvent removed under reduced pressure. The residue was chromatographed on a silica gel column using hexane and ethyl acetate (90/10) as eluents to afford the title compound as colourless crystals.

Refinement

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

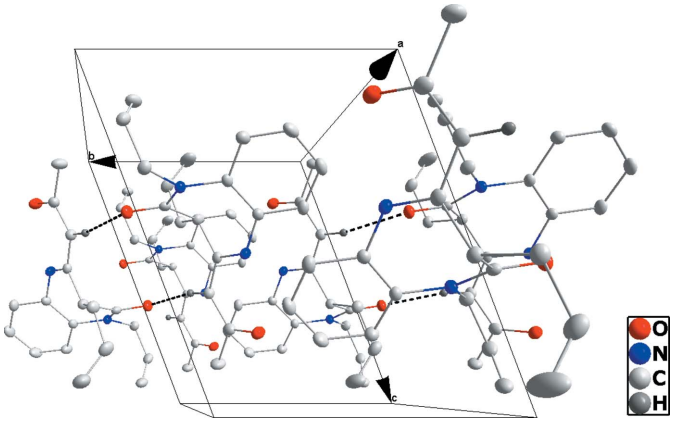


Figure 2
Packing projected onto (001) with intermolecular C—H···O hydrogen bonds shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.910 (17)	1.878 (16)	2.6308 (12)	138.6 (14)
C10—H10···O1^{i}	0.977 (14)	2.567 (14)	3.5316 (13)	168.9 (11)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{20}N_2O_2$
M_r	296.36
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	8.6864 (6), 8.9925 (6), 10.9872 (7)
α, β, γ (°)	110.653 (1), 95.111 (1), 104.723 (1)
V (Å^3)	761.42 (9)
Z	2
Radiation type	Mo *Kα*
μ (mm^{-1})	0.09
Crystal size (mm)	0.36 × 0.25 × 0.25
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.88, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14767, 4041, 3219
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.685
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.128, 1.09
No. of reflections	4041
No. of parameters	279
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.24

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012)and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

JTM thanks Tulane University for support of the Tulane Crystallography Laboratory.

References

Ahabchane, N. H., Ibrahimi, S., Salem, M., Essassi, E. M., Amzazi, S. & Benjouad, A. (2001). *C. R. Chem.* **4**, 917–924.
Ben-Cherif, W., Gharbi, R., Sebai, H., Dridi, D., Boughattas, N. A. & Ben-Attia, M. (2010). *C. R. Biol.* **333**, 214–219.
Brandenburg, K. & Putz, H. (2012). *DIAMOND*, Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hamor, T. A. & Martin, I. I. (1984). *Structure–activity relationships in a series of 5-phenyl-1,4-benzodiazepines.* In *X-ray crystallography and drug action* edited by A. S. Horn & C. J. Ranter, pp. 275–301. Oxford: Clarendon press.
Landquist, J. K., Katritzky, A. R. & Rees, C. W. (1984). In *Comprehensive Heterocyclic Chemistry*, Vol. 1, pp. 166–170. Oxford: Pergamon.

Minnih, M. S., Kandri Rodi, Y. & Essassi, E. M. (2014). *J. Marocain. Chim. Heterocycl.* **13**, 1–24.
Sebhaoui, J., El Bakri, Y., Rayni, I., Essassi, E. M. & Mague, J. T. (2016). *IUCrData*, **1**, x161013.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2017). **2**, x170493 [https://doi.org/10.1107/S241431461700493X]

(4*Z*)-4-(2-Oxopropylidene)-1,3-bis(prop-2-en-1-yl)-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepin-2-one

Jihad Sebhaoui, Youness El Bakri, Ibtissam Rayni, Khadija El Bourakadi, El Mokhtar Essassi and Joel T. Mague

(4*Z*)-4-(2-Oxopropylidene)-1,3-bis(prop-2-en-1-yl)-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepin-2-one

Crystal data

$C_{18}H_{20}N_2O_2$
M_r = 296.36
Triclinic, $P\overline{1}$
a = 8.6864 (6) Å
b = 8.9925 (6) Å
c = 10.9872 (7) Å
α = 110.653 (1)°
β = 95.111 (1)°
γ = 104.723 (1)°
V = 761.42 (9) Å^3
Z = 2
$F(000)$ = 316
D_x = 1.293 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6420 reflections
θ = 2.5–29.2°
μ = 0.09 mm^{-1}
T = 100 K
Block, colourless
0.36 × 0.25 × 0.25 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.88, T_{max} = 0.98
14767 measured reflections
4041 independent reflections
3219 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 29.2°, θ_{min} = 2.0°
h = −11→11
k = −12→12
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
S = 1.09
4041 reflections
279 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2 + 0.0641P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 10 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.72540 (10)	0.99583 (9)	0.37759 (8)	0.01874 (19)
O2	0.68608 (10)	0.68232 (10)	0.74999 (8)	0.0219 (2)
N1	0.73630 (11)	0.63488 (11)	0.50839 (9)	0.0149 (2)
H1	0.7503 (19)	0.6185 (19)	0.5852 (17)	0.033 (4)*
N2	0.86150 (10)	0.80420 (10)	0.33693 (9)	0.0134 (2)
C1	0.87072 (12)	0.64209 (12)	0.32073 (10)	0.0137 (2)
C2	0.95114 (13)	0.56478 (14)	0.22408 (11)	0.0183 (2)
H2	0.9908 (17)	0.6174 (17)	0.1664 (14)	0.020 (3)*
C3	0.97350 (14)	0.41321 (15)	0.21084 (12)	0.0218 (3)
H3	1.0298 (19)	0.3623 (19)	0.1449 (16)	0.032 (4)*
C4	0.91651 (14)	0.33589 (14)	0.29426 (12)	0.0205 (2)
H4	0.9307 (18)	0.2294 (19)	0.2830 (15)	0.031 (4)*
C5	0.83713 (13)	0.41063 (13)	0.39037 (11)	0.0171 (2)
H5	0.7977 (16)	0.3598 (16)	0.4529 (14)	0.018 (3)*
C6	0.81244 (12)	0.56313 (13)	0.40477 (10)	0.0137 (2)
C7	0.62363 (12)	0.71296 (12)	0.50155 (10)	0.0137 (2)
C8	0.58137 (12)	0.72269 (13)	0.36870 (10)	0.0144 (2)
H8	0.5736 (17)	0.6142 (17)	0.2981 (14)	0.022 (4)*
C9	0.72664 (12)	0.85397 (13)	0.36026 (10)	0.0135 (2)
C10	0.55651 (13)	0.77944 (13)	0.60908 (11)	0.0157 (2)
H10	0.4772 (17)	0.8366 (17)	0.5993 (14)	0.022 (3)*
C11	0.59228 (13)	0.76065 (13)	0.73184 (11)	0.0173 (2)
C12	0.51378 (16)	0.83951 (17)	0.84424 (12)	0.0249 (3)
H12A	0.469 (2)	0.760 (2)	0.881 (2)	0.059 (6)*
H12B	0.435 (2)	0.891 (2)	0.8239 (16)	0.037 (4)*
H12C	0.605 (2)	0.933 (2)	0.916 (2)	0.051 (5)*
C13	0.42116 (13)	0.75818 (14)	0.34215 (11)	0.0178 (2)
H13A	0.3311 (17)	0.6712 (17)	0.3594 (14)	0.023 (3)*
H13B	0.4255 (16)	0.8713 (17)	0.4069 (14)	0.021 (3)*
C14	0.38388 (15)	0.74770 (17)	0.20244 (13)	0.0248 (3)
H14	0.399 (2)	0.850 (3)	0.190 (2)	0.065 (6)*
C15	0.3403 (2)	0.6128 (2)	0.09694 (15)	0.0432 (4)
H15A	0.318 (3)	0.505 (3)	0.102 (3)	0.097 (8)*

H15B	0.318 (2)	0.616 (2)	0.0088 (19)	0.050 (5)*
C16	1.00249 (13)	0.92304 (13)	0.32234 (11)	0.0162 (2)
H16A	1.0122 (16)	1.0332 (17)	0.3896 (13)	0.017 (3)*
H16B	1.0997 (17)	0.8951 (17)	0.3466 (13)	0.023 (4)*
C17	0.99218 (14)	0.92956 (14)	0.18704 (11)	0.0195 (2)
H17	1.0916 (19)	1.0012 (19)	0.1798 (15)	0.033 (4)*
C18	0.86578 (16)	0.85178 (15)	0.08827 (12)	0.0234 (3)
H18A	0.762 (2)	0.7781 (19)	0.0972 (16)	0.034 (4)*
H18B	0.8730 (19)	0.8666 (18)	0.0047 (16)	0.029 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0221 (4)	0.0158 (4)	0.0216 (4)	0.0089 (3)	0.0064 (3)	0.0084 (3)
O2	0.0257 (4)	0.0262 (4)	0.0194 (4)	0.0122 (3)	0.0063 (3)	0.0118 (3)
N1	0.0165 (4)	0.0167 (4)	0.0158 (4)	0.0082 (3)	0.0050 (3)	0.0088 (4)
N2	0.0140 (4)	0.0125 (4)	0.0154 (4)	0.0049 (3)	0.0045 (3)	0.0063 (3)
C1	0.0132 (5)	0.0134 (5)	0.0147 (5)	0.0056 (4)	0.0010 (4)	0.0050 (4)
C2	0.0195 (5)	0.0215 (5)	0.0171 (5)	0.0101 (4)	0.0056 (4)	0.0080 (4)
C3	0.0236 (6)	0.0237 (6)	0.0197 (6)	0.0147 (5)	0.0057 (4)	0.0048 (4)
C4	0.0202 (5)	0.0162 (5)	0.0251 (6)	0.0098 (4)	0.0017 (4)	0.0055 (4)
C5	0.0154 (5)	0.0151 (5)	0.0220 (6)	0.0050 (4)	0.0021 (4)	0.0086 (4)
C6	0.0127 (4)	0.0144 (5)	0.0143 (5)	0.0053 (4)	0.0021 (4)	0.0051 (4)
C7	0.0121 (5)	0.0123 (4)	0.0166 (5)	0.0026 (4)	0.0024 (4)	0.0066 (4)
C8	0.0139 (5)	0.0154 (5)	0.0152 (5)	0.0055 (4)	0.0031 (4)	0.0067 (4)
C9	0.0159 (5)	0.0158 (5)	0.0101 (5)	0.0062 (4)	0.0028 (4)	0.0055 (4)
C10	0.0142 (5)	0.0160 (5)	0.0181 (5)	0.0055 (4)	0.0042 (4)	0.0072 (4)
C11	0.0165 (5)	0.0159 (5)	0.0179 (5)	0.0025 (4)	0.0045 (4)	0.0062 (4)
C12	0.0276 (6)	0.0321 (7)	0.0188 (6)	0.0135 (5)	0.0103 (5)	0.0100 (5)
C13	0.0151 (5)	0.0201 (5)	0.0197 (5)	0.0077 (4)	0.0025 (4)	0.0082 (4)
C14	0.0236 (6)	0.0300 (6)	0.0258 (6)	0.0099 (5)	0.0021 (5)	0.0160 (5)
C15	0.0613 (10)	0.0369 (8)	0.0230 (7)	0.0013 (7)	0.0004 (7)	0.0135 (6)
C16	0.0142 (5)	0.0165 (5)	0.0179 (5)	0.0028 (4)	0.0032 (4)	0.0078 (4)
C17	0.0223 (6)	0.0203 (5)	0.0212 (6)	0.0085 (4)	0.0103 (4)	0.0115 (4)
C18	0.0317 (6)	0.0260 (6)	0.0165 (6)	0.0135 (5)	0.0072 (5)	0.0091 (5)

Geometric parameters (Å, º)

O1—C9	1.2247 (13)	C8—H8	0.991 (14)
O2—C11	1.2496 (14)	C10—C11	1.4343 (16)
N1—C7	1.3527 (13)	C10—H10	0.977 (14)
N1—C6	1.4081 (14)	C11—C12	1.5070 (16)
N1—H1	0.910 (17)	C12—H12A	0.96 (2)
N2—C9	1.3701 (13)	C12—H12B	0.965 (17)
N2—C1	1.4290 (13)	C12—H12C	1.02 (2)
N2—C16	1.4690 (13)	C13—C14	1.5047 (17)
C1—C2	1.3990 (15)	C13—H13A	1.039 (14)
C1—C6	1.4058 (15)	C13—H13B	1.003 (14)

C2—C3	1.3843 (16)	C14—C15	1.287 (2)
C2—H2	0.954 (14)	C14—H14	0.96 (2)
C3—C4	1.3871 (18)	C15—H15A	0.97 (3)
C3—H3	0.958 (16)	C15—H15B	0.983 (19)
C4—C5	1.3808 (16)	C16—C17	1.5039 (16)
C4—H4	0.963 (15)	C16—H16A	0.982 (13)
C5—C6	1.3979 (15)	C16—H16B	0.980 (14)
C5—H5	0.991 (14)	C17—C18	1.3170 (17)
C7—C10	1.3765 (15)	C17—H17	0.966 (16)
C7—C8	1.5113 (15)	C18—H18A	1.010 (16)
C8—C9	1.5282 (14)	C18—H18B	0.979 (16)
C8—C13	1.5306 (14)		

C7—N1—C6	126.14 (9)	C7—C10—C11	122.55 (10)
C7—N1—H1	113.1 (10)	C7—C10—H10	118.3 (8)
C6—N1—H1	120.2 (10)	C11—C10—H10	119.0 (8)
C9—N2—C1	124.02 (9)	O2—C11—C10	122.97 (10)
C9—N2—C16	117.67 (9)	O2—C11—C12	118.49 (10)
C1—N2—C16	118.26 (8)	C10—C11—C12	118.54 (10)
C2—C1—C6	118.84 (10)	C11—C12—H12A	109.2 (12)
C2—C1—N2	118.71 (9)	C11—C12—H12B	115.9 (10)
C6—C1—N2	122.27 (9)	H12A—C12—H12B	111.7 (15)
C3—C2—C1	120.93 (11)	C11—C12—H12C	106.4 (11)
C3—C2—H2	119.7 (8)	H12A—C12—H12C	107.0 (16)
C1—C2—H2	119.4 (8)	H12B—C12—H12C	106.3 (14)
C2—C3—C4	120.12 (11)	C14—C13—C8	111.01 (9)
C2—C3—H3	120.0 (9)	C14—C13—H13A	111.2 (8)
C4—C3—H3	119.8 (9)	C8—C13—H13A	107.2 (8)
C5—C4—C3	119.71 (10)	C14—C13—H13B	109.9 (8)
C5—C4—H4	120.8 (9)	C8—C13—H13B	110.4 (8)
C3—C4—H4	119.5 (9)	H13A—C13—H13B	106.9 (11)
C4—C5—C6	121.04 (11)	C15—C14—C13	125.60 (13)
C4—C5—H5	121.5 (8)	C15—C14—H14	116.5 (13)
C6—C5—H5	117.4 (8)	C13—C14—H14	117.8 (13)
C5—C6—C1	119.36 (10)	C14—C15—H15A	121.2 (16)
C5—C6—N1	117.77 (10)	C14—C15—H15B	120.8 (10)
C1—C6—N1	122.80 (9)	H15A—C15—H15B	117.7 (19)
N1—C7—C10	121.64 (10)	N2—C16—C17	114.66 (9)
N1—C7—C8	114.62 (9)	N2—C16—H16A	106.5 (8)
C10—C7—C8	123.73 (9)	C17—C16—H16A	110.0 (8)
C7—C8—C9	105.81 (8)	N2—C16—H16B	107.8 (8)
C7—C8—C13	115.83 (9)	C17—C16—H16B	110.9 (8)
C9—C8—C13	112.20 (9)	H16A—C16—H16B	106.5 (11)
C7—C8—H8	108.3 (8)	C18—C17—C16	126.31 (11)
C9—C8—H8	107.4 (8)	C18—C17—H17	122.1 (10)
C13—C8—H8	106.9 (8)	C16—C17—H17	111.6 (10)
O1—C9—N2	121.96 (10)	C17—C18—H18A	121.5 (9)
O1—C9—C8	122.65 (9)	C17—C18—H18B	118.9 (9)

N2—C9—C8	115.34 (9)	H18A—C18—H18B	119.6 (13)
C9—N2—C1—C2	140.12 (10)	N1—C7—C8—C13	161.42 (9)
C16—N2—C1—C2	−37.25 (14)	C10—C7—C8—C13	−19.55 (14)
C9—N2—C1—C6	−44.67 (15)	C1—N2—C9—O1	177.73 (9)
C16—N2—C1—C6	137.96 (10)	C16—N2—C9—O1	−4.89 (15)
C6—C1—C2—C3	−0.03 (16)	C1—N2—C9—C8	0.13 (14)
N2—C1—C2—C3	175.35 (10)	C16—N2—C9—C8	177.51 (9)
C1—C2—C3—C4	−0.25 (18)	C7—C8—C9—O1	−103.13 (11)
C2—C3—C4—C5	0.12 (18)	C13—C8—C9—O1	24.08 (14)
C3—C4—C5—C6	0.29 (17)	C7—C8—C9—N2	74.45 (11)
C4—C5—C6—C1	−0.56 (16)	C13—C8—C9—N2	−158.34 (9)
C4—C5—C6—N1	−177.52 (10)	N1—C7—C10—C11	−4.46 (16)
C2—C1—C6—C5	0.43 (15)	C8—C7—C10—C11	176.57 (10)
N2—C1—C6—C5	−174.78 (9)	C7—C10—C11—O2	−0.30 (17)
C2—C1—C6—N1	177.22 (10)	C7—C10—C11—C12	179.43 (10)
N2—C1—C6—N1	2.01 (15)	C7—C8—C13—C14	−174.24 (9)
C7—N1—C6—C5	−139.68 (11)	C9—C8—C13—C14	64.13 (12)
C7—N1—C6—C1	43.48 (15)	C8—C13—C14—C15	71.29 (18)
C6—N1—C7—C10	−179.89 (10)	C9—N2—C16—C17	−81.22 (12)
C6—N1—C7—C8	−0.83 (14)	C1—N2—C16—C17	96.32 (11)
N1—C7—C8—C9	−73.60 (11)	N2—C16—C17—C18	6.42 (17)
C10—C7—C8—C9	105.44 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.910 (17)	1.878 (16)	2.6308 (12)	138.6 (14)
C10—H10···O1^{i}	0.977 (14)	2.567 (14)	3.5316 (13)	168.9 (11)

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.