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4-Phenyl-5a,6,7,8,9,9a-hexahydro-1*H*-1,5-benzodiazepin-2(5*H*)-one

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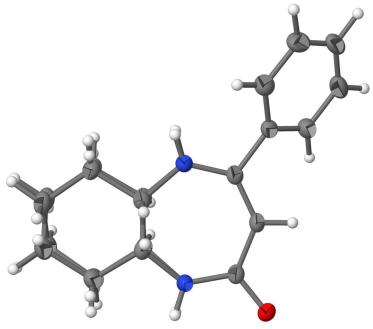
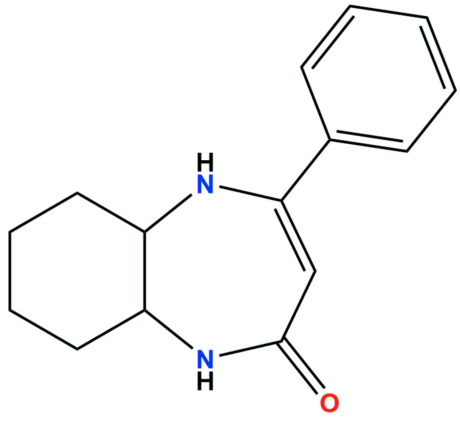
In the title compound, $C_{15}H_{18}N_2O$, the cyclohexyl portion is disordered over two alternate chair conformations in a 0.911 (2):0.089 (2) ratio. In the crystal, inversion-related pairwise N—H···O hydrogen bonds form dimers, which are connected into (100) layers by additional N—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Benzodiazepines a nowadays well known for their therapeutic virtues. These heterocylic compounds are commonly used as anti-inflammatory (Bhat & Kumar, 2016), antioxidant (Patil *et al.*, 2015) and anticancer (Chen *et al.*, 2014) agents. As part of our studies in this area, we report here the synthesis and structure of a new 1,5-benzodiazepine derivative.

The cyclohexyl ring (C1–C6) in the title molecule (Fig. 1) is disordered over two alternate chair conformations in a 0.911 (2):0.089 (2) ratio. The major component has puckering parameters Q = 0.561 (2) Å, θ = 173.1 (2)° and φ = 321.1 (19)°. A puckering analysis of the major conformation of the seven-membered ring yielded the parameters $Q(2)$ = 0.4234 (19) Å, $Q(3)$ = 0.3884 (18) Å, $\varphi(2)$ = 123.91 (2)° and $\varphi(3)$ = 40.0 (3)°, with a total puckering amplitude of 0.574 (2) Å.

In the crystal, inversion-related pairwise N2—H2···O1^{i} hydrogen bonds form dimers which are connected into (100) layers by N1—H1*B*···O1^{ii} hydrogen bonds (Table 1 and Fig. 2). These layers have the phenyl rings protruding from both surfaces.

Synthesis and crystallization

To a stirred boiling solution of 0.1 mol (11.4 g) of 1,2-diaminocyclohexane in 60 ml *p*-xylene, 0.12 mol (23.06 g) of ethyl benzoylacetate in 10 ml *p*-xylene was added dropwise and refluxed for 2 h. The reaction mixture was left at room temperature for 24 h. The

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O1^{i}	0.88	2.32	3.096 (2)	148
N2—H2···O1^{ii}	0.88	2.04	2.8936 (19)	162

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

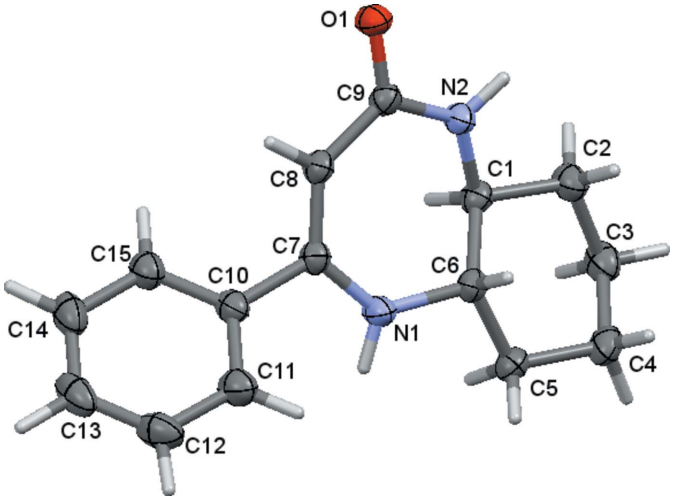


Figure 1
The title molecule, shown with 50% probability displacement ellipsoids. Only the major conformation is shown.

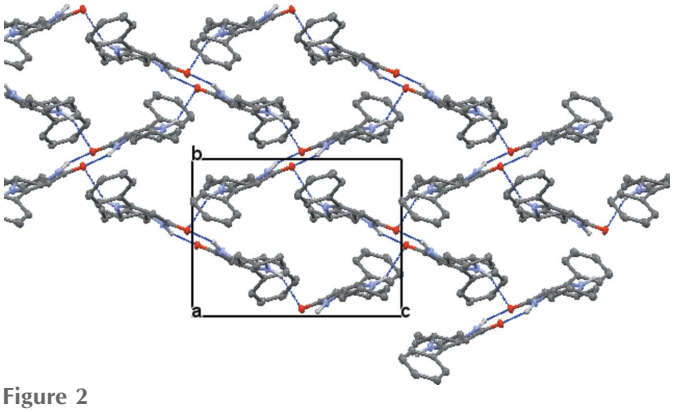


Figure 2
Packing viewed along the *a*-axis direction. N—H···O hydrogen bonds are depicted by dashed lines.

precipitated solid was collected by filtration and recrystallized from dry ethanol solution to give colourless blocks (m.p. 230–232°C).

Refinement

Crystal and refinement details are presented in Table 2. The cyclohexyl ring and its attached N atoms are disordered over two chair conformations in a 91:9 ratio. The minor component of the disorder was restrained to have a comparable geometry to that of the major one and the attached H atoms on both were included as riding contributions in idealized positions. The final model was refined as a two-component twin.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{18}N_2O$
M_r	242.31
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	11.4283 (18), 9.2294 (15), 12.3632 (19)
β (°)	96.890 (2)
V (Å^3)	1294.6 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.27 × 0.19
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.98, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	44744, 44744, 25002
R_{int}	0.046
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.686
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.152, 0.93
No. of reflections	44744
No. of parameters	207
No. of restraints	18
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.24

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2008) and *SHELXTL* (Bruker, 2016).

Acknowledgements

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full crystallographic data

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4-Phenyl-5a,6,7,8,9,9a-hexahydro-1*H*-1,5-benzodiazepin-2(5*H*)-one

Crystal data

$C_{15}H_{18}N_2O$
M_r = 242.31
Monoclinic, $P2_1/c$
a = 11.4283 (18) Å
b = 9.2294 (15) Å
c = 12.3632 (19) Å
β = 96.890 (2)°
V = 1294.6 (4) Å^3
Z = 4
$F(000)$ = 520
D_x = 1.243 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9967 reflections
θ = 2.8–29.2°
μ = 0.08 mm^{-1}
T = 100 K
Block, colourless
0.30 × 0.27 × 0.19 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.98, T_{max} = 0.99
44744 measured reflections
44744 independent reflections
25002 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 29.2°, θ_{min} = 1.8°
h = −15→15
k = −12→12
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.152
S = 0.93
44744 reflections
207 parameters
18 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
$w = 1/[\sigma^2(F_o^2) + (0.0804P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 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 deg. in omega, colllected at phi = 0.00, 90.00 and 180.00 deg. and 2 sets of 800 frames, each of width 0.45 deg in phi, collected at omega = -30.00 and 210.00 deg. The scan time was 30 sec/frame. Analysis of 1323 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about *b*. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

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. The cyclohexyl ring and its attached nitrogen atoms are disordered over two chair conformations in a 91:9 ratio. The minor component of the disorder was restrained to have a comparable geometry to that of the major one and the attached hydrogens on both were included as riding contributions in idealized positions. The final model was refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.35039 (10)	0.54728 (14)	0.97683 (10)	0.0323 (4)	
N1	0.35229 (12)	0.69692 (17)	0.63902 (12)	0.0309 (4)	0.911 (2)
H1B	0.336391	0.742292	0.576378	0.037*	0.911 (2)
N2	0.48216 (12)	0.58638 (16)	0.85897 (12)	0.0291 (4)	0.911 (2)
H2	0.530411	0.528523	0.899541	0.035*	0.911 (2)
C1	0.53237 (16)	0.6625 (2)	0.77215 (16)	0.0264 (5)	0.911 (2)
H1	0.527560	0.769274	0.784632	0.032*	0.911 (2)
C2	0.66216 (17)	0.6171 (3)	0.78221 (19)	0.0338 (7)	0.911 (2)
H2A	0.702263	0.651335	0.853023	0.041*	0.911 (2)
H2B	0.666875	0.510004	0.781610	0.041*	0.911 (2)
C3	0.72628 (18)	0.6767 (3)	0.69142 (18)	0.0359 (6)	0.911 (2)
H3A	0.809178	0.643256	0.701073	0.043*	0.911 (2)
H3B	0.726174	0.783939	0.693833	0.043*	0.911 (2)
C4	0.66544 (18)	0.6250 (3)	0.58212 (19)	0.0367 (6)	0.911 (2)
H4A	0.668078	0.517946	0.578709	0.044*	0.911 (2)
H4B	0.706872	0.664164	0.522574	0.044*	0.911 (2)
C5	0.53792 (17)	0.6761 (2)	0.56791 (17)	0.0303 (6)	0.911 (2)
H5A	0.498609	0.639623	0.497463	0.036*	0.911 (2)
H5B	0.536658	0.783314	0.564929	0.036*	0.911 (2)
C6	0.46797 (16)	0.6259 (2)	0.65916 (16)	0.0259 (5)	0.911 (2)
H6	0.456677	0.518621	0.653614	0.031*	0.911 (2)
N1A	0.35229 (12)	0.69692 (17)	0.63902 (12)	0.0309 (4)	0.089 (2)
H1C	0.331921	0.683920	0.568769	0.037*	0.089 (2)
N2A	0.48216 (12)	0.58638 (16)	0.85897 (12)	0.0291 (4)	0.089 (2)
H2C	0.538385	0.583969	0.914203	0.035*	0.089 (2)
C1A	0.5210 (11)	0.5822 (19)	0.7504 (9)	0.0264 (5)	0.089 (2)
H1A	0.489134	0.492652	0.712003	0.032*	0.089 (2)

C2A	0.6553 (12)	0.573 (3)	0.7681 (15)	0.0338 (7)	0.089 (2)
H2AA	0.685897	0.652867	0.816838	0.041*	0.089 (2)
H2AB	0.678265	0.480545	0.805409	0.041*	0.089 (2)
C3A	0.7129 (15)	0.581 (2)	0.6642 (16)	0.0359 (6)	0.089 (2)
H3AA	0.688596	0.496789	0.617389	0.043*	0.089 (2)
H3AB	0.799659	0.578199	0.681997	0.043*	0.089 (2)
C4A	0.6773 (13)	0.720 (2)	0.6032 (18)	0.0367 (6)	0.089 (2)
H4AA	0.712770	0.723251	0.533981	0.044*	0.089 (2)
H4AB	0.706448	0.804972	0.647678	0.044*	0.089 (2)
C5A	0.5437 (12)	0.727 (3)	0.5796 (14)	0.0303 (6)	0.089 (2)
H5AA	0.516753	0.646747	0.529269	0.036*	0.089 (2)
H5AB	0.521217	0.819029	0.542015	0.036*	0.089 (2)
C6A	0.4795 (8)	0.7153 (18)	0.6810 (11)	0.0259 (5)	0.089 (2)
H6A	0.491302	0.805811	0.725432	0.031*	0.089 (2)
C7	0.26759 (14)	0.69980 (19)	0.70681 (15)	0.0251 (4)	
C8	0.27531 (16)	0.65248 (19)	0.81167 (15)	0.0264 (4)	
C9	0.37109 (15)	0.59344 (19)	0.88495 (15)	0.0255 (4)	
C10	0.15212 (15)	0.7588 (2)	0.65637 (16)	0.0284 (4)	
H10	0.1482 (17)	0.650 (2)	0.5102 (16)	0.039 (6)*	
C11	0.10522 (17)	0.7196 (2)	0.55146 (18)	0.0376 (5)	
H11	−0.0345 (19)	0.738 (2)	0.4304 (18)	0.052 (6)*	
C12	−0.00385 (18)	0.7731 (3)	0.5068 (2)	0.0456 (6)	
H12	−0.1426 (19)	0.906 (2)	0.5324 (17)	0.047 (6)*	
C13	−0.06599 (18)	0.8668 (3)	0.5657 (2)	0.0447 (6)	
H13	−0.0647 (19)	0.971 (2)	0.7134 (17)	0.048 (6)*	
C14	−0.02046 (18)	0.9060 (2)	0.6693 (2)	0.0426 (6)	
H14	0.2059 (16)	0.6540 (19)	0.8426 (14)	0.028 (5)*	
C15	0.08779 (16)	0.8525 (2)	0.71489 (18)	0.0346 (5)	
H15	0.1212 (17)	0.881 (2)	0.7891 (17)	0.038 (6)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0263 (7)	0.0473 (9)	0.0239 (8)	0.0017 (6)	0.0055 (5)	0.0068 (6)
N1	0.0225 (8)	0.0477 (10)	0.0230 (9)	0.0055 (7)	0.0040 (7)	0.0068 (7)
N2	0.0214 (8)	0.0412 (10)	0.0253 (9)	0.0048 (6)	0.0052 (6)	0.0079 (7)
C1	0.0227 (10)	0.0308 (12)	0.0265 (12)	−0.0013 (8)	0.0063 (8)	0.0017 (9)
C2	0.0228 (10)	0.0436 (17)	0.0351 (13)	0.0008 (9)	0.0038 (9)	0.0074 (11)
C3	0.0234 (10)	0.0419 (15)	0.0433 (15)	0.0004 (9)	0.0080 (10)	0.0096 (11)
C4	0.0312 (11)	0.0425 (14)	0.0391 (14)	0.0049 (10)	0.0156 (10)	0.0048 (11)
C5	0.0284 (10)	0.0371 (15)	0.0265 (12)	0.0026 (9)	0.0087 (8)	0.0015 (10)
C6	0.0222 (10)	0.0296 (12)	0.0264 (12)	0.0024 (8)	0.0049 (8)	0.0009 (9)
N1A	0.0225 (8)	0.0477 (10)	0.0230 (9)	0.0055 (7)	0.0040 (7)	0.0068 (7)
N2A	0.0214 (8)	0.0412 (10)	0.0253 (9)	0.0048 (6)	0.0052 (6)	0.0079 (7)
C1A	0.0227 (10)	0.0308 (12)	0.0265 (12)	−0.0013 (8)	0.0063 (8)	0.0017 (9)
C2A	0.0228 (10)	0.0436 (17)	0.0351 (13)	0.0008 (9)	0.0038 (9)	0.0074 (11)
C3A	0.0234 (10)	0.0419 (15)	0.0433 (15)	0.0004 (9)	0.0080 (10)	0.0096 (11)
C4A	0.0312 (11)	0.0425 (14)	0.0391 (14)	0.0049 (10)	0.0156 (10)	0.0048 (11)

C5A	0.0284 (10)	0.0371 (15)	0.0265 (12)	0.0026 (9)	0.0087 (8)	0.0015 (10)
C6A	0.0222 (10)	0.0296 (12)	0.0264 (12)	0.0024 (8)	0.0049 (8)	0.0009 (9)
C7	0.0200 (8)	0.0286 (10)	0.0269 (11)	−0.0008 (7)	0.0036 (7)	0.0002 (8)
C8	0.0195 (9)	0.0338 (11)	0.0269 (11)	0.0004 (7)	0.0062 (8)	0.0020 (8)
C9	0.0224 (9)	0.0303 (10)	0.0241 (10)	−0.0008 (7)	0.0048 (7)	−0.0018 (8)
C10	0.0206 (9)	0.0361 (11)	0.0287 (11)	−0.0005 (7)	0.0041 (8)	0.0078 (8)
C11	0.0279 (10)	0.0523 (14)	0.0326 (13)	0.0006 (9)	0.0032 (9)	0.0050 (10)
C12	0.0295 (11)	0.0690 (16)	0.0362 (14)	−0.0041 (10)	−0.0042 (10)	0.0123 (11)
C13	0.0202 (10)	0.0603 (15)	0.0533 (16)	0.0024 (9)	0.0036 (10)	0.0244 (12)
C14	0.0281 (11)	0.0490 (14)	0.0525 (16)	0.0097 (9)	0.0117 (10)	0.0143 (11)
C15	0.0261 (10)	0.0423 (12)	0.0359 (13)	0.0037 (8)	0.0054 (9)	0.0068 (9)

Geometric parameters (Å, º)

O1—C9	1.262 (2)	C1A—C6A	1.541 (10)
N1—C7	1.354 (2)	C1A—H1A	1.0000
N1—C6	1.470 (2)	C2A—C3A	1.514 (10)
N1—H1B	0.8800	C2A—H2AA	0.9900
N2—C9	1.348 (2)	C2A—H2AB	0.9900
N2—C1	1.457 (2)	C3A—C4A	1.519 (10)
N2—H2	0.8800	C3A—H3AA	0.9900
C1—C2	1.532 (3)	C3A—H3AB	0.9900
C1—C6	1.536 (3)	C4A—C5A	1.521 (10)
C1—H1	1.0000	C4A—H4AA	0.9900
C2—C3	1.515 (3)	C4A—H4AB	0.9900
C2—H2A	0.9900	C5A—C6A	1.529 (10)
C2—H2B	0.9900	C5A—H5AA	0.9900
C3—C4	1.520 (3)	C5A—H5AB	0.9900
C3—H3A	0.9900	C6A—H6A	1.0000
C3—H3B	0.9900	C7—C8	1.361 (2)
C4—C5	1.522 (3)	C7—C10	1.493 (2)
C4—H4A	0.9900	C8—C9	1.441 (2)
C4—H4B	0.9900	C8—H14	0.922 (18)
C5—C6	1.531 (3)	C10—C11	1.391 (3)
C5—H5A	0.9900	C10—C15	1.392 (3)
C5—H5B	0.9900	C11—C12	1.392 (3)
C6—H6	1.0000	C11—H10	0.99 (2)
N1A—C7	1.354 (2)	C12—C13	1.381 (3)
N1A—C6A	1.494 (9)	C12—H11	1.02 (2)
N1A—H1C	0.8800	C13—C14	1.372 (3)
N2A—C9	1.348 (2)	C13—H12	0.99 (2)
N2A—C1A	1.464 (9)	C14—C15	1.388 (3)
N2A—H2C	0.8800	C14—H13	0.99 (2)
C1A—C2A	1.526 (10)	C15—H15	0.99 (2)
C7—N1—C6	126.79 (15)	C1A—C2A—H2AB	108.7
C7—N1—H1B	116.6	H2AA—C2A—H2AB	107.6
C6—N1—H1B	116.6	C2A—C3A—C4A	110.2 (12)

C9—N2—C1	128.15 (15)	C2A—C3A—H3AA	109.6
C9—N2—H2	115.9	C4A—C3A—H3AA	109.6
C1—N2—H2	115.9	C2A—C3A—H3AB	109.6
N2—C1—C2	105.75 (16)	C4A—C3A—H3AB	109.6
N2—C1—C6	112.07 (16)	H3AA—C3A—H3AB	108.1
C2—C1—C6	111.55 (16)	C3A—C4A—C5A	109.3 (12)
N2—C1—H1	109.1	C3A—C4A—H4AA	109.8
C2—C1—H1	109.1	C5A—C4A—H4AA	109.8
C6—C1—H1	109.1	C3A—C4A—H4AB	109.8
C3—C2—C1	112.96 (18)	C5A—C4A—H4AB	109.8
C3—C2—H2A	109.0	H4AA—C4A—H4AB	108.3
C1—C2—H2A	109.0	C4A—C5A—C6A	114.2 (11)
C3—C2—H2B	109.0	C4A—C5A—H5AA	108.7
C1—C2—H2B	109.0	C6A—C5A—H5AA	108.7
H2A—C2—H2B	107.8	C4A—C5A—H5AB	108.7
C2—C3—C4	109.52 (18)	C6A—C5A—H5AB	108.7
C2—C3—H3A	109.8	H5AA—C5A—H5AB	107.6
C4—C3—H3A	109.8	N1A—C6A—C5A	105.4 (9)
C2—C3—H3B	109.8	N1A—C6A—C1A	108.9 (10)
C4—C3—H3B	109.8	C5A—C6A—C1A	111.4 (11)
H3A—C3—H3B	108.2	N1A—C6A—H6A	110.3
C3—C4—C5	109.57 (18)	C5A—C6A—H6A	110.3
C3—C4—H4A	109.8	C1A—C6A—H6A	110.3
C5—C4—H4A	109.8	N1A—C7—C8	127.86 (16)
C3—C4—H4B	109.8	N1—C7—C8	127.86 (16)
C5—C4—H4B	109.8	N1A—C7—C10	114.21 (15)
H4A—C4—H4B	108.2	N1—C7—C10	114.21 (15)
C4—C5—C6	113.50 (18)	C8—C7—C10	117.90 (15)
C4—C5—H5A	108.9	C7—C8—C9	132.66 (17)
C6—C5—H5A	108.9	C7—C8—H14	115.5 (11)
C4—C5—H5B	108.9	C9—C8—H14	111.8 (11)
C6—C5—H5B	108.9	O1—C9—N2A	118.81 (16)
H5A—C5—H5B	107.7	O1—C9—N2	118.81 (16)
N1—C6—C5	106.19 (15)	O1—C9—C8	118.89 (16)
N1—C6—C1	112.28 (15)	N2A—C9—C8	122.30 (16)
C5—C6—C1	111.59 (16)	N2—C9—C8	122.30 (16)
N1—C6—H6	108.9	C11—C10—C15	118.54 (18)
C5—C6—H6	108.9	C11—C10—C7	121.13 (17)
C1—C6—H6	108.9	C15—C10—C7	120.31 (18)
C7—N1A—C6A	121.4 (6)	C10—C11—C12	120.3 (2)
C7—N1A—H1C	119.3	C10—C11—H10	119.4 (11)
C6A—N1A—H1C	119.3	C12—C11—H10	120.2 (11)
C9—N2A—C1A	128.1 (5)	C13—C12—C11	120.4 (2)
C9—N2A—H2C	115.9	C13—C12—H11	123.1 (12)
C1A—N2A—H2C	115.9	C11—C12—H11	116.5 (12)
N2A—C1A—C2A	106.3 (9)	C14—C13—C12	119.7 (2)
N2A—C1A—C6A	112.5 (10)	C14—C13—H12	120.5 (12)
C2A—C1A—C6A	111.2 (11)	C12—C13—H12	119.8 (12)

N2A—C1A—H1A	108.9	C13—C14—C15	120.4 (2)
C2A—C1A—H1A	108.9	C13—C14—H13	120.9 (12)
C6A—C1A—H1A	108.9	C15—C14—H13	118.7 (13)
C3A—C2A—C1A	114.1 (12)	C14—C15—C10	120.7 (2)
C3A—C2A—H2AA	108.7	C14—C15—H15	120.5 (11)
C1A—C2A—H2AA	108.7	C10—C15—H15	118.8 (11)
C3A—C2A—H2AB	108.7		

C9—N2—C1—C2	178.49 (18)	C2A—C1A—C6A—C5A	47.7 (17)
C9—N2—C1—C6	−59.8 (3)	C6A—N1A—C7—C8	−33.3 (8)
N2—C1—C2—C3	175.09 (18)	C6A—N1A—C7—C10	148.6 (7)
C6—C1—C2—C3	53.0 (3)	C6—N1—C7—C8	7.9 (3)
C1—C2—C3—C4	−58.6 (3)	C6—N1—C7—C10	−170.20 (17)
C2—C3—C4—C5	59.2 (2)	N1A—C7—C8—C9	3.5 (3)
C3—C4—C5—C6	−57.0 (2)	N1—C7—C8—C9	3.5 (3)
C7—N1—C6—C5	−170.40 (17)	C10—C7—C8—C9	−178.47 (19)
C7—N1—C6—C1	−48.2 (2)	C1A—N2A—C9—O1	155.9 (9)
C4—C5—C6—N1	174.11 (17)	C1A—N2A—C9—C8	−24.4 (9)
C4—C5—C6—C1	51.5 (2)	C1—N2—C9—O1	−163.67 (18)
N2—C1—C6—N1	74.5 (2)	C1—N2—C9—C8	16.0 (3)
C2—C1—C6—N1	−167.09 (16)	C7—C8—C9—O1	−174.44 (19)
N2—C1—C6—C5	−166.35 (16)	C7—C8—C9—N2A	5.9 (3)
C2—C1—C6—C5	−48.0 (2)	C7—C8—C9—N2	5.9 (3)
C9—N2A—C1A—C2A	−179.4 (11)	N1A—C7—C10—C11	43.1 (2)
C9—N2A—C1A—C6A	58.6 (15)	N1—C7—C10—C11	43.1 (2)
N2A—C1A—C2A—C3A	−174.7 (17)	C8—C7—C10—C11	−135.20 (19)
C6A—C1A—C2A—C3A	−52 (2)	N1A—C7—C10—C15	−138.29 (18)
C1A—C2A—C3A—C4A	57 (2)	N1—C7—C10—C15	−138.29 (18)
C2A—C3A—C4A—C5A	−57 (2)	C8—C7—C10—C15	43.4 (2)
C3A—C4A—C5A—C6A	57 (2)	C15—C10—C11—C12	−0.2 (3)
C7—N1A—C6A—C5A	−172.4 (10)	C7—C10—C11—C12	178.49 (18)
C7—N1A—C6A—C1A	67.9 (12)	C10—C11—C12—C13	0.7 (3)
C4A—C5A—C6A—N1A	−170.1 (15)	C11—C12—C13—C14	−0.7 (3)
C4A—C5A—C6A—C1A	−52 (2)	C12—C13—C14—C15	0.3 (3)
N2A—C1A—C6A—N1A	−77.3 (15)	C13—C14—C15—C10	0.3 (3)
C2A—C1A—C6A—N1A	163.6 (13)	C11—C10—C15—C14	−0.3 (3)
N2A—C1A—C6A—C5A	166.9 (13)	C7—C10—C15—C14	−178.97 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O1^{i}	0.88	2.32	3.096 (2)	148
N2—H2···O1^{ii}	0.88	2.04	2.8936 (19)	162

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