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1-Benzyl-3-hydroxy-4-phenyl-2,3,4,5-tetrahydro-1*H*-1,5-benzodiazepin-2-one

Mohammed Rida,[a]* Youness El Bakri,[a] Mohamadou Lamine Doumbia,[b] El Mokhtar Essassi[a] and Joel T. Mague[c]

[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, [b]UFR–Environnement, UNIV Jean Lorougnon Guédé, BP 150, Daloa, Ivory Coast, and [c]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: rida.m.b@hotmail.com

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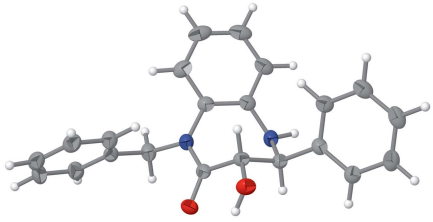
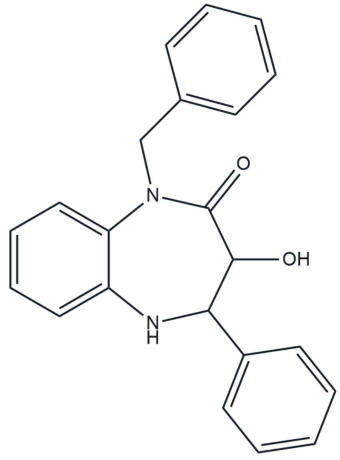
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{22}H_{20}N_2O_2$, forms chains in the [001] direction in the monoclinic crystal, through N—H···O hydrogen bonding. The chains are associated *via* O—H···π(ring) and C—H···π(ring) interactions involving one phenyl ring and the benzene ring of the benzodiazepine as acceptors. For these intermolecular contacts, the H···π separations are close to 2.7 Å.

3D view



Chemical scheme



Structure description

1,5-Benzodiazepine derivatives have been used as therapeutics for viral infection, cardiovascular disorder (Jacob *et al.*, 2011; Maleki *et al.*, 2014) and as antimicrobial agents against some microorganisms (An *et al.*, 2016). They are active against peptide hormones and potassium blockers (Claremon *et al.*, 1996). They are also employed as intermediates for the synthesis of several heterocyclic compounds (Minnih *et al.*, 2014).

As part of our studies in this area, we now describe the synthesis and structure of the title compound. In the molecular structure, the dihedral angle between the C1–C6 and C10–C15 rings is 42.57 (5)°, while the angle between the former and the C17–C22 ring is 81.24 (4)°. A puckering analysis of the seven-membered diazepine ring yielded parameters q_2 = 0.992 (1) Å, q_3 = 0.183 (1) Å, φ_2 = 11.81 (6)° and φ_3 = 98.4 (3)°, for a total puckering amplitude of 1.009 (1) Å. There is likely an intramolecular O1—H1*A*···O2 hydrogen bond forming an *S*(5) ring (Fig. 1 and Table 1), but because of the acute O1—H1*A*···O2 angle of 115 (1)° and the rather long H1*A*···O2 separation of 2.166 (17) Å, it should be considered as a weak interaction.

In the crystal, intermolecular N1—H1···O2^{i} hydrogen bonds [symmetry code: (i) x, $-y+\frac{1}{2}$, $z-\frac{1}{2}$; see Table 1 and Fig. 2] form chains parallel to [001]. The cohesion is

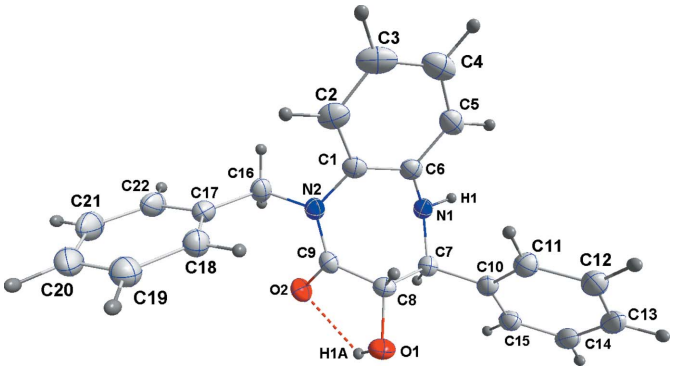


Figure 1
The title molecule, showing the labelling scheme and 50% probability ellipsoids for non-H atoms. The intramolecular hydrogen bond is shown as a dotted line.

reinforced by O1—H1*A*···π(ring) interactions involving the C10–C15 ring at $x, -y+\frac{1}{2}, z+\frac{1}{2}$ (see Table 1). The chains are further associated through contact C13—H13···π(ring), involving the C1–C6 benzene ring of the benzodiazepine as acceptor, with symmetry code $(1+x, y, z)$ (Fig. 3 and Table 1).

Synthesis and crystallization

To a solution of 3-hydroxy-4-phenyl-4,5-dihydro-1*H*-1,5-benzodiazepin-2(3*H*)-one (1 g, 3.94 mmol) in dimethylformamide (20 ml) were added benzyl chloride (0.95 g, 7.88 mmol), potassium carbonate (1 g, 7.4 mmol) and a catalytic amount of tetra-*n*-butylammonium bromide. The mixture was stirred at room temperature for 48 h. The solution was filtered and the solvent removed under reduced pressure. The residue was recrystallized from ethanol to afford the title compound as colourless crystals.

Refinement

Crystal and refinement details appear in Table 2.

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C10–C15 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2	0.878 (18)	2.166 (17)	2.6601 (12)	115.1 (14)
N1—H1···O2^{i}	0.918 (15)	2.045 (16)	2.9531 (12)	169.5 (13)
O1—H1*A*···*Cg*2^{ii}	0.878 (18)	2.719 (18)	3.4636 (10)	143.4 (16)
C13—H13···*Cg*1^{iii}	0.984 (15)	2.699 (15)	3.3283 (14)	122.1 (10)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{20}N_2O_2$
M_r	344.40
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	8.9169 (2), 17.6360 (5), 11.7937 (3)
β (°)	109.199 (1)
V (Å^3)	1751.51 (8)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	0.67
Crystal size (mm)	0.20 × 0.18 × 0.17
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.82, 0.89
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37686, 3413, 3177
R_{int}	0.037
(sin θ/λ)$_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.092, 1.04
No. of reflections	3413
No. of parameters	316
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.17

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

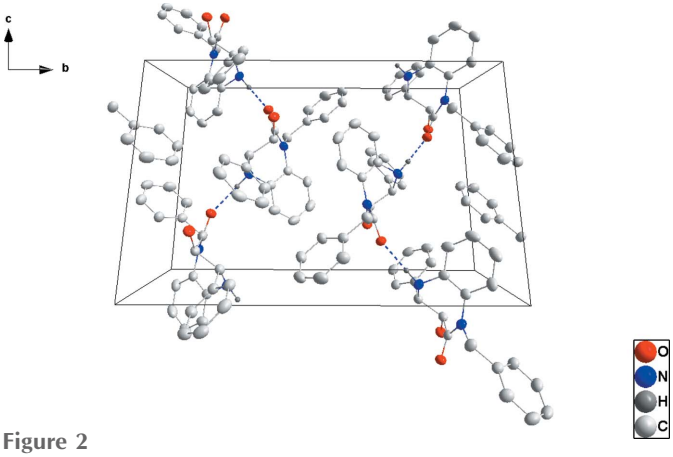


Figure 2
Packing viewed along the *a* axis, with the N—H···O hydrogen bonds shown as dotted lines.

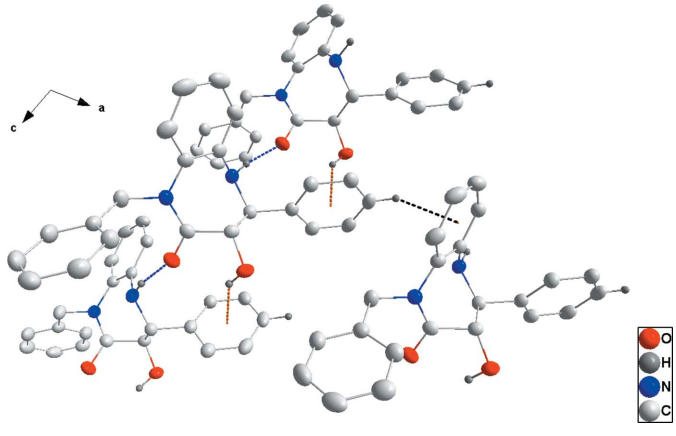


Figure 3
A portion of one chain, showing the N—H···O (blue dotted line) and O—H···π(ring) (orange dotted line) interactions on the left and one of the C—H···π(ring) interactions (black dotted line) between the chains.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{22}H_{20}N_2O_2$
M_r = 344.40
Monoclinic, $P2_1/c$
a = 8.9169 (2) Å
b = 17.6360 (5) Å
c = 11.7937 (3) Å
β = 109.199 (1)°
V = 1751.51 (8) Å^3
Z = 4
$F(000)$ = 728
D_x = 1.306 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9851 reflections
θ = 2.5–71.9°
μ = 0.67 mm^{-1}
T = 150 K
Block, colourless
0.20 × 0.18 × 0.17 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.82, T_{max} = 0.89
37686 measured reflections
3413 independent reflections
3177 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 72.1°, θ_{min} = 4.7°
h = −10→10
k = −21→19
l = −11→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.092
S = 1.04
3413 reflections
316 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
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.4657P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0054 (4)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.81338 (9)	0.35773 (5)	0.75652 (7)	0.0327 (2)
H1A	0.799 (2)	0.3328 (10)	0.8165 (16)	0.056 (5)*
O2	0.55542 (10)	0.32787 (5)	0.81467 (7)	0.0331 (2)
N1	0.50274 (11)	0.27320 (5)	0.49763 (8)	0.0276 (2)
H1	0.5059 (17)	0.2401 (9)	0.4383 (13)	0.041 (4)*
N2	0.38729 (11)	0.37324 (5)	0.63890 (8)	0.0270 (2)
C1	0.35548 (12)	0.38753 (6)	0.51424 (9)	0.0269 (2)
C2	0.25775 (14)	0.44790 (7)	0.45973 (11)	0.0342 (3)
H2	0.2182 (16)	0.4807 (8)	0.5110 (12)	0.035 (3)*
C3	0.21116 (15)	0.45795 (7)	0.33638 (12)	0.0409 (3)
H3	0.1424 (18)	0.4987 (9)	0.2997 (14)	0.048 (4)*
C4	0.26397 (15)	0.40804 (8)	0.26721 (11)	0.0401 (3)
H4	0.2317 (17)	0.4149 (9)	0.1785 (14)	0.046 (4)*
C5	0.36499 (14)	0.34917 (7)	0.32094 (10)	0.0337 (3)
H5	0.4051 (17)	0.3133 (9)	0.2716 (13)	0.042 (4)*
C6	0.41277 (12)	0.33759 (6)	0.44519 (9)	0.0266 (2)
C7	0.66430 (13)	0.28233 (6)	0.58467 (9)	0.0260 (2)
H7	0.6833 (14)	0.2386 (7)	0.6399 (11)	0.024 (3)*
C8	0.66829 (12)	0.35285 (6)	0.66149 (9)	0.0254 (2)
H8	0.6564 (14)	0.3996 (7)	0.6109 (10)	0.022 (3)*
C9	0.53102 (13)	0.34961 (6)	0.71094 (9)	0.0258 (2)
C10	0.79289 (13)	0.28501 (6)	0.52625 (10)	0.0273 (2)
C11	0.78566 (14)	0.33802 (7)	0.43669 (10)	0.0316 (3)
H11	0.6959 (17)	0.3749 (9)	0.4111 (12)	0.041 (4)*
C12	0.89886 (14)	0.33828 (7)	0.37932 (10)	0.0353 (3)
H12	0.8903 (17)	0.3761 (9)	0.3147 (13)	0.043 (4)*
C13	1.02100 (14)	0.28571 (7)	0.41097 (11)	0.0360 (3)
H13	1.0997 (18)	0.2848 (8)	0.3689 (13)	0.044 (4)*
C14	1.03167 (14)	0.23378 (7)	0.50135 (11)	0.0348 (3)
H14	1.1170 (17)	0.1974 (9)	0.5247 (12)	0.039 (4)*
C15	0.91782 (13)	0.23347 (7)	0.55894 (10)	0.0305 (3)
H15	0.9247 (15)	0.1973 (8)	0.6224 (12)	0.031 (3)*
C16	0.25895 (14)	0.37887 (7)	0.69117 (11)	0.0316 (3)
H16A	0.2569 (16)	0.3305 (8)	0.7363 (12)	0.037 (4)*
H16B	0.1580 (17)	0.3833 (8)	0.6241 (12)	0.038 (4)*
C17	0.27738 (12)	0.44490 (6)	0.77704 (9)	0.0279 (2)
C18	0.38682 (14)	0.50269 (6)	0.78820 (10)	0.0318 (3)
H18	0.4578 (17)	0.5021 (8)	0.7375 (13)	0.043 (4)*
C19	0.40120 (15)	0.56106 (7)	0.87057 (11)	0.0365 (3)
H19	0.4842 (18)	0.6010 (9)	0.8800 (13)	0.048 (4)*
C20	0.30586 (16)	0.56241 (7)	0.94175 (11)	0.0391 (3)
H20	0.3194 (18)	0.6011 (9)	1.0033 (14)	0.048 (4)*
C21	0.19464 (16)	0.50561 (8)	0.92981 (12)	0.0422 (3)
H21	0.126 (2)	0.5057 (9)	0.9811 (15)	0.058 (5)*
C22	0.18007 (14)	0.44702 (7)	0.84832 (11)	0.0357 (3)

H22	0.1029 (17)	0.4053 (8)	0.8402 (12)	0.040 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0286 (4)	0.0352 (4)	0.0286 (4)	−0.0020 (3)	0.0017 (3)	0.0018 (3)
O2	0.0426 (5)	0.0318 (4)	0.0265 (4)	0.0005 (3)	0.0132 (3)	0.0030 (3)
N1	0.0271 (5)	0.0266 (5)	0.0297 (5)	−0.0033 (4)	0.0101 (4)	−0.0053 (4)
N2	0.0281 (5)	0.0262 (5)	0.0275 (5)	−0.0009 (3)	0.0103 (4)	−0.0034 (4)
C1	0.0251 (5)	0.0259 (5)	0.0274 (5)	−0.0045 (4)	0.0056 (4)	−0.0005 (4)
C2	0.0291 (6)	0.0264 (6)	0.0416 (6)	−0.0026 (4)	0.0042 (5)	−0.0006 (5)
C3	0.0327 (6)	0.0331 (6)	0.0454 (7)	−0.0059 (5)	−0.0027 (5)	0.0110 (5)
C4	0.0387 (7)	0.0455 (7)	0.0299 (6)	−0.0135 (5)	0.0029 (5)	0.0078 (5)
C5	0.0318 (6)	0.0412 (7)	0.0279 (6)	−0.0106 (5)	0.0093 (5)	−0.0004 (5)
C6	0.0233 (5)	0.0287 (5)	0.0271 (5)	−0.0069 (4)	0.0072 (4)	−0.0006 (4)
C7	0.0273 (5)	0.0241 (5)	0.0270 (5)	−0.0006 (4)	0.0097 (4)	0.0012 (4)
C8	0.0259 (5)	0.0238 (5)	0.0242 (5)	−0.0014 (4)	0.0052 (4)	0.0011 (4)
C9	0.0327 (6)	0.0198 (5)	0.0251 (5)	−0.0013 (4)	0.0096 (4)	−0.0021 (4)
C10	0.0262 (5)	0.0284 (5)	0.0274 (5)	−0.0045 (4)	0.0089 (4)	−0.0038 (4)
C11	0.0288 (6)	0.0341 (6)	0.0321 (6)	−0.0040 (5)	0.0103 (5)	0.0014 (5)
C12	0.0317 (6)	0.0440 (7)	0.0304 (6)	−0.0114 (5)	0.0105 (5)	−0.0020 (5)
C13	0.0269 (6)	0.0492 (7)	0.0336 (6)	−0.0122 (5)	0.0124 (5)	−0.0131 (5)
C14	0.0254 (6)	0.0397 (7)	0.0378 (6)	−0.0018 (5)	0.0084 (5)	−0.0107 (5)
C15	0.0292 (6)	0.0302 (6)	0.0308 (6)	−0.0024 (4)	0.0081 (5)	−0.0038 (4)
C16	0.0292 (6)	0.0324 (6)	0.0356 (6)	−0.0045 (4)	0.0143 (5)	−0.0058 (5)
C17	0.0254 (5)	0.0304 (6)	0.0269 (5)	0.0028 (4)	0.0074 (4)	−0.0006 (4)
C18	0.0326 (6)	0.0301 (6)	0.0339 (6)	−0.0002 (4)	0.0128 (5)	−0.0028 (4)
C19	0.0385 (7)	0.0307 (6)	0.0367 (6)	0.0017 (5)	0.0072 (5)	−0.0038 (5)
C20	0.0444 (7)	0.0384 (7)	0.0298 (6)	0.0123 (5)	0.0058 (5)	−0.0057 (5)
C21	0.0414 (7)	0.0540 (8)	0.0355 (6)	0.0113 (6)	0.0184 (6)	−0.0020 (6)
C22	0.0296 (6)	0.0435 (7)	0.0361 (6)	0.0014 (5)	0.0136 (5)	−0.0005 (5)

Geometric parameters (Å, º)

O1—C8	1.4084 (13)	C10—C11	1.3961 (16)
O1—H1A	0.878 (18)	C11—C12	1.3877 (16)
O2—C9	1.2312 (13)	C11—H11	0.998 (15)
N1—C6	1.4104 (14)	C12—C13	1.3849 (18)
N1—C7	1.4774 (14)	C12—H12	0.997 (15)
N1—H1	0.918 (15)	C13—C14	1.3846 (19)
N2—C9	1.3498 (14)	C13—H13	0.984 (15)
N2—C1	1.4253 (14)	C14—C15	1.3947 (16)
N2—C16	1.4708 (14)	C14—H14	0.963 (15)
C1—C2	1.3920 (16)	C15—H15	0.971 (14)
C1—C6	1.4047 (15)	C16—C17	1.5164 (15)
C2—C3	1.3866 (18)	C16—H16A	1.009 (15)
C2—H2	0.983 (14)	C16—H16B	0.987 (14)
C3—C4	1.384 (2)	C17—C18	1.3871 (16)

C3—H3	0.951 (16)	C17—C22	1.3931 (16)
C4—C5	1.3840 (18)	C18—C19	1.3921 (16)
C4—H4	0.997 (15)	C18—H18	1.003 (15)
C5—C6	1.4000 (15)	C19—C20	1.3774 (18)
C5—H5	1.002 (15)	C19—H19	1.001 (16)
C7—C10	1.5203 (15)	C20—C21	1.384 (2)
C7—C8	1.5321 (14)	C20—H20	0.974 (16)
C7—H7	0.988 (13)	C21—C22	1.3878 (18)
C8—C9	1.5202 (15)	C21—H21	0.994 (18)
C8—H8	1.003 (12)	C22—H22	0.990 (15)
C10—C15	1.3906 (16)		

C8—O1—H1A	105.7 (11)	C15—C10—C7	120.59 (10)
C6—N1—C7	120.06 (8)	C11—C10—C7	120.64 (10)
C6—N1—H1	109.5 (9)	C12—C11—C10	120.74 (11)
C7—N1—H1	109.4 (9)	C12—C11—H11	119.3 (8)
C9—N2—C1	121.98 (9)	C10—C11—H11	119.9 (8)
C9—N2—C16	117.75 (9)	C13—C12—C11	120.00 (11)
C1—N2—C16	120.13 (9)	C13—C12—H12	120.6 (8)
C2—C1—C6	120.24 (10)	C11—C12—H12	119.4 (8)
C2—C1—N2	119.58 (10)	C14—C13—C12	119.95 (11)
C6—C1—N2	120.01 (9)	C14—C13—H13	119.8 (9)
C3—C2—C1	120.55 (12)	C12—C13—H13	120.2 (9)
C3—C2—H2	121.8 (8)	C13—C14—C15	120.05 (11)
C1—C2—H2	117.6 (8)	C13—C14—H14	120.5 (8)
C4—C3—C2	119.64 (12)	C15—C14—H14	119.5 (8)
C4—C3—H3	120.4 (9)	C10—C15—C14	120.49 (11)
C2—C3—H3	120.0 (9)	C10—C15—H15	119.0 (8)
C3—C4—C5	120.24 (11)	C14—C15—H15	120.5 (8)
C3—C4—H4	120.3 (9)	N2—C16—C17	113.79 (9)
C5—C4—H4	119.4 (9)	N2—C16—H16A	108.4 (8)
C4—C5—C6	121.12 (12)	C17—C16—H16A	108.3 (8)
C4—C5—H5	120.7 (8)	N2—C16—H16B	107.4 (8)
C6—C5—H5	118.2 (8)	C17—C16—H16B	110.1 (8)
C5—C6—C1	118.15 (10)	H16A—C16—H16B	108.7 (12)
C5—C6—N1	120.65 (10)	C18—C17—C22	118.77 (10)
C1—C6—N1	120.89 (9)	C18—C17—C16	123.09 (10)
N1—C7—C10	113.39 (9)	C22—C17—C16	118.13 (10)
N1—C7—C8	109.09 (8)	C17—C18—C19	120.67 (11)
C10—C7—C8	111.62 (9)	C17—C18—H18	119.9 (8)
N1—C7—H7	106.9 (7)	C19—C18—H18	119.5 (8)
C10—C7—H7	109.4 (7)	C20—C19—C18	120.29 (12)
C8—C7—H7	106.2 (7)	C20—C19—H19	120.1 (9)
O1—C8—C9	109.99 (8)	C18—C19—H19	119.5 (9)
O1—C8—C7	110.90 (9)	C19—C20—C21	119.39 (11)
C9—C8—C7	109.35 (8)	C19—C20—H20	121.1 (9)
O1—C8—H8	108.2 (7)	C21—C20—H20	119.4 (9)
C9—C8—H8	108.6 (7)	C20—C21—C22	120.68 (12)

C7—C8—H8	109.8 (7)	C20—C21—H21	120.2 (10)
O2—C9—N2	122.85 (10)	C22—C21—H21	119.1 (10)
O2—C9—C8	119.44 (10)	C21—C22—C17	120.19 (12)
N2—C9—C8	117.68 (9)	C21—C22—H22	121.6 (8)
C15—C10—C11	118.75 (10)	C17—C22—H22	118.2 (8)
C9—N2—C1—C2	−142.60 (10)	C7—C8—C9—O2	99.40 (11)
C16—N2—C1—C2	41.75 (14)	O1—C8—C9—N2	155.42 (9)
C9—N2—C1—C6	42.15 (14)	C7—C8—C9—N2	−82.57 (11)
C16—N2—C1—C6	−133.50 (10)	N1—C7—C10—C15	−122.85 (11)
C6—C1—C2—C3	2.31 (16)	C8—C7—C10—C15	113.45 (11)
N2—C1—C2—C3	−172.93 (10)	N1—C7—C10—C11	55.54 (13)
C1—C2—C3—C4	−0.80 (18)	C8—C7—C10—C11	−68.16 (13)
C2—C3—C4—C5	−1.13 (18)	C15—C10—C11—C12	1.45 (16)
C3—C4—C5—C6	1.57 (18)	C7—C10—C11—C12	−176.98 (10)
C4—C5—C6—C1	−0.08 (16)	C10—C11—C12—C13	−0.18 (17)
C4—C5—C6—N1	173.66 (10)	C11—C12—C13—C14	−1.16 (17)
C2—C1—C6—C5	−1.84 (15)	C12—C13—C14—C15	1.22 (17)
N2—C1—C6—C5	173.38 (9)	C11—C10—C15—C14	−1.38 (16)
C2—C1—C6—N1	−175.56 (9)	C7—C10—C15—C14	177.04 (10)
N2—C1—C6—N1	−0.35 (15)	C13—C14—C15—C10	0.07 (17)
C7—N1—C6—C5	117.83 (11)	C9—N2—C16—C17	72.54 (13)
C7—N1—C6—C1	−68.60 (13)	C1—N2—C16—C17	−111.63 (11)
C6—N1—C7—C10	−88.73 (11)	N2—C16—C17—C18	11.59 (16)
C6—N1—C7—C8	36.34 (13)	N2—C16—C17—C22	−168.02 (10)
N1—C7—C8—O1	171.71 (8)	C22—C17—C18—C19	1.11 (17)
C10—C7—C8—O1	−62.20 (11)	C16—C17—C18—C19	−178.49 (11)
N1—C7—C8—C9	50.25 (11)	C17—C18—C19—C20	−0.41 (18)
C10—C7—C8—C9	176.34 (8)	C18—C19—C20—C21	−0.61 (18)
C1—N2—C9—O2	−170.58 (10)	C19—C20—C21—C22	0.92 (19)
C16—N2—C9—O2	5.17 (15)	C20—C21—C22—C17	−0.21 (19)
C1—N2—C9—C8	11.46 (14)	C18—C17—C22—C21	−0.80 (17)
C16—N2—C9—C8	−172.79 (9)	C16—C17—C22—C21	178.82 (11)
O1—C8—C9—O2	−22.61 (13)		

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C1–C6 and C10–C15 phenyl rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2	0.878 (18)	2.166 (17)	2.6601 (12)	115.1 (14)
N1—H1···O2^{i}	0.918 (15)	2.045 (16)	2.9531 (12)	169.5 (13)
O1—H1*A*···*Cg*2^{ii}	0.878 (18)	2.719 (18)	3.4636 (10)	143.4 (16)
C13—H13···*Cg*1^{iii}	0.984 (15)	2.699 (15)	3.3283 (14)	122.1 (10)

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