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1-Benzyl-4-phenyl-1*H*-1,5-benzodiazepin-2(3*H*)-one

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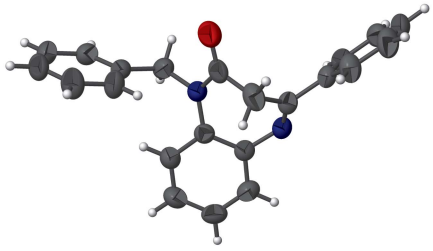
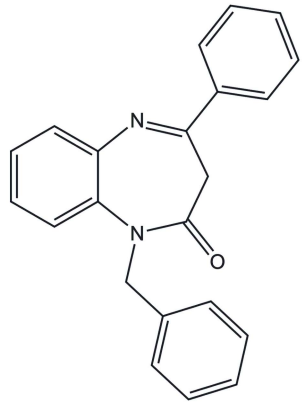
In the title molecule, $C_{22}H_{18}N_2O$, the seven-membered ring adopts a boat conformation with the planes of the pendant phenyl rings nearly perpendicular to the plane of the aromatic portion of the benzodiazepine core. Pairwise C—H$\cdots\pi$(ring) interactions form inversion dimers which pack in zigzag layers associated through weak C—H$\cdots$O hydrogen bonds.

3D view



Chemical scheme



Structure description

Benzodiazepines have attracted attention as an important class of heterocyclic compounds in the field of drugs and pharmaceuticals. These compounds are widely used as anti-anxiety agents (Kusanur *et al.*, 2004) and hypnotic agents (Zellou *et al.*, 1998). The present work is a continuation of our work on 1,5-benzodiazepin-2-one derivatives (Ballo *et al.*, 2010).

In the title compound (Fig. 1), the dihedral angle between the mean planes of the C10–C15 and C1–C6 rings is 83.82 (6)° while that between the mean planes of the C1–C6 and C17–C22 rings is 87.32 (6)°. A conformational analysis of the seven-membered ring yielded the puckering parameters $Q(2)$ = 0.879 (1) Å, $Q(3)$ = 0.219 (1) Å, $\varphi(2)$ = 207.53 (8)° and $\varphi(3)$ = 307.8 (3)°, which indicates a boat conformation.

In the crystal, the molecules form inversion dimers through pairwise C4—H4$\cdots\pi$ interactions (Table 1 and Fig. 2). These dimers pack in zigzag layers which are associated through weak C14—H14$\cdots$O1^{ii} hydrogen bonds (Table 1 and Figs. 2 and 3).

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

*Cg*1 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1^{i}	0.93	2.47	3.281 (2)	145
C4—H4···*Cg*1^{ii}	0.93	2.98	3.767 (2)	143

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

Synthesis and crystallization

To a solution of 4-phenyl-1,5-benzodiazepin-2-one (2.36 g, 10 mmol) in DMF (40 ml) was added benzyl chloride (2.3 ml, 20 mmol), potassium carbonate (2.77 g, 20 mmol) and a catalytic quantity of tetra-*n*-butylammonium bromide. The mixture was stirred at room temperature for 24 h. The solution was filtered and the solvent removed under reduced pressure. The residue was recrystallized from ethanol solution to afford the title compound as colourless crystals (yield: 68%).

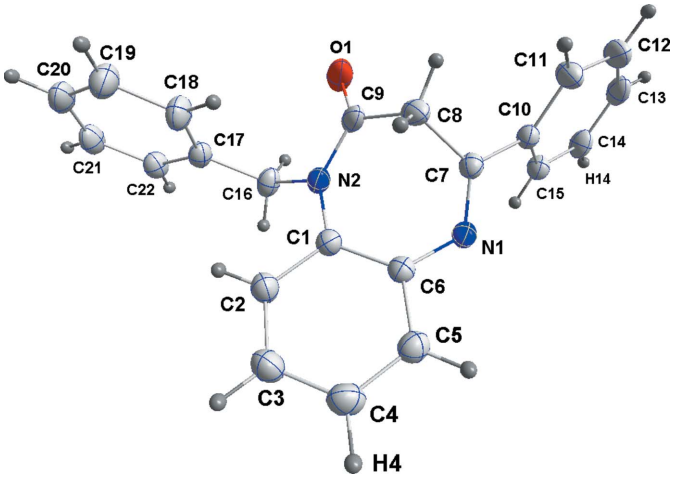


Figure 1
The title molecule with the labeling scheme and 50% probability ellipsoids.

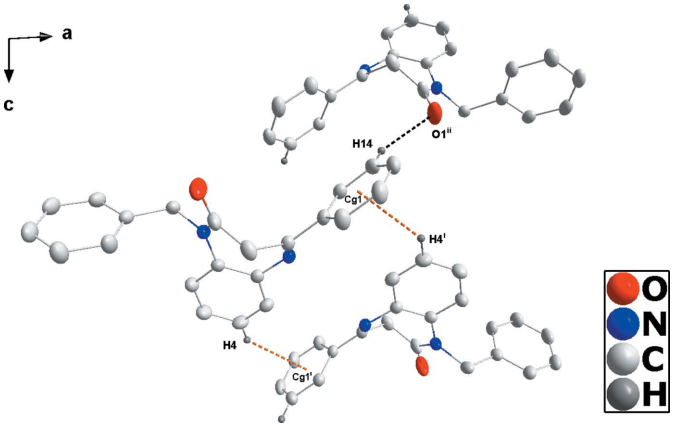


Figure 2
Detail of the intermolecular interactions with the C—H···O and C—H···π(ring) interactions shown, respectively, as black and orange dotted lines [symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; *Cg*1 is the centroid of the C10–C15 ring].

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}N_2O$
M_r	326.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	14.6973 (7), 5.9179 (3), 19.8537 (9)
β (°)	93.461 (1)
V (Å^3)	1723.67 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.43 × 0.30 × 0.22
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.87, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30265, 4261, 3110
R_{int}	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.139, 1.07
No. of reflections	4261
No. of parameters	226
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.15

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

Refinement

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

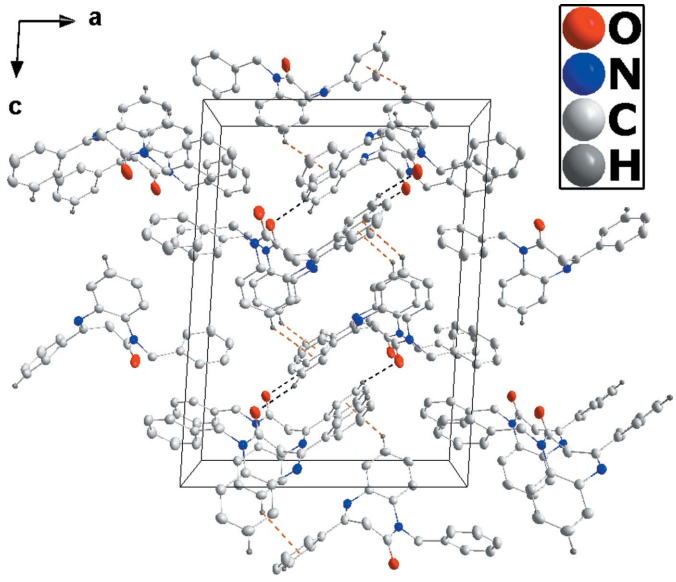


Figure 3
Packing viewed along the *b* axis showing the zigzag layers. The intermolecular interactions are represented as in Fig. 2. H atoms not involved in interactions have been omitted for clarity.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161988 [https://doi.org/10.1107/S241431461601988X]

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Crystal data

$C_{22}H_{18}N_2O$
M_r = 326.38
Monoclinic, $P2_1/c$
a = 14.6973 (7) Å
b = 5.9179 (3) Å
c = 19.8537 (9) Å
β = 93.461 (1)°
V = 1723.67 (14) Å^3
Z = 4
$F(000)$ = 688
D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9683 reflections
θ = 2.4–27.5°
μ = 0.08 mm^{-1}
T = 296 K
Block, colourless
0.43 × 0.30 × 0.22 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} = 0.87, T_{max} = 0.98
30265 measured reflections
4261 independent reflections
3110 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.3°, θ_{min} = 2.1°
h = −19→19
k = −7→7
l = −26→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.139
S = 1.07
4261 reflections
226 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0823P)^2 + 0.065P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, collected 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 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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.24295 (7)	0.5688 (2)	0.31026 (6)	0.0954 (4)
N1	0.40947 (6)	0.15215 (15)	0.42752 (5)	0.0473 (2)
N2	0.22089 (6)	0.26574 (17)	0.37616 (4)	0.0514 (3)
C1	0.24093 (7)	0.13976 (19)	0.43604 (5)	0.0458 (3)
C2	0.16861 (8)	0.0487 (2)	0.46964 (6)	0.0577 (3)
H2	0.1091	0.0767	0.4532	0.069*
C3	0.18363 (10)	−0.0813 (2)	0.52644 (7)	0.0663 (4)
H3	0.1346	−0.1407	0.5481	0.080*
C4	0.27189 (10)	−0.1238 (3)	0.55135 (7)	0.0663 (4)
H4	0.2823	−0.2090	0.5904	0.080*
C5	0.34419 (9)	−0.0404 (2)	0.51839 (6)	0.0565 (3)
H5	0.4033	−0.0731	0.5349	0.068*
C6	0.33060 (7)	0.09273 (18)	0.46054 (5)	0.0449 (3)
C7	0.41683 (7)	0.35018 (18)	0.40285 (6)	0.0459 (3)
C8	0.34347 (8)	0.5261 (2)	0.40845 (7)	0.0596 (3)
H8A	0.3241	0.5320	0.4543	0.071*
H8B	0.3663	0.6739	0.3968	0.071*
C9	0.26510 (8)	0.4603 (2)	0.36051 (7)	0.0602 (3)
C10	0.49709 (7)	0.40460 (19)	0.36411 (6)	0.0466 (3)
C11	0.53994 (8)	0.6133 (2)	0.36959 (7)	0.0624 (3)
H11	0.5181	0.7232	0.3980	0.075*
C12	0.61486 (9)	0.6586 (2)	0.33306 (8)	0.0720 (4)
H12	0.6442	0.7974	0.3379	0.086*
C13	0.64630 (8)	0.5000 (3)	0.28976 (7)	0.0673 (4)
H13	0.6957	0.5331	0.2643	0.081*
C14	0.60475 (8)	0.2924 (3)	0.28393 (6)	0.0627 (3)
H14	0.6264	0.1845	0.2548	0.075*
C15	0.53077 (7)	0.2438 (2)	0.32134 (6)	0.0522 (3)
H15	0.5034	0.1022	0.3178	0.063*
C16	0.14258 (8)	0.1991 (3)	0.33137 (6)	0.0593 (3)
H16A	0.1336	0.0375	0.3358	0.071*
H16B	0.1571	0.2284	0.2852	0.071*
C17	0.05352 (7)	0.3175 (2)	0.34414 (5)	0.0513 (3)
C18	0.04870 (9)	0.5022 (2)	0.38589 (7)	0.0662 (4)
H18	0.1013	0.5564	0.4088	0.079*

C19	−0.03416 (9)	0.6081 (3)	0.39392 (8)	0.0759 (4)
H19	−0.0369	0.7328	0.4223	0.091*
C20	−0.11235 (9)	0.5294 (3)	0.36009 (8)	0.0704 (4)
H20	−0.1677	0.6016	0.3651	0.084*
C21	−0.10814 (8)	0.3448 (3)	0.31912 (7)	0.0668 (4)
H21	−0.1609	0.2900	0.2966	0.080*
C22	−0.02581 (8)	0.2394 (2)	0.31100 (6)	0.0595 (3)
H22	−0.0236	0.1141	0.2829	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0594 (6)	0.1204 (9)	0.1077 (8)	0.0146 (6)	0.0168 (5)	0.0682 (8)
N1	0.0425 (5)	0.0469 (5)	0.0521 (5)	0.0025 (4)	−0.0001 (4)	−0.0024 (4)
N2	0.0423 (5)	0.0628 (6)	0.0491 (5)	0.0057 (4)	0.0040 (4)	0.0092 (4)
C1	0.0478 (6)	0.0463 (6)	0.0433 (6)	0.0023 (4)	0.0036 (4)	−0.0003 (4)
C2	0.0487 (6)	0.0674 (8)	0.0574 (7)	−0.0014 (5)	0.0064 (5)	0.0068 (6)
C3	0.0657 (8)	0.0745 (9)	0.0599 (8)	−0.0073 (7)	0.0126 (6)	0.0125 (7)
C4	0.0775 (9)	0.0708 (9)	0.0499 (7)	−0.0024 (7)	−0.0010 (6)	0.0141 (6)
C5	0.0583 (7)	0.0589 (7)	0.0510 (6)	0.0010 (5)	−0.0066 (5)	0.0023 (5)
C6	0.0467 (6)	0.0418 (5)	0.0458 (6)	0.0002 (4)	0.0011 (4)	−0.0044 (5)
C7	0.0418 (5)	0.0434 (6)	0.0524 (6)	0.0024 (4)	0.0010 (4)	−0.0064 (5)
C8	0.0548 (7)	0.0426 (6)	0.0835 (9)	0.0056 (5)	0.0222 (6)	−0.0005 (6)
C9	0.0434 (6)	0.0668 (8)	0.0720 (8)	0.0152 (5)	0.0177 (5)	0.0207 (7)
C10	0.0374 (5)	0.0482 (6)	0.0539 (6)	0.0029 (4)	−0.0006 (4)	−0.0008 (5)
C11	0.0507 (7)	0.0514 (7)	0.0857 (9)	−0.0045 (5)	0.0089 (6)	−0.0081 (6)
C12	0.0495 (7)	0.0635 (8)	0.1033 (11)	−0.0066 (6)	0.0073 (7)	0.0098 (8)
C13	0.0400 (6)	0.0891 (10)	0.0731 (8)	0.0042 (6)	0.0065 (5)	0.0194 (8)
C14	0.0490 (6)	0.0831 (9)	0.0564 (7)	0.0137 (6)	0.0056 (5)	−0.0032 (6)
C15	0.0456 (6)	0.0552 (7)	0.0554 (6)	0.0037 (5)	−0.0007 (5)	−0.0048 (5)
C16	0.0504 (6)	0.0810 (9)	0.0461 (6)	0.0112 (6)	0.0013 (5)	−0.0011 (6)
C17	0.0446 (6)	0.0645 (7)	0.0447 (6)	0.0044 (5)	0.0023 (4)	0.0066 (5)
C18	0.0435 (6)	0.0796 (9)	0.0752 (8)	0.0022 (6)	0.0003 (6)	−0.0129 (7)
C19	0.0575 (8)	0.0770 (9)	0.0942 (11)	0.0082 (7)	0.0112 (7)	−0.0135 (8)
C20	0.0439 (6)	0.0825 (10)	0.0852 (10)	0.0103 (6)	0.0087 (6)	0.0155 (8)
C21	0.0440 (6)	0.0875 (10)	0.0680 (8)	−0.0048 (6)	−0.0034 (5)	0.0127 (7)
C22	0.0543 (7)	0.0705 (8)	0.0531 (7)	−0.0039 (6)	−0.0012 (5)	0.0025 (6)

Geometric parameters (Å, º)

O1—C9	1.2139 (15)	C11—C12	1.3808 (18)
N1—C7	1.2773 (14)	C11—H11	0.9300
N1—C6	1.4103 (13)	C12—C13	1.372 (2)
N2—C9	1.3672 (16)	C12—H12	0.9300
N2—C1	1.4190 (14)	C13—C14	1.374 (2)
N2—C16	1.4653 (15)	C13—H13	0.9300
C1—C2	1.3969 (16)	C14—C15	1.3836 (17)
C1—C6	1.4048 (15)	C14—H14	0.9300

C2—C3	1.3719 (18)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.5193 (16)
C3—C4	1.383 (2)	C16—H16A	0.9700
C3—H3	0.9300	C16—H16B	0.9700
C4—C5	1.3731 (19)	C17—C18	1.3766 (18)
C4—H4	0.9300	C17—C22	1.3832 (17)
C5—C6	1.3971 (16)	C18—C19	1.3873 (18)
C5—H5	0.9300	C18—H18	0.9300
C7—C10	1.4820 (15)	C19—C20	1.377 (2)
C7—C8	1.5078 (15)	C19—H19	0.9300
C8—C9	1.5007 (19)	C20—C21	1.366 (2)
C8—H8A	0.9700	C20—H20	0.9300
C8—H8B	0.9700	C21—C22	1.3795 (18)
C10—C15	1.3865 (15)	C21—H21	0.9300
C10—C11	1.3879 (17)	C22—H22	0.9300

C7—N1—C6	119.87 (9)	C12—C11—H11	119.9
C9—N2—C1	123.75 (10)	C10—C11—H11	119.9
C9—N2—C16	117.08 (10)	C13—C12—C11	120.40 (13)
C1—N2—C16	118.87 (10)	C13—C12—H12	119.8
C2—C1—C6	118.89 (10)	C11—C12—H12	119.8
C2—C1—N2	118.52 (10)	C12—C13—C14	119.99 (12)
C6—C1—N2	122.49 (10)	C12—C13—H13	120.0
C3—C2—C1	121.31 (12)	C14—C13—H13	120.0
C3—C2—H2	119.3	C13—C14—C15	120.03 (12)
C1—C2—H2	119.3	C13—C14—H14	120.0
C2—C3—C4	119.79 (12)	C15—C14—H14	120.0
C2—C3—H3	120.1	C14—C15—C10	120.48 (12)
C4—C3—H3	120.1	C14—C15—H15	119.8
C5—C4—C3	120.02 (12)	C10—C15—H15	119.8
C5—C4—H4	120.0	N2—C16—C17	115.33 (10)
C3—C4—H4	120.0	N2—C16—H16A	108.4
C4—C5—C6	121.21 (11)	C17—C16—H16A	108.4
C4—C5—H5	119.4	N2—C16—H16B	108.4
C6—C5—H5	119.4	C17—C16—H16B	108.4
C5—C6—C1	118.75 (10)	H16A—C16—H16B	107.5
C5—C6—N1	116.23 (9)	C18—C17—C22	118.64 (11)
C1—C6—N1	124.74 (10)	C18—C17—C16	122.87 (11)
N1—C7—C10	119.13 (9)	C22—C17—C16	118.47 (11)
N1—C7—C8	121.86 (10)	C17—C18—C19	120.36 (12)
C10—C7—C8	118.90 (10)	C17—C18—H18	119.8
C9—C8—C7	107.40 (10)	C19—C18—H18	119.8
C9—C8—H8A	110.2	C20—C19—C18	120.24 (14)
C7—C8—H8A	110.2	C20—C19—H19	119.9
C9—C8—H8B	110.2	C18—C19—H19	119.9
C7—C8—H8B	110.2	C21—C20—C19	119.65 (12)
H8A—C8—H8B	108.5	C21—C20—H20	120.2
O1—C9—N2	121.64 (14)	C19—C20—H20	120.2

O1—C9—C8	122.78 (13)	C20—C21—C22	120.21 (12)
N2—C9—C8	115.56 (10)	C20—C21—H21	119.9
C15—C10—C11	118.80 (11)	C22—C21—H21	119.9
C15—C10—C7	119.57 (10)	C21—C22—C17	120.89 (13)
C11—C10—C7	121.63 (10)	C21—C22—H22	119.6
C12—C11—C10	120.27 (13)	C17—C22—H22	119.6
C9—N2—C1—C2	139.33 (12)	C7—C8—C9—N2	66.58 (13)
C16—N2—C1—C2	−34.13 (15)	N1—C7—C10—C15	38.62 (15)
C9—N2—C1—C6	−44.34 (16)	C8—C7—C10—C15	−137.79 (12)
C16—N2—C1—C6	142.19 (11)	N1—C7—C10—C11	−141.23 (12)
C6—C1—C2—C3	1.24 (19)	C8—C7—C10—C11	42.37 (16)
N2—C1—C2—C3	177.70 (12)	C15—C10—C11—C12	−0.15 (19)
C1—C2—C3—C4	0.1 (2)	C7—C10—C11—C12	179.70 (11)
C2—C3—C4—C5	−1.5 (2)	C10—C11—C12—C13	1.6 (2)
C3—C4—C5—C6	1.6 (2)	C11—C12—C13—C14	−1.8 (2)
C4—C5—C6—C1	−0.32 (18)	C12—C13—C14—C15	0.5 (2)
C4—C5—C6—N1	−174.53 (12)	C13—C14—C15—C10	1.00 (18)
C2—C1—C6—C5	−1.09 (17)	C11—C10—C15—C14	−1.16 (17)
N2—C1—C6—C5	−177.40 (10)	C7—C10—C15—C14	178.99 (10)
C2—C1—C6—N1	172.58 (11)	C9—N2—C16—C17	−81.50 (13)
N2—C1—C6—N1	−3.73 (17)	C1—N2—C16—C17	92.40 (13)
C7—N1—C6—C5	−140.63 (11)	N2—C16—C17—C18	11.36 (18)
C7—N1—C6—C1	45.55 (15)	N2—C16—C17—C22	−170.31 (11)
C6—N1—C7—C10	−175.68 (9)	C22—C17—C18—C19	−0.5 (2)
C6—N1—C7—C8	0.61 (16)	C16—C17—C18—C19	177.85 (13)
N1—C7—C8—C9	−73.35 (14)	C17—C18—C19—C20	−0.1 (2)
C10—C7—C8—C9	102.95 (11)	C18—C19—C20—C21	0.7 (2)
C1—N2—C9—O1	−176.47 (11)	C19—C20—C21—C22	−0.8 (2)
C16—N2—C9—O1	−2.89 (17)	C20—C21—C22—C17	0.2 (2)
C1—N2—C9—C8	4.97 (16)	C18—C17—C22—C21	0.41 (19)
C16—N2—C9—C8	178.55 (9)	C16—C17—C22—C21	−177.99 (12)
C7—C8—C9—O1	−111.96 (14)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1^{i}	0.93	2.47	3.2808 (17)	145
C4—H4···*Cg*1^{ii}	0.93	2.98	3.767 (2)	143

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