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(*E*)-*N*′-Benzylidene-2-phenylquinoline-4-carbohydrazide

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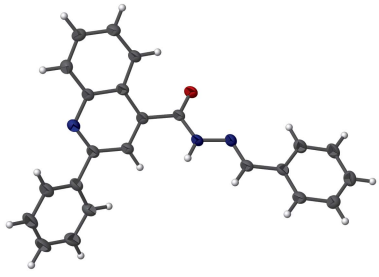
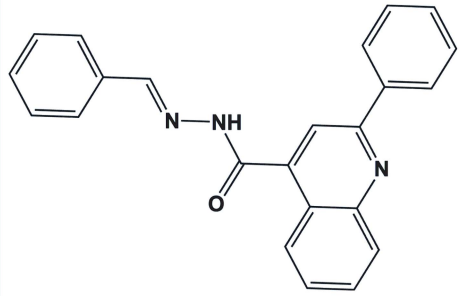
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{23}H_{17}N_3O$, there is a short intramolecular C—H···O contact present, and the conformation about the C=N bond is *E*. The phenyl and benzylidene rings make dihedral angles of 28.21 (15) and 37.65 (14)° with the mean plane of the quinoline moiety. In the crystal, molecules are linked by N—H···O and C—H···O hydrogen bonds, forming chains propagating along [001], with the O atom accepting three hydrogen bonds.

3D view



Chemical scheme



Structure description

It has been reported that quinoline derivatives serve as antagonists (Bennacef *et al.*, 2007), analgesic agents (Gopalsamy & Pallai, 1997), 5HT3 antagonists (Anzini *et al.*, 1995) and structural subunits of natural products (Sivaprasad *et al.*, 2006). Among the compounds of a quinoline series, Atophan and its derivatives have shown a variety of biological effects (Muscia *et al.*, 2008; Wang *et al.*, 2009). Moreover, hydrazide-hydrazone compounds are found to be associated with various biological activities such as antimicrobial, anticonvulsant, analgesic, anti-inflammatory, anti-platelet, anti-tubercular and anti-tumour properties (Mohamed *et al.*, 2015). As part of our studies in this area, we now report the crystal structure of the title compound.

The molecular structure of the title compound is illustrated in Fig. 1. The quinoline moiety is slightly twisted as indicated by the dihedral angle of 2.27 (16)° between the C1–C6 and N1/C6–C9 rings. The phenyl (C10–C15) and benzylidene (C18–C23) rings make dihedral angles of 28.21 (15) and 37.65 (14)°, respectively, with the mean plane of the

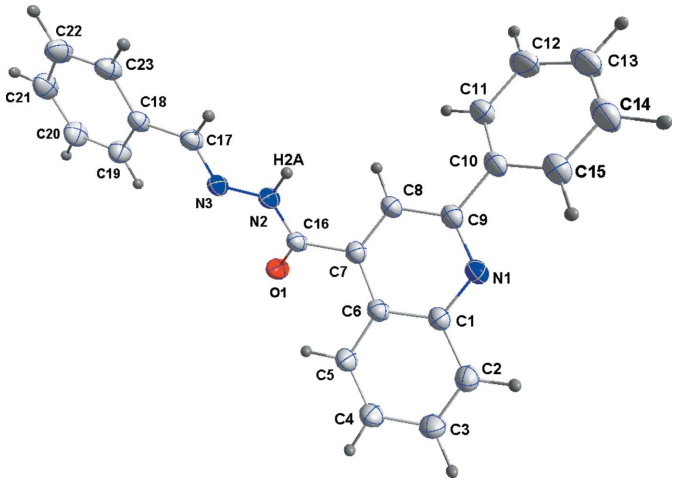


Figure 1
The molecular structure of the title compound, showing the atom labelling and 50% probability displacement ellipsoids.

quinoline moiety. The conformation about the C17═N3 bond is *E* and there is a short C5—H5···O1 contact in the molecule (Table 1).

In the crystal, N2—H2*A*···O1^{i}, C8—H8···O1^{i} and C17—H17···O1^{i} [symmetry code: (i) x, $-y+1$, $z-\frac{1}{2}$] hydrogen bonds link the molecules into chains along the *c*-axis direction (Table 1 and Fig. 2).

Synthesis and crystallization

The title compound was prepared in 89% yield according to a reported procedure (Mohamed *et al.*, 2016). Colourless needle-like crystals of the title compound were obtained by recrystallization from ethanol solution (m.p. 515–518 K).

Refinement

Crystal and refinement details are given in Table 2.

Acknowledgements

The support of NSF–MRI Grant No. 1228232 for the purchase of the diffractometer and Tulane University for support of the Tulane Crystallography Laboratory are gratefully acknowledged.

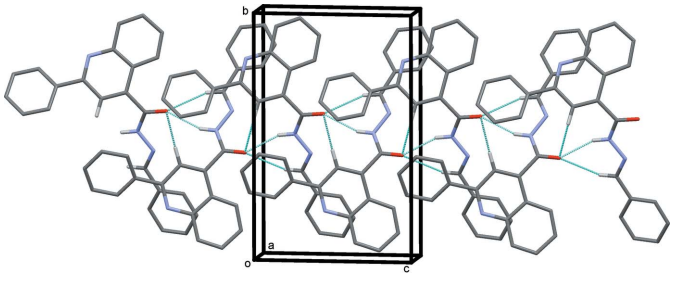


Figure 2
A view along the *a* axis of the crystal packing of the title compound. The N—H···O and C—H···O hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only H atoms H26, H8 and H17 have been included.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1	0.95	2.34	2.939 (3)	121
N2—H2*A*···O1^{i}	0.88 (4)	2.08 (4)	2.907 (3)	155 (4)
C8—H8···O1^{i}	0.95	2.50	3.288 (3)	140
C17—H17···O1^{i}	0.95	2.52	3.268 (3)	136

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{17}N_3O$
M_r	351.39
Crystal system, space group	Monoclinic, *Pc*
Temperature (K)	150
a, *b*, *c* (Å)	7.6704 (8), 13.2898 (13), 9.0627 (9)
β (°)	107.220 (6)
V (Å^3)	882.42 (16)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.66
Crystal size (mm)	0.24 × 0.07 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.83, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6668, 2637, 2394
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.087, 1.07
No. of reflections	2637
No. of parameters	250
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.16

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

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full crystallographic data

IUCrData (2016). **1**, x161544 [https://doi.org/10.1107/S2414314616015443]

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Crystal data

$C_{23}H_{17}N_3O$
M_r = 351.39
Monoclinic, *Pc*
a = 7.6704 (8) Å
b = 13.2898 (13) Å
c = 9.0627 (9) Å
β = 107.220 (6)°
V = 882.42 (16) Å^3
Z = 2
F(000) = 368
D_x = 1.323 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54178 Å
Cell parameters from 5448 reflections
θ = 3.3–72.3°
μ = 0.66 mm^{-1}
T = 150 K
Needles, colourless
0.24 × 0.07 × 0.04 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC I*μ*S micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.83, T_{max} = 0.97
6668 measured reflections
2637 independent reflections
2394 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 72.3°, θ_{min} = 3.3°
h = −9→8
k = −16→15
l = −10→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.087
S = 1.07
2637 reflections
250 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 0.1673P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0046 (8)
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.2 (4)

Special details

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. Refined as a 2-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5328 (3)	0.41857 (14)	0.9098 (2)	0.0351 (5)
N1	0.3365 (4)	0.19467 (18)	0.4307 (3)	0.0312 (5)
N2	0.6135 (4)	0.50398 (17)	0.7228 (3)	0.0296 (5)
H2A	0.604 (5)	0.510 (3)	0.624 (4)	0.045 (10)*
N3	0.6784 (3)	0.58400 (17)	0.8203 (3)	0.0296 (5)
C1	0.4132 (4)	0.1685 (2)	0.5821 (3)	0.0290 (6)
C2	0.4235 (4)	0.0645 (2)	0.6177 (3)	0.0344 (7)
H2	0.3728	0.0170	0.5384	0.041*
C3	0.5054 (5)	0.0318 (2)	0.7645 (3)	0.0361 (7)
H3	0.5112	−0.0382	0.7874	0.043*
C4	0.5811 (5)	0.1021 (2)	0.8818 (3)	0.0360 (7)
H4	0.6419	0.0790	0.9832	0.043*
C5	0.5688 (4)	0.2030 (2)	0.8526 (3)	0.0331 (7)
H5	0.6186	0.2492	0.9343	0.040*
C6	0.4826 (4)	0.2396 (2)	0.7019 (3)	0.0282 (6)
C7	0.4633 (4)	0.3437 (2)	0.6587 (3)	0.0280 (6)
C8	0.3796 (4)	0.3683 (2)	0.5077 (3)	0.0294 (6)
H8	0.3617	0.4370	0.4780	0.035*
C9	0.3195 (4)	0.2915 (2)	0.3955 (3)	0.0296 (6)
C10	0.2341 (4)	0.3167 (2)	0.2296 (3)	0.0318 (7)
C11	0.1402 (5)	0.4069 (2)	0.1854 (4)	0.0373 (7)
H11	0.1363	0.4552	0.2616	0.045*
C12	0.0520 (5)	0.4267 (3)	0.0301 (4)	0.0460 (8)
H12	−0.0135	0.4877	0.0007	0.055*
C13	0.0603 (5)	0.3570 (3)	−0.0810 (4)	0.0479 (9)
H13	−0.0009	0.3698	−0.1868	0.058*
C14	0.1574 (6)	0.2689 (3)	−0.0383 (4)	0.0477 (9)
H14	0.1659	0.2224	−0.1155	0.057*
C15	0.2429 (5)	0.2475 (3)	0.1164 (4)	0.0400 (8)
H15	0.3071	0.1859	0.1449	0.048*
C16	0.5387 (4)	0.4248 (2)	0.7759 (3)	0.0278 (6)
C17	0.7413 (4)	0.6576 (2)	0.7606 (3)	0.0293 (6)
H17	0.7424	0.6530	0.6563	0.035*
C18	0.8117 (4)	0.7491 (2)	0.8492 (3)	0.0278 (6)

C19	0.8098 (5)	0.7608 (2)	1.0015 (3)	0.0349 (7)
H19	0.7640	0.7083	1.0510	0.042*
C20	0.8744 (5)	0.8485 (2)	1.0807 (4)	0.0381 (7)
H20	0.8715	0.8565	1.1841	0.046*
C21	0.9431 (5)	0.9247 (2)	1.0102 (4)	0.0381 (7)
H21	0.9869	0.9850	1.0653	0.046*
C22	0.9483 (5)	0.9136 (2)	0.8603 (4)	0.0371 (7)
H22	0.9976	0.9655	0.8125	0.044*
C23	0.8806 (4)	0.8257 (2)	0.7794 (3)	0.0328 (7)
H23	0.8818	0.8184	0.6755	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0532 (14)	0.0323 (11)	0.0202 (10)	0.0008 (10)	0.0114 (9)	−0.0002 (8)
N1	0.0352 (15)	0.0334 (13)	0.0238 (12)	−0.0015 (11)	0.0065 (10)	0.0007 (10)
N2	0.0400 (15)	0.0293 (12)	0.0177 (10)	−0.0012 (10)	0.0058 (9)	−0.0007 (9)
N3	0.0354 (15)	0.0285 (12)	0.0223 (11)	−0.0006 (10)	0.0044 (10)	−0.0023 (9)
C1	0.0334 (16)	0.0288 (14)	0.0237 (13)	0.0004 (12)	0.0070 (11)	−0.0004 (11)
C2	0.0410 (19)	0.0311 (15)	0.0302 (16)	−0.0017 (14)	0.0093 (14)	−0.0037 (12)
C3	0.045 (2)	0.0270 (15)	0.0353 (16)	0.0014 (13)	0.0107 (14)	0.0043 (12)
C4	0.047 (2)	0.0327 (16)	0.0254 (15)	0.0025 (14)	0.0064 (13)	0.0031 (11)
C5	0.0429 (19)	0.0321 (15)	0.0218 (14)	0.0003 (13)	0.0058 (13)	0.0000 (12)
C6	0.0323 (17)	0.0297 (15)	0.0222 (13)	0.0016 (12)	0.0076 (11)	0.0011 (11)
C7	0.0326 (17)	0.0275 (14)	0.0233 (13)	0.0008 (12)	0.0075 (11)	−0.0006 (11)
C8	0.0361 (17)	0.0291 (14)	0.0213 (13)	0.0004 (12)	0.0057 (11)	0.0015 (11)
C9	0.0308 (17)	0.0338 (15)	0.0229 (13)	−0.0011 (13)	0.0059 (12)	−0.0002 (11)
C10	0.0309 (17)	0.0399 (17)	0.0219 (14)	−0.0039 (13)	0.0038 (12)	0.0002 (12)
C11	0.0402 (19)	0.0422 (17)	0.0254 (15)	0.0001 (14)	0.0034 (12)	0.0025 (13)
C12	0.044 (2)	0.052 (2)	0.0355 (18)	0.0004 (16)	0.0009 (14)	0.0093 (15)
C13	0.049 (2)	0.065 (2)	0.0227 (16)	−0.0093 (18)	0.0005 (14)	0.0049 (15)
C14	0.054 (2)	0.061 (2)	0.0237 (15)	−0.0054 (18)	0.0058 (14)	−0.0045 (15)
C15	0.046 (2)	0.0445 (18)	0.0262 (15)	−0.0002 (15)	0.0060 (13)	−0.0019 (13)
C16	0.0352 (17)	0.0272 (14)	0.0192 (14)	0.0029 (12)	0.0049 (11)	0.0004 (10)
C17	0.0337 (17)	0.0315 (15)	0.0214 (13)	0.0016 (12)	0.0060 (11)	0.0018 (11)
C18	0.0279 (16)	0.0308 (14)	0.0220 (13)	0.0019 (12)	0.0033 (11)	0.0000 (11)
C19	0.0392 (18)	0.0399 (17)	0.0260 (15)	−0.0053 (14)	0.0103 (13)	−0.0014 (12)
C20	0.043 (2)	0.0463 (18)	0.0248 (14)	−0.0055 (15)	0.0104 (13)	−0.0066 (13)
C21	0.0415 (19)	0.0350 (17)	0.0349 (17)	−0.0007 (14)	0.0068 (14)	−0.0077 (13)
C22	0.0451 (19)	0.0302 (15)	0.0341 (16)	−0.0011 (13)	0.0090 (13)	0.0016 (12)
C23	0.0398 (19)	0.0330 (15)	0.0236 (14)	0.0033 (13)	0.0065 (12)	0.0022 (11)

Geometric parameters (Å, º)

O1—C16	1.231 (3)	C10—C15	1.395 (4)
N1—C9	1.324 (3)	C11—C12	1.394 (4)
N1—C1	1.367 (4)	C11—H11	0.9500
N2—C16	1.353 (4)	C12—C13	1.382 (5)

N2—N3	1.378 (3)	C12—H12	0.9500
N2—H2A	0.88 (4)	C13—C14	1.381 (5)
N3—C17	1.279 (4)	C13—H13	0.9500
C1—C2	1.416 (4)	C14—C15	1.390 (5)
C1—C6	1.418 (4)	C14—H14	0.9500
C2—C3	1.363 (4)	C15—H15	0.9500
C2—H2	0.9500	C17—C18	1.469 (4)
C3—C4	1.406 (4)	C17—H17	0.9500
C3—H3	0.9500	C18—C23	1.383 (4)
C4—C5	1.365 (4)	C18—C19	1.393 (4)
C4—H4	0.9500	C19—C20	1.382 (4)
C5—C6	1.416 (4)	C19—H19	0.9500
C5—H5	0.9500	C20—C21	1.383 (5)
C6—C7	1.434 (4)	C20—H20	0.9500
C7—C8	1.367 (4)	C21—C22	1.379 (4)
C7—C16	1.504 (4)	C21—H21	0.9500
C8—C9	1.418 (4)	C22—C23	1.395 (4)
C8—H8	0.9500	C22—H22	0.9500
C9—C10	1.489 (4)	C23—H23	0.9500
C10—C11	1.395 (4)		

C9—N1—C1	118.1 (2)	C10—C11—H11	119.8
C16—N2—N3	118.8 (2)	C13—C12—C11	119.7 (3)
C16—N2—H2A	121 (2)	C13—C12—H12	120.1
N3—N2—H2A	119 (2)	C11—C12—H12	120.1
C17—N3—N2	115.4 (2)	C14—C13—C12	120.1 (3)
N1—C1—C2	117.1 (2)	C14—C13—H13	120.0
N1—C1—C6	123.4 (2)	C12—C13—H13	120.0
C2—C1—C6	119.5 (3)	C13—C14—C15	120.7 (3)
C3—C2—C1	120.9 (3)	C13—C14—H14	119.7
C3—C2—H2	119.6	C15—C14—H14	119.7
C1—C2—H2	119.6	C14—C15—C10	119.7 (3)
C2—C3—C4	119.6 (3)	C14—C15—H15	120.1
C2—C3—H3	120.2	C10—C15—H15	120.1
C4—C3—H3	120.2	O1—C16—N2	123.2 (3)
C5—C4—C3	121.2 (3)	O1—C16—C7	122.0 (3)
C5—C4—H4	119.4	N2—C16—C7	114.9 (2)
C3—C4—H4	119.4	N3—C17—C18	121.7 (2)
C4—C5—C6	120.6 (3)	N3—C17—H17	119.1
C4—C5—H5	119.7	C18—C17—H17	119.1
C6—C5—H5	119.7	C23—C18—C19	119.2 (3)
C5—C6—C1	118.2 (2)	C23—C18—C17	119.2 (2)
C5—C6—C7	125.1 (3)	C19—C18—C17	121.6 (3)
C1—C6—C7	116.6 (2)	C20—C19—C18	120.1 (3)
C8—C7—C6	118.9 (3)	C20—C19—H19	120.0
C8—C7—C16	120.2 (3)	C18—C19—H19	120.0
C6—C7—C16	120.8 (3)	C19—C20—C21	120.4 (3)
C7—C8—C9	120.2 (3)	C19—C20—H20	119.8

C7—C8—H8	119.9	C21—C20—H20	119.8
C9—C8—H8	119.9	C22—C21—C20	120.2 (3)
N1—C9—C8	122.6 (3)	C22—C21—H21	119.9
N1—C9—C10	116.4 (2)	C20—C21—H21	119.9
C8—C9—C10	121.0 (3)	C21—C22—C23	119.5 (3)
C11—C10—C15	119.3 (3)	C21—C22—H22	120.2
C11—C10—C9	121.2 (3)	C23—C22—H22	120.2
C15—C10—C9	119.5 (3)	C18—C23—C22	120.6 (3)
C12—C11—C10	120.4 (3)	C18—C23—H23	119.7
C12—C11—H11	119.8	C22—C23—H23	119.7

C16—N2—N3—C17	−177.6 (3)	C8—C9—C10—C15	154.4 (3)
C9—N1—C1—C2	177.6 (3)	C15—C10—C11—C12	1.6 (5)
C9—N1—C1—C6	−2.9 (4)	C9—C10—C11—C12	−176.2 (3)
N1—C1—C2—C3	177.0 (3)	C10—C11—C12—C13	−1.0 (5)
C6—C1—C2—C3	−2.5 (5)	C11—C12—C13—C14	−0.8 (6)
C1—C2—C3—C4	−0.2 (5)	C12—C13—C14—C15	2.1 (6)
C2—C3—C4—C5	2.2 (5)	C13—C14—C15—C10	−1.5 (5)
C3—C4—C5—C6	−1.4 (5)	C11—C10—C15—C14	−0.4 (5)
C4—C5—C6—C1	−1.4 (4)	C9—C10—C15—C14	177.5 (3)
C4—C5—C6—C7	−179.6 (3)	N3—N2—C16—O1	−3.3 (4)
N1—C1—C6—C5	−176.2 (3)	N3—N2—C16—C7	177.0 (3)
C2—C1—C6—C5	3.3 (4)	C8—C7—C16—O1	144.0 (3)
N1—C1—C6—C7	2.2 (4)	C6—C7—C16—O1	−37.9 (4)
C2—C1—C6—C7	−178.3 (3)	C8—C7—C16—N2	−36.4 (4)
C5—C6—C7—C8	178.8 (3)	C6—C7—C16—N2	141.7 (3)
C1—C6—C7—C8	0.5 (4)	N2—N3—C17—C18	178.7 (3)
C5—C6—C7—C16	0.6 (4)	N3—C17—C18—C23	179.0 (3)
C1—C6—C7—C16	−177.6 (3)	N3—C17—C18—C19	−1.3 (5)
C6—C7—C8—C9	−2.4 (4)	C23—C18—C19—C20	0.7 (5)
C16—C7—C8—C9	175.8 (3)	C17—C18—C19—C20	−179.0 (3)
C1—N1—C9—C8	0.9 (4)	C18—C19—C20—C21	−0.7 (5)
C1—N1—C9—C10	−179.6 (3)	C19—C20—C21—C22	−0.2 (5)
C7—C8—C9—N1	1.8 (5)	C20—C21—C22—C23	1.2 (5)
C7—C8—C9—C10	−177.8 (3)	C19—C18—C23—C22	0.3 (5)
N1—C9—C10—C11	152.7 (3)	C17—C18—C23—C22	179.9 (3)
C8—C9—C10—C11	−27.8 (4)	C21—C22—C23—C18	−1.2 (5)
N1—C9—C10—C15	−25.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1	0.95	2.34	2.939 (3)	121
N2—H2*A*···O1^{i}	0.88 (4)	2.08 (4)	2.907 (3)	155 (4)
C8—H8···O1^{i}	0.95	2.50	3.288 (3)	140
C17—H17···O1^{i}	0.95	2.52	3.268 (3)	136

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