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1-Benzyl-3-[(4-methoxyphenyl)imino]indolin-2-one

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Keywords: crystal structure; *N*-benzylisatin; *p*-arnisidine; Schiff base.

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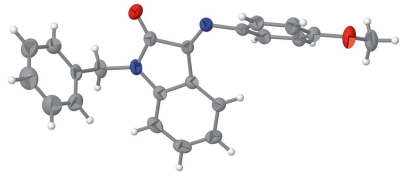
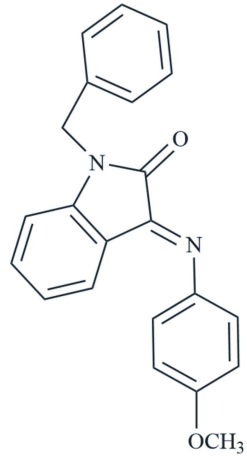
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{22}H_{18}N_2O_2$, is a Schiff base obtained by condensing *p*-arnisidine (4-methoxyaniline) with *N*-benzylisatin (1-benzyl-1*H*-indole-2,3-dione), which crystallizes in the triclinic $P\overline{1}$ space group. The benzyl and phenyl rings subtend dihedral angles of 76.08 (7) and 60.70 (6)°, respectively, with the isatin group. The imino C═N double bond exists in an *E* conformation.

3D view



Chemical scheme



Structure description

Isatin (1*H*, indole-2,3-dione), an indole, and its analogs are an important class of heterocyclic compounds due to the presence of the indole ring structure, which is common to many pharmaceutical agents (Visagaperumal *et al.*, 2018). Isatin and its derivatives have served as starting materials for several organic, metal–organic and organometallic syntheses (Garima & Sumitra 2014; Ikotun *et al.*, 2015, 2019). These compounds attract great interest because of their potent pharmacological and biological activities (Guo, 2019; Czeleń *et al.*, 2022; Ikotun *et al.*, 2022). *N*-Benzylisatin is a biologically potent derivative of isatin that has been used to prepare many new biologically potent Schiff bases and complexes suitable for medicinal purposes (Shakir & Al-Mudhafar, 2020; Banerjee, 2021). The crystal structure of *N*-benzylisatin has been determined (Akkurt *et al.*, 2006; Schutte *et al.*, 2012). We have previously reported the synthesis and crystal structure of the Schiff base prepared from *N*-benzylisatin and *p*-toluidine (Ikotun *et al.*, 2012). The crystal structure of 1-benzyl-3-[(4-methoxyphenyl)imino]indolin-2-one (Fig. 1) is hereby reported.

In the title compound, the asymmetric unit of compound contains one independent molecule crystallizing in the triclinic space group $P\overline{1}$. The crystal disintegrated at 300 K and the X-ray structure was acquired at room temperature. The benzyl and phenyl rings subtend dihedral angles of 76.08 (7) and 60.70 (6)°, respectively, with the isatin group.

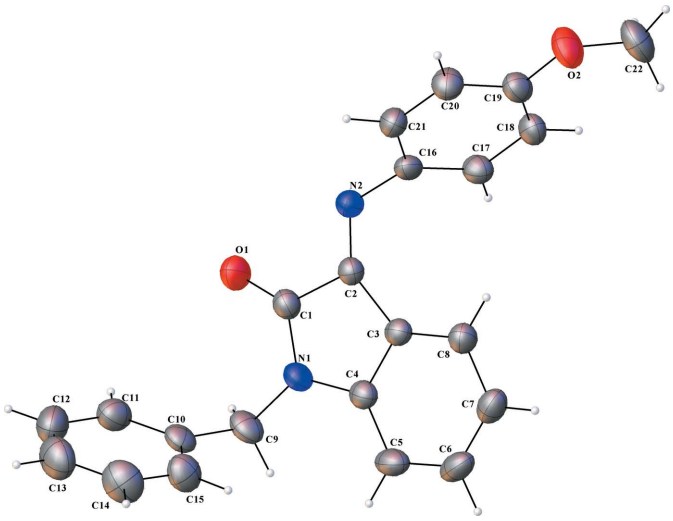


Figure 1
The molecular structure of 1-benzyl-3-[(4-methoxyphenyl)imino]indolin-2-one showing the atomic labelling; displacement ellipsoids are drawn at the 50% probability level.

Synthesis and crystallization

N-benzylisatin was prepared according to a literature method (Ikotun *et al.*, 2012). *N*-Benzylisatin (1.000 g, 4.2194 mmol) was dissolved in 20 ml of methanol. 4-Methoxylaniline (0.5196 g, 4.2194 mmol) was also dissolved in 10 ml of methanol. The two solutions were mixed together while stirring at room temperature with the addition of 6 drops of glacial acetic acid for 8 h. The precipitate was filtered under vacuum, dried and the weight was determined to be 1.0566 g (73%). X-ray-suitable crystals were obtained by recrystallization from dimethylformamide solution after about two weeks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}N_2O_2$
M_r	342.38
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	300
a, b, c (Å)	8.8872 (19), 8.8922 (19), 11.772 (3)
α, β, γ (°)	94.374 (6), 110.139 (6), 93.747 (6)
V (Å^3)	866.7 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.55 × 0.53 × 0.44
Data collection	
Diffractometer	Bruker APEXII DUO (PHOTON 100)
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.358, 0.431
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24116, 4003, 3219
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.109, 1.03
No. of reflections	4003
No. of parameters	237
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.18

Computer programs: *APEX2* and *SAINT* (Bruker, 2018), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *PLATON* (Spek, 2020).

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References

Akkurt, M., Türktekin, S., Jarrahpour, A. A., Khalili, D. & Büyükgüngör, O. (2006). *Acta Cryst.* E**62**, o1575–o1577.
Banerjee, S. (2021). *Int. J. Biol. Macromol.* **187**, 341–349.
Bruker (2018). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Czeleń, P., Skotnicka, A. & Szefler, B. (2022). *Int. J. Mol. Sci.* **23**, 8046.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Garima, M. & Sumitra, N. (2014). *Med. Chem.* **4**, 417–427.
Guo, H. (2019). *Eur. J. Med. Chem.* **164**, 678–688.
Ikotun, A. A., Adelani, P. O. & Egharevba, G. O. (2012). *Acta Cryst.* E**68**, o2098.
Ikotun, A. A., Babajide, E. E., Omolekan, T. O. & Ajaelu, C. J. (2022). Trop. J. Nat. Prod. Res., **6**, 1723-1726.
Ikotun, A. A., Coogan, M. P., Owoseni, A. A., Bhuvanesh, N. & Egharevba, G. O. (2015). *Acta Cryst.* E**71**, m106–m107.
Ikotun, A. A., Coogan, M. P., Owoseni, A. A. & Egharevba, G. O. (2019). *J. Chem Soc. Nigeria*, **44**, 948–958.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Schutte, M., Visser, H. G., Roodt, A. & Braband, H. (2012). *Acta Cryst.* E**68**, o777.
Shakir, T. H. & Al-Mudhafar, M. M. J. (2020). *Sys. Rev. Pharm.* **11**, 1950–1955.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.
Visagaperumal, S., Ezekwem, J. E., Munji, H. & Chandy, V. (2018). *Pharma Tutor.* **6**, 38-47.

full crystallographic data

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Crystal data

$C_{22}H_{18}N_2O_2$
M_r = 342.38
Triclinic, $P\overline{1}$
a = 8.8872 (19) Å
b = 8.8922 (19) Å
c = 11.772 (3) Å
α = 94.374 (6)°
β = 110.139 (6)°
γ = 93.747 (6)°
V = 866.7 (3) Å^3
Z = 2
$F(000)$ = 360
D_x = 1.312 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9907 reflections
θ = 2.5–27.5°
μ = 0.09 mm^{-1}
T = 300 K
Block, orange
0.55 × 0.53 × 0.44 mm

Data collection

Bruker APEXII DUO (PHOTON 100) diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.358, T_{max} = 0.431
24116 measured reflections
4003 independent reflections
3219 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −11→11
k = −11→11
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.109
S = 1.02
4003 reflections
237 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.2626P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL2018/3* (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.184 (7)

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. Systematic reflection conditions and statistical tests of the data suggested the space group P-1. A solution was obtained readily using XT/XS in APEX2. Hydrogen atoms were placed in idealized positions and were set riding on the respective parent atoms. All non-hydrogen atoms were refined with anisotropic thermal parameters. Absence of additional symmetry and voids were confirmed using PLATON. The structure was refined (weighted least squares refinement on F2) to convergence (Sheldrick, 2008, 2015; Dolomanov, *et al.*, 2009).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.32465 (13)	0.09548 (11)	0.17890 (9)	0.0467 (3)
O2	0.15900 (14)	0.09727 (14)	0.84290 (10)	0.0546 (3)
N1	0.33951 (14)	0.35590 (13)	0.20515 (10)	0.0367 (3)
N2	0.28029 (13)	0.11348 (12)	0.40997 (10)	0.0340 (3)
C1	0.32025 (15)	0.21291 (15)	0.23706 (12)	0.0336 (3)
C2	0.28984 (14)	0.23196 (14)	0.35726 (11)	0.0290 (3)
C3	0.29136 (14)	0.39654 (14)	0.38541 (11)	0.0295 (3)
C4	0.32480 (15)	0.46621 (15)	0.29236 (12)	0.0324 (3)
C5	0.34166 (17)	0.62236 (16)	0.29431 (14)	0.0429 (3)
H5	0.363199	0.667768	0.232234	0.051*
C6	0.32539 (17)	0.70910 (16)	0.39198 (15)	0.0455 (4)
H6	0.335311	0.814188	0.394595	0.055*
C7	0.29483 (17)	0.64298 (16)	0.48527 (14)	0.0429 (3)
H7	0.286015	0.703664	0.550177	0.051*
C8	0.27719 (16)	0.48616 (15)	0.48251 (12)	0.0355 (3)
H8	0.256098	0.441593	0.545095	0.043*
C9	0.37347 (17)	0.38347 (18)	0.09473 (13)	0.0426 (3)
H9A	0.352646	0.486352	0.076706	0.051*
H9B	0.300810	0.315234	0.027033	0.051*
C10	0.54526 (17)	0.36126 (16)	0.10615 (12)	0.0364 (3)
C11	0.5760 (2)	0.24368 (17)	0.03577 (14)	0.0458 (4)
H11	0.490557	0.178863	−0.017936	0.055*
C12	0.7322 (2)	0.2210 (2)	0.04411 (17)	0.0576 (4)
H12	0.751328	0.142265	−0.004234	0.069*
C13	0.8587 (2)	0.3160 (2)	0.12445 (18)	0.0634 (5)
H13	0.963785	0.301025	0.130876	0.076*
C14	0.8301 (2)	0.4332 (2)	0.19530 (17)	0.0612 (5)
H14	0.916046	0.496349	0.250138	0.073*
C15	0.67396 (19)	0.45734 (19)	0.18531 (14)	0.0484 (4)
H15	0.655276	0.538342	0.231865	0.058*
C16	0.24553 (15)	0.11827 (14)	0.51921 (11)	0.0311 (3)
C17	0.10870 (16)	0.17623 (15)	0.52979 (12)	0.0360 (3)
H17	0.039392	0.220029	0.465081	0.043*
C18	0.07458 (16)	0.16936 (16)	0.63595 (13)	0.0372 (3)
H18	−0.017670	0.207542	0.641944	0.045*
C19	0.17839 (17)	0.10545 (15)	0.73296 (12)	0.0370 (3)
C20	0.31359 (17)	0.04389 (16)	0.72204 (13)	0.0403 (3)
H20	0.382694	−0.000043	0.786762	0.048*
C21	0.34513 (16)	0.04796 (15)	0.61558 (12)	0.0360 (3)

H21	0.433457	0.003537	0.607830	0.043*
C22	0.0133 (2)	0.1394 (2)	0.85474 (16)	0.0595 (5)
H22A	−0.076403	0.080458	0.793597	0.089*
H22B	0.005243	0.245081	0.844710	0.089*
H22C	0.012674	0.121264	0.933923	0.089*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0621 (7)	0.0413 (6)	0.0439 (6)	0.0032 (5)	0.0297 (5)	−0.0034 (5)
O2	0.0610 (7)	0.0759 (8)	0.0391 (6)	0.0185 (6)	0.0293 (5)	0.0136 (5)
N1	0.0435 (6)	0.0387 (6)	0.0353 (6)	0.0060 (5)	0.0217 (5)	0.0099 (5)
N2	0.0413 (6)	0.0296 (6)	0.0364 (6)	0.0042 (5)	0.0197 (5)	0.0051 (4)
C1	0.0334 (7)	0.0367 (7)	0.0335 (7)	0.0044 (5)	0.0151 (5)	0.0045 (5)
C2	0.0283 (6)	0.0302 (6)	0.0306 (6)	0.0040 (5)	0.0125 (5)	0.0035 (5)
C3	0.0267 (6)	0.0293 (6)	0.0335 (6)	0.0047 (5)	0.0109 (5)	0.0060 (5)
C4	0.0285 (6)	0.0342 (7)	0.0368 (7)	0.0063 (5)	0.0130 (5)	0.0084 (5)
C5	0.0419 (8)	0.0374 (8)	0.0553 (9)	0.0070 (6)	0.0212 (7)	0.0185 (7)
C6	0.0401 (8)	0.0275 (7)	0.0694 (10)	0.0055 (6)	0.0193 (7)	0.0067 (7)
C7	0.0409 (8)	0.0341 (7)	0.0533 (9)	0.0053 (6)	0.0175 (7)	−0.0032 (6)
C8	0.0370 (7)	0.0341 (7)	0.0374 (7)	0.0035 (5)	0.0159 (6)	0.0017 (5)
C9	0.0452 (8)	0.0564 (9)	0.0318 (7)	0.0070 (7)	0.0178 (6)	0.0154 (6)
C10	0.0448 (7)	0.0424 (8)	0.0281 (6)	0.0042 (6)	0.0188 (6)	0.0116 (5)
C11	0.0556 (9)	0.0420 (8)	0.0424 (8)	0.0003 (7)	0.0214 (7)	0.0037 (6)
C12	0.0699 (11)	0.0520 (10)	0.0632 (11)	0.0179 (8)	0.0368 (9)	0.0071 (8)
C13	0.0488 (9)	0.0777 (13)	0.0722 (12)	0.0166 (9)	0.0287 (9)	0.0157 (10)
C14	0.0473 (9)	0.0743 (12)	0.0554 (10)	−0.0031 (8)	0.0124 (8)	0.0016 (9)
C15	0.0524 (9)	0.0552 (9)	0.0375 (8)	0.0015 (7)	0.0179 (7)	−0.0024 (7)
C16	0.0382 (7)	0.0240 (6)	0.0341 (6)	0.0004 (5)	0.0172 (5)	0.0031 (5)
C17	0.0364 (7)	0.0363 (7)	0.0376 (7)	0.0058 (5)	0.0142 (6)	0.0096 (6)
C18	0.0329 (7)	0.0392 (7)	0.0442 (8)	0.0048 (5)	0.0193 (6)	0.0043 (6)
C19	0.0429 (7)	0.0380 (7)	0.0336 (7)	0.0012 (6)	0.0183 (6)	0.0027 (5)
C20	0.0449 (8)	0.0434 (8)	0.0349 (7)	0.0121 (6)	0.0143 (6)	0.0099 (6)
C21	0.0391 (7)	0.0323 (7)	0.0415 (7)	0.0082 (5)	0.0191 (6)	0.0055 (6)
C22	0.0575 (10)	0.0811 (13)	0.0523 (10)	0.0020 (9)	0.0361 (8)	0.0053 (9)

Geometric parameters (Å, º)

O1—C1	1.2147 (16)	C10—C15	1.387 (2)
O2—C19	1.3697 (16)	C11—H11	0.9300
O2—C22	1.4197 (19)	C11—C12	1.387 (2)
N1—C1	1.3695 (17)	C12—H12	0.9300
N1—C4	1.4102 (17)	C12—C13	1.376 (3)
N1—C9	1.4663 (17)	C13—H13	0.9300
N2—C2	1.2753 (16)	C13—C14	1.376 (3)
N2—C16	1.4205 (16)	C14—H14	0.9300
C1—C2	1.5286 (17)	C14—C15	1.384 (2)
C2—C3	1.4739 (17)	C15—H15	0.9300

C3—C4	1.4056 (18)	C16—C17	1.3915 (18)
C3—C8	1.3895 (18)	C16—C21	1.3966 (19)
C4—C5	1.3843 (19)	C17—H17	0.9300
C5—H5	0.9300	C17—C18	1.3884 (19)
C5—C6	1.390 (2)	C18—H18	0.9300
C6—H6	0.9300	C18—C19	1.386 (2)
C6—C7	1.381 (2)	C19—C20	1.3934 (19)
C7—H7	0.9300	C20—H20	0.9300
C7—C8	1.3897 (19)	C20—C21	1.3776 (19)
C8—H8	0.9300	C21—H21	0.9300
C9—H9A	0.9700	C22—H22A	0.9600
C9—H9B	0.9700	C22—H22B	0.9600
C9—C10	1.513 (2)	C22—H22C	0.9600
C10—C11	1.384 (2)		

C19—O2—C22	118.34 (12)	C10—C11—C12	121.00 (15)
C1—N1—C4	110.94 (10)	C12—C11—H11	119.5
C1—N1—C9	122.28 (12)	C11—C12—H12	120.2
C4—N1—C9	126.77 (12)	C13—C12—C11	119.51 (16)
C2—N2—C16	122.11 (11)	C13—C12—H12	120.2
O1—C1—N1	125.81 (12)	C12—C13—H13	119.9
O1—C1—C2	127.73 (12)	C14—C13—C12	120.16 (16)
N1—C1—C2	106.44 (11)	C14—C13—H13	119.9
N2—C2—C1	117.81 (11)	C13—C14—H14	119.9
N2—C2—C3	136.54 (12)	C13—C14—C15	120.28 (16)
C3—C2—C1	105.47 (10)	C15—C14—H14	119.9
C4—C3—C2	106.74 (11)	C10—C15—H15	119.9
C8—C3—C2	133.75 (12)	C14—C15—C10	120.27 (15)
C8—C3—C4	119.38 (12)	C14—C15—H15	119.9
C3—C4—N1	110.38 (11)	C17—C16—N2	122.85 (12)
C5—C4—N1	128.15 (12)	C17—C16—C21	118.87 (12)
C5—C4—C3	121.46 (12)	C21—C16—N2	117.96 (11)
C4—C5—H5	121.1	C16—C17—H17	119.7
C4—C5—C6	117.89 (13)	C18—C17—C16	120.69 (12)
C6—C5—H5	121.1	C18—C17—H17	119.7
C5—C6—H6	119.2	C17—C18—H18	120.1
C7—C6—C5	121.59 (13)	C19—C18—C17	119.80 (12)
C7—C6—H6	119.2	C19—C18—H18	120.1
C6—C7—H7	119.9	O2—C19—C18	124.58 (12)
C6—C7—C8	120.26 (13)	O2—C19—C20	115.57 (12)
C8—C7—H7	119.9	C18—C19—C20	119.85 (12)
C3—C8—C7	119.41 (13)	C19—C20—H20	119.9
C3—C8—H8	120.3	C21—C20—C19	120.15 (13)
C7—C8—H8	120.3	C21—C20—H20	119.9
N1—C9—H9A	109.0	C16—C21—H21	119.7
N1—C9—H9B	109.0	C20—C21—C16	120.53 (12)
N1—C9—C10	112.92 (11)	C20—C21—H21	119.7
H9A—C9—H9B	107.8	O2—C22—H22A	109.5

C10—C9—H9A	109.0	O2—C22—H22B	109.5
C10—C9—H9B	109.0	O2—C22—H22C	109.5
C11—C10—C9	119.80 (13)	H22A—C22—H22B	109.5
C11—C10—C15	118.76 (14)	H22A—C22—H22C	109.5
C15—C10—C9	121.44 (13)	H22B—C22—H22C	109.5
C10—C11—H11	119.5		

O1—C1—C2—N2	6.2 (2)	C5—C6—C7—C8	−0.9 (2)
O1—C1—C2—C3	−177.95 (13)	C6—C7—C8—C3	0.3 (2)
O2—C19—C20—C21	−179.24 (13)	C8—C3—C4—N1	178.07 (11)
N1—C1—C2—N2	−174.78 (11)	C8—C3—C4—C5	−0.95 (19)
N1—C1—C2—C3	1.07 (13)	C9—N1—C1—O1	−1.9 (2)
N1—C4—C5—C6	−178.48 (13)	C9—N1—C1—C2	179.07 (11)
N1—C9—C10—C11	113.49 (15)	C9—N1—C4—C3	179.82 (12)
N1—C9—C10—C15	−67.07 (18)	C9—N1—C4—C5	−1.2 (2)
N2—C2—C3—C4	172.91 (14)	C9—C10—C11—C12	179.78 (14)
N2—C2—C3—C8	−2.5 (2)	C9—C10—C15—C14	179.05 (14)
N2—C16—C17—C18	175.73 (12)	C10—C11—C12—C13	0.6 (3)
N2—C16—C21—C20	−177.48 (12)	C11—C10—C15—C14	−1.5 (2)
C1—N1—C4—C3	−1.19 (15)	C11—C12—C13—C14	−0.4 (3)
C1—N1—C4—C5	177.75 (13)	C12—C13—C14—C15	−0.7 (3)
C1—N1—C9—C10	−74.72 (17)	C13—C14—C15—C10	1.7 (3)
C1—C2—C3—C4	−1.74 (13)	C15—C10—C11—C12	0.3 (2)
C1—C2—C3—C8	−177.20 (13)	C16—N2—C2—C1	−177.27 (11)
C2—N2—C16—C17	56.00 (18)	C16—N2—C2—C3	8.6 (2)
C2—N2—C16—C21	−130.53 (13)	C16—C17—C18—C19	0.6 (2)
C2—C3—C4—N1	1.84 (14)	C17—C16—C21—C20	−3.7 (2)
C2—C3—C4—C5	−177.19 (12)	C17—C18—C19—O2	177.83 (13)
C2—C3—C8—C7	175.61 (13)	C17—C18—C19—C20	−2.1 (2)
C3—C4—C5—C6	0.4 (2)	C18—C19—C20—C21	0.7 (2)
C4—N1—C1—O1	179.06 (13)	C19—C20—C21—C16	2.3 (2)
C4—N1—C1—C2	0.02 (14)	C21—C16—C17—C18	2.3 (2)
C4—N1—C9—C10	104.17 (15)	C22—O2—C19—C18	8.2 (2)
C4—C3—C8—C7	0.60 (19)	C22—O2—C19—C20	−171.81 (14)
C4—C5—C6—C7	0.6 (2)		