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(2*Z*)-*N*-(4-Methoxyphenyl)-2-(4-methoxyphenylimino)-2*H*-1,4-benzoxazin-3-amine

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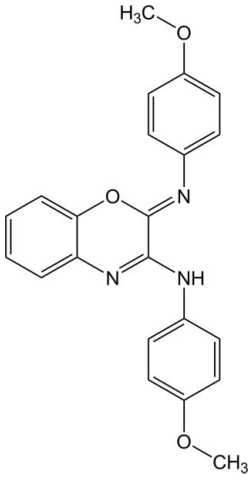
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.083; wR factor = 0.195; data-to-parameter ratio = 19.3.

In the crystal structure of the title compound, $C_{22}H_{19}N_3O_3$, intermolecular C—H···O hydrogen bonds link the molecules into a zigzag chain parallel to the face diagonal of the *ac* plane. The methoxy phenyl rings make a dihdral angle of 32.38 (7)° and form dihedral angles of 0.66 (8) and 24.17 (7)° with the fused benzooxazine ring system.

Related literature

For the Baeyer–Villiger oxidation of 1-alkyl-3-arylimino-2-indolinone with *m*-chloroperbenzoic acid to afford 1-alkyl-4-(arylimino)-1*H* benzo[*d*][1,3]oxazin-2(4*H*)-one, see: Mehrdad *et al.* (2011); Azizian *et al.* (2000); Jadidi *et al.* (2008). For a related structure, see: Asgari *et al.* (2011).



Experimental

Crystal data

$C_{22}H_{19}N_3O_3$
M_r = 373.40
Monoclinic, $P2_1/n$
a = 14.4225 (14) Å
b = 8.0836 (5) Å
c = 16.2749 (14) Å
β = 107.263 (7)°
V = 1811.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.60 × 0.13 × 0.04 mm

Data collection

Stoe IPDS II diffractometer
21467 measured reflections
4893 independent reflections
3190 reflections with $I > 2\sigma(I)$
R_{int} = 0.111

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.195
S = 1.15
4893 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O3^{i}	0.93	2.59	3.423 (3)	149

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

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5425).

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supporting information

Acta Cryst. (2011). E**67**, o49 [https://doi.org/10.1107/S1600536810050294]

(2*Z*)-*N*-(4-Methoxyphenyl)-2-(4-methoxyphenylimino)-2*H*-1,4-benzoxazin-3-amine

Morteza Mehrdad, Mohammad Ghanbari, Khosrow Jadidi, Amir Salemi and Hamid Reza Khavasi

S1. Comment

Recently, we reported a Baeyer–Villiger oxidation of 1-alkyl-3-arylimino-2-indolinone with *m*-chloroperbenzoic acid to afford 1-alkyl-4-(arylimino)-1H benzo[*d*][1,3]oxazin-2(4*H*)-one (Azizian *et al.*, 2000; Jadidi *et al.*, 2008). As a continuation of this work, 2-arylimino-*N*-aryl-2*H*-benzo[*b*][1,4]oxazin-3-amines (2) or *N*-aryl-*N*-(2-arylamino-3*H*-indol-3-ylidene)amine N-oxides (3) were obtained in two different temperatures by Baeyer-Villiger oxidation reaction (Fig. 1) of *N*-aryl-3-(arylimino)-3*H*-indol-2-amines (1) (Mehrdad *et al.*, 2011). In this paper, we report the structure of (2*Z*)-2-(4-methoxyphenylimino)-*N*-(4-methoxyphenyl)- 2*H*-benzo[*b*][1,4]oxazin-3-amine (2a). The molecular structure of the title compound is shown in Fig. 2.

The methoxy phenyl rings, A (C2—C7) and B (C16—C21) and benzooxazine ring C (C9—C14/C8/O2/N2/C15) enclose the dihedral angles: A/B = 32.38 (7)°, A/C = 10.66 (8)° and B/C = 24.17 (7)°. Intermolecular C—H···O interactions (Table 1) stabilize the crystal structure.

S2. Experimental

The solution of *N*-Aryl-3-(Arylimino)-3*H*-indol-2-amine (1a) (1.0 mmol) in 25 ml CH_2Cl_2 was cooled to 253K. Then, *m*-CPBA (1.5 mmol) dissolved in 25 ml CH_2Cl_2 was added dropwise to the stirred solution of (1a). After stirring for 6 h at 253K, product (2a) was formed (monitoring by TLC). The crude product was poured into water and extracted with CH_2Cl_2 (60 ml). The organic layer was dried over Na_2SO_4, and evaporation of the solvent afforded the crude product (2a), which was purified on silica gel by column chromatography using 90:10 n-hexane:ethyl acetate as eluent to afford (2a) as a light yellow solid (90%); m.p. = 169–171°C (Mehrdad *et al.*, 2011).

S3. Refinement

All H atoms were positioned geometrically, with N—H=0.86 Å, C_{methyl}—H=0.96Å and $C_{aromatic}$—H=0.93Å and constrained to ride on their parent atoms, with U_{iso}(H)=1.2U_{eq}(C,N).

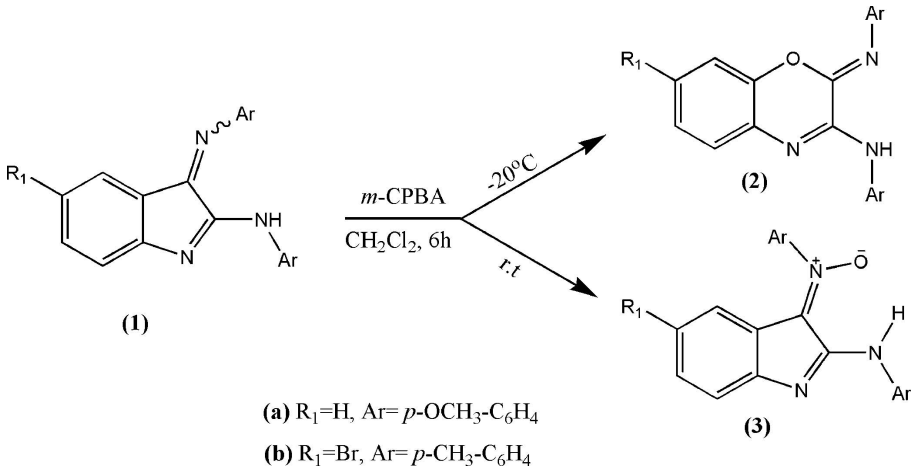

Figure 1

Reaction scheme.

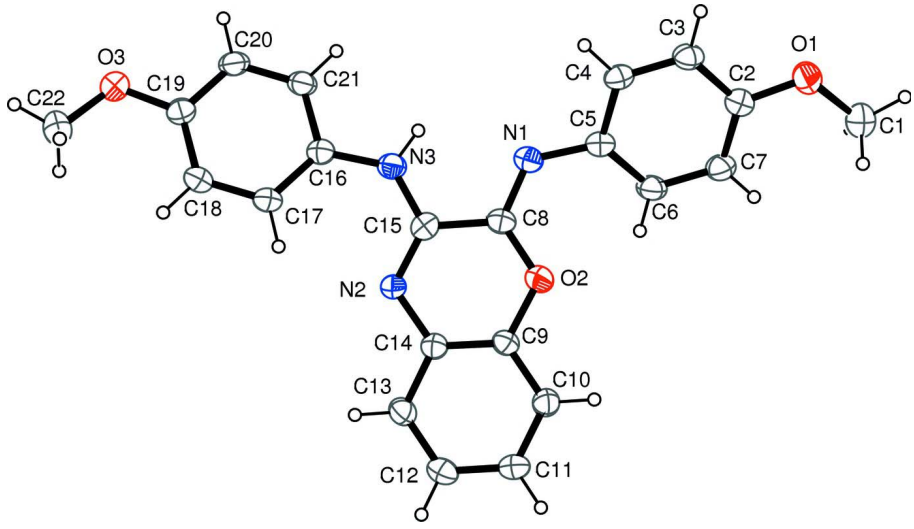

Figure 2

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

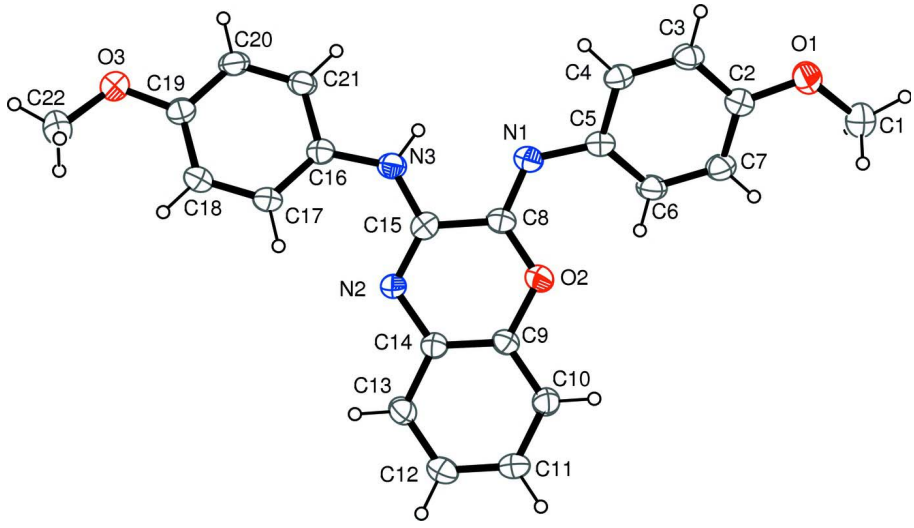

Figure 3

Unit-cell packing diagram for (I).

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Crystal data

$C_{22}H_{19}N_3O_3$
$M_r = 373.40$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 14.4225\ (14)$ Å
$b = 8.0836\ (5)$ Å
$c = 16.2749\ (14)$ Å
$\beta = 107.263\ (7)°$
$V = 1811.9\ (3)$ Å^3
$Z = 4$
$F(000) = 784$
$D_x = 1.369$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 21467 reflections
$\theta = 1.7–29.3°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Needle, yellow
0.60 × 0.13 × 0.04 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0.15 mm pixels mm^{-1}
rotation method scans
21467 measured reflections
4893 independent reflections
3190 reflections with $I > 2\sigma(I)$
$R_{int} = 0.111$
$\theta_{max} = 29.3°$, $\theta_{min} = 1.7°$
$h = -18\rightarrow19$
$k = -10\rightarrow11$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.083$
$wR(F^2) = 0.195$
$S = 1.15$
4893 reflections
253 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
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.8502P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0070 (3)	0.2134 (5)	0.0453 (2)	0.0719 (9)
H1A	−0.0208	0.3142	0.0707	0.086*
H1B	0.0435	0.1542	0.0866	0.086*
H1C	−0.0645	0.1464	0.0281	0.086*
C2	0.1045 (2)	0.3483 (3)	−0.01638 (17)	0.0497 (6)
C3	0.1271 (2)	0.3897 (3)	−0.09054 (17)	0.0521 (7)
H3	0.0870	0.3551	−0.1437	0.063*
C4	0.2088 (2)	0.4820 (3)	−0.08625 (16)	0.0476 (6)
H4	0.2224	0.5109	−0.1368	0.057*
C5	0.27136 (19)	0.5328 (3)	−0.00716 (16)	0.0459 (6)
C6	0.2465 (2)	0.4957 (4)	0.06647 (17)	0.0557 (7)
H6	0.2861	0.5319	0.1196	0.067*
C7	0.1629 (2)	0.4047 (4)	0.06239 (18)	0.0570 (7)
H7	0.1465	0.3822	0.1124	0.068*
C8	0.43609 (19)	0.6338 (3)	0.05119 (16)	0.0446 (6)
C9	0.54000 (18)	0.5791 (3)	0.18936 (16)	0.0436 (6)
C10	0.5543 (2)	0.5004 (4)	0.26776 (18)	0.0518 (6)
H10	0.5058	0.4342	0.2773	0.062*
C11	0.6412 (2)	0.5210 (4)	0.33167 (17)	0.0536 (7)
H11	0.6514	0.4685	0.3844	0.064*
C12	0.7131 (2)	0.6199 (4)	0.31721 (18)	0.0554 (7)
H12	0.7713	0.6340	0.3606	0.066*
C13	0.6990 (2)	0.6979 (4)	0.23896 (17)	0.0525 (7)
H13	0.7476	0.7644	0.2298	0.063*
C14	0.61137 (18)	0.6767 (3)	0.17343 (15)	0.0428 (6)
C15	0.5157 (2)	0.7295 (3)	0.03396 (16)	0.0447 (6)
C16	0.55436 (18)	0.8817 (3)	−0.08379 (15)	0.0435 (6)
C17	0.6539 (2)	0.9088 (4)	−0.04862 (17)	0.0536 (7)
H17	0.6862	0.8660	0.0053	0.064*
C18	0.7048 (2)	0.9990 (4)	−0.09332 (18)	0.0578 (7)
H18	0.7713	1.0150	−0.0693	0.069*
C19	0.6583 (2)	1.0656 (3)	−0.17326 (17)	0.0487 (6)
C20	0.5592 (2)	1.0388 (4)	−0.20832 (17)	0.0548 (7)
H20	0.5268	1.0827	−0.2620	0.066*
C21	0.5087 (2)	0.9484 (4)	−0.16457 (16)	0.0505 (6)

H21	0.4425	0.9312	−0.1894	0.061*
C22	0.8046 (2)	1.1618 (5)	−0.1983 (2)	0.0777 (10)
H22A	0.8289	1.0517	−0.1997	0.093*
H22B	0.8296	1.2060	−0.1412	0.093*
H22C	0.8250	1.2305	−0.2379	0.093*
N1	0.35461 (16)	0.6221 (3)	−0.01063 (14)	0.0499 (5)
N2	0.59911 (15)	0.7521 (3)	0.09392 (12)	0.0413 (5)
N3	0.49602 (16)	0.7909 (3)	−0.04487 (13)	0.0494 (5)
H3A	0.4381	0.7720	−0.0774	0.059*
O1	0.02353 (17)	0.2511 (3)	−0.02758 (14)	0.0700 (6)
O2	0.45078 (13)	0.5596 (3)	0.12731 (12)	0.0556 (5)
O3	0.70194 (16)	1.1580 (3)	−0.22196 (13)	0.0655 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.066 (2)	0.077 (2)	0.076 (2)	−0.0097 (17)	0.0262 (17)	0.0031 (18)
C2	0.0490 (15)	0.0481 (15)	0.0498 (14)	0.0023 (12)	0.0114 (12)	−0.0024 (12)
C3	0.0606 (17)	0.0492 (15)	0.0416 (13)	−0.0021 (13)	0.0074 (12)	−0.0070 (12)
C4	0.0567 (16)	0.0476 (15)	0.0367 (12)	0.0030 (12)	0.0111 (11)	−0.0008 (11)
C5	0.0479 (14)	0.0464 (14)	0.0405 (12)	0.0063 (11)	0.0088 (11)	−0.0015 (11)
C6	0.0488 (15)	0.075 (2)	0.0393 (13)	−0.0014 (14)	0.0072 (11)	−0.0043 (13)
C7	0.0549 (17)	0.075 (2)	0.0414 (13)	−0.0001 (15)	0.0143 (12)	0.0018 (13)
C8	0.0438 (13)	0.0448 (14)	0.0420 (13)	0.0052 (11)	0.0077 (11)	−0.0031 (11)
C9	0.0378 (13)	0.0457 (14)	0.0445 (13)	0.0027 (10)	0.0079 (10)	0.0008 (11)
C10	0.0464 (14)	0.0535 (16)	0.0554 (15)	0.0022 (12)	0.0147 (12)	0.0093 (13)
C11	0.0533 (16)	0.0587 (17)	0.0434 (13)	0.0080 (13)	0.0061 (12)	0.0054 (13)
C12	0.0479 (15)	0.0627 (18)	0.0486 (14)	−0.0022 (13)	0.0035 (12)	−0.0079 (13)
C13	0.0467 (15)	0.0584 (17)	0.0499 (15)	−0.0085 (12)	0.0104 (12)	−0.0057 (13)
C14	0.0438 (13)	0.0431 (13)	0.0414 (12)	0.0015 (11)	0.0125 (10)	−0.0020 (10)
C15	0.0531 (15)	0.0393 (13)	0.0443 (13)	0.0065 (11)	0.0186 (11)	−0.0017 (10)
C16	0.0440 (13)	0.0461 (14)	0.0400 (12)	0.0054 (11)	0.0119 (11)	−0.0026 (10)
C17	0.0440 (14)	0.0676 (18)	0.0433 (14)	0.0022 (13)	0.0036 (12)	0.0082 (13)
C18	0.0421 (14)	0.075 (2)	0.0497 (14)	−0.0037 (14)	0.0041 (12)	0.0031 (15)
C19	0.0533 (15)	0.0501 (15)	0.0423 (13)	0.0014 (12)	0.0136 (12)	−0.0018 (11)
C20	0.0530 (16)	0.0699 (19)	0.0372 (12)	0.0059 (14)	0.0068 (12)	0.0054 (13)
C21	0.0422 (13)	0.0640 (18)	0.0408 (13)	0.0028 (12)	0.0052 (11)	−0.0016 (12)
C22	0.0560 (19)	0.095 (3)	0.084 (2)	−0.0101 (18)	0.0233 (18)	0.012 (2)
N1	0.0459 (12)	0.0551 (14)	0.0447 (11)	−0.0003 (10)	0.0071 (10)	−0.0023 (10)
N2	0.0417 (11)	0.0446 (12)	0.0361 (10)	−0.0024 (9)	0.0095 (8)	−0.0002 (9)
N3	0.0446 (12)	0.0576 (14)	0.0431 (11)	0.0033 (10)	0.0087 (9)	0.0008 (10)
O1	0.0668 (14)	0.0815 (15)	0.0617 (13)	−0.0229 (12)	0.0193 (11)	−0.0067 (11)
O2	0.0446 (10)	0.0604 (12)	0.0558 (11)	−0.0025 (9)	0.0058 (9)	0.0078 (9)
O3	0.0595 (13)	0.0817 (15)	0.0544 (11)	−0.0078 (11)	0.0157 (10)	0.0101 (11)

Geometric parameters (Å, º)

C1—O1	1.416 (4)	C11—H11	0.9300
C1—H1A	0.9600	C12—C13	1.381 (4)
C1—H1B	0.9600	C12—H12	0.9300
C1—H1C	0.9600	C13—C14	1.402 (4)
C2—O1	1.374 (3)	C13—H13	0.9300
C2—C3	1.382 (4)	C14—N2	1.393 (3)
C2—C7	1.386 (4)	C15—N2	1.318 (3)
C3—C4	1.378 (4)	C15—N3	1.325 (3)
C3—H3	0.9300	C16—C21	1.393 (4)
C4—C5	1.397 (3)	C16—C17	1.396 (4)
C4—H4	0.9300	C16—N3	1.401 (3)
C5—C6	1.382 (4)	C17—C18	1.385 (4)
C5—N1	1.417 (4)	C17—H17	0.9300
C6—C7	1.397 (4)	C18—C19	1.384 (4)
C6—H6	0.9300	C18—H18	0.9300
C7—H7	0.9300	C19—O3	1.370 (3)
C8—N1	1.304 (3)	C19—C20	1.390 (4)
C8—O2	1.336 (3)	C20—C21	1.371 (4)
C8—C15	1.479 (4)	C20—H20	0.9300
C9—C14	1.381 (4)	C21—H21	0.9300
C9—C10	1.385 (4)	C22—O3	1.415 (4)
C9—O2	1.389 (3)	C22—H22A	0.9600
C10—C11	1.381 (4)	C22—H22B	0.9600
C10—H10	0.9300	C22—H22C	0.9600
C11—C12	1.384 (4)	N3—H3A	0.8600
O1—C1—H1A	109.5	C12—C13—H13	120.1
O1—C1—H1B	109.5	C14—C13—H13	120.1
H1A—C1—H1B	109.5	C9—C14—N2	121.9 (2)
O1—C1—H1C	109.5	C9—C14—C13	118.8 (2)
H1A—C1—H1C	109.5	N2—C14—C13	119.4 (2)
H1B—C1—H1C	109.5	N2—C15—N3	123.5 (2)
O1—C2—C3	115.8 (2)	N2—C15—C8	121.4 (2)
O1—C2—C7	124.8 (3)	N3—C15—C8	115.1 (2)
C3—C2—C7	119.5 (3)	C21—C16—C17	117.8 (2)
C4—C3—C2	120.5 (2)	C21—C16—N3	116.8 (2)
C4—C3—H3	119.8	C17—C16—N3	125.4 (2)
C2—C3—H3	119.8	C18—C17—C16	120.6 (2)
C3—C4—C5	121.0 (2)	C18—C17—H17	119.7
C3—C4—H4	119.5	C16—C17—H17	119.7
C5—C4—H4	119.5	C19—C18—C17	120.9 (3)
C6—C5—C4	118.2 (3)	C19—C18—H18	119.5
C6—C5—N1	125.9 (2)	C17—C18—H18	119.5
C4—C5—N1	115.9 (2)	O3—C19—C18	125.3 (3)
C5—C6—C7	121.0 (3)	O3—C19—C20	116.1 (2)
C5—C6—H6	119.5	C18—C19—C20	118.5 (3)

C7—C6—H6	119.5	C21—C20—C19	120.7 (2)
C2—C7—C6	119.8 (3)	C21—C20—H20	119.7
C2—C7—H7	120.1	C19—C20—H20	119.7
C6—C7—H7	120.1	C20—C21—C16	121.4 (2)
N1—C8—O2	122.8 (2)	C20—C21—H21	119.3
N1—C8—C15	117.7 (2)	C16—C21—H21	119.3
O2—C8—C15	119.5 (2)	O3—C22—H22A	109.5
C14—C9—C10	121.3 (2)	O3—C22—H22B	109.5
C14—C9—O2	120.6 (2)	H22A—C22—H22B	109.5
C10—C9—O2	118.1 (2)	O3—C22—H22C	109.5
C11—C10—C9	119.5 (3)	H22A—C22—H22C	109.5
C11—C10—H10	120.3	H22B—C22—H22C	109.5
C9—C10—H10	120.3	C8—N1—C5	125.9 (2)
C10—C11—C12	120.0 (3)	C15—N2—C14	117.6 (2)
C10—C11—H11	120.0	C15—N3—C16	130.4 (2)
C12—C11—H11	120.0	C15—N3—H3A	114.8
C13—C12—C11	120.6 (3)	C16—N3—H3A	114.8
C13—C12—H12	119.7	C2—O1—C1	118.4 (2)
C11—C12—H12	119.7	C8—O2—C9	118.8 (2)
C12—C13—C14	119.9 (3)	C19—O3—C22	118.5 (2)

O1—C2—C3—C4	−177.7 (3)	C17—C18—C19—O3	179.2 (3)
C7—C2—C3—C4	2.0 (4)	C17—C18—C19—C20	−0.6 (5)
C2—C3—C4—C5	1.3 (4)	O3—C19—C20—C21	−179.8 (3)
C3—C4—C5—C6	−3.4 (4)	C18—C19—C20—C21	0.0 (4)
C3—C4—C5—N1	177.9 (2)	C19—C20—C21—C16	0.5 (5)
C4—C5—C6—C7	2.3 (4)	C17—C16—C21—C20	−0.4 (4)
N1—C5—C6—C7	−179.3 (3)	N3—C16—C21—C20	−179.8 (3)
O1—C2—C7—C6	176.6 (3)	O2—C8—N1—C5	0.2 (4)
C3—C2—C7—C6	−3.2 (4)	C15—C8—N1—C5	178.3 (2)
C5—C6—C7—C2	1.0 (5)	C6—C5—N1—C8	25.8 (4)
C14—C9—C10—C11	0.6 (4)	C4—C5—N1—C8	−155.7 (3)
O2—C9—C10—C11	−178.2 (3)	N3—C15—N2—C14	−178.2 (2)
C9—C10—C11—C12	0.1 (4)	C8—C15—N2—C14	2.6 (3)
C10—C11—C12—C13	−0.4 (5)	C9—C14—N2—C15	1.1 (4)
C11—C12—C13—C14	−0.1 (4)	C13—C14—N2—C15	−179.9 (2)
C10—C9—C14—N2	177.9 (2)	N2—C15—N3—C16	3.1 (4)
O2—C9—C14—N2	−3.4 (4)	C8—C15—N3—C16	−177.7 (2)
C10—C9—C14—C13	−1.1 (4)	C21—C16—N3—C15	−171.6 (3)
O2—C9—C14—C13	177.7 (2)	C17—C16—N3—C15	9.0 (5)
C12—C13—C14—C9	0.9 (4)	C3—C2—O1—C1	−176.0 (3)
C12—C13—C14—N2	−178.1 (3)	C7—C2—O1—C1	4.3 (5)
N1—C8—C15—N2	177.6 (2)	N1—C8—O2—C9	−180.0 (2)
O2—C8—C15—N2	−4.3 (4)	C15—C8—O2—C9	2.0 (3)
N1—C8—C15—N3	−1.7 (3)	C14—C9—O2—C8	1.6 (4)
O2—C8—C15—N3	176.5 (2)	C10—C9—O2—C8	−179.6 (2)
C21—C16—C17—C18	−0.2 (4)	C18—C19—O3—C22	12.6 (5)
N3—C16—C17—C18	179.2 (3)	C20—C19—O3—C22	−167.6 (3)

C16—C17—C18—C19	0.7 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O3^{i}	0.93	2.59	3.423 (3)	149

Symmetry code: (i) $x-1/2, -y+3/2, z+1/2$.