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2-[3-(2-Acetoxyphenyl)quinoxalin-2-yl]-phenyl acetate

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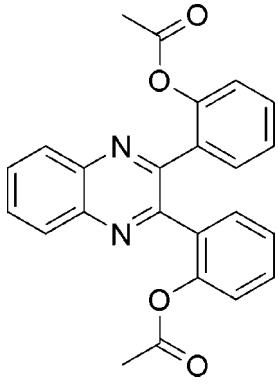
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.117; data-to-parameter ratio = 13.3.

The title compound, $C_{24}H_{18}N_2O_4$, crystallizes as a *syn*-conformer, with dihedral angles between the quinoxaline moiety and the acetoxy-substituted benzene rings of 53.46 (3)° and 54.78 (3)°. In the crystal, the molecules form chains along [100] *via* C—H···O interactions.

Related literature

For general background to quinoxaline derivatives, see: Brasche & Buchwald (2008); Do & Daugulis (2008); He *et al.* (2003); Kim *et al.* (2004); Lyons & Sanford (2010). For quinoxaline-directed C—H activation, see: Reddy *et al.* (2011). For a related structure, see: Rajnikant *et al.* (2006).



Experimental

Crystal data

$C_{24}H_{18}N_2O_4$
M_r = 398.40
Monoclinic, $P2_1/c$
a = 9.5723 (5) Å
b = 16.7309 (8) Å
c = 13.0555 (6) Å
β = 92.929 (2)°
V = 2088.15 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.48 × 0.46 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID/ZJUG diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.959, T_{max} = 0.983
15632 measured reflections
3646 independent reflections
2553 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.00
3646 reflections
274 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O4^{i}	0.93	2.43	3.329 (2)	164

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

Data collection: *PROCESS-AUTO* (Rigaku, 2006); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2007); 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, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

We thank Professor Jian-Ming Gu of Zhejiang University for his help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2099).

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supporting information

Acta Cryst. (2013). E**69**, o764 [https://doi.org/10.1107/S1600536813009161]

2-[3-(2-Acetoxyphenyl)quinoxalin-2-yl]phenyl acetate

Dan-Feng Shen, Shao-Jie Lou and Dan-Qian Xu

S1. Comment

Quinoxaline derivatives have received considerable interest from chemists because of their pharmacological properties such as antiviral, antibacterial, anti-inflammatory, and antiprotozoal activities, and as kinase inhibitors. C—H activation is a versatile approach for the direct functionalization of aromatic C—H bonds using transition metal catalysis. Palladium complexes are particularly attractive catalysts for such transformations. The molecular structure of the title compound is presented on Fig. 1. The plane of the quinoxaline moiety makes angles of 53.46 (3)°, 54.78 (3)° with the planes of phenyl rings. The torsion angle C9—C1—C8—C17 is 4.91 (3)°.

S2. Experimental

A mixture of 2,3-diphenylquinoxaline (282 mg,1.0 mmol), phenyliodine diacetate (805 mg, 2.5 mmol), and Palladium acetate (34 mg, 0.15 mmol) in acetic acid-acetic anhydride (3.0 ml-3.0 ml) was stirred at room temperature for 10 min, then the resulting mixture was heated to 120 degrees for 4hr. After completion of reaction as indicated by TLC, the reaction mixture was filtered, diluted with water and extracted with dichloromethane. The combined organic layers were dried over anhydrous sodium sulfate salt, concentrated *in vacuo*, and purified by column chromatography on silica gel (eluent:petroleum ether-ethyl acetate) to afford pure product with a 90 percent yield. Suitable crystals were obtained by slow evaporation of an ethanol solution.

S3. Refinement

H atoms were placed in calculated position with C—H ranging from 0.93 Å to 0.98 Å. All H atoms included in the final cycles of refinement as riding mode, with U_{iso}(H)=1.2U_{eq} of the carrier atoms. Positions of hydrogens of the methyl groups awere optimized rotationally.

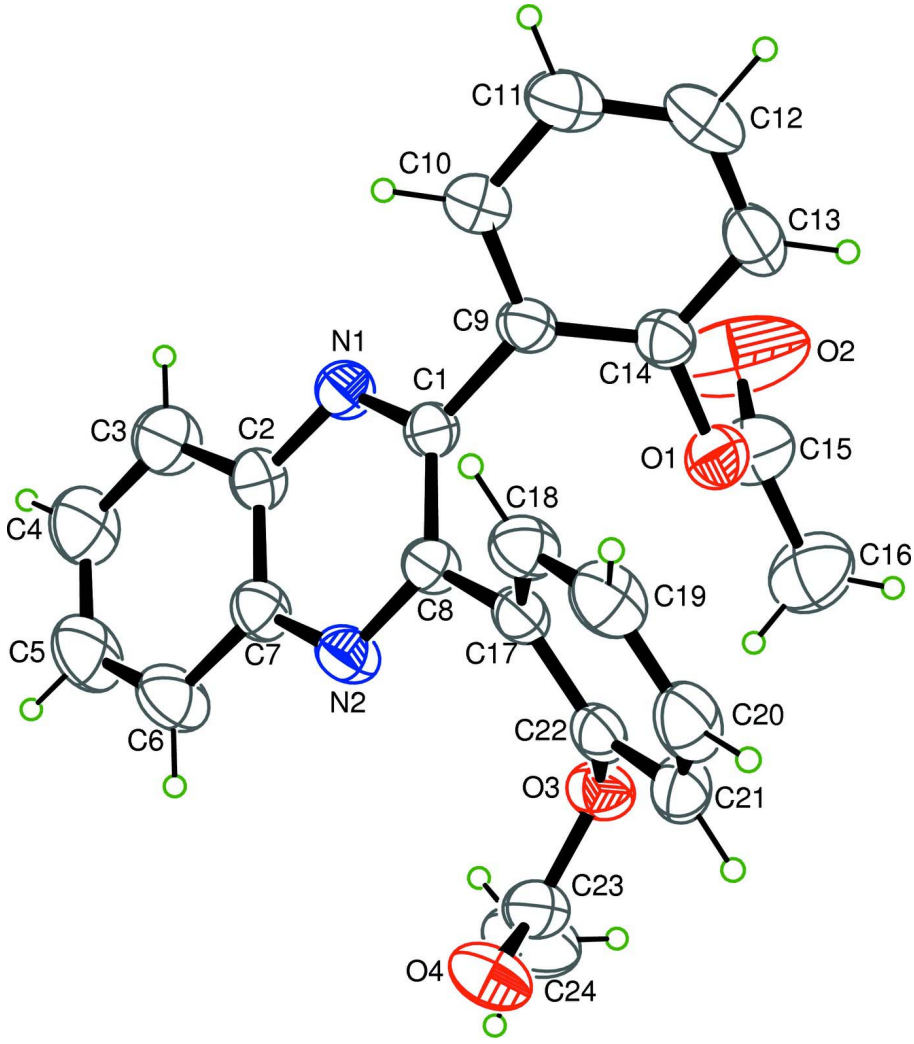

Figure 1

The molecule of the title compound, with the atomic labeling scheme. Displacement ellipsoids are drawn at the 40% probability level.

2-[3-(2-Acetoxyphenyl)quinoxalin-2-yl]phenyl acetate

Crystal data

$C_{24}H_{18}N_2O_4$
$M_r = 398.40$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.5723\ (5)$ Å
$b = 16.7309\ (8)$ Å
$c = 13.0555\ (6)$ Å
$\beta = 92.929\ (2)°$
$V = 2088.15\ (18)$ Å^3
$Z = 4$
$F(000) = 832$
$D_x = 1.267$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 11299 reflections
$\theta = 3.1–27.4°$
$\mu = 0.09$ mm^{-1}
$T = 296$ K
Platelet, yellow
0.48 × 0.46 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID/ZJUG diffractometer
Radiation source: rotating anode
Graphite monochromator
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.959, T_{max} = 0.983
15632 measured reflections
3646 independent reflections
2553 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.0°, θ_{min} = 3.1°
h = −11→11
k = −19→19
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.117
S = 1.00
3646 reflections
274 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
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.7545P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.045 (2)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.57616 (19)	0.12138 (11)	0.27152 (13)	0.0401 (4)
C2	0.7311 (2)	0.02174 (11)	0.31884 (15)	0.0467 (5)
C3	0.7625 (3)	−0.04950 (13)	0.37296 (19)	0.0678 (6)
H3	0.6940	−0.0747	0.4093	0.081*
C4	0.8934 (3)	−0.08127 (15)	0.3718 (2)	0.0778 (7)
H4	0.9141	−0.1280	0.4080	0.093*
C5	0.9964 (3)	−0.04432 (15)	0.3169 (2)	0.0783 (7)
H5	1.0850	−0.0671	0.3166	0.094*
C6	0.9699 (2)	0.02435 (14)	0.2639 (2)	0.0704 (7)
H6	1.0394	0.0480	0.2270	0.085*
C7	0.8360 (2)	0.05939 (12)	0.26533 (15)	0.0494 (5)
C8	0.68513 (19)	0.16210 (11)	0.22108 (14)	0.0429 (5)
C9	0.43173 (19)	0.15473 (11)	0.27655 (14)	0.0438 (5)
C10	0.3759 (2)	0.16739 (13)	0.37183 (17)	0.0586 (6)

H10	0.4290	0.1545	0.4312	0.070*
C11	0.2436 (3)	0.19857 (15)	0.3797 (2)	0.0714 (7)
H11	0.2083	0.2068	0.4439	0.086*
C12	0.1641 (2)	0.21744 (15)	0.2926 (2)	0.0731 (7)
H12	0.0751	0.2389	0.2980	0.088*
C13	0.2152 (2)	0.20474 (14)	0.19734 (19)	0.0628 (6)
H13	0.1610	0.2171	0.1383	0.075*
C14	0.3478 (2)	0.17335 (12)	0.19050 (15)	0.0473 (5)
C15	0.3570 (3)	0.09580 (15)	0.04113 (19)	0.0727 (7)
C16	0.4121 (3)	0.09362 (19)	−0.0632 (2)	0.0940 (9)
H16A	0.3871	0.0438	−0.0956	0.141*
H16B	0.5121	0.0987	−0.0581	0.141*
H16C	0.3727	0.1369	−0.1033	0.141*
C17	0.66704 (19)	0.24376 (11)	0.17661 (15)	0.0432 (5)
C18	0.6188 (2)	0.30646 (12)	0.23494 (17)	0.0537 (5)
H18	0.5930	0.2967	0.3015	0.064*
C19	0.6084 (2)	0.38308 (13)	0.19573 (19)	0.0622 (6)
H19	0.5755	0.4244	0.2357	0.075*
C20	0.6466 (2)	0.39806 (14)	0.09761 (19)	0.0650 (6)
H20	0.6390	0.4495	0.0710	0.078*
C21	0.6961 (2)	0.33717 (13)	0.03828 (17)	0.0577 (6)
H21	0.7231	0.3475	−0.0279	0.069*
C22	0.70544 (19)	0.26088 (11)	0.07788 (15)	0.0448 (5)
C23	0.8838 (2)	0.19247 (13)	−0.00467 (16)	0.0554 (5)
C24	0.9139 (3)	0.11638 (17)	−0.0569 (2)	0.0940 (9)
H24A	1.0092	0.1164	−0.0765	0.141*
H24B	0.8524	0.1108	−0.1169	0.141*
H24C	0.8997	0.0726	−0.0111	0.141*
N1	0.59936 (17)	0.05326 (9)	0.32027 (12)	0.0467 (4)
N2	0.81105 (17)	0.13064 (10)	0.21658 (13)	0.0513 (4)
O1	0.40006 (15)	0.16132 (9)	0.09276 (10)	0.0569 (4)
O2	0.2849 (3)	0.04774 (14)	0.0780 (2)	0.1502 (12)
O3	0.74576 (14)	0.19711 (8)	0.01622 (10)	0.0536 (4)
O4	0.96565 (16)	0.24378 (10)	0.01729 (13)	0.0718 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0399 (11)	0.0407 (10)	0.0397 (9)	−0.0011 (8)	0.0016 (8)	−0.0007 (8)
C2	0.0485 (12)	0.0394 (11)	0.0519 (11)	0.0026 (9)	−0.0016 (9)	0.0003 (8)
C3	0.0670 (16)	0.0531 (13)	0.0834 (16)	0.0067 (11)	0.0054 (12)	0.0188 (12)
C4	0.0777 (19)	0.0577 (15)	0.0972 (19)	0.0184 (13)	−0.0026 (15)	0.0172 (13)
C5	0.0593 (16)	0.0675 (16)	0.108 (2)	0.0249 (13)	−0.0009 (14)	0.0111 (14)
C6	0.0494 (14)	0.0646 (15)	0.0979 (18)	0.0147 (11)	0.0098 (12)	0.0115 (13)
C7	0.0457 (12)	0.0445 (11)	0.0580 (12)	0.0051 (9)	0.0015 (9)	0.0023 (9)
C8	0.0384 (11)	0.0427 (11)	0.0477 (11)	0.0002 (8)	0.0036 (8)	0.0007 (8)
C9	0.0381 (11)	0.0445 (11)	0.0492 (11)	−0.0024 (8)	0.0060 (9)	0.0029 (8)
C10	0.0454 (13)	0.0746 (15)	0.0564 (12)	0.0038 (11)	0.0086 (10)	0.0019 (10)

C11	0.0522 (15)	0.0910 (18)	0.0725 (16)	0.0059 (13)	0.0183 (12)	−0.0046 (13)
C12	0.0405 (13)	0.0788 (17)	0.101 (2)	0.0113 (11)	0.0109 (13)	−0.0055 (14)
C13	0.0432 (13)	0.0661 (15)	0.0781 (16)	0.0040 (10)	−0.0068 (11)	0.0070 (11)
C14	0.0409 (12)	0.0490 (12)	0.0520 (11)	−0.0037 (9)	0.0017 (9)	0.0033 (9)
C15	0.0844 (18)	0.0636 (15)	0.0710 (16)	−0.0143 (14)	0.0131 (14)	−0.0085 (12)
C16	0.115 (2)	0.103 (2)	0.0653 (16)	−0.0082 (18)	0.0090 (16)	−0.0149 (15)
C17	0.0332 (10)	0.0432 (11)	0.0529 (11)	−0.0009 (8)	0.0005 (8)	0.0054 (8)
C18	0.0493 (13)	0.0485 (12)	0.0640 (13)	0.0034 (9)	0.0088 (10)	0.0036 (10)
C19	0.0546 (14)	0.0455 (13)	0.0865 (17)	0.0056 (10)	0.0044 (12)	0.0014 (11)
C20	0.0543 (14)	0.0490 (13)	0.0905 (17)	0.0007 (11)	−0.0080 (12)	0.0190 (12)
C21	0.0513 (13)	0.0609 (14)	0.0600 (13)	−0.0052 (10)	−0.0063 (10)	0.0185 (11)
C22	0.0328 (10)	0.0477 (11)	0.0531 (11)	−0.0055 (8)	−0.0048 (8)	0.0040 (9)
C23	0.0490 (13)	0.0624 (14)	0.0552 (12)	−0.0057 (11)	0.0080 (10)	0.0018 (10)
C24	0.0787 (19)	0.088 (2)	0.118 (2)	−0.0099 (15)	0.0290 (17)	−0.0343 (17)
N1	0.0458 (10)	0.0428 (9)	0.0517 (9)	−0.0007 (7)	0.0033 (7)	0.0048 (7)
N2	0.0399 (10)	0.0489 (10)	0.0656 (11)	0.0035 (7)	0.0075 (8)	0.0065 (8)
O1	0.0542 (9)	0.0661 (10)	0.0501 (8)	−0.0107 (7)	−0.0014 (7)	0.0030 (7)
O2	0.218 (3)	0.0990 (16)	0.142 (2)	−0.0865 (18)	0.092 (2)	−0.0508 (14)
O3	0.0461 (8)	0.0589 (9)	0.0562 (8)	−0.0123 (6)	0.0052 (6)	−0.0055 (6)
O4	0.0485 (10)	0.0730 (11)	0.0944 (12)	−0.0164 (8)	0.0085 (8)	−0.0079 (9)

Geometric parameters (Å, º)

C1—N1	1.319 (2)	C13—H13	0.9300
C1—C8	1.434 (2)	C14—O1	1.409 (2)
C1—C9	1.495 (3)	C15—O2	1.178 (3)
C2—N1	1.368 (2)	C15—O1	1.341 (3)
C2—C7	1.401 (3)	C15—C16	1.486 (3)
C2—C3	1.410 (3)	C16—H16A	0.9600
C3—C4	1.362 (3)	C16—H16B	0.9600
C3—H3	0.9300	C16—H16C	0.9600
C4—C5	1.393 (4)	C17—C22	1.388 (3)
C4—H4	0.9300	C17—C18	1.389 (3)
C5—C6	1.359 (3)	C18—C19	1.382 (3)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.410 (3)	C19—C20	1.373 (3)
C6—H6	0.9300	C19—H19	0.9300
C7—N2	1.367 (2)	C20—C21	1.379 (3)
C8—N2	1.319 (2)	C20—H20	0.9300
C8—C17	1.491 (3)	C21—C22	1.378 (3)
C9—C14	1.383 (3)	C21—H21	0.9300
C9—C10	1.395 (3)	C22—O3	1.403 (2)
C10—C11	1.378 (3)	C23—O4	1.188 (2)
C10—H10	0.9300	C23—O3	1.365 (2)
C11—C12	1.372 (4)	C23—C24	1.479 (3)
C11—H11	0.9300	C24—H24A	0.9600
C12—C13	1.376 (3)	C24—H24B	0.9600
C12—H12	0.9300	C24—H24C	0.9600

C13—C14	1.381 (3)		
N1—C1—C8	121.58 (17)	C9—C14—O1	119.04 (17)
N1—C1—C9	115.76 (16)	O2—C15—O1	121.6 (2)
C8—C1—C9	122.60 (16)	O2—C15—C16	126.9 (3)
N1—C2—C7	121.18 (17)	O1—C15—C16	111.5 (2)
N1—C2—C3	119.48 (18)	C15—C16—H16A	109.5
C7—C2—C3	119.34 (19)	C15—C16—H16B	109.5
C4—C3—C2	119.8 (2)	H16A—C16—H16B	109.5
C4—C3—H3	120.1	C15—C16—H16C	109.5
C2—C3—H3	120.1	H16A—C16—H16C	109.5
C3—C4—C5	120.6 (2)	H16B—C16—H16C	109.5
C3—C4—H4	119.7	C22—C17—C18	117.67 (18)
C5—C4—H4	119.7	C22—C17—C8	121.31 (17)
C6—C5—C4	121.2 (2)	C18—C17—C8	120.91 (17)
C6—C5—H5	119.4	C19—C18—C17	121.1 (2)
C4—C5—H5	119.4	C19—C18—H18	119.4
C5—C6—C7	119.4 (2)	C17—C18—H18	119.4
C5—C6—H6	120.3	C20—C19—C18	119.8 (2)
C7—C6—H6	120.3	C20—C19—H19	120.1
N2—C7—C2	120.79 (17)	C18—C19—H19	120.1
N2—C7—C6	119.56 (19)	C19—C20—C21	120.3 (2)
C2—C7—C6	119.63 (19)	C19—C20—H20	119.8
N2—C8—C1	121.24 (17)	C21—C20—H20	119.8
N2—C8—C17	115.87 (16)	C22—C21—C20	119.4 (2)
C1—C8—C17	122.78 (16)	C22—C21—H21	120.3
C14—C9—C10	117.21 (18)	C20—C21—H21	120.3
C14—C9—C1	123.25 (17)	C21—C22—C17	121.62 (19)
C10—C9—C1	119.53 (17)	C21—C22—O3	120.24 (18)
C11—C10—C9	121.3 (2)	C17—C22—O3	118.01 (16)
C11—C10—H10	119.4	O4—C23—O3	123.0 (2)
C9—C10—H10	119.4	O4—C23—C24	126.2 (2)
C12—C11—C10	119.9 (2)	O3—C23—C24	110.8 (2)
C12—C11—H11	120.0	C23—C24—H24A	109.5
C10—C11—H11	120.0	C23—C24—H24B	109.5
C11—C12—C13	120.3 (2)	H24A—C24—H24B	109.5
C11—C12—H12	119.8	C23—C24—H24C	109.5
C13—C12—H12	119.8	H24A—C24—H24C	109.5
C12—C13—C14	119.2 (2)	H24B—C24—H24C	109.5
C12—C13—H13	120.4	C1—N1—C2	117.34 (16)
C14—C13—H13	120.4	C8—N2—C7	117.73 (16)
C13—C14—C9	122.07 (19)	C15—O1—C14	117.26 (16)
C13—C14—O1	118.89 (18)	C23—O3—C22	117.10 (15)
N1—C2—C3—C4	179.9 (2)	C1—C8—C17—C22	−131.55 (19)
C7—C2—C3—C4	−0.7 (3)	N2—C8—C17—C18	−124.0 (2)
C2—C3—C4—C5	−0.5 (4)	C1—C8—C17—C18	52.3 (3)
C3—C4—C5—C6	0.5 (4)	C22—C17—C18—C19	0.5 (3)

C4—C5—C6—C7	0.7 (4)	C8—C17—C18—C19	176.78 (19)
N1—C2—C7—N2	2.8 (3)	C17—C18—C19—C20	−0.2 (3)
C3—C2—C7—N2	−176.6 (2)	C18—C19—C20—C21	−0.4 (3)
N1—C2—C7—C6	−178.78 (19)	C19—C20—C21—C22	0.8 (3)
C3—C2—C7—C6	1.8 (3)	C20—C21—C22—C17	−0.5 (3)
C5—C6—C7—N2	176.6 (2)	C20—C21—C22—O3	175.29 (18)
C5—C6—C7—C2	−1.9 (4)	C18—C17—C22—C21	−0.1 (3)
N1—C1—C8—N2	3.9 (3)	C8—C17—C22—C21	−176.41 (18)
C9—C1—C8—N2	−178.99 (17)	C18—C17—C22—O3	−176.01 (17)
N1—C1—C8—C17	−172.21 (17)	C8—C17—C22—O3	7.7 (3)
C9—C1—C8—C17	4.9 (3)	C8—C1—N1—C2	−1.5 (3)
N1—C1—C9—C14	−124.4 (2)	C9—C1—N1—C2	−178.85 (16)
C8—C1—C9—C14	58.4 (3)	C7—C2—N1—C1	−1.7 (3)
N1—C1—C9—C10	54.9 (2)	C3—C2—N1—C1	177.72 (19)
C8—C1—C9—C10	−122.4 (2)	C1—C8—N2—C7	−2.7 (3)
C14—C9—C10—C11	−1.2 (3)	C17—C8—N2—C7	173.69 (17)
C1—C9—C10—C11	179.5 (2)	C2—C7—N2—C8	−0.5 (3)
C9—C10—C11—C12	0.3 (4)	C6—C7—N2—C8	−178.93 (19)
C10—C11—C12—C13	0.6 (4)	O2—C15—O1—C14	−4.3 (4)
C11—C12—C13—C14	−0.5 (4)	C16—C15—O1—C14	176.0 (2)
C12—C13—C14—C9	−0.5 (3)	C13—C14—O1—C15	−79.8 (3)
C12—C13—C14—O1	−179.3 (2)	C9—C14—O1—C15	101.3 (2)
C10—C9—C14—C13	1.3 (3)	O4—C23—O3—C22	−8.4 (3)
C1—C9—C14—C13	−179.44 (19)	C24—C23—O3—C22	171.6 (2)
C10—C9—C14—O1	−179.88 (17)	C21—C22—O3—C23	74.4 (2)
C1—C9—C14—O1	−0.6 (3)	C17—C22—O3—C23	−109.70 (19)
N2—C8—C17—C22	52.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···O4^{i}	0.93	2.43	3.329 (2)	164

Symmetry code: (i) *x*−1, *y*, *z*.