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3-[2-(5*H*-Indolo[2,3-*b*]quinoxalin-5-yl)-ethyl]-1,3-oxazolidin-2-one

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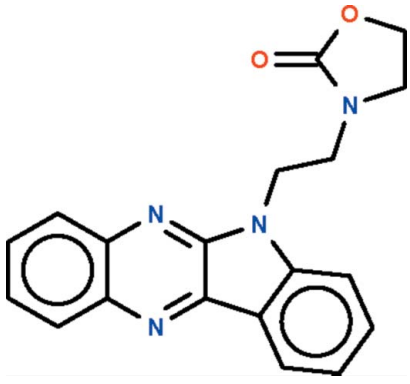
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.152; data-to-parameter ratio = 14.2.

The title compound, $C_{19}H_{16}N_4O_2$, has an almost planar fused *N*-heterocyclic system (r.m.s. deviation = 0.031 Å) and an almost planar five-membered 1,3-oxazolidine ring (r.m.s. deviation = 0.015 Å) at the ends of an ethylene chain [N—C—C—N torsion angle = −65.6 (2)°]. The ring systems are inclined at 38.1 (1)° to one another.

Related literature

For background to this class of oxindole derivatives, see: Alsubari *et al.* (2009). For a related structure, see: Alsubari *et al.* (2010)



Experimental

Crystal data

$C_{19}H_{16}N_4O_2$
M_r = 332.36
Monoclinic, $P2_1/n$
a = 14.5565 (4) Å
b = 5.8993 (2) Å
c = 18.6434 (6) Å
β = 92.393 (2)°
V = 1599.57 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.37 × 0.18 × 0.17 mm

Data collection

Bruker X8 APEXII diffractometer
19296 measured reflections
3216 independent reflections
1897 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.152
S = 0.95
3216 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2310).

References

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Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
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supporting information

Acta Cryst. (2010). E**66**, o2461 [https://doi.org/10.1107/S1600536810033222]

3-[2-(5*H*-Indolo[2,3-*b*]quinoxalin-5-yl)ethyl]-1,3-oxazolidin-2-one

Abdussalam Alsubari, Rachid Bouhfid, Hafid Zouihri, El Mokhtar Essassi and Seik Weng Ng

S1. Comment

The synthesis of new oxindole derivatives having an oxazolindin-2-one unit has been detailed in a recent report (Alsubari *et al.*, 2009). Among related compounds whose structures have been determined is 3-[2-(2,3-dioxoindolin-1-yl)ethyl]-1,3-oxazolidin-2-one (Alsubari *et al.*, 2010) in which the oxazolidinyl ring has an envelope conformation with the methylene C atom bonded to the N atom as the flap. The –CH_2–CH_2– connecting this ring to the other fused-ring system has its substituents in a *gauche* conformation [torsion angle = 62.7 (2)°]. In the tite compound (Scheme I, Fig. 1), the oxazolidinyl ring is planar (rms 0.015 Å), and there is no indication of any disorder in the ethylene portion of the ring. The fused *N*-heterocyclic system (rms 0.031 Å) is also planar and the two ring systems are inclined at 38.1 (1)° to one another. . The fused-rings are not stacked directly over one another, however, the distance between two inversion-related fused ring systems is only 3.4 Å (Fig. 2).

S2. Experimental

1-(2-(2-Oxoxazolidin-3-yl)ethyl)indoline-2,3-dione (0.5 g, 3.84 mmole) and *o*-phenylenediamine (0.41 g, 3.84 mmole) were heated in xylene (30 ml) and refluxed for twelve hours. The solvent was then removed under reduced pressure and the residue recrystallized from ethanol to afford the title compound as yellow crystals.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).

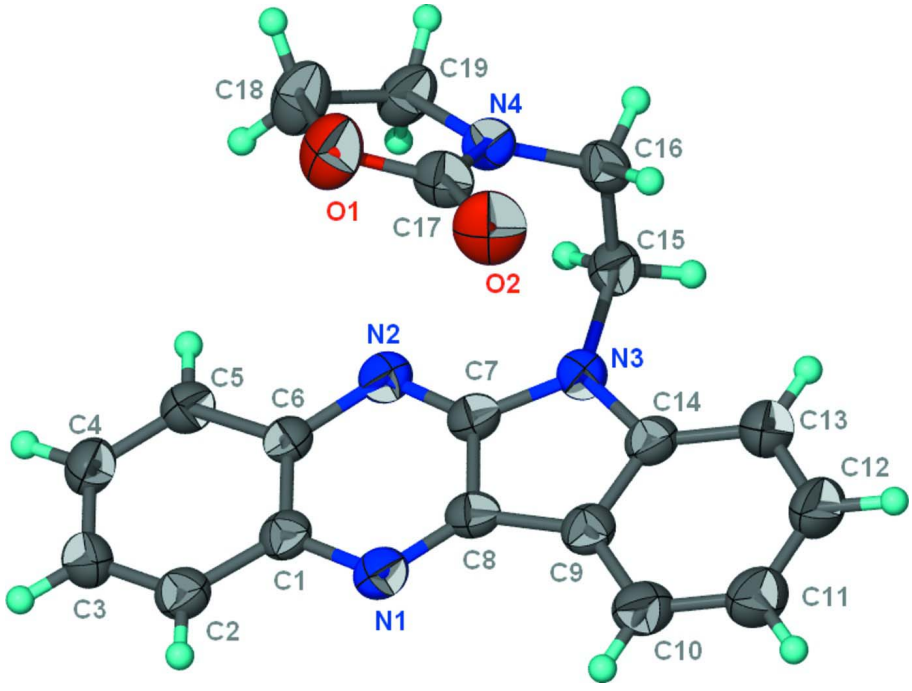

Figure 1

Thermal ellipsoid plot of the title compound at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

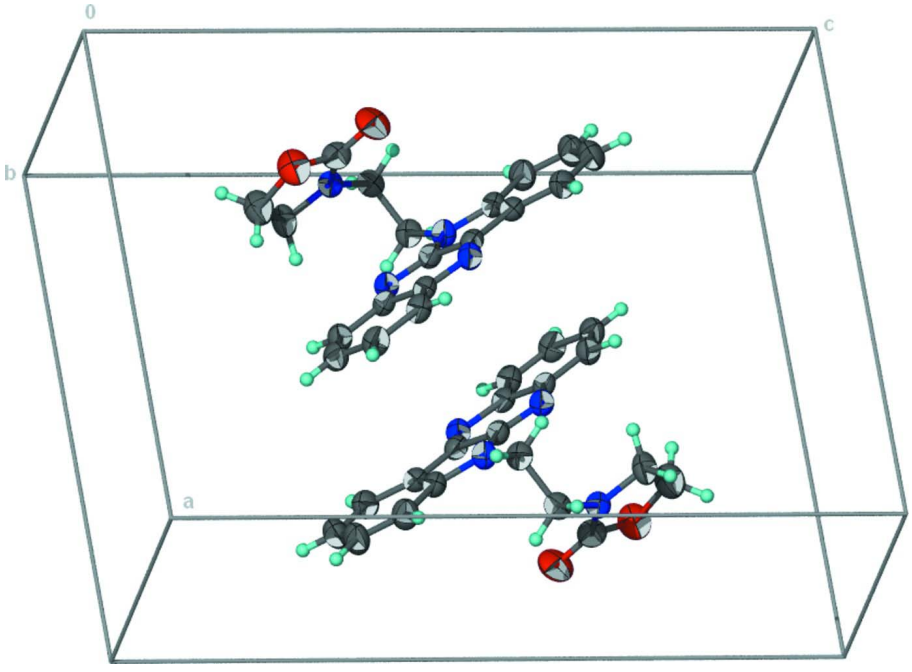

Figure 2

Two molecules disposed about a center-of-inversion.

3-[2-(5*H*-Indolo[2,3-*b*]quinoxalin-5-yl)ethyl]-1,3-oxazolidin-2-one

Crystal data

$C_{19}H_{16}N_4O_2$
$M_r = 332.36$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 14.5565$ (4) Å
$b = 5.8993$ (2) Å
$c = 18.6434$ (6) Å
$\beta = 92.393$ (2)°
$V = 1599.57$ (9) Å^3
$Z = 4$
$F(000) = 696$
$D_x = 1.380$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2575 reflections
$\theta = 2.8$–$21.3°$
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Prism, yellow
0.37 × 0.18 × 0.17 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
19296 measured reflections
3216 independent reflections
1897 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 26.3°$, $\theta_{min} = 2.8°$
$h = -18 \rightarrow 18$
$k = -7 \rightarrow 7$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.152$
$S = 0.95$
3216 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
$w = 1/[\sigma^2(F_o^2) + (0.0947P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.14976 (14)	0.4457 (3)	0.30554 (10)	0.0756 (6)
O2	0.09479 (13)	0.3291 (3)	0.41022 (10)	0.0765 (6)
N1	0.38685 (12)	0.2701 (3)	0.50246 (9)	0.0499 (5)
N2	0.32451 (12)	0.6823 (3)	0.43058 (9)	0.0493 (5)
N3	0.21587 (12)	0.6899 (3)	0.52289 (9)	0.0491 (5)
N4	0.10754 (12)	0.7065 (3)	0.38211 (9)	0.0449 (4)
C1	0.42821 (14)	0.3536 (4)	0.44272 (11)	0.0455 (5)
C2	0.50363 (16)	0.2364 (4)	0.41630 (12)	0.0536 (6)
H2	0.5235	0.1027	0.4383	0.064*
C3	0.54794 (16)	0.3169 (4)	0.35861 (12)	0.0571 (6)
H3	0.5980	0.2382	0.3418	0.069*
C4	0.51867 (16)	0.5176 (4)	0.32443 (12)	0.0573 (6)
H4	0.5496	0.5713	0.2852	0.069*
C5	0.44540 (15)	0.6342 (4)	0.34824 (12)	0.0519 (6)

H5	0.4262	0.7664	0.3249	0.062*
C6	0.39828 (14)	0.5568 (4)	0.40790 (10)	0.0434 (5)
C7	0.28851 (14)	0.5993 (4)	0.48773 (11)	0.0448 (5)
C8	0.31888 (14)	0.3950 (4)	0.52400 (11)	0.0446 (5)
C9	0.26054 (15)	0.3687 (4)	0.58425 (11)	0.0477 (5)
C10	0.25656 (16)	0.2117 (4)	0.64019 (12)	0.0593 (6)
H10	0.2985	0.0928	0.6437	0.071*
C11	0.19041 (17)	0.2347 (5)	0.68979 (14)	0.0693 (7)
H11	0.1874	0.1309	0.7272	0.083*
C12	0.12790 (18)	0.4118 (5)	0.68458 (13)	0.0713 (8)
H12	0.0829	0.4229	0.7184	0.086*
C13	0.13042 (17)	0.5719 (5)	0.63082 (12)	0.0624 (7)
H13	0.0884	0.6907	0.6282	0.075*
C14	0.19776 (15)	0.5498 (4)	0.58088 (11)	0.0480 (6)
C15	0.15862 (15)	0.8786 (4)	0.49739 (11)	0.0505 (6)
H15A	0.1961	0.9839	0.4714	0.061*
H15B	0.1353	0.9582	0.5384	0.061*
C16	0.07797 (15)	0.8028 (4)	0.44871 (12)	0.0483 (6)
H16A	0.0424	0.6908	0.4737	0.058*
H16B	0.0384	0.9317	0.4381	0.058*
C17	0.11498 (16)	0.4834 (4)	0.37101 (13)	0.0539 (6)
C18	0.1696 (2)	0.6593 (5)	0.27265 (14)	0.0742 (8)
H18A	0.1341	0.6763	0.2278	0.089*
H18B	0.2344	0.6699	0.2630	0.089*
C19	0.14339 (19)	0.8400 (4)	0.32542 (12)	0.0616 (7)
H19A	0.1965	0.9276	0.3421	0.074*
H19B	0.0971	0.9416	0.3046	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1126 (15)	0.0451 (11)	0.0699 (11)	0.0048 (9)	0.0125 (11)	−0.0150 (8)
O2	0.0993 (14)	0.0362 (10)	0.0947 (14)	−0.0026 (9)	0.0106 (11)	0.0101 (9)
N1	0.0567 (11)	0.0489 (11)	0.0437 (10)	0.0008 (9)	−0.0010 (9)	0.0018 (8)
N2	0.0515 (11)	0.0515 (11)	0.0446 (10)	0.0010 (9)	0.0001 (9)	0.0027 (8)
N3	0.0496 (11)	0.0537 (12)	0.0442 (10)	0.0081 (9)	0.0031 (9)	0.0015 (8)
N4	0.0569 (11)	0.0318 (10)	0.0459 (10)	0.0031 (8)	−0.0002 (8)	−0.0013 (8)
C1	0.0486 (12)	0.0489 (13)	0.0387 (11)	−0.0020 (10)	−0.0038 (10)	−0.0051 (9)
C2	0.0602 (14)	0.0534 (14)	0.0467 (13)	0.0070 (11)	−0.0034 (11)	−0.0031 (11)
C3	0.0562 (14)	0.0647 (16)	0.0507 (14)	0.0115 (12)	0.0040 (11)	−0.0073 (12)
C4	0.0571 (15)	0.0726 (17)	0.0426 (12)	−0.0010 (13)	0.0062 (11)	−0.0009 (12)
C5	0.0539 (13)	0.0558 (15)	0.0460 (12)	0.0022 (11)	0.0012 (11)	0.0057 (11)
C6	0.0434 (12)	0.0499 (13)	0.0366 (11)	0.0014 (10)	−0.0034 (9)	−0.0038 (9)
C7	0.0471 (12)	0.0466 (13)	0.0401 (11)	−0.0011 (10)	−0.0041 (10)	−0.0004 (10)
C8	0.0462 (12)	0.0438 (13)	0.0430 (11)	−0.0005 (10)	−0.0072 (10)	−0.0009 (10)
C9	0.0466 (12)	0.0526 (14)	0.0436 (12)	−0.0055 (10)	−0.0022 (10)	0.0002 (10)
C10	0.0585 (14)	0.0619 (16)	0.0573 (15)	−0.0005 (12)	−0.0025 (12)	0.0096 (12)
C11	0.0661 (16)	0.083 (2)	0.0587 (16)	−0.0056 (15)	0.0070 (13)	0.0199 (14)

C12	0.0602 (16)	0.102 (2)	0.0523 (14)	−0.0002 (16)	0.0111 (12)	0.0145 (15)
C13	0.0573 (15)	0.0779 (18)	0.0524 (14)	0.0068 (13)	0.0057 (12)	0.0027 (13)
C14	0.0483 (13)	0.0553 (14)	0.0401 (11)	−0.0023 (10)	−0.0031 (10)	0.0013 (10)
C15	0.0596 (14)	0.0442 (13)	0.0479 (13)	0.0055 (10)	0.0024 (11)	−0.0064 (10)
C16	0.0494 (12)	0.0401 (13)	0.0558 (13)	0.0085 (10)	0.0059 (10)	0.0024 (10)
C17	0.0604 (15)	0.0371 (13)	0.0639 (15)	0.0037 (10)	−0.0018 (12)	−0.0045 (11)
C18	0.104 (2)	0.0604 (18)	0.0588 (16)	−0.0010 (14)	0.0136 (15)	−0.0080 (12)
C19	0.0917 (18)	0.0481 (15)	0.0453 (13)	0.0035 (13)	0.0039 (12)	0.0037 (10)

Geometric parameters (Å, º)

O1—C17	1.359 (3)	C7—C8	1.442 (3)
O1—C18	1.436 (3)	C8—C9	1.445 (3)
O2—C17	1.211 (3)	C9—C10	1.398 (3)
N1—C8	1.310 (3)	C9—C14	1.406 (3)
N1—C1	1.379 (3)	C10—C11	1.369 (3)
N2—C7	1.302 (3)	C10—H10	0.9300
N2—C6	1.385 (3)	C11—C12	1.386 (4)
N3—C7	1.375 (3)	C11—H11	0.9300
N3—C14	1.395 (3)	C12—C13	1.379 (3)
N3—C15	1.458 (3)	C12—H12	0.9300
N4—C17	1.338 (3)	C13—C14	1.386 (3)
N4—C19	1.434 (3)	C13—H13	0.9300
N4—C16	1.447 (3)	C15—C16	1.521 (3)
C1—C2	1.404 (3)	C15—H15A	0.9700
C1—C6	1.423 (3)	C15—H15B	0.9700
C2—C3	1.362 (3)	C16—H16A	0.9700
C2—H2	0.9300	C16—H16B	0.9700
C3—C4	1.402 (3)	C18—C19	1.510 (3)
C3—H3	0.9300	C18—H18A	0.9700
C4—C5	1.359 (3)	C18—H18B	0.9700
C4—H4	0.9300	C19—H19A	0.9700
C5—C6	1.407 (3)	C19—H19B	0.9700
C5—H5	0.9300		

C17—O1—C18	109.19 (18)	C10—C11—C12	120.3 (2)
C8—N1—C1	114.03 (19)	C10—C11—H11	119.8
C7—N2—C6	113.11 (18)	C12—C11—H11	119.8
C7—N3—C14	108.24 (18)	C13—C12—C11	122.0 (2)
C7—N3—C15	125.57 (18)	C13—C12—H12	119.0
C14—N3—C15	125.53 (18)	C11—C12—H12	119.0
C17—N4—C19	113.09 (19)	C12—C13—C14	117.7 (2)
C17—N4—C16	123.23 (19)	C12—C13—H13	121.1
C19—N4—C16	123.19 (18)	C14—C13—H13	121.1
N1—C1—C2	118.8 (2)	C13—C14—N3	128.8 (2)
N1—C1—C6	122.26 (19)	C13—C14—C9	121.2 (2)
C2—C1—C6	118.94 (19)	N3—C14—C9	109.98 (19)
C3—C2—C1	120.5 (2)	N3—C15—C16	112.74 (18)

C3—C2—H2	119.7	N3—C15—H15A	109.0
C1—C2—H2	119.7	C16—C15—H15A	109.0
C2—C3—C4	120.5 (2)	N3—C15—H15B	109.0
C2—C3—H3	119.7	C16—C15—H15B	109.0
C4—C3—H3	119.7	H15A—C15—H15B	107.8
C5—C4—C3	120.4 (2)	N4—C16—C15	112.19 (17)
C5—C4—H4	119.8	N4—C16—H16A	109.2
C3—C4—H4	119.8	C15—C16—H16A	109.2
C4—C5—C6	120.6 (2)	N4—C16—H16B	109.2
C4—C5—H5	119.7	C15—C16—H16B	109.2
C6—C5—H5	119.7	H16A—C16—H16B	107.9
N2—C6—C5	118.5 (2)	O2—C17—N4	128.5 (2)
N2—C6—C1	122.53 (18)	O2—C17—O1	121.9 (2)
C5—C6—C1	118.95 (19)	N4—C17—O1	109.6 (2)
N2—C7—N3	126.0 (2)	O1—C18—C19	106.30 (19)
N2—C7—C8	124.87 (19)	O1—C18—H18A	110.5
N3—C7—C8	109.16 (18)	C19—C18—H18A	110.5
N1—C8—C7	123.16 (19)	O1—C18—H18B	110.5
N1—C8—C9	130.8 (2)	C19—C18—H18B	110.5
C7—C8—C9	106.00 (18)	H18A—C18—H18B	108.7
C10—C9—C14	119.3 (2)	N4—C19—C18	101.7 (2)
C10—C9—C8	134.1 (2)	N4—C19—H19A	111.4
C14—C9—C8	106.60 (18)	C18—C19—H19A	111.4
C11—C10—C9	119.4 (2)	N4—C19—H19B	111.4
C11—C10—H10	120.3	C18—C19—H19B	111.4
C9—C10—H10	120.3	H19A—C19—H19B	109.3

C8—N1—C1—C2	178.18 (19)	C14—C9—C10—C11	1.3 (3)
C8—N1—C1—C6	−0.5 (3)	C8—C9—C10—C11	−179.5 (2)
N1—C1—C2—C3	−178.2 (2)	C9—C10—C11—C12	0.0 (4)
C6—C1—C2—C3	0.6 (3)	C10—C11—C12—C13	−1.0 (4)
C1—C2—C3—C4	−0.3 (3)	C11—C12—C13—C14	0.6 (4)
C2—C3—C4—C5	−0.2 (4)	C12—C13—C14—N3	−178.6 (2)
C3—C4—C5—C6	0.6 (3)	C12—C13—C14—C9	0.9 (3)
C7—N2—C6—C5	−177.54 (18)	C7—N3—C14—C13	−179.2 (2)
C7—N2—C6—C1	2.3 (3)	C15—N3—C14—C13	−8.2 (4)
C4—C5—C6—N2	179.5 (2)	C7—N3—C14—C9	1.2 (2)
C4—C5—C6—C1	−0.4 (3)	C15—N3—C14—C9	172.27 (19)
N1—C1—C6—N2	−1.3 (3)	C10—C9—C14—C13	−1.8 (3)
C2—C1—C6—N2	179.99 (19)	C8—C9—C14—C13	178.8 (2)
N1—C1—C6—C5	178.46 (19)	C10—C9—C14—N3	177.76 (19)
C2—C1—C6—C5	−0.2 (3)	C8—C9—C14—N3	−1.6 (2)
C6—N2—C7—N3	178.79 (19)	C7—N3—C15—C16	87.4 (3)
C6—N2—C7—C8	−1.6 (3)	C14—N3—C15—C16	−82.2 (2)
C14—N3—C7—N2	179.42 (19)	C17—N4—C16—C15	98.1 (2)
C15—N3—C7—N2	8.3 (3)	C19—N4—C16—C15	−73.2 (3)
C14—N3—C7—C8	−0.3 (2)	N3—C15—C16—N4	−65.6 (2)
C15—N3—C7—C8	−171.34 (18)	C19—N4—C17—O2	176.5 (3)

C1—N1—C8—C7	1.2 (3)	C16—N4—C17—O2	4.4 (4)
C1—N1—C8—C9	−178.5 (2)	C19—N4—C17—O1	−4.0 (3)
N2—C7—C8—N1	−0.2 (3)	C16—N4—C17—O1	−176.09 (18)
N3—C7—C8—N1	179.50 (19)	C18—O1—C17—O2	−178.2 (2)
N2—C7—C8—C9	179.6 (2)	C18—O1—C17—N4	2.2 (3)
N3—C7—C8—C9	−0.7 (2)	C17—O1—C18—C19	0.2 (3)
N1—C8—C9—C10	1.9 (4)	C17—N4—C19—C18	3.8 (3)
C7—C8—C9—C10	−177.9 (2)	C16—N4—C19—C18	175.9 (2)
N1—C8—C9—C14	−178.8 (2)	O1—C18—C19—N4	−2.3 (3)
C7—C8—C9—C14	1.4 (2)		