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5,6-Dipropylphthalazino[2,3-*a*]cinnoline-8,13-dione

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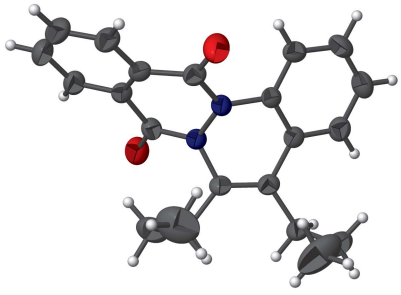
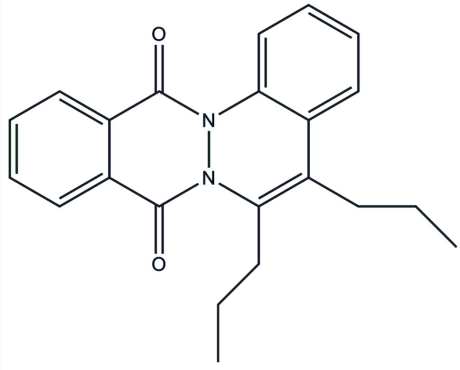
In the title compound, $C_{22}H_{22}N_2O_2$, the two central fused pyridazine rings have screw-boat conformations and the dihedral angle between their mean planes is 36.22 (8)°. The mean plane of the cinnoline ring system makes a dihedral angle of 46.56 (5)° with the mean plane of the phthalazine ring to which it is fused. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming chains along the *b* axis. The chains are reinforced by C—H···π interactions.

3D view



Chemical scheme



Structure description

Phthalazines, also called benzo-*ortho*-diazines or benzopyridazines, are a group of heterocyclic compounds, isomeric with the cinnolines. The practical interest in phthalazine derivatives is based on their widespread applications (Coates, 1999). Benzopyridazines, like other members of the isomeric diazene series, have found wide applications, including as therapeutic agents, ligands in transition metal catalysis, chemiluminescent and optical materials (Cheng *et al.*, 1999). Phthalazine derivatives have played an important role in the development of corrosion science as they can inhibit the corrosion of mild steel (Musa *et al.*, 2012). Moreover, they are of particular interest owing to their biological activity and optical properties (Caira *et al.*, 2011). Against this background, the crystal structure of the title compound has been determined and the results are presented herein.

In the title compound, Fig. 1, the two pyridazine rings (C5/C6/C7/N1/N2/C8 and N1/C9/C14–C16/N2) are conjugated and their mean planes are oriented at a dihedral angle of 36.22 (8)°. The phthalazine (N1/N2/C9–C16) unit consists of a benzene ring and a pyridazine ring which is fused with the cinnoline (N1/N2/C1–C8) ring system. The mean plane of the cinnoline ring system is inclined to the mean plane of the phthalazine ring by 46.56 (5)°.

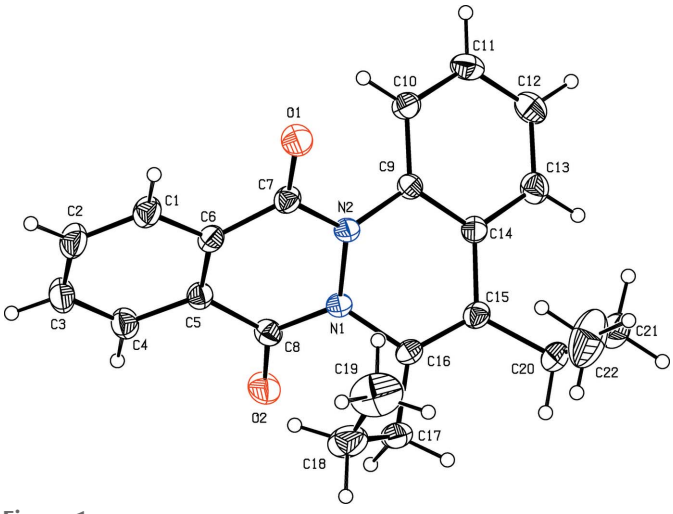


Figure 1
The molecular structure of the title compound, with atomic labelling and displacement ellipsoids drawn at the 30% probability level.

In the crystal, molecules are connected by C—H···O hydrogen bonds, leading to chains along the *b* axis (Table 1 and Fig. 2). In addition, within the chains there are C—H···π interactions, involving a benzene ring (C1–C6) H atom and the benzene ring (C9–C14) of an adjacent molecule (Table 1 and Fig. 2).

Synthesis and crystallization

2-Phenyl-2,3-dihydrophthalazine-1,4-dione (0.3 mmol) was treated with oct-4-yne (0.3 mmol) in the presence of [$RuCl_2$(*p*-cymene)$_2$] (2.5 mol%), $Cu(OAc)_2{\cdot}H_2O$ (1 equiv) and $AgSbF_6$ (0.03 mmol) in 1,2-dichloroethane at 273 K for 2.5 h in an open atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with dichloroethane, filtered through Celite and the filtrate was concentrated. The crude residue was purified through a silica gel column using petroleum ether and ethyl acetate as eluent, giving the title compound in pure form as block-like orange crystals (yield 90%).

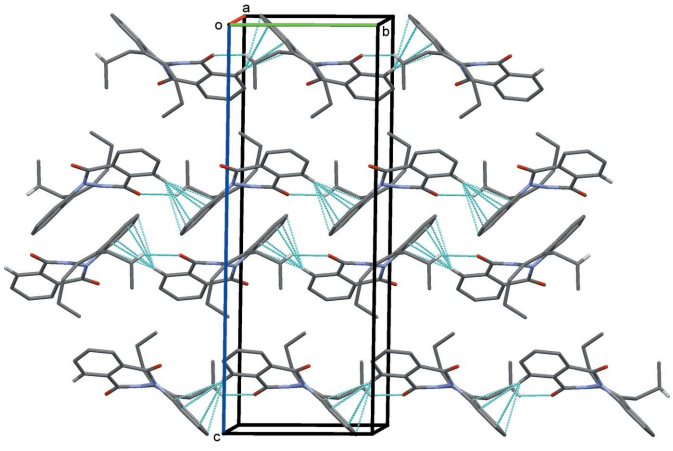


Figure 2
A view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds and C—H···π interactions are shown as dashed lines (see Table 1); C-bound H atoms not involved in these interactions have been omitted for clarity.

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

*Cg*4 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21*B*···O2^{i}	0.97	2.54	3.400 (3)	148
C4—H4···*Cg*4^{ii}	0.93	2.83	3.633	145

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{22}N_2O_2$
M_r	346.42
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, *b*, *c* (Å)	8.8711 (7), 8.6175 (6), 23.698 (2)
β (°)	99.672 (4)
V (Å^3)	1785.9 (2)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.22 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.983, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24172, 3153, 2644
R_{int}	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.148, 1.08
No. of reflections	3153
No. of parameters	235
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.30

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{22}H_{22}N_2O_2$
M_r = 346.42
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.8711 (7) Å
b = 8.6175 (6) Å
c = 23.698 (2) Å
β = 99.672 (4)°
V = 1785.9 (2) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.277 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2644 reflections
θ = 1.7–25.0°
μ = 0.08 mm^{-1}
T = 293 K
Block, orange
0.22 × 0.20 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.983, T_{max} = 0.986
24172 measured reflections
3153 independent reflections
2644 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.0°, θ_{min} = 1.7°
h = −10→10
k = −10→10
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.148
S = 1.08
3153 reflections
235 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
$w = 1/[\sigma^2(F_o^2) + (0.0908P)^2 + 0.5529P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C20	−0.0632 (2)	0.3401 (2)	0.06495 (10)	0.0484 (5)
H20A	−0.1029	0.3292	0.0244	0.058*
H20B	−0.1352	0.4034	0.0814	0.058*
C17	0.0105 (2)	0.6434 (3)	0.13449 (9)	0.0482 (5)
H17A	−0.0774	0.5785	0.1372	0.058*
H17B	−0.0267	0.7388	0.1153	0.058*
C21	−0.0576 (3)	0.1802 (3)	0.09234 (13)	0.0697 (7)
H21A	−0.1598	0.1365	0.0859	0.084*
H21B	0.0067	0.1134	0.0735	0.084*
C18	0.0925 (3)	0.6819 (3)	0.19488 (11)	0.0718 (8)
H18A	0.1694	0.7601	0.1920	0.086*
H18B	0.0188	0.7271	0.2160	0.086*
C19	0.1672 (4)	0.5497 (5)	0.22811 (11)	0.0994 (11)
H19A	0.2164	0.5854	0.2650	0.149*
H19B	0.2419	0.5047	0.2081	0.149*
H19C	0.0917	0.4731	0.2328	0.149*
C22	0.0012 (4)	0.1802 (4)	0.15434 (17)	0.1137 (14)
H22A	0.0027	0.0759	0.1687	0.171*
H22B	−0.0638	0.2430	0.1736	0.171*
H22C	0.1031	0.2218	0.1612	0.171*
N2	0.38243 (15)	0.52725 (16)	0.10830 (6)	0.0355 (4)
N1	0.25819 (16)	0.63184 (16)	0.09974 (6)	0.0363 (4)
O2	0.17675 (16)	0.87531 (16)	0.07850 (7)	0.0556 (4)
C6	0.53518 (19)	0.7336 (2)	0.15617 (7)	0.0361 (4)
C15	0.08719 (19)	0.4259 (2)	0.07134 (7)	0.0362 (4)
C5	0.4304 (2)	0.8411 (2)	0.12868 (7)	0.0356 (4)
O1	0.61735 (15)	0.47147 (16)	0.15763 (6)	0.0540 (4)
C7	0.5168 (2)	0.5669 (2)	0.14328 (8)	0.0376 (4)
C14	0.21374 (19)	0.3577 (2)	0.04659 (7)	0.0348 (4)
C8	0.2802 (2)	0.7886 (2)	0.09832 (8)	0.0376 (4)
C9	0.36383 (19)	0.40445 (19)	0.06747 (7)	0.0327 (4)
C16	0.11139 (19)	0.5610 (2)	0.09891 (8)	0.0362 (4)
C4	0.4611 (2)	0.9990 (2)	0.13425 (8)	0.0453 (5)
H4	0.3922	1.0707	0.1153	0.054*
C1	0.6675 (2)	0.7856 (2)	0.19067 (9)	0.0466 (5)
H1	0.7372	0.7146	0.2096	0.056*
C11	0.4621 (2)	0.2265 (2)	0.00602 (9)	0.0482 (5)
H11	0.5446	0.1813	−0.0073	0.058*
C10	0.4873 (2)	0.3395 (2)	0.04766 (8)	0.0414 (4)
H10	0.5863	0.3716	0.0622	0.050*

C13	0.1931 (2)	0.2441 (2)	0.00413 (8)	0.0457 (5)
H13	0.0947	0.2111	−0.0109	0.055*
C2	0.6954 (3)	0.9419 (3)	0.19691 (10)	0.0566 (6)
H2	0.7831	0.9763	0.2207	0.068*
C3	0.5940 (3)	1.0488 (2)	0.16794 (10)	0.0550 (6)
H3	0.6157	1.1543	0.1713	0.066*
C12	0.3160 (3)	0.1801 (2)	−0.01595 (9)	0.0518 (5)
H12	0.2999	0.1050	−0.0445	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C20	0.0313 (10)	0.0492 (11)	0.0627 (12)	−0.0042 (8)	0.0022 (9)	−0.0059 (10)
C17	0.0334 (10)	0.0559 (12)	0.0555 (12)	0.0040 (9)	0.0084 (8)	−0.0095 (10)
C21	0.0503 (13)	0.0545 (14)	0.106 (2)	−0.0102 (11)	0.0196 (13)	0.0052 (13)
C18	0.0545 (14)	0.103 (2)	0.0605 (14)	−0.0009 (14)	0.0172 (11)	−0.0256 (14)
C19	0.098 (2)	0.148 (3)	0.0507 (15)	0.014 (2)	0.0079 (15)	0.0010 (18)
C22	0.102 (3)	0.105 (3)	0.126 (3)	−0.040 (2)	−0.005 (2)	0.055 (2)
N2	0.0265 (7)	0.0328 (8)	0.0456 (8)	0.0040 (6)	0.0013 (6)	−0.0037 (6)
N1	0.0262 (7)	0.0328 (8)	0.0486 (9)	0.0039 (6)	0.0022 (6)	−0.0024 (6)
O2	0.0480 (8)	0.0413 (8)	0.0720 (10)	0.0112 (7)	−0.0056 (7)	0.0040 (7)
C6	0.0328 (9)	0.0407 (10)	0.0353 (9)	−0.0043 (8)	0.0071 (7)	−0.0014 (7)
C15	0.0288 (9)	0.0388 (9)	0.0390 (9)	0.0011 (7)	0.0000 (7)	0.0027 (8)
C5	0.0379 (9)	0.0362 (9)	0.0340 (9)	−0.0036 (7)	0.0099 (7)	−0.0010 (7)
O1	0.0394 (8)	0.0472 (8)	0.0683 (10)	0.0084 (6)	−0.0117 (7)	−0.0016 (7)
C7	0.0314 (9)	0.0395 (10)	0.0405 (9)	−0.0004 (8)	0.0022 (7)	0.0019 (8)
C14	0.0336 (9)	0.0330 (9)	0.0367 (9)	0.0005 (7)	0.0024 (7)	0.0018 (7)
C8	0.0393 (10)	0.0347 (9)	0.0384 (9)	0.0036 (8)	0.0051 (8)	−0.0005 (7)
C9	0.0332 (9)	0.0292 (8)	0.0355 (9)	0.0016 (7)	0.0055 (7)	0.0021 (7)
C16	0.0255 (8)	0.0401 (10)	0.0414 (9)	0.0020 (7)	0.0007 (7)	−0.0004 (8)
C4	0.0516 (12)	0.0375 (10)	0.0483 (11)	−0.0049 (9)	0.0127 (9)	−0.0009 (9)
C1	0.0385 (10)	0.0520 (12)	0.0471 (11)	−0.0068 (9)	0.0012 (8)	−0.0044 (9)
C11	0.0521 (12)	0.0479 (11)	0.0487 (11)	0.0096 (9)	0.0200 (9)	−0.0023 (9)
C10	0.0353 (10)	0.0415 (10)	0.0483 (10)	0.0011 (8)	0.0097 (8)	0.0021 (8)
C13	0.0454 (11)	0.0462 (11)	0.0431 (10)	−0.0038 (9)	0.0009 (8)	−0.0066 (9)
C2	0.0477 (12)	0.0609 (14)	0.0595 (13)	−0.0181 (11)	0.0042 (10)	−0.0158 (11)
C3	0.0621 (14)	0.0413 (11)	0.0635 (13)	−0.0153 (10)	0.0160 (11)	−0.0099 (10)
C12	0.0628 (14)	0.0485 (12)	0.0441 (11)	0.0022 (10)	0.0094 (10)	−0.0118 (9)

Geometric parameters (Å, º)

C20—C15	1.511 (2)	C6—C1	1.387 (3)
C20—C21	1.521 (3)	C6—C5	1.394 (3)
C20—H20A	0.9700	C6—C7	1.473 (3)
C20—H20B	0.9700	C15—C16	1.335 (3)
C17—C16	1.506 (3)	C15—C14	1.473 (2)
C17—C18	1.529 (3)	C5—C4	1.389 (3)
C17—H17A	0.9700	C5—C8	1.475 (2)

C17—H17B	0.9700	O1—C7	1.219 (2)
C21—C22	1.474 (4)	C14—C13	1.393 (3)
C21—H21A	0.9700	C14—C9	1.400 (2)
C21—H21B	0.9700	C9—C10	1.381 (2)
C18—C19	1.477 (4)	C4—C3	1.376 (3)
C18—H18A	0.9700	C4—H4	0.9300
C18—H18B	0.9700	C1—C2	1.373 (3)
C19—H19A	0.9600	C1—H1	0.9300
C19—H19B	0.9600	C11—C12	1.373 (3)
C19—H19C	0.9600	C11—C10	1.378 (3)
C22—H22A	0.9600	C11—H11	0.9300
C22—H22B	0.9600	C10—H10	0.9300
C22—H22C	0.9600	C13—C12	1.376 (3)
N2—C7	1.376 (2)	C13—H13	0.9300
N2—N1	1.4118 (19)	C2—C3	1.387 (3)
N2—C9	1.425 (2)	C2—H2	0.9300
N1—C8	1.366 (2)	C3—H3	0.9300
N1—C16	1.435 (2)	C12—H12	0.9300
O2—C8	1.215 (2)		

C15—C20—C21	115.80 (17)	C16—C15—C14	118.18 (16)
C15—C20—H20A	108.3	C16—C15—C20	122.84 (17)
C21—C20—H20A	108.3	C14—C15—C20	118.97 (16)
C15—C20—H20B	108.3	C6—C5—C4	120.10 (17)
C21—C20—H20B	108.3	C6—C5—C8	120.05 (16)
H20A—C20—H20B	107.4	C4—C5—C8	119.58 (17)
C16—C17—C18	113.12 (16)	O1—C7—N2	121.35 (16)
C16—C17—H17A	109.0	O1—C7—C6	123.36 (16)
C18—C17—H17A	109.0	N2—C7—C6	114.95 (15)
C16—C17—H17B	109.0	C13—C14—C9	117.34 (17)
C18—C17—H17B	109.0	C13—C14—C15	123.45 (16)
H17A—C17—H17B	107.8	C9—C14—C15	119.18 (15)
C22—C21—C20	113.9 (2)	O2—C8—N1	121.03 (17)
C22—C21—H21A	108.8	O2—C8—C5	124.17 (16)
C20—C21—H21A	108.8	N1—C8—C5	114.38 (15)
C22—C21—H21B	108.8	C10—C9—C14	121.67 (16)
C20—C21—H21B	108.8	C10—C9—N2	121.60 (15)
H21A—C21—H21B	107.7	C14—C9—N2	116.67 (15)
C19—C18—C17	115.6 (2)	C15—C16—N1	116.65 (16)
C19—C18—H18A	108.4	C15—C16—C17	128.55 (17)
C17—C18—H18A	108.4	N1—C16—C17	114.52 (15)
C19—C18—H18B	108.4	C3—C4—C5	119.72 (19)
C17—C18—H18B	108.4	C3—C4—H4	120.1
H18A—C18—H18B	107.4	C5—C4—H4	120.1
C18—C19—H19A	109.5	C2—C1—C6	120.0 (2)
C18—C19—H19B	109.5	C2—C1—H1	120.0
H19A—C19—H19B	109.5	C6—C1—H1	120.0
C18—C19—H19C	109.5	C12—C11—C10	120.46 (18)

H19A—C19—H19C	109.5	C12—C11—H11	119.8
H19B—C19—H19C	109.5	C10—C11—H11	119.8
C21—C22—H22A	109.5	C11—C10—C9	119.16 (18)
C21—C22—H22B	109.5	C11—C10—H10	120.4
H22A—C22—H22B	109.5	C9—C10—H10	120.4
C21—C22—H22C	109.5	C12—C13—C14	121.06 (19)
H22A—C22—H22C	109.5	C12—C13—H13	119.5
H22B—C22—H22C	109.5	C14—C13—H13	119.5
C7—N2—N1	120.31 (14)	C1—C2—C3	120.5 (2)
C7—N2—C9	125.69 (14)	C1—C2—H2	119.7
N1—N2—C9	112.21 (13)	C3—C2—H2	119.7
C8—N1—N2	121.55 (14)	C4—C3—C2	120.10 (19)
C8—N1—C16	123.60 (14)	C4—C3—H3	120.0
N2—N1—C16	114.53 (13)	C2—C3—H3	120.0
C1—C6—C5	119.51 (17)	C11—C12—C13	120.29 (18)
C1—C6—C7	119.38 (17)	C11—C12—H12	119.9
C5—C6—C7	120.64 (16)	C13—C12—H12	119.9

C15—C20—C21—C22	58.1 (3)	C13—C14—C9—C10	−1.0 (3)
C16—C17—C18—C19	−53.8 (3)	C15—C14—C9—C10	177.11 (16)
C7—N2—N1—C8	34.3 (2)	C13—C14—C9—N2	176.26 (16)
C9—N2—N1—C8	−131.28 (17)	C15—C14—C9—N2	−5.6 (2)
C7—N2—N1—C16	−139.42 (16)	C7—N2—C9—C10	−18.3 (3)
C9—N2—N1—C16	54.97 (19)	N1—N2—C9—C10	146.39 (16)
C21—C20—C15—C16	−118.0 (2)	C7—N2—C9—C14	164.43 (16)
C21—C20—C15—C14	61.5 (3)	N1—N2—C9—C14	−30.9 (2)
C1—C6—C5—C4	2.3 (3)	C14—C15—C16—N1	2.7 (2)
C7—C6—C5—C4	−169.90 (17)	C20—C15—C16—N1	−177.77 (16)
C1—C6—C5—C8	−171.73 (16)	C14—C15—C16—C17	−170.79 (17)
C7—C6—C5—C8	16.1 (3)	C20—C15—C16—C17	8.7 (3)
N1—N2—C7—O1	169.68 (17)	C8—N1—C16—C15	145.59 (18)
C9—N2—C7—O1	−26.8 (3)	N2—N1—C16—C15	−40.8 (2)
N1—N2—C7—C6	−16.8 (2)	C8—N1—C16—C17	−40.0 (2)
C9—N2—C7—C6	146.75 (16)	N2—N1—C16—C17	133.61 (16)
C1—C6—C7—O1	−6.0 (3)	C18—C17—C16—C15	125.2 (2)
C5—C6—C7—O1	166.16 (18)	C18—C17—C16—N1	−48.4 (2)
C1—C6—C7—N2	−179.40 (16)	C6—C5—C4—C3	−1.3 (3)
C5—C6—C7—N2	−7.2 (2)	C8—C5—C4—C3	172.72 (17)
C16—C15—C14—C13	−161.28 (18)	C5—C6—C1—C2	−0.9 (3)
C20—C15—C14—C13	19.2 (3)	C7—C6—C1—C2	171.37 (19)
C16—C15—C14—C9	20.7 (2)	C12—C11—C10—C9	0.7 (3)
C20—C15—C14—C9	−158.80 (16)	C14—C9—C10—C11	0.4 (3)
N2—N1—C8—O2	163.23 (17)	N2—C9—C10—C11	−176.71 (16)
C16—N1—C8—O2	−23.6 (3)	C9—C14—C13—C12	0.5 (3)
N2—N1—C8—C5	−23.9 (2)	C15—C14—C13—C12	−177.50 (18)
C16—N1—C8—C5	149.23 (16)	C6—C1—C2—C3	−1.4 (3)
C6—C5—C8—O2	171.95 (18)	C5—C4—C3—C2	−1.0 (3)
C4—C5—C8—O2	−2.1 (3)	C1—C2—C3—C4	2.4 (3)

C6—C5—C8—N1	−0.6 (2)	C10—C11—C12—C13	−1.1 (3)
C4—C5—C8—N1	−174.65 (16)	C14—C13—C12—C11	0.5 (3)

Hydrogen-bond geometry (Å, º)

Cg4 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21*B*···O2^{i}	0.97	2.54	3.400 (3)	148
C4—H4···*Cg*4^{ii}	0.93	2.83	3.633	145

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, *y*+1, *z*.