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N-(9-Anthrylmethyl)picolinamide

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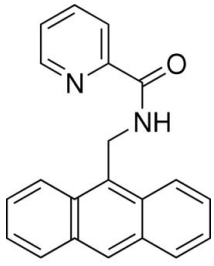
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.151; data-to-parameter ratio = 15.7.

In the title molecule, $C_{21}H_{16}N_2O$, the anthracene ring system is slightly twisted with a dihedral angle of 1.22 (1)° between the two outermost rings. The anthracene mean plane and pyridine ring make a dihedral angle of 72.6 (1)°. The $\pi\cdots\pi$ interactions [3.551 (2) Å] between the anthracene fragments form stacks of molecules parallel to the b axis.

Related literature

For crystal structures of isomers of the title compound, see: Huang *et al.* (2004); Gu *et al.* (2006); Kubo *et al.* (2007). For the applications of anthracene derivatives, see: Gunnlaugsson *et al.* (2003); Chen & Chen (2004); Kim & Yoon (2002). For related literature, see: Rowland *et al.* (2001).



Experimental

Crystal data

$C_{21}H_{16}N_2O$
M_r = 312.36
Monoclinic, $P2_1/c$
a = 10.0182 (3) Å
b = 8.1082 (3) Å
c = 19.2442 (6) Å
β = 103.0700 (10)°
V = 1522.70 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
0.25 × 0.25 × 0.06 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: none
14372 measured reflections
3479 independent reflections
2304 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.151
S = 1.01
3479 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 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
N1—H1*N*···N2	0.865 (17)	2.193 (18)	2.655 (2)	113.1 (15)
C10—H10···O1^{i}	0.95	2.59	3.533 (3)	170

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

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2255).

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supplementary materials

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N-(9-Anthrylmethyl)picolinamide

S.-J. Gu, J. Lin, L.-H. Jing, H.-X. Zhang and D.-B. Qin

Comment

Anthracene is a polycyclic aromatic hydrocarbon that has been widely used as a signaling subunit for both cation (Gunnlaugsson *et al.*, 2003) and anion (Chen & Chen, 2004; Kim & Yoon, 2002) sensing due to its well known photophysical properties and high fluorescence. We here report the crystal structure of the title compound, (I).

In (I) (Fig. 1), the bond lengths and angles are within normal ranges. The anthracene ring system is slightly twisted with a dihedral angle of 1.22 (1)° between the two utmost rings. The anthracene mean plane and pyridin ring make a dihedral angle of 72.6 (1)°. The intramolecular hydrogen bond N1—H1N···N2 (Table 1) influences molecular conformation. The short contact between the anthracene fragments of the neighbouring molecules - C9···C14^{ii} of 3.431 (2) Å and C1···C3^{iii} of 3.591 (2) Å [symmetry codes: (ii) $1-x, 2-y, 1-z$; (iii) $1-x, 1-y, 1-z$] - show an existence of π···π interactions, which form stacks of the molecules parallel to *b* axis. The crystal packing exhibits also weak intermolecular C—H···O hydrogen bonds.

Experimental

The title compound was prepared according to the reported procedure of Rowland *et al.* (2001). Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from dimethyl sulfoxide.

Refinement

C-bound H atoms were placed in calculated positions with C—H = 0.95–0.99 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C). Atom H1N was located in a difference Fourier map and refined isotropically with a bond restraint of N—H = 0.86 (2) Å.

Figures

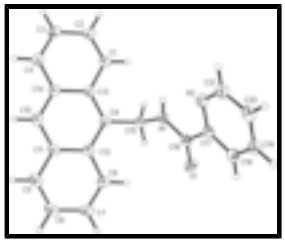


Fig. 1. The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

N-(anthracen-10-ylmethyl)picolinamide

Crystal data

$C_{21}H_{16}N_2O$ $F_{000} = 656$

M_r = 312.36	D_x = 1.363 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9693 reflections
a = 10.0182 (3) Å	θ = 3.2–27.5º
b = 8.1082 (3) Å	μ = 0.09 mm^{-1}
c = 19.2442 (6) Å	T = 153 (2) K
β = 103.0700 (10)º	Block, yellow
V = 1522.70 (9) Å^3	0.25 × 0.25 × 0.06 mm
Z = 4	

Data collection

Rigaku RAXIS-RAPID diffractometer	2304 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.032
Monochromator: graphite	θ_{max} = 27.5º
T = 153(2) K	θ_{min} = 3.3º
ω scans	h = −12→13
Absorption correction: none	k = −10→10
14372 measured reflections	l = −24→24
3479 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$w = 1/[\sigma^2(F_o^2) + (0.098P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.151	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.01	$\Delta\rho_{max}$ = 0.62 e Å^{-3}
3479 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
222 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.013 (3)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.03419 (13)	0.86927 (15)	0.62684 (7)	0.0469 (4)
N1	0.16317 (14)	0.73494 (17)	0.56145 (7)	0.0346 (3)
N2	0.07086 (15)	0.44338 (17)	0.59240 (8)	0.0389 (4)
C1	0.39511 (17)	0.70846 (19)	0.45469 (8)	0.0355 (4)
H1	0.2979	0.7049	0.4410	0.043*
C2	0.46983 (18)	0.6366 (2)	0.41213 (9)	0.0392 (4)
H2	0.4244	0.5839	0.3692	0.047*
C3	0.61427 (18)	0.6397 (2)	0.43115 (9)	0.0391 (4)
H3	0.6652	0.5910	0.4004	0.047*
C4	0.68103 (18)	0.71105 (19)	0.49267 (9)	0.0378 (4)
H4	0.7784	0.7108	0.5050	0.045*
C5	0.67089 (19)	1.0119 (2)	0.71376 (9)	0.0426 (4)
H5	0.7681	1.0085	0.7272	0.051*
C6	0.6004 (2)	1.0877 (2)	0.75709 (10)	0.0480 (5)
H6	0.6483	1.1382	0.8001	0.058*
C7	0.4556 (2)	1.0915 (2)	0.73833 (9)	0.0458 (5)
H7	0.4068	1.1448	0.7690	0.055*
C8	0.38483 (19)	1.0198 (2)	0.67683 (9)	0.0396 (4)
H8	0.2875	1.0222	0.6659	0.048*
C9	0.38519 (16)	0.86933 (18)	0.56359 (8)	0.0316 (4)
C10	0.67400 (17)	0.86240 (19)	0.60291 (9)	0.0351 (4)
H10	0.7713	0.8628	0.6156	0.042*
C11	0.60121 (17)	0.93700 (19)	0.64807 (8)	0.0345 (4)
C12	0.45425 (17)	0.94096 (18)	0.62850 (8)	0.0326 (4)
C13	0.45931 (15)	0.78882 (17)	0.51927 (8)	0.0298 (3)
C14	0.60675 (16)	0.78706 (18)	0.53946 (8)	0.0324 (4)
C15	0.23042 (16)	0.87963 (19)	0.53993 (9)	0.0343 (4)
H15A	0.1982	0.9795	0.5608	0.041*
H15B	0.2042	0.8904	0.4874	0.041*
C16	0.07404 (16)	0.74078 (19)	0.60383 (9)	0.0340 (4)
C17	0.02651 (16)	0.5742 (2)	0.62342 (8)	0.0336 (4)
C18	−0.05583 (17)	0.5611 (2)	0.67204 (9)	0.0398 (4)
H18	−0.0867	0.6568	0.6922	0.048*
C19	−0.09223 (19)	0.4049 (2)	0.69066 (10)	0.0459 (4)
H19	−0.1476	0.3916	0.7243	0.055*
C20	−0.04654 (19)	0.2690 (2)	0.65940 (10)	0.0463 (4)
H20	−0.0698	0.1605	0.6711	0.056*
C21	0.03386 (18)	0.2950 (2)	0.61073 (10)	0.0438 (4)
H21	0.0645	0.2012	0.5891	0.053*
H1N	0.1791 (18)	0.637 (2)	0.5475 (10)	0.040 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0505 (7)	0.0364 (7)	0.0597 (8)	0.0007 (5)	0.0252 (7)	−0.0038 (6)
N1	0.0384 (7)	0.0304 (7)	0.0360 (7)	−0.0010 (6)	0.0104 (6)	−0.0006 (6)
N2	0.0381 (7)	0.0342 (7)	0.0443 (8)	0.0013 (6)	0.0096 (6)	0.0027 (6)
C1	0.0410 (9)	0.0327 (8)	0.0318 (8)	−0.0006 (7)	0.0060 (7)	0.0019 (6)
C2	0.0525 (10)	0.0330 (9)	0.0329 (9)	−0.0006 (7)	0.0112 (8)	−0.0018 (7)
C3	0.0517 (10)	0.0321 (8)	0.0378 (9)	0.0073 (7)	0.0188 (8)	0.0035 (7)
C4	0.0419 (9)	0.0314 (8)	0.0422 (9)	0.0037 (7)	0.0140 (8)	0.0075 (7)
C5	0.0509 (10)	0.0377 (9)	0.0358 (9)	−0.0104 (8)	0.0028 (8)	0.0047 (7)
C6	0.0688 (13)	0.0386 (10)	0.0321 (9)	−0.0098 (9)	0.0024 (9)	−0.0012 (7)
C7	0.0735 (13)	0.0332 (9)	0.0328 (9)	0.0015 (9)	0.0162 (9)	−0.0004 (7)
C8	0.0547 (10)	0.0318 (8)	0.0339 (9)	0.0015 (7)	0.0130 (8)	0.0038 (7)
C9	0.0376 (8)	0.0269 (7)	0.0307 (8)	−0.0021 (6)	0.0088 (7)	0.0054 (6)
C10	0.0360 (8)	0.0320 (8)	0.0358 (9)	−0.0036 (6)	0.0052 (7)	0.0081 (7)
C11	0.0441 (9)	0.0281 (8)	0.0298 (8)	−0.0064 (6)	0.0051 (7)	0.0056 (6)
C12	0.0454 (9)	0.0248 (7)	0.0287 (8)	−0.0013 (6)	0.0106 (7)	0.0048 (6)
C13	0.0351 (8)	0.0252 (7)	0.0294 (8)	−0.0007 (6)	0.0080 (7)	0.0036 (6)
C14	0.0380 (9)	0.0260 (7)	0.0342 (8)	−0.0005 (6)	0.0103 (7)	0.0073 (6)
C15	0.0398 (8)	0.0310 (8)	0.0327 (8)	0.0005 (6)	0.0095 (7)	0.0034 (6)
C16	0.0328 (8)	0.0347 (8)	0.0335 (8)	0.0011 (6)	0.0056 (7)	0.0002 (6)
C17	0.0305 (7)	0.0361 (9)	0.0314 (8)	0.0015 (6)	0.0014 (7)	0.0035 (6)
C18	0.0375 (9)	0.0443 (10)	0.0373 (9)	0.0007 (7)	0.0076 (7)	0.0035 (7)
C19	0.0449 (10)	0.0540 (11)	0.0383 (9)	−0.0073 (8)	0.0087 (8)	0.0076 (8)
C20	0.0467 (10)	0.0422 (10)	0.0470 (10)	−0.0051 (8)	0.0039 (9)	0.0125 (8)
C21	0.0436 (10)	0.0342 (9)	0.0529 (11)	0.0016 (7)	0.0093 (9)	0.0037 (8)

Geometric parameters (Å, °)

O1—C16	1.2332 (18)	C8—C12	1.432 (2)
N1—C16	1.3394 (19)	C8—H8	0.9500
N1—C15	1.4587 (19)	C9—C12	1.409 (2)
N1—H1N	0.863 (19)	C9—C13	1.411 (2)
N2—C21	1.330 (2)	C9—C15	1.516 (2)
N2—C17	1.342 (2)	C10—C11	1.393 (2)
C1—C2	1.359 (2)	C10—C14	1.395 (2)
C1—C13	1.422 (2)	C10—H10	0.9500
C1—H1	0.9500	C11—C12	1.435 (2)
C2—C3	1.410 (2)	C13—C14	1.440 (2)
C2—H2	0.9500	C15—H15A	0.9900
C3—C4	1.351 (3)	C15—H15B	0.9900
C3—H3	0.9500	C16—C17	1.508 (2)
C4—C14	1.431 (2)	C17—C18	1.384 (2)
C4—H4	0.9500	C18—C19	1.387 (2)
C5—C6	1.356 (3)	C18—H18	0.9500
C5—C11	1.434 (2)	C19—C20	1.382 (3)
C5—H5	0.9500	C19—H19	0.9500

C6—C7	1.414 (3)	C20—C21	1.383 (2)
C6—H6	0.9500	C20—H20	0.9500
C7—C8	1.364 (3)	C21—H21	0.9500
C7—H7	0.9500		
C16—N1—C15	123.97 (13)	C10—C11—C12	119.79 (15)
C16—N1—H1N	114.7 (11)	C5—C11—C12	119.20 (14)
C15—N1—H1N	121.4 (11)	C9—C12—C8	123.13 (15)
C21—N2—C17	117.21 (14)	C9—C12—C11	119.50 (13)
C2—C1—C13	121.42 (16)	C8—C12—C11	117.37 (15)
C2—C1—H1	119.3	C9—C13—C1	122.99 (14)
C13—C1—H1	119.3	C9—C13—C14	119.30 (14)
C1—C2—C3	120.57 (16)	C1—C13—C14	117.71 (13)
C1—C2—H2	119.7	C10—C14—C4	121.49 (15)
C3—C2—H2	119.7	C10—C14—C13	119.65 (13)
C4—C3—C2	120.69 (14)	C4—C14—C13	118.84 (15)
C4—C3—H3	119.7	N1—C15—C9	112.15 (13)
C2—C3—H3	119.7	N1—C15—H15A	109.2
C3—C4—C14	120.73 (16)	C9—C15—H15A	109.2
C3—C4—H4	119.6	N1—C15—H15B	109.2
C14—C4—H4	119.6	C9—C15—H15B	109.2
C6—C5—C11	121.12 (17)	H15A—C15—H15B	107.9
C6—C5—H5	119.4	O1—C16—N1	124.26 (14)
C11—C5—H5	119.4	O1—C16—C17	121.37 (13)
C5—C6—C7	120.01 (17)	N1—C16—C17	114.35 (13)
C5—C6—H6	120.0	N2—C17—C18	123.21 (15)
C7—C6—H6	120.0	N2—C17—C16	116.22 (13)
C8—C7—C6	120.92 (16)	C18—C17—C16	120.55 (14)
C8—C7—H7	119.5	C17—C18—C19	118.48 (16)
C6—C7—H7	119.5	C17—C18—H18	120.8
C7—C8—C12	121.36 (17)	C19—C18—H18	120.8
C7—C8—H8	119.3	C20—C19—C18	118.88 (15)
C12—C8—H8	119.3	C20—C19—H19	120.6
C12—C9—C13	120.43 (14)	C18—C19—H19	120.6
C12—C9—C15	120.48 (13)	C19—C20—C21	118.34 (16)
C13—C9—C15	119.08 (14)	C19—C20—H20	120.8
C11—C10—C14	121.27 (15)	C21—C20—H20	120.8
C11—C10—H10	119.4	N2—C21—C20	123.87 (16)
C14—C10—H10	119.4	N2—C21—H21	118.1
C10—C11—C5	121.01 (16)	C20—C21—H21	118.1
C13—C1—C2—C3	0.1 (2)	C11—C10—C14—C4	179.64 (14)
C1—C2—C3—C4	1.3 (2)	C11—C10—C14—C13	1.2 (2)
C2—C3—C4—C14	−0.8 (2)	C3—C4—C14—C10	−179.51 (14)
C11—C5—C6—C7	1.0 (3)	C3—C4—C14—C13	−1.1 (2)
C5—C6—C7—C8	0.0 (3)	C9—C13—C14—C10	1.0 (2)
C6—C7—C8—C12	−1.2 (3)	C1—C13—C14—C10	−179.11 (13)
C14—C10—C11—C5	179.00 (14)	C9—C13—C14—C4	−177.43 (13)
C14—C10—C11—C12	−1.7 (2)	C1—C13—C14—C4	2.4 (2)
C6—C5—C11—C10	178.60 (15)	C16—N1—C15—C9	120.14 (17)

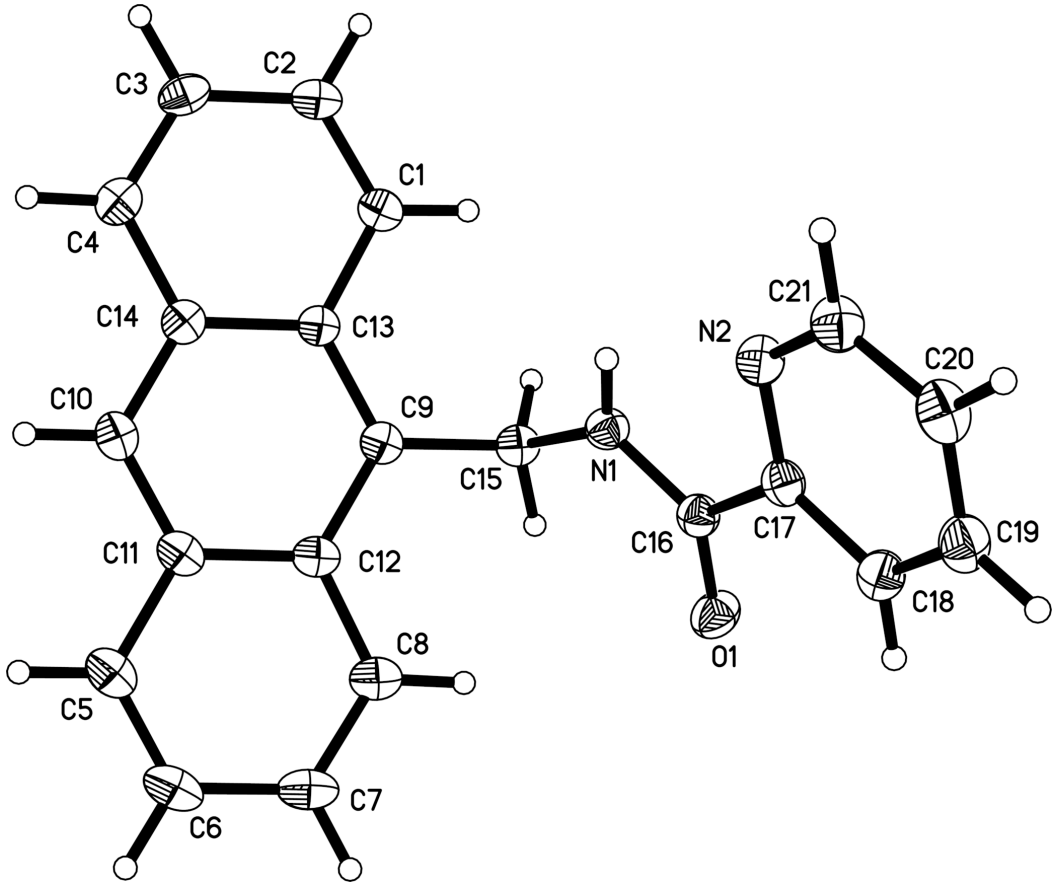
C6—C5—C11—C12	−0.7 (2)	C12—C9—C15—N1	−93.90 (16)
C13—C9—C12—C8	−177.99 (14)	C13—C9—C15—N1	86.90 (16)
C15—C9—C12—C8	2.8 (2)	C15—N1—C16—O1	3.3 (3)
C13—C9—C12—C11	2.3 (2)	C15—N1—C16—C17	−175.36 (14)
C15—C9—C12—C11	−176.84 (12)	C21—N2—C17—C18	−0.8 (2)
C7—C8—C12—C9	−178.27 (15)	C21—N2—C17—C16	177.84 (15)
C7—C8—C12—C11	1.4 (2)	O1—C16—C17—N2	176.68 (16)
C10—C11—C12—C9	−0.1 (2)	N1—C16—C17—N2	−4.6 (2)
C5—C11—C12—C9	179.22 (14)	O1—C16—C17—C18	−4.6 (3)
C10—C11—C12—C8	−179.78 (14)	N1—C16—C17—C18	174.09 (15)
C5—C11—C12—C8	−0.5 (2)	N2—C17—C18—C19	1.3 (3)
C12—C9—C13—C1	177.34 (13)	C16—C17—C18—C19	−177.33 (16)
C15—C9—C13—C1	−3.5 (2)	C17—C18—C19—C20	−0.8 (3)
C12—C9—C13—C14	−2.8 (2)	C18—C19—C20—C21	0.0 (3)
C15—C9—C13—C14	176.40 (12)	C17—N2—C21—C20	−0.1 (3)
C2—C1—C13—C9	177.87 (14)	C19—C20—C21—N2	0.5 (3)
C2—C1—C13—C14	−2.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···N2	0.865 (17)	2.193 (18)	2.655 (2)	113.1 (15)
C10—H10···O1^{i}	0.95	2.59	3.533 (3)	170

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

Fig. 1


C3
C2
C1
C4
C14
C13
C10
C9
C15
N1
C21
N2
C20
C16
C17
C19
C11
C12
C18
O1
C8
C5
C7
C6