IUCrData

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(*Z*)-2-(4-Nitrophenyl)-3-[4-(pyridin-4-ylmethoxy)-phenyl]acrylonitrile

Qingpeng Rao,[a] Zepeng Wang,[a] Mingdi Yang[b] and Zhichao Wu[a,c]*

[a]Department of Chemistry, Anhui University, Hefei 230601, People's Republic of China, [b]College of Chemistry and Chemical Engineering, Anhui University, and Anhui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, Hefei, 230601, People's Republic of China, and [c]Key Laboratory of Functional Inorganic Materials Chemistry, Hefei 230601, People's Republic of China. *Correspondence e-mail: wu_zhichao63@sina.com

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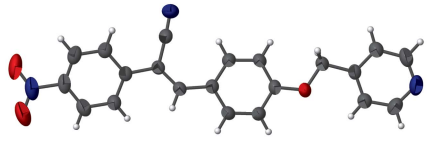
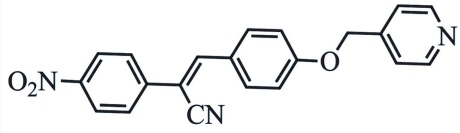
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{21}H_{15}N_3O_3$, features an essentially planar molecule (r.m.s. deviation for all non-H atoms = 0.090 Å). An intramolecular C—H···N hydrogen bond occurs. In the crystal, the molecules are connected by C—H···N and C—H···O hydrogen bonds into layers parallel to (102).

3D view



Chemical scheme



Structure description

We are interested in the title compound as it is a potential aggregation-induced emission (AIE) material (Liu & Fujiki, 2016). The molecule (Fig. 1) is almost planar (r.m.s. deviation for all non-H atoms = 0.090 Å). An intramolecular C—H···N hydrogen bond occurs (Table 1).

In the crystal, the molecules are connected by C—H···O and C—H···N hydrogen bonds into layers parallel to (102) (Table 1, Fig. 2).

Synthesis and crystallization

Firstly, 1.24 g (4.90 mmol) of 4-(bromomethyl)pyridine hydrobromide and 0.50 g (4.10 mmol) of 4-hydroxybenzaldehyde were added to a flask equipped with 50 ml acetonitrile. And then anhydrous potassium carbonate (3.24 g, 23.44 mmol) and 18-crown-6 (1 g) were added and refluxed at 353 K overnight. Subsequently, the mixture was filtered and the solvent was removed under reduced pressure. Finally, the white product was obtained by column chromatography with petroleum petroleum ether/ethyl acetate (2:1, *v*/*v*). Then, the white product (0.20 g, 0.94 mmol) of the previous step and 0.15 g (0.95 mmol) of 2-(4-nitrophenyl)acetonitrile were dissolved in 20 ml ethanol into a flask equipped with a magnetic stirrer for 5 h. Subsequently, the yellow solid was filtered.

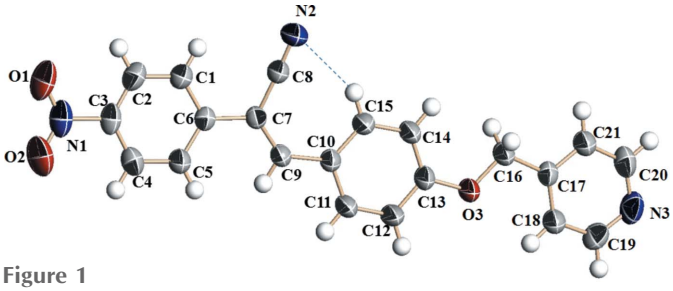


Figure 1
The structure of title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is indicated by a dashed line.

Yellow crystals suitable for X-ray analysis were obtained by recrystallization from ethanol solution.

Refinement

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

Funding information

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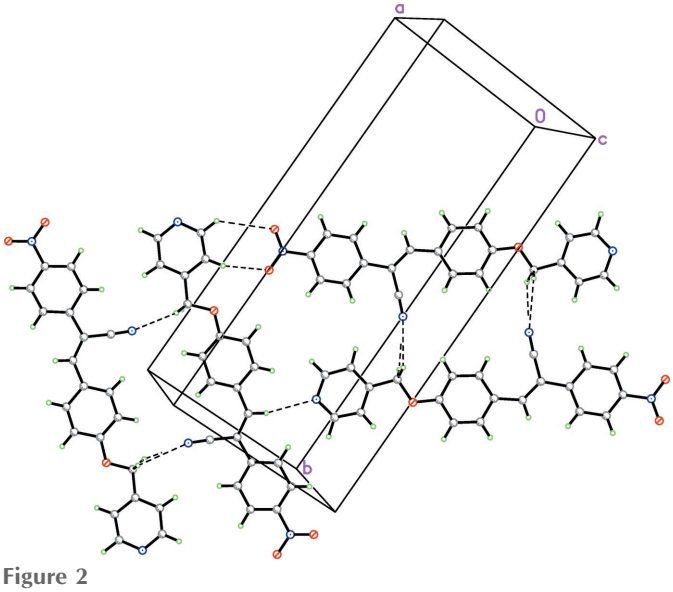

Figure 2
C—H···N and C—H···O hydrogen bonds connect the molecules into layers parallel to (102).

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···N2	0.93	2.58	3.417 (2)	149
C1—H1···N3^{i}	0.93	2.97	3.468 (2)	115
C16—H16A···N2^{ii}	0.97	2.83	3.261 (2)	107
C4—H4···O2^{iii}	0.93	2.63	3.502 (3)	156
C18—H18···O1^{iv}	0.93	2.47	3.362 (2)	162

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x, -y+1, -z+2$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{15}N_3O_3$
M_r	357.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	10.1759 (15), 23.521 (4), 7.4038 (11)
β (°)	95.674 (2)
V (Å^3)	1763.4 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.21 × 0.20 × 0.19
Data collection	
Diffractometer	Bruker SMART CCD area detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12823, 3270, 2621
R_{int}	0.021
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.113, 1.01
No. of reflections	3270
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.18

Computer programs: *SMART* (Bruker, 2004), *SAINT* (Bruker, 2004), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2008), *SHELXTL* (Sheldrick, 2008).

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Liu, B. & Fujiki, M. (2016). *_Aggregation-Induced Emission: Materials and Applications*, Vol. 1, edited by M. Fujiki, B. Liu and B. Z. Tang, ch. 1. ACS Symposium Series. Washington, DC: American Chemical Society.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

full crystallographic data

IUCrData (2018). **3**, x181328 [https://doi.org/10.1107/S2414314618013287]

(*Z*)-2-(4-Nitrophenyl)-3-[4-(pyridin-4-ylmethoxy)phenyl]acrylonitrile

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Crystal data

$C_{21}H_{15}N_3O_3$
M_r = 357.36
Monoclinic, $P2_1/c$
a = 10.1759 (15) Å
b = 23.521 (4) Å
c = 7.4038 (11) Å
β = 95.674 (2)°
V = 1763.4 (5) Å^3
Z = 4
$F(000)$ = 744
D_x = 1.346 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4694 reflections
θ = 2.2–27.0°
μ = 0.09 mm^{-1}
T = 296 K
Block, yellow
0.21 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
12823 measured reflections
3270 independent reflections
2621 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.5°, θ_{min} = 1.7°
h = −12→12
k = −28→28
l = −8→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 1.01
3270 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.3275P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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. All H atoms were placed in geometrically calculated positions and refined using a riding model with C–H distances of 0.93 Å for all H atoms bound to C(sp^2) atoms and 0.97 Å for H atoms bound to secondary C(sp^3) atoms. Isotropic displacement parameters for H atoms were calculated as $U_{iso}(H) = 1.2U_{eq}(C)$.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.90163 (15)	0.59837 (8)	0.5910 (2)	0.0760 (5)
N2	0.26154 (15)	0.56478 (6)	0.8779 (2)	0.0798 (5)
N3	−0.40049 (15)	0.17881 (7)	1.0732 (2)	0.0745 (4)
O1	0.90200 (15)	0.65022 (7)	0.5838 (2)	0.1062 (5)
O2	0.99589 (15)	0.56935 (8)	0.5654 (3)	0.1137 (6)
O3	−0.00447 (10)	0.29351 (4)	0.96989 (17)	0.0635 (3)
C1	0.55913 (15)	0.57655 (6)	0.7070 (2)	0.0533 (4)
H1	0.4858	0.5987	0.7251	0.064*
C2	0.67248 (17)	0.60273 (7)	0.6613 (2)	0.0613 (4)
H2	0.6758	0.6420	0.6486	0.074*
C3	0.77981 (15)	0.57002 (7)	0.6351 (2)	0.0567 (4)
C4	0.77684 (15)	0.51182 (7)	0.6501 (2)	0.0604 (4)
H4	0.8504	0.4902	0.6296	0.072*
C5	0.66288 (14)	0.48595 (6)	0.6962 (2)	0.0539 (4)
H5	0.6602	0.4466	0.7070	0.065*
C6	0.55184 (13)	0.51786 (6)	0.72667 (18)	0.0428 (3)
C7	0.42900 (13)	0.49128 (6)	0.78063 (18)	0.0417 (3)
C8	0.33306 (14)	0.53124 (6)	0.8334 (2)	0.0521 (4)
C9	0.40641 (13)	0.43488 (6)	0.78435 (18)	0.0440 (3)
H9	0.4751	0.4128	0.7487	0.053*
C10	0.29350 (13)	0.40227 (6)	0.83428 (18)	0.0440 (3)
C11	0.30583 (15)	0.34322 (6)	0.8376 (2)	0.0597 (4)
H11	0.3842	0.3270	0.8077	0.072*
C12	0.20650 (16)	0.30814 (6)	0.8833 (3)	0.0661 (5)
H12	0.2181	0.2689	0.8843	0.079*
C13	0.08860 (14)	0.33152 (6)	0.9280 (2)	0.0500 (4)
C14	0.07328 (14)	0.38986 (6)	0.9266 (2)	0.0530 (4)
H14	−0.0051	0.4059	0.9573	0.064*
C15	0.17420 (14)	0.42453 (6)	0.8797 (2)	0.0525 (4)
H15	0.1622	0.4637	0.8785	0.063*
C16	−0.12520 (14)	0.31518 (6)	1.0222 (2)	0.0525 (4)
H16A	−0.1632	0.3419	0.9317	0.063*
H16B	−0.1095	0.3350	1.1372	0.063*
C17	−0.21847 (13)	0.26665 (6)	1.03973 (19)	0.0446 (3)
C18	−0.18182 (15)	0.21070 (6)	1.0301 (2)	0.0548 (4)
H18	−0.0952	0.2010	1.0136	0.066*
C19	−0.27535 (18)	0.16909 (7)	1.0453 (3)	0.0700 (5)

H19	−0.2491	0.1314	1.0354	0.084*
C20	−0.43400 (16)	0.23323 (8)	1.0816 (2)	0.0667 (5)
H20	−0.5211	0.2417	1.0994	0.080*
C21	−0.34893 (15)	0.27792 (7)	1.0658 (2)	0.0560 (4)
H21	−0.3785	0.3152	1.0724	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0579 (10)	0.0991 (13)	0.0716 (10)	−0.0312 (9)	0.0090 (7)	0.0036 (9)
N2	0.0692 (9)	0.0503 (8)	0.1253 (14)	0.0098 (7)	0.0371 (9)	0.0006 (8)
N3	0.0680 (9)	0.0672 (10)	0.0908 (11)	−0.0271 (7)	0.0199 (8)	−0.0032 (8)
O1	0.0915 (11)	0.0937 (11)	0.1359 (14)	−0.0495 (9)	0.0244 (9)	0.0119 (10)
O2	0.0546 (8)	0.1344 (14)	0.1563 (16)	−0.0212 (9)	0.0321 (9)	0.0062 (11)
O3	0.0458 (6)	0.0438 (6)	0.1057 (9)	−0.0047 (4)	0.0305 (6)	−0.0001 (5)
C1	0.0515 (8)	0.0476 (8)	0.0617 (10)	−0.0046 (6)	0.0106 (7)	0.0026 (7)
C2	0.0654 (10)	0.0525 (9)	0.0668 (10)	−0.0167 (8)	0.0099 (8)	0.0045 (7)
C3	0.0476 (8)	0.0713 (11)	0.0513 (9)	−0.0220 (7)	0.0049 (7)	0.0020 (7)
C4	0.0432 (8)	0.0721 (11)	0.0672 (10)	−0.0046 (7)	0.0123 (7)	−0.0011 (8)
C5	0.0475 (8)	0.0493 (8)	0.0667 (10)	−0.0040 (6)	0.0144 (7)	0.0000 (7)
C6	0.0425 (7)	0.0458 (8)	0.0404 (7)	−0.0051 (6)	0.0050 (6)	−0.0008 (6)
C7	0.0398 (7)	0.0436 (7)	0.0422 (7)	−0.0010 (5)	0.0074 (6)	−0.0003 (6)
C8	0.0483 (8)	0.0433 (8)	0.0666 (10)	−0.0030 (6)	0.0148 (7)	0.0022 (7)
C9	0.0400 (7)	0.0446 (7)	0.0488 (8)	−0.0003 (5)	0.0107 (6)	−0.0017 (6)
C10	0.0421 (7)	0.0422 (7)	0.0489 (8)	−0.0028 (6)	0.0099 (6)	−0.0018 (6)
C11	0.0456 (8)	0.0458 (8)	0.0916 (12)	0.0018 (6)	0.0262 (8)	−0.0022 (8)
C12	0.0531 (9)	0.0386 (8)	0.1111 (15)	0.0001 (7)	0.0309 (9)	−0.0004 (8)
C13	0.0418 (7)	0.0450 (8)	0.0650 (9)	−0.0070 (6)	0.0148 (7)	−0.0010 (7)
C14	0.0400 (7)	0.0461 (8)	0.0754 (10)	−0.0004 (6)	0.0186 (7)	−0.0046 (7)
C15	0.0475 (8)	0.0391 (7)	0.0730 (10)	−0.0023 (6)	0.0167 (7)	−0.0030 (7)
C16	0.0434 (8)	0.0466 (8)	0.0698 (10)	−0.0037 (6)	0.0174 (7)	−0.0061 (7)
C17	0.0428 (7)	0.0472 (8)	0.0449 (8)	−0.0078 (6)	0.0094 (6)	−0.0032 (6)
C18	0.0506 (8)	0.0499 (9)	0.0660 (10)	−0.0030 (7)	0.0161 (7)	−0.0026 (7)
C19	0.0784 (12)	0.0450 (9)	0.0894 (13)	−0.0119 (8)	0.0220 (10)	−0.0038 (8)
C20	0.0449 (9)	0.0792 (12)	0.0780 (12)	−0.0130 (8)	0.0167 (8)	0.0004 (9)
C21	0.0486 (8)	0.0541 (9)	0.0671 (10)	−0.0020 (7)	0.0144 (7)	−0.0011 (7)

Geometric parameters (Å, º)

O3—C13	1.3603 (17)	C17—C18	1.372 (2)
O3—C16	1.4188 (17)	C17—C21	1.386 (2)
C7—C9	1.3472 (19)	C17—C16	1.4983 (19)
C7—C8	1.4370 (19)	C11—C12	1.373 (2)
C7—C6	1.4873 (18)	C11—H11	0.9300
C6—C1	1.391 (2)	C18—C19	1.378 (2)
C6—C5	1.393 (2)	C18—H18	0.9300
C10—C15	1.3935 (19)	C16—H16A	0.9700
C10—C11	1.395 (2)	C16—H16B	0.9700

C10—C9	1.4590 (18)	C2—C1	1.379 (2)
C9—H9	0.9300	C2—H2	0.9300
C14—C13	1.381 (2)	C12—H12	0.9300
C14—C15	1.3822 (19)	C4—H4	0.9300
C14—H14	0.9300	C1—H1	0.9300
C5—C4	1.382 (2)	N1—O2	1.208 (2)
C5—H5	0.9300	N1—O1	1.221 (2)
C8—N2	1.1436 (19)	N3—C20	1.328 (2)
C3—C2	1.366 (2)	N3—C19	1.330 (2)
C3—C4	1.374 (2)	C21—C20	1.374 (2)
C3—N1	1.4723 (19)	C21—H21	0.9300
C15—H15	0.9300	C20—H20	0.9300
C13—C12	1.389 (2)	C19—H19	0.9300

C13—O3—C16	117.86 (11)	C17—C18—C19	118.93 (15)
C9—C7—C8	121.11 (12)	C17—C18—H18	120.5
C9—C7—C6	124.69 (12)	C19—C18—H18	120.5
C8—C7—C6	114.19 (11)	O3—C16—C17	108.85 (11)
C1—C6—C5	117.73 (13)	O3—C16—H16A	109.9
C1—C6—C7	120.02 (13)	C17—C16—H16A	109.9
C5—C6—C7	122.25 (12)	O3—C16—H16B	109.9
C15—C10—C11	116.68 (12)	C17—C16—H16B	109.9
C15—C10—C9	126.19 (13)	H16A—C16—H16B	108.3
C11—C10—C9	117.14 (12)	C3—C2—C1	118.92 (15)
C7—C9—C10	131.53 (12)	C3—C2—H2	120.5
C7—C9—H9	114.2	C1—C2—H2	120.5
C10—C9—H9	114.2	C11—C12—C13	119.67 (14)
C13—C14—C15	120.13 (13)	C11—C12—H12	120.2
C13—C14—H14	119.9	C13—C12—H12	120.2
C15—C14—H14	119.9	C3—C4—C5	118.97 (15)
C4—C5—C6	121.10 (14)	C3—C4—H4	120.5
C4—C5—H5	119.5	C5—C4—H4	120.5
C6—C5—H5	119.5	C2—C1—C6	121.56 (15)
N2—C8—C7	176.74 (17)	C2—C1—H1	119.2
C2—C3—C4	121.71 (14)	C6—C1—H1	119.2
C2—C3—N1	118.63 (16)	O2—N1—O1	123.50 (16)
C4—C3—N1	119.66 (16)	O2—N1—C3	118.56 (18)
C14—C15—C10	121.71 (13)	O1—N1—C3	117.94 (17)
C14—C15—H15	119.1	C20—N3—C19	115.30 (14)
C10—C15—H15	119.1	C20—C21—C17	119.06 (15)
O3—C13—C14	125.04 (13)	C20—C21—H21	120.5
O3—C13—C12	115.55 (13)	C17—C21—H21	120.5
C14—C13—C12	119.41 (13)	N3—C20—C21	124.52 (16)
C18—C17—C21	117.38 (13)	N3—C20—H20	117.7
C18—C17—C16	123.27 (13)	C21—C20—H20	117.7
C21—C17—C16	119.34 (13)	N3—C19—C18	124.79 (16)
C12—C11—C10	122.39 (13)	N3—C19—H19	117.6
C12—C11—H11	118.8	C18—C19—H19	117.6

C10—C11—H11	118.8		
C9—C7—C6—C1	172.46 (14)	C18—C17—C16—O3	8.2 (2)
C8—C7—C6—C1	−8.53 (19)	C21—C17—C16—O3	−171.38 (13)
C9—C7—C6—C5	−8.3 (2)	C4—C3—C2—C1	1.1 (2)
C8—C7—C6—C5	170.74 (14)	N1—C3—C2—C1	−178.40 (14)
C8—C7—C9—C10	0.6 (2)	C10—C11—C12—C13	0.1 (3)
C6—C7—C9—C10	179.53 (13)	O3—C13—C12—C11	179.45 (16)
C15—C10—C9—C7	5.0 (3)	C14—C13—C12—C11	−0.3 (3)
C11—C10—C9—C7	−174.82 (16)	C2—C3—C4—C5	−1.2 (3)
C1—C6—C5—C4	0.7 (2)	N1—C3—C4—C5	178.31 (14)
C7—C6—C5—C4	−178.54 (14)	C6—C5—C4—C3	0.2 (2)
C9—C7—C8—N2	152 (3)	C3—C2—C1—C6	−0.1 (2)
C6—C7—C8—N2	−27 (3)	C5—C6—C1—C2	−0.8 (2)
C13—C14—C15—C10	−0.5 (2)	C7—C6—C1—C2	178.46 (13)
C11—C10—C15—C14	0.3 (2)	C2—C3—N1—O2	−178.99 (17)
C9—C10—C15—C14	−179.48 (14)	C4—C3—N1—O2	1.5 (2)
C16—O3—C13—C14	−2.2 (2)	C2—C3—N1—O1	1.5 (2)
C16—O3—C13—C12	178.05 (15)	C4—C3—N1—O1	−177.97 (17)
C15—C14—C13—O3	−179.23 (15)	C18—C17—C21—C20	0.4 (2)
C15—C14—C13—C12	0.5 (3)	C16—C17—C21—C20	179.94 (15)
C15—C10—C11—C12	−0.1 (3)	C19—N3—C20—C21	−0.8 (3)
C9—C10—C11—C12	179.69 (16)	C17—C21—C20—N3	−0.2 (3)
C21—C17—C18—C19	0.4 (2)	C20—N3—C19—C18	1.7 (3)
C16—C17—C18—C19	−179.10 (15)	C17—C18—C19—N3	−1.6 (3)
C13—O3—C16—C17	173.17 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···N2	0.93	2.58	3.417 (2)	149
C1—H1···N3^{i}	0.93	2.97	3.468 (2)	115
C16—H16*A*···N2^{ii}	0.97	2.83	3.261 (2)	107
C4—H4···O2^{iii}	0.93	2.63	3.502 (3)	156
C18—H18···O1^{iv}	0.93	2.47	3.362 (2)	162

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+3/2; (ii) −*x*, −*y*+1, −*z*+2; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) −*x*+1, *y*−1/2, −*z*+3/2.