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6-Nicotinamido-2-naphthoic acid

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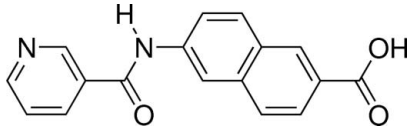
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.092; data-to-parameter ratio = 8.2.

In the title molecule, $C_{17}H_{12}N_2O_3$, the naphthalene ring system and the pyridin-3-yl rings are nearly coplanar with a dihedral angle between them of 2.28 (8)°. In the crystal, the hydroxy and amide N atoms participate in hydrogen bonds, which connect the molecules into a two-dimensional network parallel to (101).

Related literature

For coordination polymers based on linking ligands with O- and N-donors see: Robin & Fromm, 2006. For *d–f* coordination polymers based on linking ligands with pyridyl–carboxylate terminals see: Hu *et al.* (2012); Chen *et al.* (2010); Tang *et al.* (2010); Yue *et al.* (2011); Zhu *et al.* (2010). For related potential linking ligands see: Han & Lee, 2012; Zheng & Lee, 2012.



Experimental

Crystal data

$C_{17}H_{12}N_2O_3$
M_r = 292.29
Monoclinic, *Cc*
a = 25.901 (3) Å
b = 6.2097 (7) Å
c = 8.6080 (9) Å
β = 103.258 (9)°
V = 1347.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.40 × 0.20 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.992
11725 measured reflections
1693 independent reflections
2845 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.05
1693 reflections
207 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*···O1^{i}	0.92 (3)	2.01 (3)	2.926 (2)	170 (2)
O2—H2*O*···N1^{ii}	0.84 (3)	1.88 (4)	2.708 (2)	170 (3)

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

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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2071).

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supporting information

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6-Nicotinamido-2-naphthoic acid

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S1. Comment

Bis(pyridyl)- and dicarboxylate-type linking ligands have been typically employed for the preparation of coordination polymers (Robin & Fromm, 2006). The vast majority of known coordination polymers contain either a *d*- or an *f*-block metal. However, several research groups recently prepared polymers containing both *d*- and *f*-block metals within their frameworks by utilizing linking ligands possessing pyridyl–carboxylate terminal groups (Hu *et al.*, 2012; Chen *et al.*, 2010; Tang *et al.*, 2010; Yue *et al.*, 2011; Zhu *et al.*, 2010). Consistent with the hard–soft acid–base concept, the harder oxygen atoms are bonded to the *f*-block metals and the softer nitrogen atoms are bonded to the *d*-block metals in these polymers. Our research group recently reported the structures of two potential linking ligands with pyridyl–carboxylate terminal groups (Han & Lee, 2012; Zheng & Lee, 2012) and here we report the structure of third.

The molecular structure of the title molecule with the atom-labeling scheme is given in Figure 1. The naphthalene and 3-pyridyl rings are nearly coplanar with a dihedral angle between them of 2.28 (8)°. The N2–C6 bond length (1.343 (2) Å) indicates a C–N single bond. The intermolecular O–H···N and N–H···O (carbonyl) hydrogen bonds (Table 1) connect the molecules along the *a*- and *c*-axes, respectively, leading to a 2-D network in the [101] direction (Figure 2).

S2. Experimental

A stirred mixture of 6-amino-2-naphthoic acid (0.94 g, 5 mmol) and *N*,*N*-dimethyl-4-aminopyridine (0.02 g, 0.17 mmol) in dimethylacetamide (15 mL) was heated at 80 °C for 30 min under argon. The solution was cooled to 10 °C, and nicotinoyl chloride hydrochloride (0.89 g, 5 mmol) was added. The temperature was then raised slowly to 50 °C and was maintained there for 8 h. On addition of dichloromethane to the resulting mixture, a precipitate was formed, which was filtered off and dried under vacuum at 100°C. The product was recrystallized from methanol to give crystals of the title compound (1.22 g, 4.2 mmol, 83.9% yield). mp: 593–595 K (decomp). ^{1}H NMR (500 MHz, DMSO-d$_6$, d) 11.06 (s, 1H, carboxylic acid OH), 9.35 (s, 1H, amide NH), 8.93 (d, 1H, pyridine proton), 8.71 (d, 1H, pyridine proton), 8.56 (s, 2H, naphthalene proton), 8.14 (d, 1H, pyridine proton), 7.96–7.94 (m, 4H, naphthalene proton), 7.88 (t, 1H, pyridine proton). ^{13}C{^{1}H} NMR (125 MHz, DMSO-d$_6$, d) 167.3, 163.1, 148.7, 145.7, 139.5, 138.4, 135.4, 131.6, 130.2, 129.9, 129.1, 127.8, 127.0, 125.75, 125.0, 121.3, 116.2. IR (KBr, cm^{-1}): 3623 (w), 3328 (w), 2925 (*s*), 2640 (*s*), 2372 (*s*), 2075 (*s*), 1800 (*m*), 1621 (*m*), 1551 (*m*), 1291 (*m*), 1195 (*m*), 1018 (*m*), 773 (*m*), 724 (*m*), 678 (*m*), 633 (*m*), 494 (*s*).

S3. Refinement

All non-hydrogen atoms were refined anisotropically. C-bound H atoms were positioned geometrically [C–H = 0.93–0.97 A] and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). The hydrogen atoms attached to N and O were located in a difference Fourier map and refined isotropically.

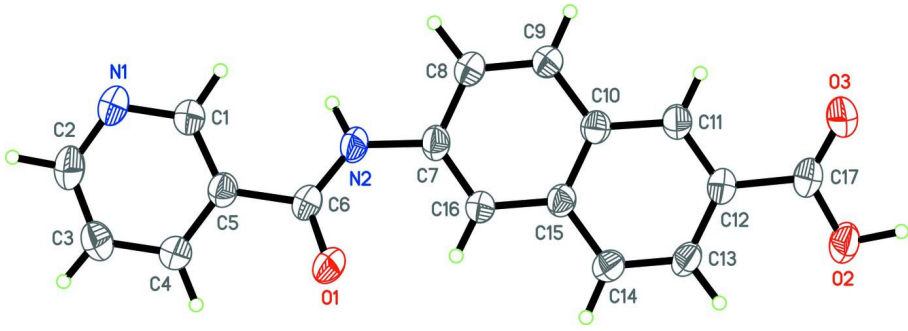

Figure 1

The molecular structure of the title compound showing the atomic numbering and 50% probability displacement ellipsoids.

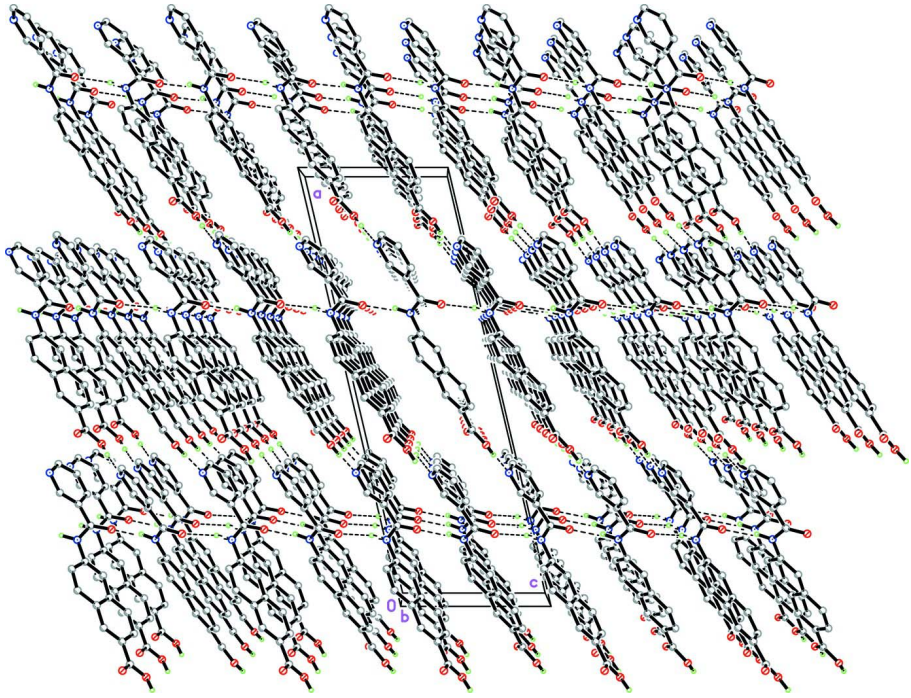

Figure 2

A portion of the crystal packing showing a 2-D H-bonded (dashed lines) network.

6-Nicotinamido-2-naphthoic acid

Crystal data

$C_{17}H_{12}N_2O_3$
$M_r = 292.29$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 25.901\ (3)$ Å
$b = 6.2097\ (7)$ Å
$c = 8.6080\ (9)$ Å
$\beta = 103.258\ (9)°$
$V = 1347.6\ (3)$ Å^3
$Z = 4$

$F(000) = 608$
$D_x = 1.441$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6523 reflections
$\theta = 3.2–28.5°$
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Plate, yellow
0.40 × 0.20 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.992
11725 measured reflections
1693 independent reflections
2845 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.5°, θ_{min} = 1.6°
h = −34→34
k = −8→8
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.05
1693 reflections
207 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.0998P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Absolute structure: The absolute structure could not be determined with certainty

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 $F^2 > \sigma(F^2)$ 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}
O1	0.31793 (6)	−0.2140 (2)	0.26571 (17)	0.0391 (3)
O2	0.62483 (6)	0.3924 (3)	0.1855 (2)	0.0454 (4)
H2O	0.6456 (12)	0.485 (6)	0.163 (4)	0.059 (8)*
O3	0.59863 (7)	0.6936 (3)	0.2841 (3)	0.0583 (5)
N1	0.19038 (7)	−0.1634 (3)	0.5762 (2)	0.0406 (4)
N2	0.33612 (6)	0.0227 (3)	0.47225 (19)	0.0354 (4)
H2N	0.3278 (9)	0.070 (4)	0.565 (3)	0.037 (6)*
C1	0.23346 (8)	−0.0931 (3)	0.5307 (2)	0.0359 (4)
H1	0.2453	0.0463	0.5580	0.043*
C2	0.17334 (8)	−0.3618 (4)	0.5349 (3)	0.0432 (5)
H2	0.1435	−0.4116	0.5666	0.052*
C3	0.19787 (9)	−0.4971 (4)	0.4473 (3)	0.0430 (5)
H3	0.1846	−0.6346	0.4200	0.052*
C4	0.24257 (8)	−0.4253 (4)	0.4005 (2)	0.0386 (4)
H4	0.2598	−0.5133	0.3409	0.046*

C5	0.26131 (7)	−0.2192 (3)	0.4442 (2)	0.0301 (4)
C6	0.30789 (7)	−0.1368 (3)	0.3864 (2)	0.0301 (4)
C7	0.38118 (7)	0.1288 (3)	0.4401 (2)	0.0307 (4)
C8	0.39174 (8)	0.3389 (3)	0.5049 (2)	0.0340 (4)
H8	0.3691	0.4013	0.5616	0.041*
C9	0.43521 (7)	0.4492 (3)	0.4839 (2)	0.0320 (4)
H9	0.4420	0.5865	0.5270	0.038*
C10	0.47019 (7)	0.3577 (3)	0.3975 (2)	0.0283 (4)
C11	0.51502 (7)	0.4691 (3)	0.3710 (2)	0.0308 (4)
H11	0.5221	0.6080	0.4106	0.037*
C12	0.54815 (7)	0.3749 (3)	0.2878 (2)	0.0311 (4)
C13	0.53849 (8)	0.1624 (3)	0.2294 (2)	0.0350 (4)
H13	0.5618	0.0978	0.1757	0.042*
C14	0.49520 (7)	0.0515 (3)	0.2513 (2)	0.0338 (4)
H14	0.4890	−0.0876	0.2113	0.041*
C15	0.45962 (7)	0.1469 (3)	0.3345 (2)	0.0285 (4)
C16	0.41444 (7)	0.0333 (3)	0.3574 (2)	0.0317 (4)
H16	0.4074	−0.1050	0.3166	0.038*
C17	0.59290 (7)	0.5052 (4)	0.2540 (2)	0.0356 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0371 (7)	0.0478 (8)	0.0382 (6)	−0.0070 (6)	0.0207 (5)	−0.0074 (6)
O2	0.0352 (8)	0.0457 (9)	0.0632 (9)	−0.0036 (7)	0.0274 (7)	0.0042 (7)
O3	0.0498 (10)	0.0452 (10)	0.0917 (13)	−0.0172 (8)	0.0405 (9)	−0.0099 (8)
N1	0.0283 (8)	0.0505 (10)	0.0483 (9)	−0.0018 (7)	0.0197 (7)	−0.0032 (8)
N2	0.0312 (8)	0.0458 (10)	0.0353 (8)	−0.0097 (7)	0.0200 (6)	−0.0055 (7)
C1	0.0283 (9)	0.0382 (10)	0.0452 (10)	−0.0026 (8)	0.0166 (8)	−0.0032 (8)
C2	0.0282 (9)	0.0566 (14)	0.0485 (11)	−0.0062 (9)	0.0166 (8)	0.0062 (10)
C3	0.0375 (11)	0.0382 (11)	0.0551 (12)	−0.0114 (8)	0.0142 (9)	−0.0017 (9)
C4	0.0340 (10)	0.0398 (11)	0.0450 (10)	−0.0033 (7)	0.0156 (8)	−0.0053 (8)
C5	0.0232 (8)	0.0363 (10)	0.0334 (8)	−0.0031 (7)	0.0120 (6)	0.0016 (7)
C6	0.0252 (8)	0.0366 (9)	0.0318 (8)	−0.0011 (7)	0.0132 (6)	0.0023 (7)
C7	0.0255 (9)	0.0385 (11)	0.0308 (8)	−0.0060 (7)	0.0123 (6)	0.0013 (7)
C8	0.0332 (9)	0.0383 (10)	0.0348 (9)	−0.0001 (8)	0.0169 (7)	−0.0021 (7)
C9	0.0334 (10)	0.0317 (9)	0.0343 (8)	−0.0025 (7)	0.0149 (7)	−0.0030 (7)
C10	0.0267 (8)	0.0318 (9)	0.0285 (7)	−0.0003 (7)	0.0109 (6)	0.0021 (6)
C11	0.0281 (9)	0.0324 (9)	0.0337 (8)	−0.0057 (7)	0.0109 (7)	0.0004 (7)
C12	0.0244 (8)	0.0351 (10)	0.0357 (9)	−0.0022 (7)	0.0110 (7)	0.0052 (7)
C13	0.0295 (9)	0.0368 (10)	0.0429 (10)	0.0014 (7)	0.0171 (8)	0.0008 (8)
C14	0.0318 (10)	0.0324 (9)	0.0414 (10)	0.0003 (7)	0.0171 (8)	−0.0022 (7)
C15	0.0266 (9)	0.0331 (9)	0.0289 (7)	−0.0031 (7)	0.0124 (6)	0.0009 (6)
C16	0.0296 (9)	0.0336 (9)	0.0346 (9)	−0.0057 (7)	0.0130 (7)	−0.0013 (7)
C17	0.0256 (9)	0.0445 (12)	0.0392 (9)	−0.0064 (8)	0.0126 (7)	0.0031 (8)

Geometric parameters (Å, º)

O1—C6	1.225 (2)	C7—C16	1.372 (3)
O2—C17	1.321 (2)	C7—C8	1.421 (3)
O2—H2O	0.84 (3)	C8—C9	1.365 (3)
O3—C17	1.200 (3)	C8—H8	0.9300
N1—C2	1.330 (3)	C9—C10	1.416 (2)
N1—C1	1.338 (2)	C9—H9	0.9300
N2—C6	1.347 (3)	C10—C11	1.414 (2)
N2—C7	1.422 (2)	C10—C15	1.420 (2)
N2—H2N	0.92 (3)	C11—C12	1.369 (3)
C1—C5	1.391 (2)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.413 (3)
C2—C3	1.378 (3)	C12—C17	1.496 (2)
C2—H2	0.9300	C13—C14	1.365 (3)
C3—C4	1.384 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.420 (2)
C4—C5	1.389 (3)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.418 (2)
C5—C6	1.497 (2)	C16—H16	0.9300
C17—O2—H2O	104 (2)	C7—C8—H8	120.0
C2—N1—C1	118.18 (17)	C8—C9—C10	120.97 (17)
C6—N2—C7	126.92 (15)	C8—C9—H9	119.5
C6—N2—H2N	120.2 (15)	C10—C9—H9	119.5
C7—N2—H2N	112.9 (15)	C11—C10—C9	122.43 (17)
N1—C1—C5	122.86 (18)	C11—C10—C15	118.87 (15)
N1—C1—H1	118.6	C9—C10—C15	118.69 (15)
C5—C1—H1	118.6	C12—C11—C10	120.79 (18)
N1—C2—C3	123.04 (18)	C12—C11—H11	119.6
N1—C2—H2	118.5	C10—C11—H11	119.6
C3—C2—H2	118.5	C11—C12—C13	120.25 (17)
C2—C3—C4	119.0 (2)	C11—C12—C17	118.50 (18)
C2—C3—H3	120.5	C13—C12—C17	121.19 (17)
C4—C3—H3	120.5	C14—C13—C12	120.39 (17)
C3—C4—C5	118.79 (18)	C14—C13—H13	119.8
C3—C4—H4	120.6	C12—C13—H13	119.8
C5—C4—H4	120.6	C13—C14—C15	120.52 (17)
C4—C5—C1	118.16 (16)	C13—C14—H14	119.7
C4—C5—C6	118.87 (16)	C15—C14—H14	119.7
C1—C5—C6	122.81 (16)	C16—C15—C10	119.90 (15)
O1—C6—N2	123.99 (16)	C16—C15—C14	120.97 (17)
O1—C6—C5	119.50 (17)	C10—C15—C14	119.13 (15)
N2—C6—C5	116.51 (15)	C7—C16—C15	119.58 (18)
C16—C7—C8	120.89 (16)	C7—C16—H16	120.2
C16—C7—N2	122.82 (17)	C15—C16—H16	120.2
C8—C7—N2	116.24 (16)	O3—C17—O2	123.64 (17)
C9—C8—C7	119.96 (16)	O3—C17—C12	123.26 (18)

C9—C8—H8	120.0	O2—C17—C12	113.08 (18)
C2—N1—C1—C5	−0.8 (3)	C9—C10—C11—C12	179.58 (16)
C1—N1—C2—C3	−0.2 (3)	C15—C10—C11—C12	−0.8 (3)
N1—C2—C3—C4	0.5 (3)	C10—C11—C12—C13	−1.2 (3)
C2—C3—C4—C5	0.3 (3)	C10—C11—C12—C17	176.03 (16)
C3—C4—C5—C1	−1.2 (3)	C11—C12—C13—C14	2.0 (3)
C3—C4—C5—C6	−176.77 (19)	C17—C12—C13—C14	−175.16 (19)
N1—C1—C5—C4	1.6 (3)	C12—C13—C14—C15	−0.7 (3)
N1—C1—C5—C6	176.89 (18)	C11—C10—C15—C16	−179.01 (19)
C7—N2—C6—O1	0.2 (3)	C9—C10—C15—C16	0.6 (2)
C7—N2—C6—C5	−178.98 (17)	C11—C10—C15—C14	2.0 (2)
C4—C5—C6—O1	23.5 (3)	C9—C10—C15—C14	−178.39 (19)
C1—C5—C6—O1	−151.76 (19)	C13—C14—C15—C16	179.77 (17)
C4—C5—C6—N2	−157.19 (18)	C13—C14—C15—C10	−1.2 (3)
C1—C5—C6—N2	27.5 (3)	C8—C7—C16—C15	−0.8 (3)
C6—N2—C7—C16	−26.4 (3)	N2—C7—C16—C15	−177.94 (16)
C6—N2—C7—C8	156.33 (19)	C10—C15—C16—C7	0.2 (3)
C16—C7—C8—C9	0.6 (3)	C14—C15—C16—C7	179.18 (17)
N2—C7—C8—C9	177.93 (17)	C11—C12—C17—O3	−6.6 (3)
C7—C8—C9—C10	0.2 (3)	C13—C12—C17—O3	170.6 (2)
C8—C9—C10—C11	178.80 (17)	C11—C12—C17—O2	174.43 (16)
C8—C9—C10—C15	−0.8 (3)	C13—C12—C17—O2	−8.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O1^{i}	0.92 (3)	2.01 (3)	2.926 (2)	170 (2)
O2—H2*O*···N1^{ii}	0.84 (3)	1.88 (4)	2.708 (2)	170 (3)

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