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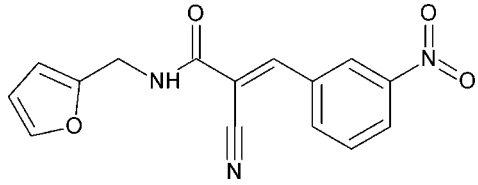

# Crystal structure of 2-cyano-*N*-(furan-2-ylmethyl)-3-(3-nitrophenyl)propanamide

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In the title compound, $C_{15}H_{11}N_3O_4$, the acetamide group is inclined to the furan ring by 66.5 (1)°. The dihedral angle between the furan ring and the benzene ring is 66.8 (1)°. In the crystal, molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(12)$ ring motif. The dimers are linked *via* two pairs of C—H···O hydrogen bonds to the same acceptor oxygen atom, enclosing $R_2^1(6)$ ring motifs, forming chains along the [101] direction.

**Keywords:** crystal structure; furan; acetamide; N—H···N hydrogen bonds; inversion dimers.

**CCDC reference**: 1410650

## 1. Related literature

For examples of biological properties of furan derivatives, see: Anupam *et al.* (2011). For the biological activities of some heterocyclic derivatives containing the acetamide moiety, see: Fallah-Tafti *et al.* (2011); Shams *et al.* (2011). For the crystal structure of the similar compound 2-cyano-*N*-furfuryl-3-(2-furyl)acrylamide, see: Pomés Hernández *et al.* (1996).

## 2. Experimental

### 2.1. Crystal data

$C_{15}H_{11}N_3O_4$
$M_r$ = 297.27
Triclinic, $P\overline{1}$
$a$ = 7.4358 (3) Å
$b$ = 9.4165 (5) Å
$c$ = 10.3934 (5) Å
$\alpha$ = 90.938 (2)°
$\beta$ = 96.910 (2)°
$\gamma$ = 105.872 (2)°
$V$ = 693.98 (6) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.20 mm

### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.942, $T_{max}$ = 0.983
12708 measured reflections
2442 independent reflections
2055 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.116
$S$ = 1.02
2442 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$A$···N2$^{i}$ | 0.86 | 2.27 | 3.056 (2) | 152 |
| C5—H5···O3$^{ii}$ | 0.93 | 2.49 | 3.337 (2) | 151 |
| C7—H7···O3$^{ii}$ | 0.93 | 2.49 | 3.362 (2) | 156 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014* and *PLATON*.

## Acknowledgements

We thank Dr Babu Varghese for the XRD data collection at the Sophisticated Analytical Instrument Facility (SAIF), Indian Institute of Technology, Madras.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5161).

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# supporting information

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## Crystal structure of 2-cyano-*N*-(furan-2-ylmethyl)-3-(3-nitrophenyl)-propanamide

**Shivanna Subhadramma, Budanur Papaiah Siddaraju, Naveen Chandra, Janardhanan Saravanan and Dasararaju Gayathri**

### S1. Comment

Furan is one of the most important five-membered heterocyclic ring systems and its derivatives are well known to possess various biological properties, such as antibacterial, antitumor, anti-inflammatory, antifungal, anticonvulsant, and analgesic (Anupam *et al.*, 2011). Acetamide derivatives possess a wide range of pharmacological properties (Fallah-Tafti *et al.*, 2011; Shams *et al.*, 2011). In view of the biological importance of furan and acetamide derivatives, we have synthesized the title compound and report herein on its crystal structure.

In the title compound, Fig. 1, the acetamide group is inclined to the furan ring by 66.5 (1)°. Torsion angles N3—C9—C8—C15 [-5.4 (2)°] and O3—C9—C8—C15 [174.6 (2)°] indicate that the acetonitrile and acetamide moieties are almost planar. The dihedral angle between the furan ring and the benzene ring is 66.8 (1)°. The bond lengths and bond angles are comparable with those reported for a similar structure, *viz.* 2-cyano-*N*-furfuryl-3-(2-furyl)acrylamide (Pomés Hernández *et al.*, 1996).

In the crystal (Table 1 and Fig. 2), molecules are linked by pairs of N-H···N hydrogen bonds forming inversion dimers with an $R_2^2(12)$ ring motif. The dimers are linked *via* two pairs of bifurcated C-H···O hydrogen bonds, enclosing $R_2^1(6)$ ring motifs, forming chains along direction [101].

### S2. Experimental

An equimolar mixture of furfuryl amine and ethyl cyano acetate was mixed in a conical flask and the mixture was heated under microwave irradiation at 700 W for 3 min with an interval of 20 s each time. The mixture was then poured into a beaker and cooled giving a solid that was washed with ethanol. The furfuryl cyano acetamide product so obtained was treated with an equi-molar ratio of 3-nitro benzaldehyde in the presence of glacial acetic acid and refluxed for 3 h. On cooling, colourless crystals of the title compound were obtained.

### S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NH and C-bound H atoms were included in calculated positions and refined using a riding model: N—H = 0.86 Å, C—H = 0.93 - 0.97 Å with $U_{iso}(H) = 1.2U_{eq}(N,C)$.

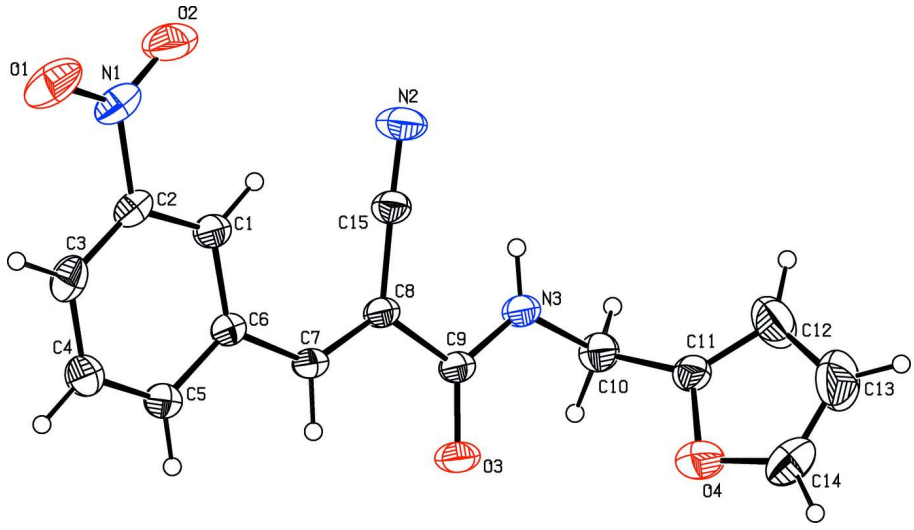


**Figure 1**

The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

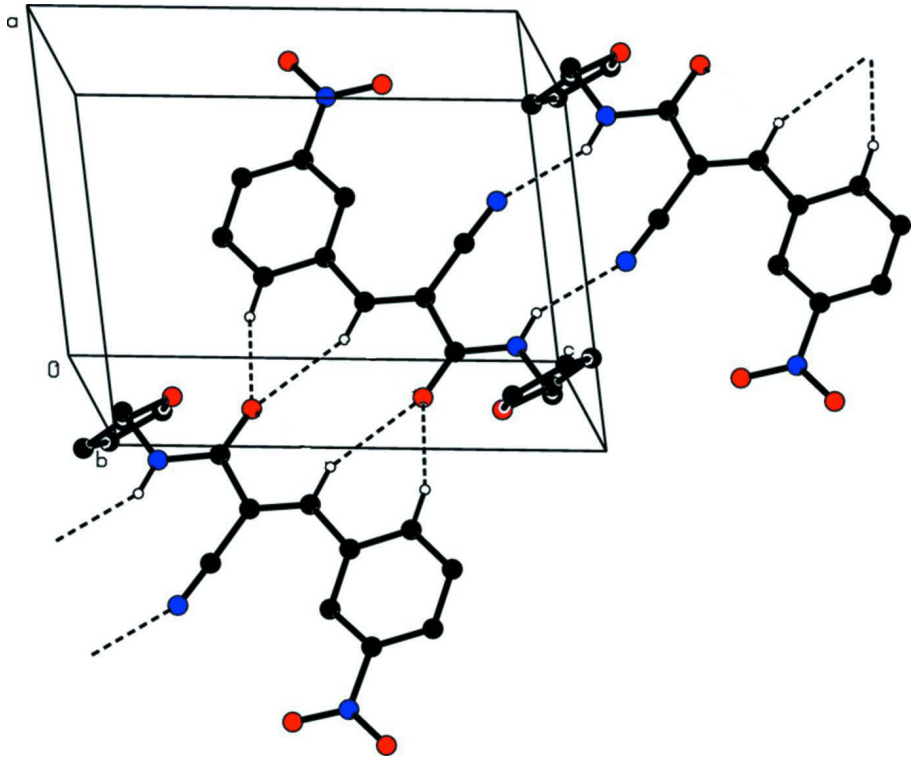


**Figure 2**

A view along the *b* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1 for details). For clarity, H atoms not involved in hydrogen bonding have been omitted.

**2-Cyano-*N*-(furan-2-ylmethyl)-3-(3-nitrophenyl)propanamide**

*Crystal data*

$C_{15}H_{11}N_3O_4$
$M_r = 297.27$
Triclinic, $P\overline{1}$
$a = 7.4358$ (3) Å
$b = 9.4165$ (5) Å
$c = 10.3934$ (5) Å
$\alpha = 90.938$ (2)°
$\beta = 96.910$ (2)°
$\gamma = 105.872$ (2)°
$V = 693.98$ (6) Å$^3$
$Z = 2$
$F(000) = 308$
$D_x = 1.423$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6452 reflections
$\theta = 2.8$–$25.6°$
$\mu = 0.11$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.942$, $T_{max} = 0.983$
12708 measured reflections
2442 independent reflections
2055 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 10$
$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.116$
$S = 1.02$
2442 reflections
200 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
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.2005P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{min} = -0.16$ e Å$^{-3}$
Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.030 (5)

*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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.5353 (2) | 0.28891 (17) | 0.58091 (15) | 0.0437 (4) |
| H1 | 0.5862 | 0.3239 | 0.6654 | 0.052* |
| C2 | 0.6211 (2) | 0.20823 (17) | 0.51113 (16) | 0.0450 (4) |
| C3 | 0.5534 (3) | 0.15471 (19) | 0.38555 (17) | 0.0548 (5) |
| H3 | 0.6160 | 0.1015 | 0.3400 | 0.066* |
| C4 | 0.3898 (3) | 0.1826 (2) | 0.32955 (17) | 0.0576 (5) |

| | | | | |
|---|---|---|---|---|
| H4 | 0.3401 | 0.1470 | 0.2450 | 0.069* |
| C5 | 0.2988 (2) | 0.26268 (18) | 0.39767 (15) | 0.0479 (4) |
| H5 | 0.1879 | 0.2798 | 0.3586 | 0.057* |
| C6 | 0.3703 (2) | 0.31818 (16) | 0.52382 (14) | 0.0389 (4) |
| C7 | 0.2662 (2) | 0.40380 (16) | 0.58752 (14) | 0.0392 (4) |
| H7 | 0.1617 | 0.4177 | 0.5360 | 0.047* |
| C8 | 0.2965 (2) | 0.46539 (16) | 0.70769 (14) | 0.0380 (4) |
| C9 | 0.1628 (2) | 0.54718 (17) | 0.74909 (14) | 0.0404 (4) |
| C10 | 0.0773 (2) | 0.67695 (19) | 0.92842 (16) | 0.0486 (4) |
| H10A | 0.0750 | 0.6564 | 1.0194 | 0.058* |
| H10B | −0.0509 | 0.6412 | 0.8851 | 0.058* |
| C11 | 0.1429 (2) | 0.83840 (19) | 0.91721 (15) | 0.0474 (4) |
| C12 | 0.2518 (5) | 0.9468 (3) | 0.9961 (2) | 0.1020 (10) |
| H12 | 0.3096 | 0.9378 | 1.0788 | 0.122* |
| C13 | 0.2647 (5) | 1.0791 (3) | 0.9319 (3) | 0.1089 (10) |
| H13 | 0.3310 | 1.1739 | 0.9645 | 0.131* |
| C14 | 0.1663 (3) | 1.0432 (3) | 0.8186 (3) | 0.0790 (7) |
| H14 | 0.1519 | 1.1094 | 0.7553 | 0.095* |
| C15 | 0.4516 (2) | 0.45908 (19) | 0.80123 (14) | 0.0447 (4) |
| N1 | 0.7935 (2) | 0.17794 (17) | 0.57526 (18) | 0.0592 (4) |
| N2 | 0.5728 (2) | 0.4565 (2) | 0.87857 (14) | 0.0667 (5) |
| N3 | 0.19322 (18) | 0.59563 (15) | 0.87343 (12) | 0.0439 (3) |
| H3A | 0.2851 | 0.5781 | 0.9231 | 0.053* |
| O1 | 0.8792 (2) | 0.1167 (2) | 0.51177 (17) | 0.0881 (5) |
| O2 | 0.8406 (2) | 0.2139 (2) | 0.69036 (16) | 0.0840 (5) |
| O3 | 0.03619 (18) | 0.56592 (15) | 0.67145 (11) | 0.0609 (4) |
| O4 | 0.0876 (2) | 0.89464 (16) | 0.80594 (13) | 0.0724 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0448 (9) | 0.0476 (9) | 0.0417 (8) | 0.0195 (7) | 0.0013 (7) | 0.0035 (7) |
| C2 | 0.0437 (9) | 0.0420 (9) | 0.0556 (10) | 0.0200 (7) | 0.0106 (7) | 0.0120 (7) |
| C3 | 0.0667 (11) | 0.0488 (10) | 0.0584 (11) | 0.0261 (9) | 0.0212 (9) | 0.0027 (8) |
| C4 | 0.0688 (12) | 0.0622 (11) | 0.0452 (9) | 0.0268 (9) | 0.0017 (8) | −0.0086 (8) |
| C5 | 0.0490 (9) | 0.0522 (10) | 0.0439 (9) | 0.0201 (8) | −0.0023 (7) | −0.0022 (7) |
| C6 | 0.0395 (8) | 0.0396 (8) | 0.0392 (8) | 0.0148 (6) | 0.0023 (6) | 0.0039 (6) |
| C7 | 0.0376 (8) | 0.0436 (8) | 0.0381 (8) | 0.0172 (7) | −0.0022 (6) | 0.0032 (6) |
| C8 | 0.0375 (8) | 0.0413 (8) | 0.0369 (8) | 0.0159 (6) | −0.0002 (6) | 0.0053 (6) |
| C9 | 0.0415 (8) | 0.0445 (9) | 0.0379 (8) | 0.0191 (7) | −0.0009 (6) | 0.0030 (6) |
| C10 | 0.0509 (9) | 0.0579 (10) | 0.0426 (9) | 0.0227 (8) | 0.0099 (7) | 0.0007 (7) |
| C11 | 0.0511 (9) | 0.0554 (10) | 0.0414 (8) | 0.0257 (8) | 0.0035 (7) | −0.0015 (7) |
| C12 | 0.159 (3) | 0.0602 (14) | 0.0657 (14) | 0.0154 (15) | −0.0330 (15) | −0.0052 (11) |
| C13 | 0.153 (3) | 0.0523 (14) | 0.107 (2) | 0.0143 (15) | −0.008 (2) | −0.0025 (13) |
| C14 | 0.0888 (16) | 0.0643 (14) | 0.0948 (17) | 0.0370 (12) | 0.0152 (13) | 0.0253 (12) |
| C15 | 0.0470 (9) | 0.0588 (10) | 0.0342 (8) | 0.0262 (8) | 0.0012 (7) | −0.0008 (7) |
| N1 | 0.0539 (9) | 0.0598 (9) | 0.0764 (11) | 0.0323 (8) | 0.0161 (8) | 0.0197 (8) |
| N2 | 0.0628 (10) | 0.1065 (14) | 0.0412 (8) | 0.0480 (9) | −0.0084 (7) | −0.0060 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.0474 (7) | 0.0536 (8) | 0.0364 (7) | 0.0261 (6) | −0.0006 (5) | 0.0010 (6) |
| O1 | 0.0840 (11) | 0.1097 (13) | 0.1024 (12) | 0.0702 (10) | 0.0338 (9) | 0.0228 (9) |
| O2 | 0.0720 (10) | 0.1099 (13) | 0.0829 (11) | 0.0555 (9) | −0.0105 (8) | 0.0032 (9) |
| O3 | 0.0626 (8) | 0.0875 (9) | 0.0446 (6) | 0.0495 (7) | −0.0111 (6) | −0.0084 (6) |
| O4 | 0.0791 (9) | 0.0714 (9) | 0.0649 (8) | 0.0266 (7) | −0.0123 (7) | 0.0114 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.367 (2) | C9—N3 | 1.3354 (19) |
| C1—C6 | 1.396 (2) | C10—N3 | 1.4564 (19) |
| C1—H1 | 0.9300 | C10—C11 | 1.475 (2) |
| C2—C3 | 1.376 (2) | C10—H10A | 0.9700 |
| C2—N1 | 1.472 (2) | C10—H10B | 0.9700 |
| C3—C4 | 1.377 (3) | C11—C12 | 1.315 (3) |
| C3—H3 | 0.9300 | C11—O4 | 1.346 (2) |
| C4—C5 | 1.380 (2) | C12—C13 | 1.408 (4) |
| C4—H4 | 0.9300 | C12—H12 | 0.9300 |
| C5—C6 | 1.390 (2) | C13—C14 | 1.296 (4) |
| C5—H5 | 0.9300 | C13—H13 | 0.9300 |
| C6—C7 | 1.461 (2) | C14—O4 | 1.358 (3) |
| C7—C8 | 1.336 (2) | C14—H14 | 0.9300 |
| C7—H7 | 0.9300 | C15—N2 | 1.139 (2) |
| C8—C15 | 1.432 (2) | N1—O1 | 1.210 (2) |
| C8—C9 | 1.509 (2) | N1—O2 | 1.220 (2) |
| C9—O3 | 1.2170 (18) | N3—H3A | 0.8600 |
| | | | |
| C2—C1—C6 | 119.19 (15) | N3—C10—C11 | 114.03 (14) |
| C2—C1—H1 | 120.4 | N3—C10—H10A | 108.7 |
| C6—C1—H1 | 120.4 | C11—C10—H10A | 108.7 |
| C1—C2—C3 | 123.02 (15) | N3—C10—H10B | 108.7 |
| C1—C2—N1 | 117.60 (15) | C11—C10—H10B | 108.7 |
| C3—C2—N1 | 119.38 (15) | H10A—C10—H10B | 107.6 |
| C2—C3—C4 | 117.80 (15) | C12—C11—O4 | 109.03 (18) |
| C2—C3—H3 | 121.1 | C12—C11—C10 | 132.98 (17) |
| C4—C3—H3 | 121.1 | O4—C11—C10 | 117.98 (15) |
| C3—C4—C5 | 120.64 (16) | C11—C12—C13 | 107.3 (2) |
| C3—C4—H4 | 119.7 | C11—C12—H12 | 126.4 |
| C5—C4—H4 | 119.7 | C13—C12—H12 | 126.4 |
| C4—C5—C6 | 121.02 (15) | C14—C13—C12 | 106.8 (2) |
| C4—C5—H5 | 119.5 | C14—C13—H13 | 126.6 |
| C6—C5—H5 | 119.5 | C12—C13—H13 | 126.6 |
| C5—C6—C1 | 118.31 (14) | C13—C14—O4 | 109.9 (2) |
| C5—C6—C7 | 117.18 (13) | C13—C14—H14 | 125.0 |
| C1—C6—C7 | 124.50 (13) | O4—C14—H14 | 125.0 |
| C8—C7—C6 | 130.56 (13) | N2—C15—C8 | 177.71 (16) |
| C8—C7—H7 | 114.7 | O1—N1—O2 | 123.45 (16) |
| C6—C7—H7 | 114.7 | O1—N1—C2 | 118.39 (17) |
| C7—C8—C15 | 123.40 (13) | O2—N1—C2 | 118.15 (14) |

| | | | |
|---|---|---|---|
| C7—C8—C9 | 119.37 (13) | C9—N3—C10 | 122.71 (13) |
| C15—C8—C9 | 117.24 (12) | C9—N3—H3A | 118.6 |
| O3—C9—N3 | 123.55 (14) | C10—N3—H3A | 118.6 |
| O3—C9—C8 | 120.49 (13) | C11—O4—C14 | 106.99 (16) |
| N3—C9—C8 | 115.97 (12) | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.6 (3) | C15—C8—C9—N3 | −5.4 (2) |
| C6—C1—C2—N1 | −179.20 (14) | N3—C10—C11—C12 | −94.5 (3) |
| C1—C2—C3—C4 | −1.1 (3) | N3—C10—C11—O4 | 84.68 (19) |
| N1—C2—C3—C4 | 178.69 (15) | O4—C11—C12—C13 | 0.6 (3) |
| C2—C3—C4—C5 | 0.5 (3) | C10—C11—C12—C13 | 179.9 (2) |
| C3—C4—C5—C6 | 0.5 (3) | C11—C12—C13—C14 | −0.9 (4) |
| C4—C5—C6—C1 | −1.0 (3) | C12—C13—C14—O4 | 0.9 (4) |
| C4—C5—C6—C7 | 178.99 (15) | C1—C2—N1—O1 | −174.37 (16) |
| C2—C1—C6—C5 | 0.5 (2) | C3—C2—N1—O1 | 5.9 (2) |
| C2—C1—C6—C7 | −179.50 (14) | C1—C2—N1—O2 | 6.8 (2) |
| C5—C6—C7—C8 | 177.38 (16) | C3—C2—N1—O2 | −172.96 (17) |
| C1—C6—C7—C8 | −2.6 (3) | O3—C9—N3—C10 | −0.3 (3) |
| C6—C7—C8—C15 | 1.2 (3) | C8—C9—N3—C10 | 179.74 (14) |
| C6—C7—C8—C9 | −179.14 (15) | C11—C10—N3—C9 | −88.52 (19) |
| C7—C8—C9—O3 | −5.1 (2) | C12—C11—O4—C14 | −0.1 (3) |
| C15—C8—C9—O3 | 174.61 (15) | C10—C11—O4—C14 | −179.50 (16) |
| C7—C8—C9—N3 | 174.88 (14) | C13—C14—O4—C11 | −0.5 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*A*···N2$^{i}$ | 0.86 | 2.27 | 3.056 (2) | 152 |
| C5—H5···O3$^{ii}$ | 0.93 | 2.49 | 3.337 (2) | 151 |
| C7—H7···O3$^{ii}$ | 0.93 | 2.49 | 3.362 (2) | 156 |

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