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# *N*-Methyl-3,5-dinitrobenzamide

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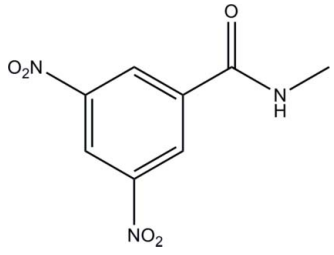
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.067; $wR$ factor = 0.162; data-to-parameter ratio = 11.8.

The asymmetric unit of the title compound, $C_8H_7N_3O_5$, contains two independent molecules in which the amide plane is oriented at dihedral angles of 29.82 (2) and 31.17 (2)° with respect to the benzene ring. In the crystal, molecules are connected *via* intermolecular N—H···O hydrogen bonds, forming chains running along the *b* axis.

## Related literature

For general background to the biological activity of benzamide derivatives, see: Lee *et al.* (2009). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### *Crystal data*

$C_8H_7N_3O_5$
$M_r$ = 225.16
Orthorhombic, *Pbca*
$a$ = 10.716 (2) Å
$b$ = 10.057 (2) Å
$c$ = 36.101 (7) Å
$V$ = 3890.6 (13) Å$^3$
$Z$ = 16
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.10 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.962, $T_{max}$ = 0.987
4711 measured reflections
3402 independent reflections
1653 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.0582
3 standard reflections every 200 reflections
intensity decay: 1%

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.162
$S$ = 0.96
3402 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$A$···O5$^{i}$ | 0.86 | 2.06 | 2.900 (4) | 165 |
| N6—H6$A$···O10$^{i}$ | 0.86 | 2.12 | 2.955 (4) | 164 |

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5409).

## References

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# supporting information

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## *N*-Methyl-3,5-dinitrobenzamide

**Gui-Ming Deng, Chao-Run Wang, Zhen Chen and He-Ming Zhang**

### S1. Comment

Benzamide derivatives exhibit interesting biological activities such as antibacterial and antifungal effects (Lee *et al.*., 2009). We report here the crystal structure of the title compound (Fig. 1). Bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

In the crystal packing of (I) the molecules are connected together *via* N—H···O intermolecular hydrogen bonds to form a one-dimensional chains in the *b* direction (Table 1, graph set C1,1(4)), which seems to be very effective in the stabilization of the crystal structure.

### S2. Experimental

A 1:1 mixture of N,N′-dimethylurea (0.088 g, 1 mmol), 3,5-dinitrobenzoic acid (0.212 g, 1 mmol) and $ZrOCl_2.8H_2O$ (0.032 g, 1 mmol) were ground in a mortar, placed in a 50 ml conical flask and irradiated in a microwave oven. The progress of the reaction was monitored by TLC. After completion of the reaction, the contents were extracted with EtOAc (3 × 10 ml) and filtered to remove the catalyst. To remove unreacted acid, the organic layer was washed with a $NaHCO_3$ solution followed by water. Evaporating the organic solvent provided the crystals.

### S3. Refinement

All H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.93 Å for aromatic H, 0.96 Å for methyl H and 0.86 Å for N—H. $U_{iso}$(H)= 1.2$U_{eq}$(C) and 1.5$U_{eq}$(N).

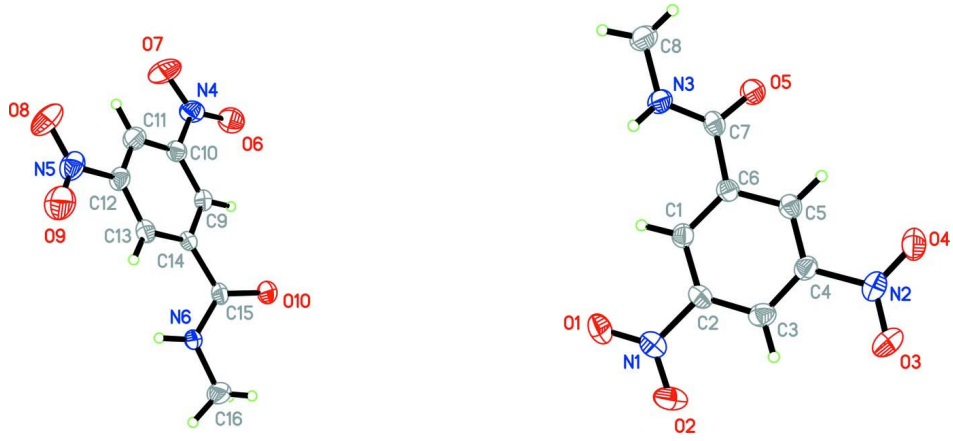


**Figure 1**

The molecular structure of (I) (thermal ellipsoids are shown at 30% probability levels).

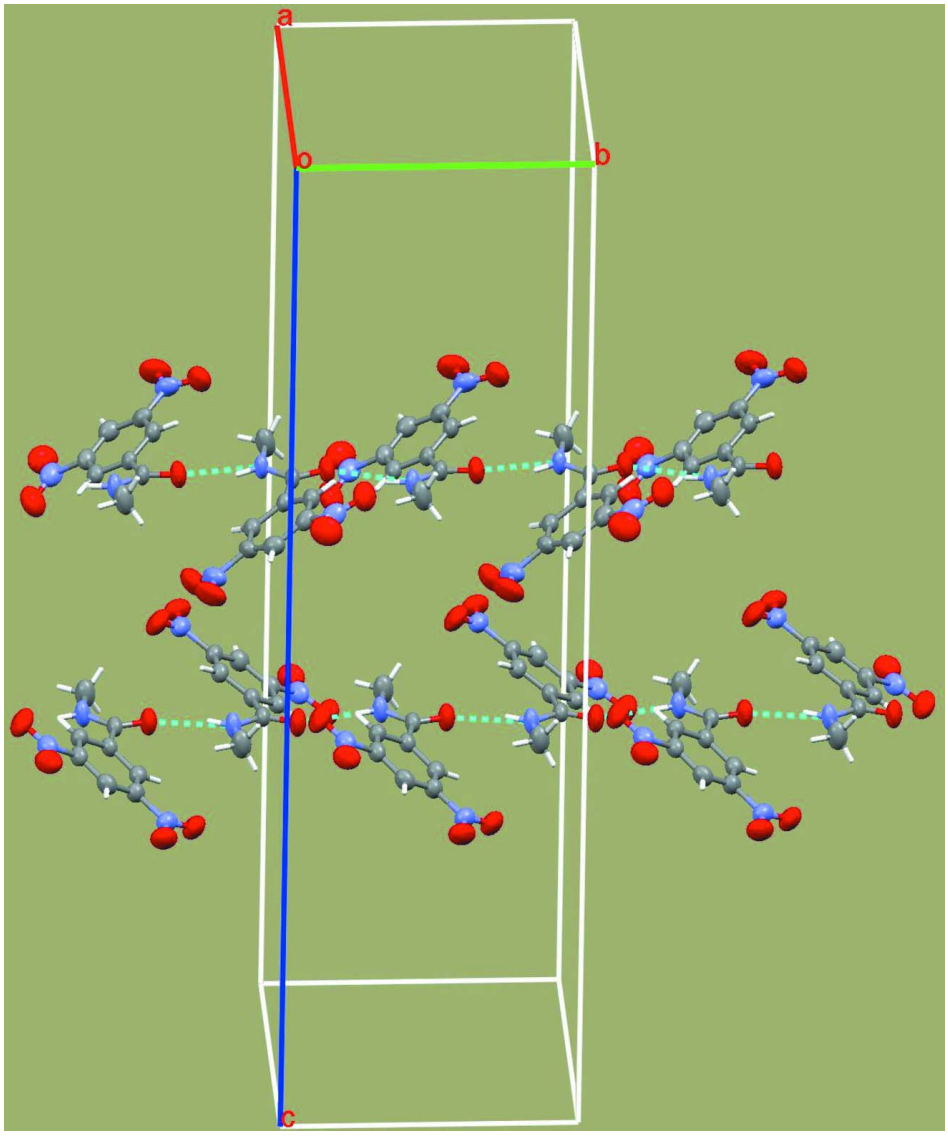


**Figure 2**

The packing of (I), viewed down the *b* axis. The dashed lines represent the hydrogen bonding interactions.

### *N*-Methyl-3,5-dinitrobenzamide

*Crystal data*

$C_8H_7N_3O_5$
$M_r$ = 225.16
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
*a* = 10.716 (2) Å
*b* = 10.057 (2) Å
*c* = 36.101 (7) Å
*V* = 3890.6 (13) Å$^3$
*Z* = 16

*F*(000) = 1856
$D_x$ = 1.538 Mg m$^{-3}$
Mo *Kα* radiation, $\lambda$ = 0.71073 Å
Cell parameters from 25 reflections
$\theta$ = 9–13°
$\mu$ = 0.13 mm$^{-1}$
*T* = 293 K
Block, yellow
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.962, $T_{max}$ = 0.987
4711 measured reflections
3402 independent reflections
1653 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.058
$\theta_{max}$ = 25.1°, $\theta_{min}$ = 2.2°
$h$ = 0→12
$k$ = 0→11
$l$ = 0→42
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.162
$S$ = 0.96
3402 reflections
289 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
$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 1.1588 (3) | 0.7222 (4) | 0.65015 (10) | 0.0554 (9) |
| C1 | 0.9707 (3) | 0.8426 (4) | 0.67035 (11) | 0.0444 (10) |
| H1A | 0.9221 | 0.7795 | 0.6582 | 0.053* |
| O1 | 1.0927 (3) | 0.6404 (3) | 0.63547 (10) | 0.0798 (11) |
| O2 | 1.2734 (2) | 0.7187 (3) | 0.64960 (8) | 0.0716 (9) |
| C2 | 1.0989 (3) | 0.8326 (4) | 0.67030 (11) | 0.0462 (10) |
| N2 | 1.1949 (4) | 1.1247 (4) | 0.72609 (10) | 0.0571 (10) |
| N3 | 0.7009 (3) | 0.8718 (3) | 0.68582 (10) | 0.0568 (10) |
| H3A | 0.7314 | 0.7927 | 0.6850 | 0.068* |
| O3 | 1.3077 (3) | 1.1073 (3) | 0.72618 (9) | 0.0726 (10) |
| C3 | 1.1751 (3) | 0.9227 (4) | 0.68860 (12) | 0.0521 (11) |
| H3B | 1.2616 | 0.9148 | 0.6885 | 0.063* |
| O4 | 1.1423 (3) | 1.2198 (3) | 0.74015 (10) | 0.0745 (10) |
| C4 | 1.1155 (3) | 1.0243 (4) | 0.70688 (12) | 0.0461 (10) |
| O5 | 0.7395 (2) | 1.0907 (2) | 0.68914 (9) | 0.0636 (9) |

| | | | | |
|---|---|---|---|---|
| C5 | 0.9889 (3) | 1.0400 (4) | 0.70711 (11) | 0.0437 (10) |
| H5A | 0.9527 | 1.1114 | 0.7194 | 0.052* |
| C6 | 0.9151 (3) | 0.9481 (3) | 0.68874 (10) | 0.0413 (10) |
| C7 | 0.7776 (3) | 0.9749 (4) | 0.68801 (11) | 0.0445 (10) |
| C8 | 0.5670 (3) | 0.8895 (4) | 0.68472 (14) | 0.0705 (14) |
| H8A | 0.5272 | 0.8042 | 0.6832 | 0.106* |
| H8B | 0.5450 | 0.9416 | 0.6634 | 0.106* |
| H8C | 0.5401 | 0.9344 | 0.7068 | 0.106* |
| O6 | 0.3317 (3) | 0.2716 (3) | 0.39302 (10) | 0.0788 (11) |
| O7 | 0.1844 (3) | 0.1345 (4) | 0.40663 (10) | 0.0918 (12) |
| O8 | 0.2726 (3) | −0.2445 (4) | 0.48397 (10) | 0.0938 (12) |
| O9 | 0.4620 (4) | −0.2891 (4) | 0.49911 (11) | 0.0952 (12) |
| O10 | 0.7598 (2) | 0.1750 (2) | 0.42863 (8) | 0.0614 (9) |
| N4 | 0.2939 (3) | 0.1676 (4) | 0.40662 (11) | 0.0617 (11) |
| N5 | 0.3840 (4) | −0.2228 (4) | 0.48302 (11) | 0.0669 (11) |
| N6 | 0.8109 (3) | −0.0414 (3) | 0.43239 (9) | 0.0503 (10) |
| H6A | 0.7843 | −0.1212 | 0.4356 | 0.060* |
| C9 | 0.5097 (3) | 0.1061 (4) | 0.42133 (11) | 0.0452 (10) |
| H9A | 0.5364 | 0.1806 | 0.4083 | 0.054* |
| C10 | 0.3841 (3) | 0.0788 (4) | 0.42467 (12) | 0.0501 (11) |
| C11 | 0.3408 (4) | −0.0288 (4) | 0.44465 (12) | 0.0560 (11) |
| H11A | 0.2558 | −0.0460 | 0.4469 | 0.067* |
| C12 | 0.4279 (3) | −0.1087 (4) | 0.46088 (11) | 0.0481 (10) |
| C13 | 0.5549 (3) | −0.0875 (3) | 0.45744 (11) | 0.0468 (10) |
| H13A | 0.6116 | −0.1457 | 0.4683 | 0.056* |
| C14 | 0.5960 (3) | 0.0213 (3) | 0.43772 (11) | 0.0390 (9) |
| C15 | 0.7307 (3) | 0.0574 (3) | 0.43282 (11) | 0.0435 (10) |
| C16 | 0.9431 (3) | −0.0190 (4) | 0.42662 (15) | 0.0718 (14) |
| H16A | 0.9863 | −0.1025 | 0.4270 | 0.108* |
| H16B | 0.9748 | 0.0372 | 0.4460 | 0.108* |
| H16C | 0.9557 | 0.0234 | 0.4031 | 0.108* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.063 (2) | 0.052 (2) | 0.051 (3) | 0.010 (2) | 0.003 (2) | −0.001 (2) |
| C1 | 0.046 (2) | 0.039 (2) | 0.048 (3) | −0.0017 (18) | −0.004 (2) | −0.002 (2) |
| O1 | 0.082 (2) | 0.064 (2) | 0.093 (3) | −0.0010 (18) | 0.012 (2) | −0.035 (2) |
| O2 | 0.0549 (19) | 0.091 (2) | 0.069 (2) | 0.0238 (17) | 0.0071 (17) | −0.0031 (19) |
| C2 | 0.052 (2) | 0.038 (2) | 0.049 (3) | 0.0070 (19) | 0.003 (2) | −0.001 (2) |
| N2 | 0.058 (2) | 0.057 (2) | 0.056 (3) | −0.012 (2) | −0.010 (2) | 0.000 (2) |
| N3 | 0.0419 (17) | 0.0308 (16) | 0.098 (3) | −0.0009 (15) | −0.0010 (18) | 0.007 (2) |
| O3 | 0.0486 (17) | 0.091 (2) | 0.078 (2) | −0.0116 (17) | −0.0149 (17) | 0.003 (2) |
| C3 | 0.043 (2) | 0.052 (2) | 0.061 (3) | 0.005 (2) | −0.003 (2) | 0.009 (2) |
| O4 | 0.077 (2) | 0.0621 (19) | 0.085 (3) | −0.0036 (18) | −0.0174 (18) | −0.021 (2) |
| C4 | 0.042 (2) | 0.042 (2) | 0.055 (3) | −0.0048 (19) | −0.004 (2) | 0.002 (2) |
| O5 | 0.0520 (16) | 0.0334 (15) | 0.106 (3) | 0.0035 (13) | −0.0022 (17) | −0.0014 (15) |
| C5 | 0.048 (2) | 0.040 (2) | 0.043 (2) | −0.0008 (19) | 0.0021 (19) | 0.001 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.042 (2) | 0.034 (2) | 0.048 (3) | 0.0019 (18) | 0.000 (2) | 0.004 (2) |
| C7 | 0.054 (2) | 0.031 (2) | 0.049 (3) | 0.001 (2) | 0.001 (2) | 0.001 (2) |
| C8 | 0.045 (2) | 0.051 (2) | 0.116 (4) | −0.001 (2) | 0.000 (3) | 0.002 (3) |
| O6 | 0.068 (2) | 0.066 (2) | 0.102 (3) | 0.0145 (19) | −0.019 (2) | 0.010 (2) |
| O7 | 0.0410 (17) | 0.129 (3) | 0.106 (3) | −0.0026 (19) | −0.0210 (18) | 0.015 (2) |
| O8 | 0.072 (2) | 0.117 (3) | 0.092 (3) | −0.041 (2) | 0.016 (2) | 0.019 (2) |
| O9 | 0.099 (3) | 0.079 (3) | 0.108 (3) | −0.009 (2) | 0.016 (2) | 0.032 (2) |
| O10 | 0.0528 (16) | 0.0324 (14) | 0.099 (2) | −0.0012 (13) | 0.0006 (17) | 0.0076 (16) |
| N4 | 0.046 (2) | 0.075 (3) | 0.064 (3) | 0.010 (2) | −0.016 (2) | −0.014 (2) |
| N5 | 0.073 (3) | 0.069 (3) | 0.058 (3) | −0.020 (2) | 0.014 (2) | 0.000 (2) |
| N6 | 0.0394 (17) | 0.0264 (16) | 0.085 (3) | −0.0011 (14) | 0.0063 (17) | 0.0019 (18) |
| C9 | 0.046 (2) | 0.035 (2) | 0.055 (3) | −0.0028 (18) | 0.000 (2) | −0.003 (2) |
| C10 | 0.046 (2) | 0.049 (2) | 0.056 (3) | 0.003 (2) | −0.008 (2) | −0.014 (2) |
| C11 | 0.051 (2) | 0.061 (3) | 0.055 (3) | −0.007 (2) | 0.005 (2) | −0.009 (2) |
| C12 | 0.053 (2) | 0.044 (2) | 0.047 (3) | −0.010 (2) | 0.009 (2) | 0.001 (2) |
| C13 | 0.055 (2) | 0.037 (2) | 0.049 (3) | −0.0001 (19) | 0.002 (2) | −0.004 (2) |
| C14 | 0.040 (2) | 0.0296 (18) | 0.047 (2) | 0.0027 (17) | −0.0007 (18) | −0.0053 (19) |
| C15 | 0.048 (2) | 0.027 (2) | 0.056 (3) | −0.0007 (18) | −0.003 (2) | −0.0014 (19) |
| C16 | 0.045 (2) | 0.049 (2) | 0.121 (4) | −0.002 (2) | 0.007 (3) | 0.016 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—O1 | 1.207 (4) | O6—N4 | 1.224 (4) |
| N1—O2 | 1.229 (4) | O7—N4 | 1.221 (4) |
| N1—C2 | 1.475 (5) | O8—N5 | 1.214 (4) |
| C1—C2 | 1.378 (5) | O9—N5 | 1.217 (4) |
| C1—C6 | 1.386 (5) | O10—C15 | 1.232 (4) |
| C1—H1A | 0.9300 | N4—C10 | 1.468 (5) |
| C2—C3 | 1.387 (5) | N5—C12 | 1.475 (5) |
| N2—O4 | 1.221 (4) | N6—C15 | 1.314 (4) |
| N2—O3 | 1.221 (4) | N6—C16 | 1.449 (4) |
| N2—C4 | 1.491 (5) | N6—H6A | 0.8600 |
| N3—C7 | 1.325 (4) | C9—C10 | 1.379 (5) |
| N3—C8 | 1.446 (4) | C9—C14 | 1.391 (5) |
| N3—H3A | 0.8600 | C9—H9A | 0.9300 |
| C3—C4 | 1.374 (5) | C10—C11 | 1.381 (5) |
| C3—H3B | 0.9300 | C11—C12 | 1.364 (5) |
| C4—C5 | 1.366 (5) | C11—H11A | 0.9300 |
| O5—C7 | 1.234 (4) | C12—C13 | 1.383 (5) |
| C5—C6 | 1.385 (5) | C13—C14 | 1.378 (5) |
| C5—H5A | 0.9300 | C13—H13A | 0.9300 |
| C6—C7 | 1.498 (5) | C14—C15 | 1.498 (5) |
| C8—H8A | 0.9600 | C16—H16A | 0.9600 |
| C8—H8B | 0.9600 | C16—H16B | 0.9600 |
| C8—H8C | 0.9600 | C16—H16C | 0.9600 |
| | | | |
| O1—N1—O2 | 124.0 (4) | O7—N4—O6 | 123.5 (4) |
| O1—N1—C2 | 118.3 (3) | O7—N4—C10 | 117.8 (4) |

| | | | |
|---|---|---|---|
| O2—N1—C2 | 117.6 (4) | O6—N4—C10 | 118.7 (3) |
| C2—C1—C6 | 119.0 (3) | O8—N5—O9 | 124.3 (4) |
| C2—C1—H1A | 120.5 | O8—N5—C12 | 118.0 (4) |
| C6—C1—H1A | 120.5 | O9—N5—C12 | 117.7 (4) |
| C1—C2—C3 | 122.6 (4) | C15—N6—C16 | 121.6 (3) |
| C1—C2—N1 | 119.3 (4) | C15—N6—H6A | 119.2 |
| C3—C2—N1 | 118.1 (3) | C16—N6—H6A | 119.2 |
| O4—N2—O3 | 124.6 (4) | C10—C9—C14 | 119.4 (4) |
| O4—N2—C4 | 117.4 (3) | C10—C9—H9A | 120.3 |
| O3—N2—C4 | 118.0 (4) | C14—C9—H9A | 120.3 |
| C7—N3—C8 | 121.3 (3) | C9—C10—C11 | 122.0 (4) |
| C7—N3—H3A | 119.3 | C9—C10—N4 | 118.8 (4) |
| C8—N3—H3A | 119.3 | C11—C10—N4 | 119.2 (4) |
| C4—C3—C2 | 116.2 (3) | C12—C11—C10 | 117.1 (4) |
| C4—C3—H3B | 121.9 | C12—C11—H11A | 121.4 |
| C2—C3—H3B | 121.9 | C10—C11—H11A | 121.4 |
| C5—C4—C3 | 123.4 (4) | C11—C12—C13 | 122.9 (4) |
| C5—C4—N2 | 119.1 (4) | C11—C12—N5 | 118.2 (4) |
| C3—C4—N2 | 117.5 (3) | C13—C12—N5 | 118.9 (4) |
| C4—C5—C6 | 119.2 (4) | C14—C13—C12 | 119.0 (4) |
| C4—C5—H5A | 120.4 | C14—C13—H13A | 120.5 |
| C6—C5—H5A | 120.4 | C12—C13—H13A | 120.5 |
| C5—C6—C1 | 119.6 (3) | C13—C14—C9 | 119.6 (3) |
| C5—C6—C7 | 116.7 (3) | C13—C14—C15 | 124.2 (3) |
| C1—C6—C7 | 123.5 (3) | C9—C14—C15 | 116.2 (3) |
| O5—C7—N3 | 122.4 (3) | O10—C15—N6 | 123.9 (3) |
| O5—C7—C6 | 119.6 (3) | O10—C15—C14 | 119.4 (3) |
| N3—C7—C6 | 118.0 (3) | N6—C15—C14 | 116.6 (3) |
| N3—C8—H8A | 109.5 | N6—C16—H16A | 109.5 |
| N3—C8—H8B | 109.5 | N6—C16—H16B | 109.5 |
| H8A—C8—H8B | 109.5 | H16A—C16—H16B | 109.5 |
| N3—C8—H8C | 109.5 | N6—C16—H16C | 109.5 |
| H8A—C8—H8C | 109.5 | H16A—C16—H16C | 109.5 |
| H8B—C8—H8C | 109.5 | H16B—C16—H16C | 109.5 |

| | | | |
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| C6—C1—C2—C3 | 1.3 (6) | C14—C9—C10—C11 | 1.7 (6) |
| C6—C1—C2—N1 | −178.8 (3) | C14—C9—C10—N4 | −178.8 (3) |
| O1—N1—C2—C1 | −2.9 (6) | O7—N4—C10—C9 | 172.6 (4) |
| O2—N1—C2—C1 | 177.6 (4) | O6—N4—C10—C9 | −8.7 (6) |
| O1—N1—C2—C3 | 177.0 (4) | O7—N4—C10—C11 | −7.8 (6) |
| O2—N1—C2—C3 | −2.5 (5) | O6—N4—C10—C11 | 170.8 (4) |
| C1—C2—C3—C4 | −0.4 (6) | C9—C10—C11—C12 | −0.6 (6) |
| N1—C2—C3—C4 | 179.7 (3) | N4—C10—C11—C12 | 179.9 (4) |
| C2—C3—C4—C5 | −1.0 (6) | C10—C11—C12—C13 | −1.3 (6) |
| C2—C3—C4—N2 | −178.6 (3) | C10—C11—C12—N5 | 178.8 (4) |
| O4—N2—C4—C5 | −2.6 (6) | O8—N5—C12—C11 | 4.2 (6) |
| O3—N2—C4—C5 | 178.6 (4) | O9—N5—C12—C11 | −175.9 (4) |
| O4—N2—C4—C3 | 175.1 (4) | O8—N5—C12—C13 | −175.8 (4) |

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|---|---|---|---|
| O3—N2—C4—C3 | −3.8 (6) | O9—N5—C12—C13 | 4.1 (6) |
| C3—C4—C5—C6 | 1.4 (6) | C11—C12—C13—C14 | 2.0 (6) |
| N2—C4—C5—C6 | 178.9 (3) | N5—C12—C13—C14 | −178.1 (3) |
| C4—C5—C6—C1 | −0.3 (5) | C12—C13—C14—C9 | −0.8 (5) |
| C4—C5—C6—C7 | −176.4 (3) | C12—C13—C14—C15 | 178.3 (4) |
| C2—C1—C6—C5 | −1.0 (5) | C10—C9—C14—C13 | −0.9 (6) |
| C2—C1—C6—C7 | 174.8 (4) | C10—C9—C14—C15 | 179.9 (3) |
| C8—N3—C7—O5 | −0.2 (7) | C16—N6—C15—O10 | −0.3 (7) |
| C8—N3—C7—C6 | −179.6 (4) | C16—N6—C15—C14 | 177.9 (3) |
| C5—C6—C7—O5 | 29.1 (5) | C13—C14—C15—O10 | −151.0 (4) |
| C1—C6—C7—O5 | −146.9 (4) | C9—C14—C15—O10 | 28.1 (5) |
| C5—C6—C7—N3 | −151.5 (4) | C13—C14—C15—N6 | 30.6 (6) |
| C1—C6—C7—N3 | 32.5 (6) | C9—C14—C15—N6 | −150.3 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*A*···O5$^{i}$ | 0.86 | 2.06 | 2.900 (4) | 165 |
| N6—H6*A*···O10$^{i}$ | 0.86 | 2.12 | 2.955 (4) | 164 |

Symmetry code: (i) −*x*+3/2, *y*−1/2, *z*.