Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4-Nitro-*N*-(4-nitrobenzoyl)benzamide

**Sohail Saeed,[a]‡ Naghmana Rashid,[a] Seik Weng Ng[b] and Edward R. T. Tiekink[b]***

[a]Department of Chemistry, Research Complex, Allama Iqbal Open University, Islamabad 44000, Pakistan, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: edward.tiekink@gmail.com

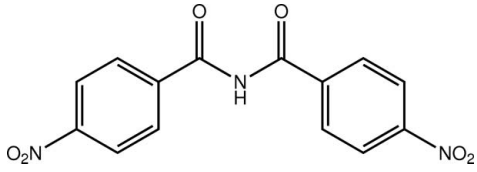
Received 16 April 2011; accepted 18 April 2011

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.005 Å; disorder in main residue; $R$ factor = 0.065; $wR$ factor = 0.217; data-to-parameter ratio = 11.3.

The central acetylacetamide moiety in the title compound, $C_{14}H_9N_3O_6$, is buckled [*e.g.* the C—N—C—O torsion angle is 14.3 (6)°] but the r.m.s. deviation for the five atoms is 0.044 Å. The benzene rings lie on the same side of the central plane, forming dihedral angles of 37.17 (15) and 28.58 (19)° with it. The dihedral angle between the two rings is 17.8 (2)° indicating that the molecule is curved. The carbonyl groups are *syn* to each other and *anti* to the amino H atom. This allows for the formation of N—H···O hydrogen bonds in the crystal, which leads to twisted chains along the *b* axis. Positional disorder (50:50) of the O atoms was modelled for both the nitro groups.

## Related literature

For background to high-temperature polymers for replacement of ceramics and metals, see: Ataei *et al.* (2005); Im & Jung, (2000); Yang *et al.* (2002).




## Experimental

### Crystal data

$C_{14}H_9N_3O_6$
$M_r$ = 315.24
Orthorhombic, *Pbca*
$a$ = 13.4757 (7) Å
$b$ = 8.5170 (6) Å
$c$ = 24.6285 (17) Å
$V$ = 2826.7 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.12 mm$^{-1}$
$T$ = 295 K
0.30 × 0.15 × 0.05 mm

### Data collection

Agilent Technologies SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.965, $T_{max}$ = 0.994
13745 measured reflections
2487 independent reflections
1433 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.217
$S$ = 1.02
2487 reflections
221 parameters
40 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O3$^{i}$ | 0.88 | 2.08 | 2.951 (4) | 170 |

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors are grateful to Allama Iqbal Open University, Islamabad, Pakistan, for the allocation of research and analytical laboratory facilities. The authors also thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5852).

## References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
Ataei, S. M., Sarrafi, Y., Hatami, M. & Faizi, L. A. (2005). *Eur. Polym. J.* **41**, 491–499.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Im, J. K. & Jung, J. C. (2000). *Polymers*, **41**, 8709–8716.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yang, C.-P., Chen, R.-S. & Hsu, M.-F. (2002). *J. Polym. Res.* **9**, 245–250.

‡ Additional correspondence author, e-mail: sohail262001@yahoo.com.

# supporting information

*Acta Cryst.* (2011). E**67**, o1194 [doi:10.1107/S1600536811014450]

## 4-Nitro-*N*-(4-nitrobenzoyl)benzamide

**Sohail Saeed, Naghmana Rashid, Seik Weng Ng and Edward R. T. Tiekink**

### S1. Comment

High-temperature polymers have received much attention owing to interest in the replacement of ceramics and metals (Ataei *et al.*, 2005). However, in many cases they are insoluble and do not melt below their decomposition temperature, a feature that restricts their applications (Im & Jung, 2000). Many studies have therefore focused upon obtaining aromatic polymers that are processable by conventional techniques (Yang *et al.*, 2002). The title compound, (I), is a logical precursor for an attempt to synthesize polyamides and polyimides having excellent thermal and mechanical properties.

Small twists are evident in the central acetylacetamide moiety as seen in the values of the C8—N2—C7—O3 and C7—N2—C8—O4 torsion angles of -4.9 (6) and 14.3 (6) °, respectively. Despite this, the r.m.s. of the fitted atoms from their least-squares plane = 0.0438 Å with the major deviations of 0.0473 (16) and -0.0708 (23) Å being for the O4 and C8 atoms, respectively. The C1- and C9-benzene rings form dihedral angles of 37.17 (15) and 28.58 (19) ° with the central plane, respectively, and form a dihedral angle of 17.8 (2) ° with each other. As the benzene rings lie to the same side of the central plane, overall, the molecule of (I) is curved, Fig. 1. The carbonyl groups are *syn* and the amino-H atom is directed towards the other side of the molecule, *i.e. anti* to the carbonyls. This arrangmement allows for the formation of N—H···O hydorgen bonds leading to a highly twisted chain, Fig. 2 and Table 1. Globally, molecules pack into undulating layers as shown in Fig. 3.

### S2. Experimental

All the reagents and organic solvents were of analytical grade and commercially available. The title compound was accidentally generated during the reaction of 4-nitrobenzoyl chloride with imidazole; it was isolated from the reaction mixture by column chromatography in 45% yield and then purified by re-crystallization from ethanol to give colourless prisms of (I). *M*.pt. 438–439 K; Anal.: C, 53.34; H, 2.88; N, 13.33%. $C_{14}H_9N_3O_6$ requires: C, 53.41; H, 2.87; N, 13.36%.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.93 Å, $U_{iso}$(H) 1.2$U_{eq}$(C)] and were included in the refinement in the riding model approximation. The amino H-atom was similarly placed [N–H 0.88 Å, $U_{iso}$(H) 1.2$U_{eq}$(N)].

The nitro groups are disordered over two positions in respect of the O atoms; the disorder could not be refined, and was assumed to be a 1:1 type of disorder. For each group, the N—O distances were restrained to within ±0.01 Å of each other, and the four-atom $CNO_2$ unit was restrained to be nearly flat. The displacement parameters were restrained to be nearly isotropic.

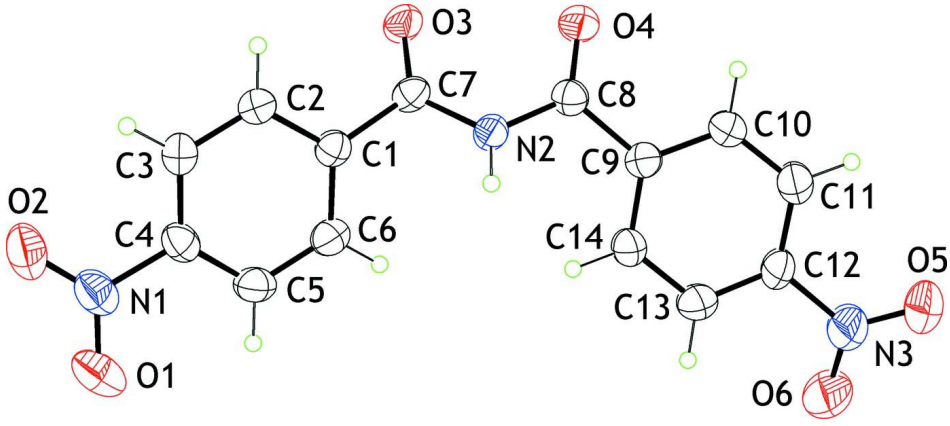



**Figure 1**

The molecular structure of (I) showing displacement ellipsoids at the 35% probability level.

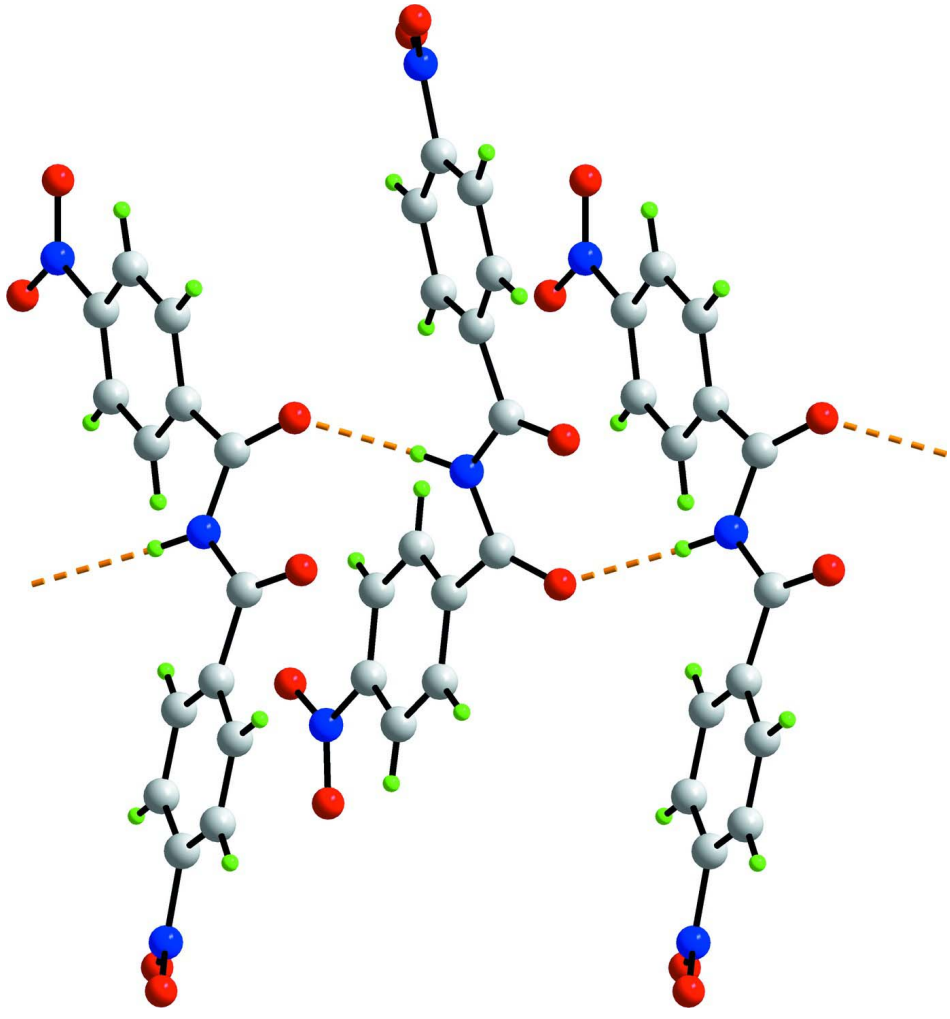


**Figure 2**

Supramolecular chain aligned along the *b* axis in (I) mediated by N—H···O hydrogen bonding shown as orange dashed lines.

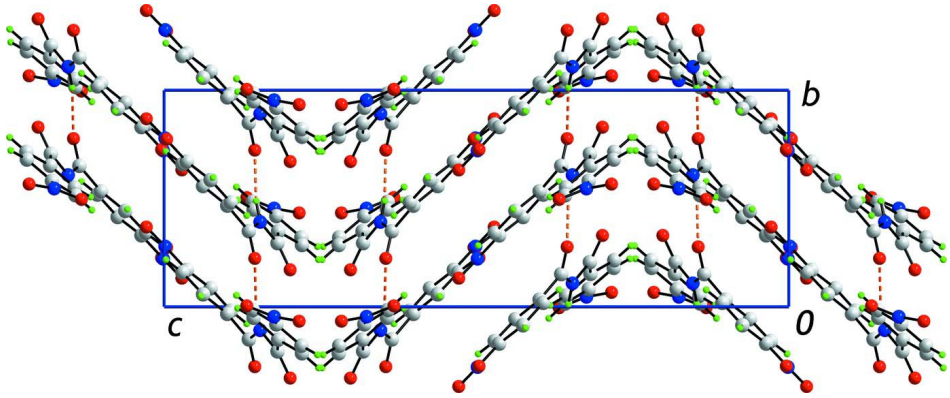



**Figure 3**

A view in projection down the *a* axis of the crystal packing in (I), highlighting the undulating layers. The N—H···O hydrogen bonding is shown as orange dashed lines.

### 4-Nitro-*N*-(4-nitrobenzoyl)benzamide

*Crystal data*

$C_{14}H_9N_3O_6$
$M_r$ = 315.24
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
*a* = 13.4757 (7) Å
*b* = 8.5170 (6) Å
*c* = 24.6285 (17) Å
*V* = 2826.7 (3) Å$^3$
*Z* = 8
*F*(000) = 1296
$D_x$ = 1.482 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 2137 reflections
*θ* = 2.4–29.3°
*μ* = 0.12 mm$^{-1}$
*T* = 295 K
Prism, colorless
0.30 × 0.15 × 0.05 mm

*Data collection*

Agilent Technologies SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
*ω* scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.965, $T_{max}$ = 0.994
13745 measured reflections
2487 independent reflections
1433 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067
$\theta_{max}$ = 25.1°, $\theta_{min}$ = 3.0°
*h* = −16→16
*k* = −10→8
*l* = −29→29

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.217
*S* = 1.02
2487 reflections
221 parameters
40 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
$w = 1/[\sigma^2(F_o^2) + (0.0936P)^2 + 1.8503P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0036 (11)

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.975 (3) | 0.868 (3) | 0.4716 (10) | 0.092 (4) | 0.50 |
| O2 | 1.1108 (6) | 0.774 (4) | 0.5041 (14) | 0.087 (3) | 0.50 |
| O1′ | 0.974 (3) | 0.835 (3) | 0.4633 (9) | 0.092 (4) | 0.50 |
| O2′ | 1.1072 (6) | 0.804 (4) | 0.5128 (14) | 0.087 (3) | 0.50 |
| O3 | 0.84634 (19) | 0.2233 (3) | 0.64513 (11) | 0.0615 (8) | |
| O4 | 0.67456 (19) | 0.1707 (3) | 0.70172 (11) | 0.0596 (8) | |
| O5 | 0.1877 (10) | 0.4334 (12) | 0.7162 (4) | 0.100 (3) | 0.50 |
| O6 | 0.2086 (12) | 0.5041 (11) | 0.6323 (4) | 0.112 (3) | 0.50 |
| O5′ | 0.1823 (10) | 0.3657 (12) | 0.6995 (4) | 0.100 (3) | 0.50 |
| O6′ | 0.2166 (12) | 0.5728 (10) | 0.6491 (4) | 0.112 (3) | 0.50 |
| N1 | 1.0204 (3) | 0.7784 (4) | 0.50161 (13) | 0.0710 (11) | |
| N2 | 0.71486 (19) | 0.3916 (4) | 0.65368 (12) | 0.0489 (8) | |
| H2 | 0.6951 | 0.4882 | 0.6471 | 0.059* | |
| N3 | 0.2410 (3) | 0.4541 (4) | 0.67600 (15) | 0.0986 (15) | |
| C1 | 0.8597 (2) | 0.4671 (4) | 0.60108 (14) | 0.0462 (9) | |
| C2 | 0.9620 (3) | 0.4820 (5) | 0.60666 (15) | 0.0518 (10) | |
| H2A | 0.9955 | 0.4218 | 0.6323 | 0.062* | |
| C3 | 1.0139 (3) | 0.5855 (5) | 0.57437 (15) | 0.0524 (10) | |
| H3 | 1.0821 | 0.5976 | 0.5784 | 0.063* | |
| C4 | 0.9630 (3) | 0.6702 (4) | 0.53628 (14) | 0.0525 (10) | |
| C5 | 0.8623 (3) | 0.6587 (5) | 0.52915 (15) | 0.0576 (11) | |
| H5 | 0.8299 | 0.7174 | 0.5027 | 0.069* | |
| C6 | 0.8110 (3) | 0.5574 (5) | 0.56230 (15) | 0.0546 (10) | |
| H6 | 0.7425 | 0.5492 | 0.5587 | 0.066* | |
| C7 | 0.8080 (3) | 0.3493 (4) | 0.63559 (15) | 0.0468 (9) | |
| C8 | 0.6499 (3) | 0.2939 (5) | 0.68146 (14) | 0.0475 (9) | |
| C9 | 0.5444 (2) | 0.3483 (4) | 0.68244 (14) | 0.0458 (9) | |
| C10 | 0.4802 (3) | 0.2851 (5) | 0.72057 (15) | 0.0578 (11) | |
| H10 | 0.5048 | 0.2180 | 0.7471 | 0.069* | |
| C11 | 0.3815 (3) | 0.3200 (6) | 0.71968 (17) | 0.0691 (13) | |
| H11 | 0.3385 | 0.2783 | 0.7454 | 0.083* | |
| C12 | 0.3472 (3) | 0.4188 (5) | 0.67959 (17) | 0.0628 (11) | |
| C13 | 0.4080 (3) | 0.4851 (5) | 0.64193 (17) | 0.0628 (11) | |
| H13 | 0.3828 | 0.5532 | 0.6158 | 0.075* | |
| C14 | 0.5079 (3) | 0.4492 (5) | 0.64323 (15) | 0.0532 (10) | |
| H14 | 0.5507 | 0.4929 | 0.6177 | 0.064* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.125 (3) | 0.080 (8) | 0.071 (6) | −0.005 (6) | 0.007 (5) | 0.026 (5) |
| O2 | 0.083 (2) | 0.087 (9) | 0.093 (8) | −0.014 (2) | 0.032 (3) | 0.006 (5) |
| O1′ | 0.125 (3) | 0.080 (8) | 0.071 (6) | −0.005 (6) | 0.007 (5) | 0.026 (5) |
| O2′ | 0.083 (2) | 0.087 (9) | 0.093 (8) | −0.014 (2) | 0.032 (3) | 0.006 (5) |
| O3 | 0.0501 (15) | 0.0421 (17) | 0.092 (2) | 0.0075 (12) | 0.0066 (14) | 0.0080 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4 | 0.0601 (17) | 0.0487 (17) | 0.0699 (17) | 0.0045 (13) | 0.0018 (13) | 0.0090 (14) |
| O5 | 0.059 (2) | 0.131 (8) | 0.109 (6) | 0.003 (5) | 0.022 (4) | 0.021 (5) |
| O6 | 0.066 (3) | 0.164 (7) | 0.105 (5) | 0.017 (6) | −0.015 (4) | 0.031 (5) |
| O5′ | 0.059 (2) | 0.131 (8) | 0.109 (6) | 0.003 (5) | 0.022 (4) | 0.021 (5) |
| O6′ | 0.066 (3) | 0.164 (7) | 0.105 (5) | 0.017 (6) | −0.015 (4) | 0.031 (5) |
| N1 | 0.088 (3) | 0.064 (3) | 0.061 (2) | −0.001 (2) | 0.018 (2) | 0.007 (2) |
| N2 | 0.0411 (16) | 0.0393 (18) | 0.066 (2) | 0.0004 (14) | 0.0043 (14) | 0.0044 (15) |
| N3 | 0.054 (2) | 0.150 (4) | 0.091 (3) | 0.011 (3) | 0.005 (2) | 0.040 (3) |
| C1 | 0.045 (2) | 0.043 (2) | 0.051 (2) | 0.0012 (16) | 0.0009 (16) | −0.0034 (17) |
| C2 | 0.047 (2) | 0.055 (2) | 0.053 (2) | 0.0058 (18) | −0.0012 (17) | 0.0064 (19) |
| C3 | 0.047 (2) | 0.055 (2) | 0.055 (2) | −0.0038 (18) | 0.0067 (18) | −0.0019 (19) |
| C4 | 0.063 (3) | 0.049 (2) | 0.045 (2) | −0.0002 (19) | 0.0097 (18) | 0.0019 (18) |
| C5 | 0.065 (3) | 0.060 (3) | 0.048 (2) | 0.013 (2) | −0.0016 (19) | 0.0076 (19) |
| C6 | 0.048 (2) | 0.059 (3) | 0.057 (2) | 0.0057 (19) | −0.0044 (18) | 0.001 (2) |
| C7 | 0.042 (2) | 0.038 (2) | 0.060 (2) | 0.0013 (17) | −0.0050 (17) | −0.0045 (18) |
| C8 | 0.049 (2) | 0.044 (2) | 0.050 (2) | −0.0030 (18) | −0.0013 (17) | 0.0001 (18) |
| C9 | 0.044 (2) | 0.042 (2) | 0.051 (2) | −0.0036 (17) | −0.0047 (17) | −0.0007 (17) |
| C10 | 0.054 (2) | 0.069 (3) | 0.051 (2) | 0.0032 (19) | 0.0006 (18) | 0.014 (2) |
| C11 | 0.054 (2) | 0.094 (4) | 0.059 (3) | 0.001 (2) | 0.008 (2) | 0.016 (2) |
| C12 | 0.037 (2) | 0.087 (3) | 0.064 (3) | 0.000 (2) | 0.0038 (19) | 0.012 (2) |
| C13 | 0.052 (2) | 0.073 (3) | 0.063 (3) | 0.003 (2) | −0.009 (2) | 0.015 (2) |
| C14 | 0.046 (2) | 0.056 (2) | 0.058 (2) | −0.0063 (18) | 0.0020 (18) | 0.0086 (19) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—N1 | 1.228 (7) | C2—H2A | 0.9300 |
| O2—N1 | 1.221 (7) | C3—C4 | 1.367 (5) |
| O1′—N1 | 1.228 (7) | C3—H3 | 0.9300 |
| O2′—N1 | 1.222 (7) | C4—C5 | 1.372 (5) |
| O3—C7 | 1.214 (4) | C5—C6 | 1.374 (5) |
| O4—C8 | 1.209 (4) | C5—H5 | 0.9300 |
| O5—N3 | 1.235 (7) | C6—H6 | 0.9300 |
| O6—N3 | 1.237 (7) | C8—C9 | 1.496 (5) |
| O5′—N3 | 1.236 (7) | C9—C14 | 1.383 (5) |
| O6′—N3 | 1.254 (7) | C9—C10 | 1.385 (5) |
| N1—C4 | 1.475 (5) | C10—C11 | 1.363 (5) |
| N2—C7 | 1.380 (4) | C10—H10 | 0.9300 |
| N2—C8 | 1.388 (4) | C11—C12 | 1.377 (6) |
| N2—H2 | 0.8800 | C11—H11 | 0.9300 |
| N3—C12 | 1.466 (5) | C12—C13 | 1.360 (6) |
| C1—C2 | 1.391 (5) | C13—C14 | 1.381 (5) |
| C1—C6 | 1.391 (5) | C13—H13 | 0.9300 |
| C1—C7 | 1.488 (5) | C14—H14 | 0.9300 |
| C2—C3 | 1.378 (5) | | |
| | | | |
| O2—N1—O1 | 123 (3) | C4—C5—H5 | 121.1 |
| O2′—N1—O1′ | 126 (3) | C6—C5—H5 | 121.1 |
| O2—N1—C4 | 118.4 (19) | C5—C6—C1 | 121.2 (4) |

| | | | |
|---|---|---|---|
| O2′—N1—C4 | 118.9 (19) | C5—C6—H6 | 119.4 |
| O1—N1—C4 | 118 (2) | C1—C6—H6 | 119.4 |
| O1′—N1—C4 | 115 (2) | O3—C7—N2 | 123.7 (3) |
| C7—N2—C8 | 125.2 (3) | O3—C7—C1 | 120.5 (3) |
| C7—N2—H2 | 117.4 | N2—C7—C1 | 115.7 (3) |
| C8—N2—H2 | 117.4 | O4—C8—N2 | 123.4 (3) |
| O5—N3—O6 | 122.7 (12) | O4—C8—C9 | 121.6 (3) |
| O5—N3—O6′ | 112.7 (10) | N2—C8—C9 | 115.0 (3) |
| O5′—N3—O6′ | 124.8 (12) | C14—C9—C10 | 119.5 (3) |
| O5—N3—C12 | 119.4 (8) | C14—C9—C8 | 121.2 (3) |
| O6—N3—C12 | 117.9 (9) | C10—C9—C8 | 119.0 (3) |
| O5′—N3—C12 | 118.2 (8) | C11—C10—C9 | 120.9 (4) |
| O6′—N3—C12 | 117.0 (9) | C11—C10—H10 | 119.5 |
| C2—C1—C6 | 119.0 (3) | C9—C10—H10 | 119.5 |
| C2—C1—C7 | 118.0 (3) | C10—C11—C12 | 118.2 (4) |
| C6—C1—C7 | 123.0 (3) | C10—C11—H11 | 120.9 |
| C3—C2—C1 | 120.3 (3) | C12—C11—H11 | 120.9 |
| C3—C2—H2A | 119.9 | C13—C12—C11 | 122.7 (4) |
| C1—C2—H2A | 119.9 | C13—C12—N3 | 117.5 (4) |
| C4—C3—C2 | 118.6 (4) | C11—C12—N3 | 119.8 (3) |
| C4—C3—H3 | 120.7 | C12—C13—C14 | 118.6 (4) |
| C2—C3—H3 | 120.7 | C12—C13—H13 | 120.7 |
| C3—C4—C5 | 123.1 (3) | C14—C13—H13 | 120.7 |
| C3—C4—N1 | 117.7 (4) | C13—C14—C9 | 120.0 (3) |
| C5—C4—N1 | 119.3 (3) | C13—C14—H14 | 120.0 |
| C4—C5—C6 | 117.8 (3) | C9—C14—H14 | 120.0 |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.4 (5) | C7—N2—C8—O4 | 14.3 (6) |
| C7—C1—C2—C3 | 177.8 (3) | C7—N2—C8—C9 | −162.8 (3) |
| C1—C2—C3—C4 | −1.3 (6) | O4—C8—C9—C14 | −153.9 (4) |
| C2—C3—C4—C5 | 1.0 (6) | N2—C8—C9—C14 | 23.3 (5) |
| C2—C3—C4—N1 | −179.0 (3) | O4—C8—C9—C10 | 20.4 (5) |
| O2—N1—C4—C3 | 8.3 (14) | N2—C8—C9—C10 | −162.4 (3) |
| O2′—N1—C4—C3 | −9.7 (14) | C14—C9—C10—C11 | 0.6 (6) |
| O1—N1—C4—C3 | −171.8 (14) | C8—C9—C10—C11 | −173.8 (4) |
| O1′—N1—C4—C3 | 170.3 (14) | C9—C10—C11—C12 | 0.5 (6) |
| O2—N1—C4—C5 | −171.7 (14) | C10—C11—C12—C13 | −1.5 (7) |
| O2′—N1—C4—C5 | 170.3 (14) | C10—C11—C12—N3 | 177.6 (4) |
| O1—N1—C4—C5 | 8.2 (14) | O5—N3—C12—C13 | −160.6 (6) |
| O1′—N1—C4—C5 | −9.7 (14) | O6—N3—C12—C13 | 19.3 (6) |
| C3—C4—C5—C6 | 0.3 (6) | O5′—N3—C12—C13 | 161.1 (6) |
| N1—C4—C5—C6 | −179.7 (3) | O6′—N3—C12—C13 | −18.9 (6) |
| C4—C5—C6—C1 | −1.3 (6) | O5—N3—C12—C11 | 20.2 (6) |
| C2—C1—C6—C5 | 1.0 (6) | O6—N3—C12—C11 | −159.9 (6) |
| C7—C1—C6—C5 | −176.3 (3) | O5′—N3—C12—C11 | −18.1 (6) |
| C8—N2—C7—O3 | −4.9 (6) | O6′—N3—C12—C11 | 161.9 (6) |
| C8—N2—C7—C1 | 173.0 (3) | C11—C12—C13—C14 | 1.4 (7) |
| C2—C1—C7—O3 | −38.2 (5) | N3—C12—C13—C14 | −177.7 (4) |

| | | | |
|---|---|---|---|
| C6—C1—C7—O3 | 139.1 (4) | C12—C13—C14—C9 | −0.3 (6) |
| C2—C1—C7—N2 | 143.8 (3) | C10—C9—C14—C13 | −0.7 (6) |
| C6—C1—C7—N2 | −38.9 (5) | C8—C9—C14—C13 | 173.5 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O3$^{i}$ | 0.88 | 2.08 | 2.951 (4) | 170 |

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