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# Dimethyl 2-aminobiphenyl-4,4′-dicarboxylate

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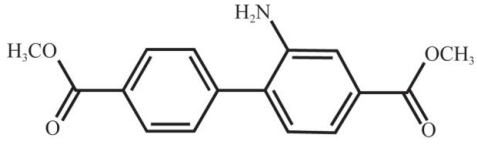
Key indicators: single-crystal X-ray study; $T$ = 90 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.045; $wR$ factor = 0.124; data-to-parameter ratio = 12.4.

The title compound, $C_{16}H_{15}NO_4$, exhibits two near-planar aromatic ester groups with a maximum aryl–ester torsion angle of 1.9 (2)°. The dihedral angle between the benzene rings is 44.7 (1)°. In the crystal, N—H···O hydrogen bonding is observed along with C—H···O contacts, forming chanins along [101]. No $\pi$–$\pi$ interactions were noted between the benzene rings.

## Related literature

For the synthesis of the title compound, see: Olkhovik *et al.* (2008). For the crystal structures of the parent dimethyl-4,4′-dicarboxylate and its structurally characterized amino derivatives, see: Ritzerfeld *et al.* (2009); Nyburg *et al.* (1988). For metal-organic framework structures with this and related linkers, see: Deshpande *et al.* (2010); Lun *et al.* (2011); Gupta *et al.* (2012); Sudik *et al.* (2005).




## Experimental

### Crystal data

$C_{16}H_{15}NO_4$
$M_r$ = 285.29
Monoclinic, $P2_1/c$
$a$ = 12.955 (3) Å
$b$ = 7.3460 (16) Å
$c$ = 14.422 (3) Å
$\beta$ = 103.263 (10)°
$V$ = 1336.0 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 90 K
0.28 × 0.12 × 0.06 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.972, $T_{max}$ = 0.994
9113 measured reflections
2463 independent reflections
1785 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
$S$ = 1.01
2463 reflections
198 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*NB*···O2$^{i}$ | 0.88 (1) | 2.54 (2) | 3.304 (3) | 146 (2) |
| N1—H1*NA*···O4$^{ii}$ | 0.88 (1) | 2.33 (1) | 3.147 (2) | 155 (2) |
| C4—H4*A*···O2$^{i}$ | 0.95 | 2.44 | 3.301 (3) | 150 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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: FF2103).

## References

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Deshpande, R. K., Minnaar, J. L. & Telfer, S. G. (2010). *Angew. Chem. Int. Ed.* **49**, 4598–4602.
Gupta, A. S., Deshpande, R. K., Liu, L., Waterhouse, G. I. N. & Telfer, S. G. (2012). *CrystEngComm*, **14**, 5701–5704.
Lun, D. J., Waterhouse, G. I. N. & Telfer, S. G. (2011). *J. Am. Chem. Soc.* **133**, 5806–5809.
Nyburg, S. C., Prasad, L., Behnam, B. A. & Hall, D. M. (1988). *J. Chem. Soc. Perkin Trans. 2*, pp. 617–623.
Olkhovik, V. K., Vasilevskii, D. A., Pap, A. A., Kalechyts, G. V., Matveienko, Y. V., Baran, A. G., Halinouski, N. A. & Petushok, V. G. (2008). *ARKIVOC*, pp. 69–93.
Ritzerfeld, V., Pyrlik, A., Wang, Y. & Englert, U. (2009). *Acta Cryst.* E**65**, o1677.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sudik, A. D., Millward, A. R., Ockwig, N. W., Cote, A. P., Kim, J. & Yaghi, O. M. (2005). *J. Am. Chem. Soc.* **127**, 7110–7118.

# supporting information

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## Dimethyl 2-aminobiphenyl-4,4′-dicarboxylate

**Ryan L. Lehane, James A. Golen, Arnold L. Rheingold and David R. Manke**

### S1. Comment

Biphenyl-4,4′-dicarboxylate and its derivatives are widely used in metal-organic (MOFs) frameworks as linkers (Sudik *et al.* 2005). One of the many advantages of MOFs is the ability to incorporate different functional groups within their pores. An area of interest is the inclusion of open Lewis base sites on the interior surfaces of MOFs. As a part of our efforts in this field, we prepared the previously reported dimethyl-2-aminobiphenyl-4,4′-dicarboxylate (Olkhovik *et al.* 2008) and report its structure herein.

The molecular structure of the title compound is shown in Figure 1. The two phenyl rings demonstrate a dihedral angle of 135.3°. In the crystal, intermolecular hydrogen bonding is observed between N1–H1NA···O4 and N1H1NB···O2. There is also a close C–H···O contact along C4H4A···O2. No $\pi$-$\pi$ interactions were noted between the phenyl rings. The packing for the title compound indicating hydrogen bonding is shown in Figure 2.

### S2. Experimental

The compound was prepared by literature procedure (Olkhovik *et al.* 2008). Crystals suitable for single-crystal X-ray analysis were grown by slow evaporation of an ethanol solution.

### S3. Refinement

All non-hydrogen atoms were refined anisotropically (*SHELXL*) by full matrix least squares on $F^2$. Hydrogen atoms H1NA and H1NB were found from a Fourier difference map and were refined with fixed distance of 0.87 (005) Å and isotropic displacement parameter of 1.20 times $U_{eq}$ of parent N atom. All other hydrogen atoms were placed in calculated positions and then refined with riding model with C—H lengths of 0.95 Å for (CH) and 0.98 Å for ($CH_3$) and with isotropic displacement parameters set to 1.20 and 1.50 times $U_{eq}$ of the parent C atom.

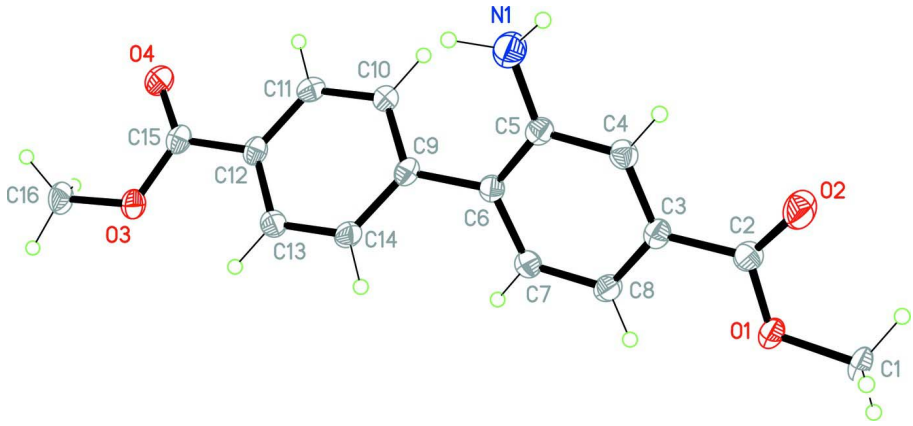


**Figure 1**

Molecular structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as spheres of arbitrary radius.

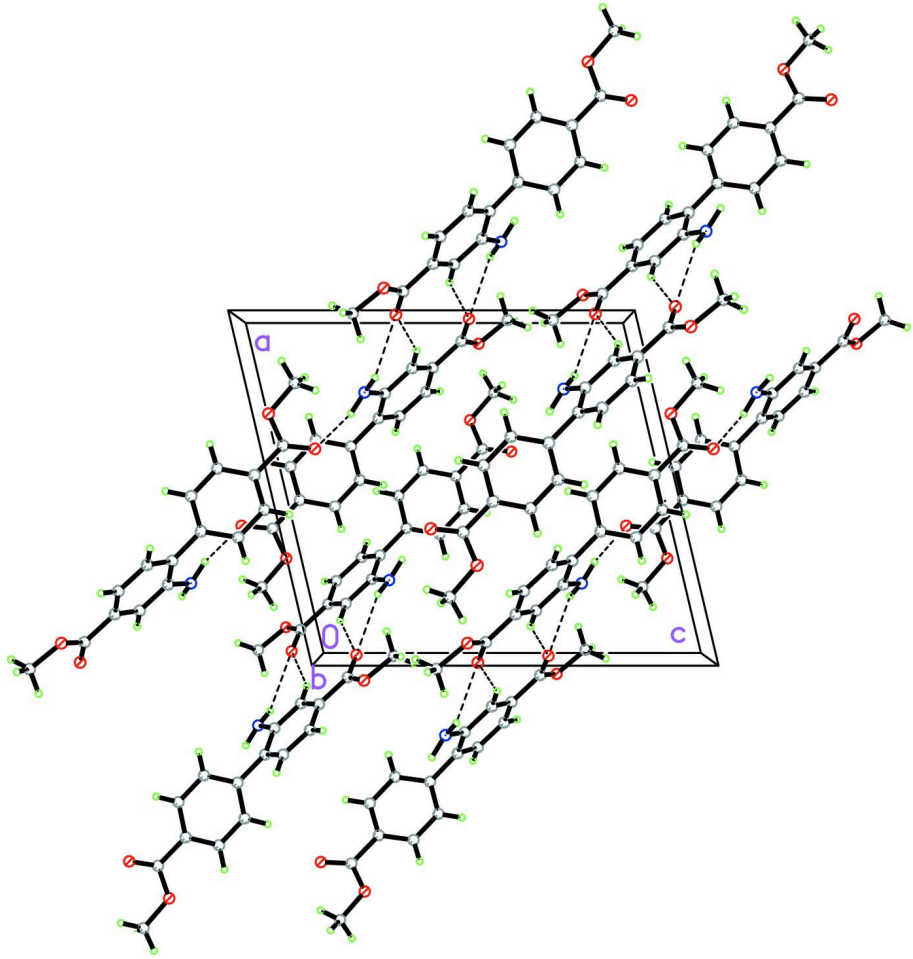


**Figure 2**

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

## Dimethyl 2-aminobiphenyl-4,4′-dicarboxylate

*Crystal data*

$C_{16}H_{15}NO_4$
$M_r = 285.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.955$ (3) Å
$b = 7.3460$ (16) Å
$c = 14.422$ (3) Å
$\beta = 103.263$ (10)°
$V = 1336.0$ (5) Å$^3$
$Z = 4$
$F(000) = 600$
$D_x = 1.418$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2401 reflections
$\theta = 2.9$–$24.9°$
$\mu = 0.10$ mm$^{-1}$
$T = 90$ K
Plate, colourless
0.28 × 0.12 × 0.06 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.972$, $T_{max} = 0.994$
9113 measured reflections
2463 independent reflections
1785 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.0°$
$h = -15 \rightarrow 15$
$k = -8 \rightarrow 8$
$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.124$
$S = 1.01$
2463 reflections
198 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
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.6328P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.06313 (12) | 0.5135 (2) | −0.10419 (10) | 0.0276 (4) |
| O2 | −0.00179 (13) | 0.7915 (2) | −0.09219 (11) | 0.0351 (4) |
| O3 | 0.71122 (11) | 0.6353 (2) | 0.53463 (9) | 0.0237 (4) |

| | | | | |
|---|---|---|---|---|
| O4 | 0.61240 (12) | 0.7629 (2) | 0.62568 (10) | 0.0280 (4) |
| N1 | 0.22094 (16) | 1.0226 (3) | 0.21975 (14) | 0.0321 (5) |
| H1NB | 0.1839 (17) | 1.109 (2) | 0.1855 (15) | 0.038* |
| H1NA | 0.2785 (12) | 1.051 (3) | 0.2629 (13) | 0.038* |
| C1 | −0.00925 (17) | 0.4946 (3) | −0.19589 (14) | 0.0277 (5) |
| H1C | −0.0122 | 0.3668 | −0.2157 | 0.042* |
| H1B | 0.0153 | 0.5695 | −0.2428 | 0.042* |
| H1A | −0.0801 | 0.5349 | −0.1915 | 0.042* |
| C2 | 0.06020 (17) | 0.6717 (3) | −0.05967 (15) | 0.0215 (5) |
| C3 | 0.14017 (16) | 0.6815 (3) | 0.03194 (14) | 0.0201 (5) |
| C4 | 0.14580 (16) | 0.8404 (3) | 0.08492 (14) | 0.0205 (5) |
| H4A | 0.0976 | 0.9367 | 0.0624 | 0.025* |
| C5 | 0.22104 (16) | 0.8614 (3) | 0.17076 (14) | 0.0190 (5) |
| C6 | 0.29167 (16) | 0.7167 (3) | 0.20412 (14) | 0.0181 (5) |
| C7 | 0.28276 (16) | 0.5577 (3) | 0.14953 (14) | 0.0206 (5) |
| H7A | 0.3294 | 0.4592 | 0.1719 | 0.025* |
| C8 | 0.20895 (17) | 0.5381 (3) | 0.06445 (14) | 0.0212 (5) |
| H8A | 0.2052 | 0.4286 | 0.0287 | 0.025* |
| C9 | 0.37584 (16) | 0.7249 (3) | 0.29319 (14) | 0.0188 (5) |
| C10 | 0.35757 (16) | 0.7869 (3) | 0.37973 (14) | 0.0198 (5) |
| H10A | 0.2899 | 0.8339 | 0.3819 | 0.024* |
| C11 | 0.43708 (17) | 0.7805 (3) | 0.46212 (14) | 0.0209 (5) |
| H11A | 0.4235 | 0.8229 | 0.5204 | 0.025* |
| C12 | 0.53657 (16) | 0.7127 (3) | 0.46029 (14) | 0.0188 (5) |
| C13 | 0.55552 (17) | 0.6511 (3) | 0.37448 (14) | 0.0211 (5) |
| H13A | 0.6233 | 0.6040 | 0.3725 | 0.025* |
| C14 | 0.47657 (16) | 0.6582 (3) | 0.29247 (14) | 0.0215 (5) |
| H14A | 0.4909 | 0.6170 | 0.2342 | 0.026* |
| C15 | 0.62115 (16) | 0.7076 (3) | 0.54930 (15) | 0.0198 (5) |
| C16 | 0.79774 (17) | 0.6225 (3) | 0.61760 (15) | 0.0258 (5) |
| H16A | 0.8590 | 0.5660 | 0.5999 | 0.039* |
| H16B | 0.7760 | 0.5480 | 0.6662 | 0.039* |
| H16C | 0.8170 | 0.7446 | 0.6431 | 0.039* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0266 (9) | 0.0302 (9) | 0.0209 (8) | 0.0058 (7) | −0.0052 (7) | −0.0085 (7) |
| O2 | 0.0427 (10) | 0.0261 (9) | 0.0284 (9) | 0.0092 (8) | −0.0087 (8) | −0.0008 (7) |
| O3 | 0.0201 (8) | 0.0284 (8) | 0.0188 (8) | 0.0022 (7) | −0.0030 (6) | −0.0014 (6) |
| O4 | 0.0283 (9) | 0.0359 (9) | 0.0183 (8) | 0.0000 (7) | 0.0019 (7) | −0.0053 (7) |
| N1 | 0.0321 (12) | 0.0302 (11) | 0.0304 (12) | 0.0010 (9) | −0.0001 (9) | −0.0020 (9) |
| C1 | 0.0267 (12) | 0.0343 (13) | 0.0168 (11) | 0.0013 (10) | −0.0059 (9) | −0.0066 (9) |
| C2 | 0.0238 (11) | 0.0199 (11) | 0.0203 (11) | 0.0008 (9) | 0.0038 (9) | 0.0003 (9) |
| C3 | 0.0204 (11) | 0.0224 (11) | 0.0171 (11) | −0.0025 (9) | 0.0033 (9) | −0.0003 (9) |
| C4 | 0.0203 (11) | 0.0193 (10) | 0.0213 (11) | 0.0015 (9) | 0.0035 (9) | 0.0018 (9) |
| C5 | 0.0204 (11) | 0.0201 (11) | 0.0175 (10) | −0.0030 (9) | 0.0062 (9) | −0.0013 (9) |
| C6 | 0.0166 (10) | 0.0229 (11) | 0.0155 (10) | −0.0017 (9) | 0.0052 (9) | 0.0000 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.0196 (11) | 0.0210 (11) | 0.0205 (11) | 0.0022 (9) | 0.0032 (9) | 0.0002 (9) |
| C8 | 0.0234 (11) | 0.0201 (11) | 0.0197 (11) | 0.0001 (9) | 0.0037 (9) | −0.0026 (9) |
| C9 | 0.0209 (11) | 0.0168 (10) | 0.0176 (10) | −0.0035 (9) | 0.0019 (9) | −0.0006 (8) |
| C10 | 0.0191 (11) | 0.0207 (11) | 0.0191 (11) | −0.0001 (9) | 0.0036 (9) | −0.0021 (9) |
| C11 | 0.0251 (12) | 0.0202 (11) | 0.0177 (11) | 0.0001 (9) | 0.0055 (9) | −0.0028 (8) |
| C12 | 0.0205 (11) | 0.0163 (10) | 0.0181 (11) | −0.0032 (9) | 0.0014 (9) | 0.0014 (8) |
| C13 | 0.0187 (11) | 0.0243 (12) | 0.0202 (11) | 0.0001 (9) | 0.0044 (9) | −0.0008 (9) |
| C14 | 0.0218 (11) | 0.0274 (12) | 0.0162 (10) | −0.0021 (9) | 0.0060 (9) | −0.0048 (9) |
| C15 | 0.0227 (12) | 0.0151 (10) | 0.0204 (11) | −0.0042 (9) | 0.0023 (9) | 0.0021 (9) |
| C16 | 0.0220 (12) | 0.0291 (12) | 0.0216 (11) | 0.0012 (10) | −0.0047 (9) | 0.0014 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.332 (2) | C6—C9 | 1.483 (3) |
| O1—C1 | 1.442 (2) | C7—C8 | 1.379 (3) |
| O2—C2 | 1.211 (2) | C7—H7A | 0.9500 |
| O3—C15 | 1.342 (2) | C8—H8A | 0.9500 |
| O3—C16 | 1.443 (2) | C9—C14 | 1.396 (3) |
| O4—C15 | 1.204 (2) | C9—C10 | 1.399 (3) |
| N1—C5 | 1.379 (3) | C10—C11 | 1.383 (3) |
| N1—H1NB | 0.877 (5) | C10—H10A | 0.9500 |
| N1—H1NA | 0.879 (5) | C11—C12 | 1.388 (3) |
| C1—H1C | 0.9800 | C11—H11A | 0.9500 |
| C1—H1B | 0.9800 | C12—C13 | 1.391 (3) |
| C1—H1A | 0.9800 | C12—C15 | 1.485 (3) |
| C2—C3 | 1.482 (3) | C13—C14 | 1.376 (3) |
| C3—C4 | 1.388 (3) | C13—H13A | 0.9500 |
| C3—C8 | 1.390 (3) | C14—H14A | 0.9500 |
| C4—C5 | 1.397 (3) | C16—H16A | 0.9800 |
| C4—H4A | 0.9500 | C16—H16B | 0.9800 |
| C5—C6 | 1.413 (3) | C16—H16C | 0.9800 |
| C6—C7 | 1.399 (3) | | |
| | | | |
| C2—O1—C1 | 116.20 (16) | C7—C8—H8A | 120.6 |
| C15—O3—C16 | 115.67 (16) | C3—C8—H8A | 120.6 |
| C5—N1—H1NB | 113.4 (17) | C14—C9—C10 | 118.07 (19) |
| C5—N1—H1NA | 117.6 (17) | C14—C9—C6 | 118.81 (18) |
| H1NB—N1—H1NA | 120 (2) | C10—C9—C6 | 123.01 (19) |
| O1—C1—H1C | 109.5 | C11—C10—C9 | 120.68 (19) |
| O1—C1—H1B | 109.5 | C11—C10—H10A | 119.7 |
| H1C—C1—H1B | 109.5 | C9—C10—H10A | 119.7 |
| O1—C1—H1A | 109.5 | C10—C11—C12 | 120.51 (18) |
| H1C—C1—H1A | 109.5 | C10—C11—H11A | 119.7 |
| H1B—C1—H1A | 109.5 | C12—C11—H11A | 119.7 |
| O2—C2—O1 | 122.46 (19) | C11—C12—C13 | 119.20 (19) |
| O2—C2—C3 | 125.17 (19) | C11—C12—C15 | 119.80 (18) |
| O1—C2—C3 | 112.37 (17) | C13—C12—C15 | 121.00 (19) |
| C4—C3—C8 | 120.21 (18) | C14—C13—C12 | 120.3 (2) |

| | | | |
|---|---|---|---|
| C4—C3—C2 | 117.99 (18) | C14—C13—H13A | 119.9 |
| C8—C3—C2 | 121.80 (18) | C12—C13—H13A | 119.9 |
| C3—C4—C5 | 121.22 (19) | C13—C14—C9 | 121.25 (18) |
| C3—C4—H4A | 119.4 | C13—C14—H14A | 119.4 |
| C5—C4—H4A | 119.4 | C9—C14—H14A | 119.4 |
| N1—C5—C4 | 117.78 (19) | O4—C15—O3 | 123.07 (19) |
| N1—C5—C6 | 123.24 (18) | O4—C15—C12 | 125.2 (2) |
| C4—C5—C6 | 118.97 (18) | O3—C15—C12 | 111.68 (17) |
| C7—C6—C5 | 118.25 (18) | O3—C16—H16A | 109.5 |
| C7—C6—C9 | 118.09 (18) | O3—C16—H16B | 109.5 |
| C5—C6—C9 | 123.65 (18) | H16A—C16—H16B | 109.5 |
| C8—C7—C6 | 122.60 (19) | O3—C16—H16C | 109.5 |
| C8—C7—H7A | 118.7 | H16A—C16—H16C | 109.5 |
| C6—C7—H7A | 118.7 | H16B—C16—H16C | 109.5 |
| C7—C8—C3 | 118.75 (19) | | |

| | | | |
|---|---|---|---|
| C1—O1—C2—O2 | 2.4 (3) | C5—C6—C9—C14 | −136.4 (2) |
| C1—O1—C2—C3 | −177.63 (17) | C7—C6—C9—C10 | −133.4 (2) |
| O2—C2—C3—C4 | −0.5 (3) | C5—C6—C9—C10 | 47.5 (3) |
| O1—C2—C3—C4 | 179.46 (17) | C14—C9—C10—C11 | −0.5 (3) |
| O2—C2—C3—C8 | −179.8 (2) | C6—C9—C10—C11 | 175.68 (19) |
| O1—C2—C3—C8 | 0.2 (3) | C9—C10—C11—C12 | 0.1 (3) |
| C8—C3—C4—C5 | 1.0 (3) | C10—C11—C12—C13 | 0.0 (3) |
| C2—C3—C4—C5 | −178.30 (18) | C10—C11—C12—C15 | 179.73 (18) |
| C3—C4—C5—N1 | −179.38 (19) | C11—C12—C13—C14 | 0.3 (3) |
| C3—C4—C5—C6 | −0.6 (3) | C15—C12—C13—C14 | −179.44 (18) |
| N1—C5—C6—C7 | 178.43 (19) | C12—C13—C14—C9 | −0.7 (3) |
| C4—C5—C6—C7 | −0.2 (3) | C10—C9—C14—C13 | 0.8 (3) |
| N1—C5—C6—C9 | −2.5 (3) | C6—C9—C14—C13 | −175.55 (18) |
| C4—C5—C6—C9 | 178.85 (18) | C16—O3—C15—O4 | 1.7 (3) |
| C5—C6—C7—C8 | 0.8 (3) | C16—O3—C15—C12 | −179.20 (16) |
| C9—C6—C7—C8 | −178.35 (19) | C11—C12—C15—O4 | −2.0 (3) |
| C6—C7—C8—C3 | −0.5 (3) | C13—C12—C15—O4 | 177.7 (2) |
| C4—C3—C8—C7 | −0.4 (3) | C11—C12—C15—O3 | 178.96 (18) |
| C2—C3—C8—C7 | 178.82 (19) | C13—C12—C15—O3 | −1.3 (3) |
| C7—C6—C9—C14 | 42.7 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*NB*···O2$^{i}$ | 0.88 (1) | 2.54 (2) | 3.304 (3) | 146 (2) |
| N1—H1*NA*···O4$^{ii}$ | 0.88 (1) | 2.33 (1) | 3.147 (2) | 155 (2) |
| C4—H4*A*···O2$^{i}$ | 0.95 | 2.44 | 3.301 (3) | 150 |

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