

4-[4-[(*E*)-(2-Hydroxyphenyl)imino-methylphenoxy]benzene-1,2-dicarbonitrile

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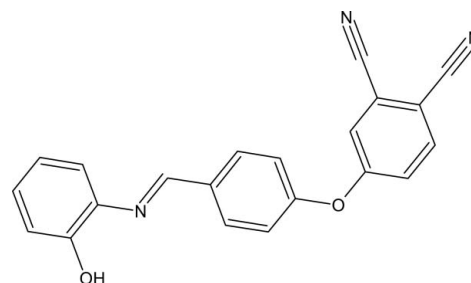
Received 24 January 2012; accepted 27 January 2012

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.052; wR factor = 0.148; data-to-parameter ratio = 17.1.

The asymmetric unit of the title compound, $\text{C}_{21}\text{H}_{13}\text{N}_3\text{O}_2$, contains two independent molecules with a similar structure. In one molecule, the central benzene ring is oriented with respect to the terminal benzene rings at 27.23 (7) and 67.96 (7)°; in the other molecule, the corresponding dihedral angles are 12.42 (7) and 64.55 (7)°. In both molecules, there is a short $\text{O}-\text{H}\cdots\text{N}$ interaction involving the OH group and the adjacent N atom. In the crystal, there are $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds, and $\text{C}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ interactions linking the molecules to form a three-dimensional network. $\pi-\pi$ stacking between the pyridine and benzene rings and between the benzene rings [centroid-centroid distances = 3.989 (2), 3.705 (2) and 3.607 (2) Å] may further stabilize the structure. A weak $\text{C}-\text{H}\cdots\pi$ interaction is present in the crystal.

Related literature

For the use of phthalonitriles for preparing symmetrically and unsymmetrically substituted phthalocyanine complexes, see: Leznoff & Lever (1996). For the widespread applications of phthalocyanines in photodynamic therapy, see: Kartal *et al.* (2006); Tüfekçi *et al.* (2009). For the fundamental optical and electronic properties of phthalocyanines, see: McKeown (1998). For related structures, see: Tuncer *et al.* (2012); Tüfekçi *et al.* (2009); Yazıcı *et al.* (2009); Kartal *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{13}\text{N}_3\text{O}_2$

$M_r = 339.34$

Triclinic, $P\bar{1}$

$a = 9.842$ (3) Å

$b = 13.448$ (4) Å

$c = 14.061$ (4) Å

$\alpha = 109.940$ (15)°

$\beta = 96.937$ (16)°

$\gamma = 104.182$ (15)°

$V = 1652.9$ (9) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 0.09$ mm⁻¹

$T = 100$ K

$0.40 \times 0.23 \times 0.13$ mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{\min} = 0.975$, $T_{\max} = 0.988$

28993 measured reflections

8180 independent reflections

4415 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.059$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.148$

$S = 1.01$

8180 reflections

478 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.25$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

C_g is the centroid of the C8–C13 ring.

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{O1}-\text{H1}\cdots\text{N1}$ | 0.84 | 2.24 | 2.713 (3) | 116 |
| $\text{O1}-\text{H1}\cdots\text{N2}^{\text{i}}$ | 0.84 | 2.50 | 2.993 (3) | 119 |
| $\text{O1}'-\text{H1}'\cdots\text{N1}'$ | 0.84 | 2.18 | 2.659 (3) | 116 |
| $\text{O1}'-\text{H1}'\cdots\text{N3}^{\text{i}}$ | 0.84 | 2.39 | 2.948 (3) | 125 |
| $\text{C3}'-\text{H3}'\cdots\text{N3}^{\text{ii}}$ | 0.95 | 2.52 | 3.344 (4) | 145 |
| $\text{C5}-\text{H5}\cdots\text{O1}^{\text{iii}}$ | 0.95 | 2.40 | 3.180 (3) | 139 |
| $\text{C12}-\text{H12}\cdots\text{O1}^{\text{iv}}$ | 0.95 | 2.35 | 3.214 (3) | 151 |
| $\text{C6}'-\text{H6}'\cdots\text{Cg}^{\text{v}}$ | 0.95 | 2.93 | 3.785 (3) | 151 |

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON (Spek, 2009).

The authors are indebted to Anadolu University and the Medicinal Plants and Medicine Research Centre of Anadolu

University, Eskişehir, Turkey, for the use of the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5458).

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supplementary materials

Acta Cryst. (2012). E68, o565–o566 [doi:10.1107/S1600536812003649]

4-{4-[(*E*)-(2-Hydroxyphenyl)iminomethyl]phenoxy}benzene-1,2-dicarbonitrile**Hülya Tuncer, Ahmet Orhan Görgülü and Tuncer Hökelek****Comment**

Phthalonitriles are used for preparing symmetrically and unsymmetrically substituted phthalocyanine complexes (Leznoff & Lever, 1996). Phthalocyanines have been of great interest to chemists, physicists and industrial scientists.

Phthalocyanines have currently been the topic of research because of their wide application fields, such as thin film fabrication, organic pigments, chemical sensors, electrochromic display devices, molecular epitaxial deposition and composites, liquid crystals, photovoltaic cells self-assembled materials. In addition to their extensive use as dyes and pigments, phthalocyanines have found widespread application, in photodynamic therapy (Kartal *et al.*, 2006; Tüfekçi *et al.*, 2009). The fundamental optical and electronic properties of these materials are explained and their potential in non-linear optics, optical data storage, electronic sensors, xerography, solar energy conversion, nuclear chemistry, molecular magnetism, electrochromic displays and heterogeneous catalysis is evaluated by McKeown (1998).

The structures of some phthalonitrile derivatives, C₁₃H₈N₂O₂ (Tuncer *et al.*, 2012), C₂₁H₁₂CIN₃O (Tüfekçi *et al.*, 2009), C₂₃H₁₇N₃O₂ (Yazıcı *et al.*, 2009) and C₁₅H₈N₂O₂ (Kartal *et al.*, 2006) have also been determined.

The asymmetric unit of the title compound, (Fig. 1) contains two crystallographically independent molecules, and the bond lengths are close to standard values (Allen *et al.*, 1987).

The dihedral angles between the hydroxyphenyl rings [A (C1—C6) and A' (C1'—C6')] and the benzene [B (C8—C13), C (C14—C19) and B' (C8'—C13'), C' (C14'—C19')] rings are A/B = 27.23 (7), A/C = 41.88 (7) and A'/B' = 12.42 (7), A'/C' = 73.19 (7) °, while those between the benzene rings B, C and B', C' are B/C = 67.96 (7) and B'/C' = 64.55 (7) °.

In the crystal, intermolecular O—H...N, C—H...O and C—H...N hydrogen bonds (Table 1) link the molecules into a three-dimensional network (Fig. 2), in which they may be effective in the stabilization of the structure. π - π Contacts between the pyridine and benzene rings and between the benzene rings, Cg1—Cg2ⁱ, Cg1—Cg6 and Cg5—Cg5ⁱⁱ [symmetry codes: (i) 1 - x, 1 - y, 1 - z, (ii) -x, -y, -z, where Cg1, Cg2, Cg5 and Cg6 are the centroids of the rings A (C1—C6), B (C8—C13), B' (C8'—C13') and C' (C14'—C19'), respectively] may further stabilize the structure, with centroid-centroid distances of 3.989 (2), 3.705 (2) and 3.607 (2) Å]. There also exists a weak C—H... π interaction (Table 1).

Experimental

The title compound has been prepared in two steps. In the first step; 4-hydroxybenzaldehyde (1.86 g, 15.2 mmol) and 4-nitrophthalonitrile (2.64 g, 15.2 mmol) were heated at 353 K in dry DMF (20 ml) with stirring under argon atmosphere. Then, dry fine powdered potassium carbonate (6.00 g, 43.47 mmol) was added in portions (14 × 3.1 mmol) every 10 min. The mixture was heated for a further 18 h. After cooling, the mixture was added into ice-water (200 g). The product was filtered off and washed with NaOH solution (10% w/w) and water until the filtrate was neutral. In the second step; 4-(4-formylphenoxy)benzene-1,2-dicarbonitrile (1.88 g, 7.6 mmol), the product obtained in the first step, and 2-hydroxyaniline (0.83 g, 7.6 mmol) were reacted at 333 K for 4 h in absolute ethanol (50 ml). Recrystallization from absolute ethanol gave a yellow product (yield: 1.55 g, 60%). Single crystals suitable for X-ray diffraction measurement were obtained by

slow evaporation of the solution in ethanol (m.p. 433 K).

Refinement

Atoms H7 and H7' (for CH) were located in a difference Fourier map and were refined by applying restraints. The remaining H-atoms were positioned geometrically with O—H = 0.84 Å for OH H-atoms, and C—H = 0.95 Å for aromatic H-atoms, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{C}, \text{O})$, where $k = 1.5$ for OH H-atoms and $k = 1.2$ for aromatic H-atoms.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

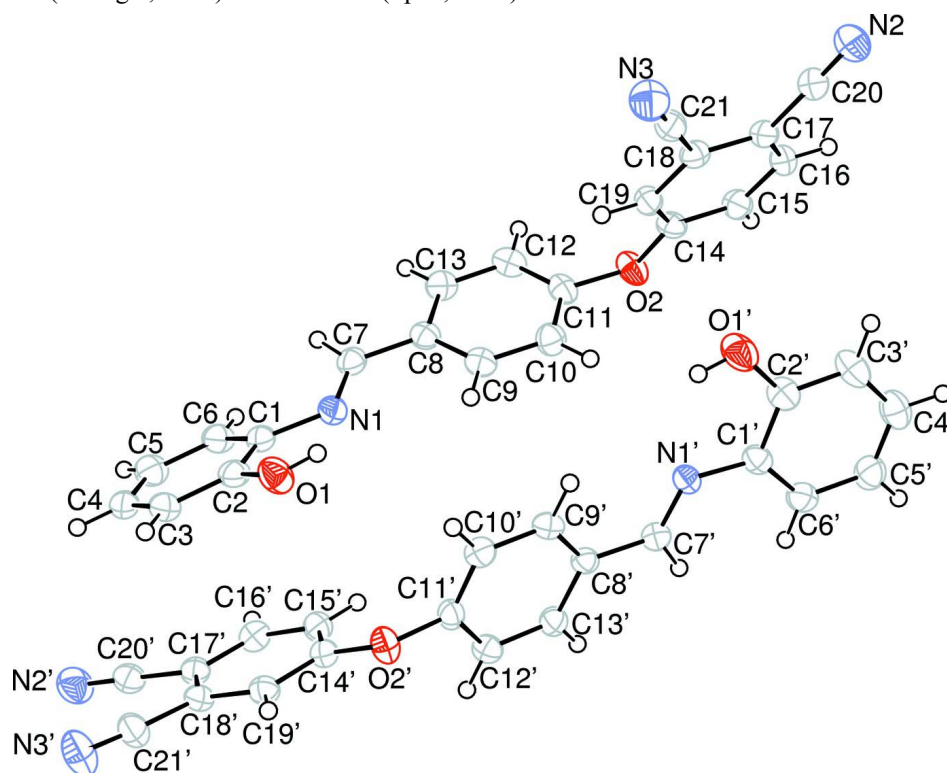
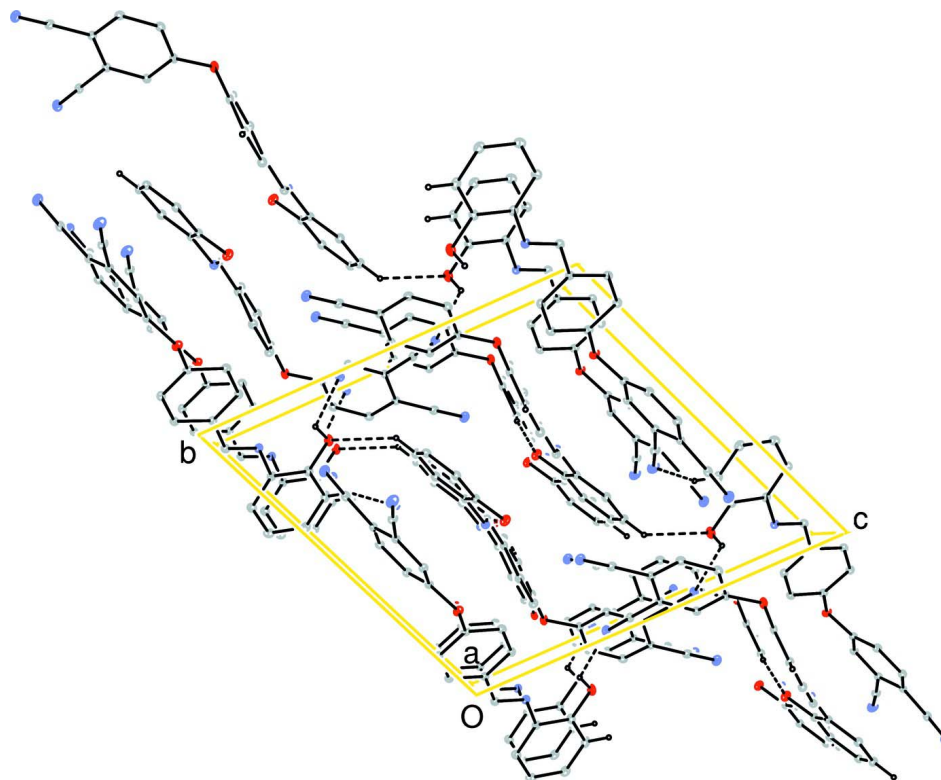


Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

A partial packing diagram. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

4-{4-[(*E*)-(2-Hydroxyphenyl)iminomethyl]phenoxy}benzene-1,2-dicarbonitrile

Crystal data

$C_{21}H_{13}N_3O_2$

$M_r = 339.34$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 9.842\ (3)\ \text{\AA}$

$b = 13.448\ (4)\ \text{\AA}$

$c = 14.061\ (4)\ \text{\AA}$

$\alpha = 109.940\ (15)^\circ$

$\beta = 96.937\ (16)^\circ$

$\gamma = 104.182\ (15)^\circ$

$V = 1652.9\ (9)\ \text{\AA}^3$

$Z = 4$

$F(000) = 704$

$D_x = 1.364\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 4598 reflections

$\theta = 2.3\text{--}23.5^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, yellow

$0.40 \times 0.23 \times 0.13\ \text{mm}$

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.975$, $T_{\max} = 0.988$

28993 measured reflections

8180 independent reflections

4415 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.059$

$\theta_{\max} = 28.5^\circ$, $\theta_{\min} = 1.6^\circ$

$h = -12 \rightarrow 13$

$k = -17 \rightarrow 17$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.148$

$S = 1.01$

8180 reflections

478 parameters

1 restraint

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

$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.3399P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0067 (11)

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|--------------|----------------------------------|
| O1 | 0.18465 (16) | 0.42838 (13) | 0.39648 (13) | 0.0415 (4) |
| H1 | 0.2341 | 0.3847 | 0.3902 | 0.062* |
| O2 | 0.81989 (17) | 0.09971 (13) | 0.27981 (12) | 0.0363 (4) |
| N1 | 0.4497 (2) | 0.44136 (14) | 0.35611 (13) | 0.0307 (4) |
| N2 | 0.8274 (2) | -0.23636 (18) | 0.53937 (17) | 0.0523 (6) |
| N3 | 0.6366 (2) | -0.00505 (17) | 0.62696 (17) | 0.0470 (6) |
| C1 | 0.3989 (2) | 0.53409 (17) | 0.36774 (16) | 0.0296 (5) |
| C2 | 0.2600 (2) | 0.52160 (18) | 0.38515 (16) | 0.0315 (5) |
| C3 | 0.1965 (3) | 0.60425 (19) | 0.39298 (17) | 0.0342 (6) |
| H3 | 0.1024 | 0.5953 | 0.4054 | 0.041* |
| C4 | 0.2708 (3) | 0.69943 (19) | 0.38268 (17) | 0.0376 (6) |
| H4 | 0.2274 | 0.7563 | 0.3878 | 0.045* |
| C5 | 0.4085 (3) | 0.71348 (19) | 0.36498 (18) | 0.0396 (6) |
| H5 | 0.4592 | 0.7798 | 0.3584 | 0.048* |
| C6 | 0.4720 (3) | 0.63074 (18) | 0.35691 (17) | 0.0351 (6) |
| H6 | 0.5659 | 0.6400 | 0.3439 | 0.042* |
| C7 | 0.5842 (3) | 0.45413 (19) | 0.37209 (17) | 0.0312 (5) |
| H7 | 0.655 (2) | 0.5282 (18) | 0.3985 (16) | 0.028 (6)* |
| C8 | 0.6422 (2) | 0.36070 (18) | 0.35210 (16) | 0.0295 (5) |
| C9 | 0.5531 (2) | 0.25160 (18) | 0.31442 (17) | 0.0338 (5) |
| H9 | 0.4519 | 0.2370 | 0.3045 | 0.041* |
| C10 | 0.6099 (2) | 0.16393 (19) | 0.29116 (18) | 0.0348 (6) |
| H10 | 0.5486 | 0.0894 | 0.2639 | 0.042* |
| C11 | 0.7580 (2) | 0.18678 (19) | 0.30826 (17) | 0.0305 (5) |

| | | | | |
|------|---------------|---------------|---------------|------------|
| C12 | 0.8491 (2) | 0.29320 (19) | 0.34658 (17) | 0.0339 (5) |
| H12 | 0.9503 | 0.3073 | 0.3584 | 0.041* |
| C13 | 0.7904 (2) | 0.37987 (19) | 0.36777 (17) | 0.0344 (5) |
| H13 | 0.8525 | 0.4541 | 0.3936 | 0.041* |
| C14 | 0.8182 (2) | 0.03424 (18) | 0.33583 (16) | 0.0290 (5) |
| C15 | 0.8887 (2) | -0.04502 (18) | 0.30548 (17) | 0.0334 (5) |
| H15 | 0.9354 | -0.0505 | 0.2494 | 0.040* |
| C16 | 0.8912 (2) | -0.11571 (18) | 0.35649 (17) | 0.0345 (6) |
| H16 | 0.9389 | -0.1703 | 0.3351 | 0.041* |
| C17 | 0.8244 (2) | -0.10786 (17) | 0.43904 (17) | 0.0300 (5) |
| C18 | 0.7555 (2) | -0.02651 (17) | 0.47002 (16) | 0.0285 (5) |
| C19 | 0.7513 (2) | 0.04448 (17) | 0.41867 (16) | 0.0282 (5) |
| H19 | 0.7036 | 0.0991 | 0.4397 | 0.034* |
| C20 | 0.8271 (3) | -0.18017 (19) | 0.49414 (19) | 0.0373 (6) |
| C21 | 0.6881 (3) | -0.01535 (18) | 0.55668 (18) | 0.0332 (5) |
| O1' | 0.48536 (19) | -0.14517 (14) | 0.22704 (13) | 0.0492 (5) |
| H1' | 0.4479 | -0.0949 | 0.2288 | 0.074* |
| O2' | -0.00214 (16) | 0.24585 (12) | 0.13213 (12) | 0.0353 (4) |
| N1' | 0.37253 (18) | -0.08750 (14) | 0.07998 (14) | 0.0281 (4) |
| N2' | 0.1000 (2) | 0.76703 (18) | 0.15817 (17) | 0.0486 (6) |
| N3' | -0.2416 (2) | 0.60508 (18) | 0.22270 (19) | 0.0549 (6) |
| C1' | 0.4335 (2) | -0.17435 (18) | 0.04730 (17) | 0.0304 (5) |
| C2' | 0.4886 (2) | -0.20314 (19) | 0.12727 (18) | 0.0354 (6) |
| C3' | 0.5463 (3) | -0.2899 (2) | 0.1072 (2) | 0.0429 (6) |
| H3' | 0.5834 | -0.3086 | 0.1621 | 0.052* |
| C4' | 0.5493 (3) | -0.3490 (2) | 0.0066 (2) | 0.0422 (6) |
| H4' | 0.5865 | -0.4101 | -0.0079 | 0.051* |
| C5' | 0.4992 (2) | -0.3211 (2) | -0.0738 (2) | 0.0402 (6) |
| H5' | 0.5044 | -0.3614 | -0.1427 | 0.048* |
| C6' | 0.4417 (2) | -0.23440 (19) | -0.05337 (18) | 0.0364 (6) |
| H6' | 0.4071 | -0.2153 | -0.1087 | 0.044* |
| C7' | 0.3167 (2) | -0.05176 (18) | 0.01768 (18) | 0.0292 (5) |
| H7' | 0.317 (2) | -0.0807 (17) | -0.0559 (13) | 0.040 (7)* |
| C8' | 0.2428 (2) | 0.03159 (17) | 0.05018 (16) | 0.0263 (5) |
| C9' | 0.2161 (2) | 0.06816 (17) | 0.14996 (16) | 0.0293 (5) |
| H9' | 0.2504 | 0.0410 | 0.1991 | 0.035* |
| C10' | 0.1404 (2) | 0.14318 (18) | 0.17726 (17) | 0.0309 (5) |
| H10' | 0.1238 | 0.1690 | 0.2454 | 0.037* |
| C11' | 0.0888 (2) | 0.18043 (17) | 0.10454 (17) | 0.0293 (5) |
| C12' | 0.1125 (2) | 0.14594 (18) | 0.00537 (17) | 0.0333 (5) |
| H12' | 0.0766 | 0.1727 | -0.0436 | 0.040* |
| C13' | 0.1897 (2) | 0.07143 (17) | -0.02080 (17) | 0.0310 (5) |
| H13' | 0.2070 | 0.0469 | -0.0888 | 0.037* |
| C14' | 0.0287 (2) | 0.34959 (17) | 0.12998 (16) | 0.0286 (5) |
| C15' | 0.1547 (2) | 0.40575 (18) | 0.11284 (17) | 0.0321 (5) |
| H15' | 0.2274 | 0.3712 | 0.0987 | 0.038* |
| C16' | 0.1749 (2) | 0.51264 (18) | 0.11636 (17) | 0.0326 (5) |
| H16' | 0.2608 | 0.5506 | 0.1030 | 0.039* |
| C17' | 0.0709 (2) | 0.56471 (17) | 0.13924 (16) | 0.0294 (5) |

| | | | | |
|------|-------------|--------------|--------------|------------|
| C18' | -0.0559 (2) | 0.50719 (18) | 0.15786 (16) | 0.0291 (5) |
| C19' | -0.0774 (2) | 0.39984 (18) | 0.15198 (16) | 0.0295 (5) |
| H19' | -0.1644 | 0.3605 | 0.1629 | 0.035* |
| C20' | 0.0907 (2) | 0.6771 (2) | 0.14833 (17) | 0.0355 (6) |
| C21' | -0.1606 (3) | 0.56133 (19) | 0.19089 (19) | 0.0372 (6) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|-------------|-------------|-------------|--------------|-------------|
| O1 | 0.0353 (10) | 0.0367 (9) | 0.0574 (11) | 0.0106 (8) | 0.0084 (8) | 0.0249 (8) |
| O2 | 0.0479 (10) | 0.0463 (10) | 0.0352 (9) | 0.0280 (8) | 0.0222 (8) | 0.0265 (8) |
| N1 | 0.0350 (11) | 0.0306 (10) | 0.0283 (10) | 0.0125 (9) | 0.0059 (8) | 0.0123 (8) |
| N2 | 0.0672 (16) | 0.0409 (12) | 0.0511 (14) | 0.0164 (12) | 0.0019 (12) | 0.0245 (11) |
| N3 | 0.0592 (15) | 0.0501 (14) | 0.0409 (13) | 0.0184 (12) | 0.0200 (11) | 0.0246 (11) |
| C1 | 0.0345 (13) | 0.0285 (12) | 0.0237 (11) | 0.0095 (10) | 0.0015 (9) | 0.0092 (9) |
| C2 | 0.0344 (13) | 0.0310 (12) | 0.0268 (12) | 0.0073 (11) | 0.0007 (10) | 0.0124 (10) |
| C3 | 0.0359 (13) | 0.0378 (13) | 0.0296 (12) | 0.0149 (11) | 0.0034 (10) | 0.0125 (11) |
| C4 | 0.0513 (16) | 0.0330 (13) | 0.0265 (12) | 0.0179 (12) | -0.0017 (11) | 0.0089 (10) |
| C5 | 0.0459 (15) | 0.0337 (13) | 0.0389 (14) | 0.0082 (12) | 0.0024 (11) | 0.0188 (11) |
| C6 | 0.0336 (13) | 0.0362 (13) | 0.0344 (13) | 0.0083 (11) | 0.0029 (10) | 0.0155 (11) |
| C7 | 0.0371 (14) | 0.0294 (13) | 0.0250 (12) | 0.0082 (11) | 0.0038 (10) | 0.0105 (10) |
| C8 | 0.0331 (13) | 0.0341 (13) | 0.0252 (11) | 0.0109 (10) | 0.0080 (9) | 0.0152 (10) |
| C9 | 0.0296 (13) | 0.0374 (13) | 0.0350 (13) | 0.0111 (11) | 0.0053 (10) | 0.0147 (11) |
| C10 | 0.0354 (14) | 0.0316 (13) | 0.0385 (14) | 0.0094 (11) | 0.0093 (11) | 0.0151 (11) |
| C11 | 0.0398 (14) | 0.0383 (13) | 0.0267 (12) | 0.0208 (11) | 0.0160 (10) | 0.0197 (10) |
| C12 | 0.0281 (12) | 0.0452 (14) | 0.0359 (13) | 0.0124 (11) | 0.0113 (10) | 0.0226 (11) |
| C13 | 0.0327 (13) | 0.0349 (13) | 0.0350 (13) | 0.0066 (11) | 0.0062 (10) | 0.0160 (11) |
| C14 | 0.0317 (12) | 0.0344 (12) | 0.0253 (12) | 0.0118 (10) | 0.0068 (9) | 0.0156 (10) |
| C15 | 0.0372 (13) | 0.0386 (13) | 0.0277 (12) | 0.0179 (11) | 0.0104 (10) | 0.0113 (10) |
| C16 | 0.0395 (14) | 0.0311 (12) | 0.0334 (13) | 0.0180 (11) | 0.0055 (11) | 0.0090 (10) |
| C17 | 0.0322 (12) | 0.0271 (12) | 0.0284 (12) | 0.0073 (10) | 0.0006 (10) | 0.0111 (10) |
| C18 | 0.0297 (12) | 0.0294 (12) | 0.0244 (11) | 0.0062 (10) | 0.0044 (9) | 0.0105 (10) |
| C19 | 0.0319 (12) | 0.0293 (12) | 0.0266 (12) | 0.0124 (10) | 0.0090 (9) | 0.0117 (10) |
| C20 | 0.0418 (15) | 0.0303 (13) | 0.0370 (14) | 0.0103 (11) | 0.0020 (11) | 0.0123 (11) |
| C21 | 0.0400 (14) | 0.0315 (13) | 0.0314 (13) | 0.0114 (11) | 0.0073 (11) | 0.0160 (11) |
| O1' | 0.0714 (13) | 0.0581 (11) | 0.0373 (10) | 0.0373 (10) | 0.0189 (9) | 0.0272 (9) |
| O2' | 0.0333 (9) | 0.0301 (9) | 0.0484 (10) | 0.0135 (7) | 0.0155 (7) | 0.0175 (8) |
| N1' | 0.0276 (10) | 0.0278 (10) | 0.0324 (10) | 0.0103 (8) | 0.0067 (8) | 0.0143 (8) |
| N2' | 0.0527 (14) | 0.0440 (13) | 0.0553 (14) | 0.0165 (11) | 0.0085 (11) | 0.0265 (11) |
| N3' | 0.0510 (14) | 0.0489 (14) | 0.0791 (18) | 0.0283 (12) | 0.0234 (13) | 0.0299 (13) |
| C1' | 0.0257 (12) | 0.0319 (12) | 0.0361 (13) | 0.0086 (10) | 0.0071 (10) | 0.0160 (11) |
| C2' | 0.0382 (14) | 0.0411 (14) | 0.0343 (14) | 0.0165 (12) | 0.0145 (11) | 0.0184 (11) |
| C3' | 0.0486 (16) | 0.0497 (15) | 0.0513 (16) | 0.0271 (13) | 0.0208 (13) | 0.0327 (13) |
| C4' | 0.0396 (15) | 0.0397 (14) | 0.0575 (17) | 0.0180 (12) | 0.0202 (13) | 0.0238 (13) |
| C5' | 0.0368 (14) | 0.0396 (14) | 0.0420 (15) | 0.0158 (12) | 0.0111 (11) | 0.0094 (12) |
| C6' | 0.0341 (13) | 0.0390 (14) | 0.0348 (13) | 0.0137 (11) | 0.0045 (10) | 0.0119 (11) |
| C7' | 0.0280 (12) | 0.0303 (12) | 0.0284 (12) | 0.0081 (10) | 0.0057 (10) | 0.0110 (10) |
| C8' | 0.0235 (11) | 0.0253 (11) | 0.0279 (12) | 0.0052 (9) | 0.0026 (9) | 0.0104 (9) |
| C9' | 0.0276 (12) | 0.0340 (12) | 0.0275 (12) | 0.0087 (10) | 0.0040 (9) | 0.0147 (10) |
| C10' | 0.0288 (12) | 0.0334 (12) | 0.0290 (12) | 0.0086 (10) | 0.0079 (10) | 0.0105 (10) |

| | | | | | | |
|------|-------------|-------------|-------------|-------------|-------------|-------------|
| C11' | 0.0253 (12) | 0.0253 (11) | 0.0356 (13) | 0.0088 (10) | 0.0067 (10) | 0.0088 (10) |
| C12' | 0.0363 (13) | 0.0334 (13) | 0.0311 (13) | 0.0116 (11) | 0.0032 (10) | 0.0144 (10) |
| C13' | 0.0359 (13) | 0.0300 (12) | 0.0271 (12) | 0.0122 (10) | 0.0067 (10) | 0.0097 (10) |
| C14' | 0.0308 (12) | 0.0263 (12) | 0.0274 (12) | 0.0090 (10) | 0.0034 (9) | 0.0095 (9) |
| C15' | 0.0291 (13) | 0.0331 (13) | 0.0332 (13) | 0.0117 (10) | 0.0074 (10) | 0.0101 (10) |
| C16' | 0.0322 (13) | 0.0334 (13) | 0.0305 (12) | 0.0071 (11) | 0.0088 (10) | 0.0116 (10) |
| C17' | 0.0338 (13) | 0.0309 (12) | 0.0246 (11) | 0.0107 (10) | 0.0049 (9) | 0.0119 (10) |
| C18' | 0.0298 (12) | 0.0322 (12) | 0.0264 (12) | 0.0124 (10) | 0.0026 (9) | 0.0117 (10) |
| C19' | 0.0253 (12) | 0.0317 (12) | 0.0304 (12) | 0.0079 (10) | 0.0053 (9) | 0.0116 (10) |
| C20' | 0.0397 (14) | 0.0377 (14) | 0.0321 (13) | 0.0133 (11) | 0.0052 (10) | 0.0171 (11) |
| C21' | 0.0366 (14) | 0.0345 (13) | 0.0455 (15) | 0.0155 (12) | 0.0092 (11) | 0.0183 (12) |

Geometric parameters (Å, °)

| | | | |
|---------|-----------|-----------|------------|
| O1—C2 | 1.362 (3) | O1'—C2' | 1.362 (3) |
| O1—H1 | 0.8400 | O1'—H1' | 0.8400 |
| O2—C11 | 1.411 (2) | O2'—C14' | 1.365 (3) |
| O2—C14 | 1.366 (2) | O2'—C11' | 1.401 (2) |
| N1—C1 | 1.420 (3) | N1'—C1' | 1.407 (3) |
| N1—C7 | 1.274 (3) | N1'—C7' | 1.265 (3) |
| N2—C20 | 1.142 (3) | C1'—C6' | 1.393 (3) |
| C1—C2 | 1.398 (3) | C2'—C1' | 1.400 (3) |
| C1—C6 | 1.390 (3) | C3'—C2' | 1.379 (3) |
| C3—C2 | 1.382 (3) | C3'—H3' | 0.9500 |
| C3—H3 | 0.9500 | C4'—C3' | 1.374 (3) |
| C4—C3 | 1.374 (3) | C4'—C5' | 1.381 (3) |
| C4—H4 | 0.9500 | C4'—H4' | 0.9500 |
| C5—C4 | 1.387 (3) | C5'—C6' | 1.377 (3) |
| C5—H5 | 0.9500 | C5'—H5' | 0.9500 |
| C6—C5 | 1.383 (3) | C6'—H6' | 0.9500 |
| C6—H6 | 0.9500 | C7'—C8' | 1.457 (3) |
| C7—H7 | 0.98 (2) | C7'—H7' | 0.974 (16) |
| C8—C7 | 1.461 (3) | C8'—C9' | 1.401 (3) |
| C8—C9 | 1.389 (3) | C8'—C13' | 1.390 (3) |
| C9—C10 | 1.383 (3) | C9'—C10' | 1.376 (3) |
| C9—H9 | 0.9500 | C9'—H9' | 0.9500 |
| C10—H10 | 0.9500 | C10'—C11' | 1.379 (3) |
| C11—C12 | 1.368 (3) | C10'—H10' | 0.9500 |
| C11—C10 | 1.386 (3) | C11'—C12' | 1.380 (3) |
| C12—C13 | 1.384 (3) | C12'—H12' | 0.9500 |
| C12—H12 | 0.9500 | C13'—C12' | 1.381 (3) |
| C13—C8 | 1.393 (3) | C13'—H13' | 0.9500 |
| C13—H13 | 0.9500 | C14'—C15' | 1.379 (3) |
| C14—C15 | 1.387 (3) | C14'—C19' | 1.387 (3) |
| C15—C16 | 1.375 (3) | C15'—C16' | 1.385 (3) |
| C15—H15 | 0.9500 | C15'—H15' | 0.9500 |
| C16—H16 | 0.9500 | C16'—C17' | 1.385 (3) |
| C17—C16 | 1.388 (3) | C16'—H16' | 0.9500 |
| C18—C17 | 1.398 (3) | C17'—C18' | 1.402 (3) |
| C18—C19 | 1.384 (3) | C17'—C20' | 1.434 (3) |

| | | | |
|-------------|-------------|----------------|-------------|
| C18—C21 | 1.437 (3) | C18'—C19' | 1.379 (3) |
| C19—C14 | 1.389 (3) | C18'—C21' | 1.436 (3) |
| C19—H19 | 0.9500 | C19'—H19' | 0.9500 |
| C20—C17 | 1.438 (3) | C20'—N2' | 1.148 (3) |
| C21—N3 | 1.147 (3) | C21'—N3' | 1.148 (3) |
| C2—O1—H1 | 109.5 | C2'—O1'—H1' | 109.5 |
| C14—O2—C11 | 120.14 (16) | C14'—O2'—C11' | 121.23 (17) |
| C7—N1—C1 | 120.25 (19) | C7'—N1'—C1' | 122.54 (19) |
| C2—C1—N1 | 115.60 (19) | C2'—C1'—N1' | 114.24 (19) |
| C6—C1—N1 | 125.4 (2) | C6'—C1'—N1' | 127.7 (2) |
| C6—C1—C2 | 118.8 (2) | C6'—C1'—C2' | 118.0 (2) |
| O1—C2—C1 | 120.78 (19) | O1'—C2'—C1' | 119.9 (2) |
| O1—C2—C3 | 118.4 (2) | O1'—C2'—C3' | 118.8 (2) |
| C3—C2—C1 | 120.8 (2) | C3'—C2'—C1' | 121.3 (2) |
| C2—C3—H3 | 120.3 | C2'—C3'—H3' | 120.5 |
| C4—C3—C2 | 119.4 (2) | C4'—C3'—C2' | 119.1 (2) |
| C4—C3—H3 | 120.3 | C4'—C3'—H3' | 120.5 |
| C3—C4—C5 | 120.7 (2) | C3'—C4'—C5' | 121.2 (2) |
| C3—C4—H4 | 119.6 | C3'—C4'—H4' | 119.4 |
| C5—C4—H4 | 119.6 | C5'—C4'—H4' | 119.4 |
| C4—C5—H5 | 120.1 | C4'—C5'—H5' | 120.2 |
| C6—C5—C4 | 119.9 (2) | C6'—C5'—C4' | 119.5 (2) |
| C6—C5—H5 | 120.1 | C6'—C5'—H5' | 120.2 |
| C1—C6—H6 | 119.9 | C1'—C6'—H6' | 119.5 |
| C5—C6—C1 | 120.3 (2) | C5'—C6'—C1' | 120.9 (2) |
| C5—C6—H6 | 119.9 | C5'—C6'—H6' | 119.5 |
| N1—C7—C8 | 122.6 (2) | N1'—C7'—C8' | 122.4 (2) |
| N1—C7—H7 | 121.4 (12) | N1'—C7'—H7' | 121.7 (13) |
| C8—C7—H7 | 116.0 (12) | C8'—C7'—H7' | 115.8 (13) |
| C9—C8—C7 | 121.7 (2) | C9'—C8'—C7' | 121.56 (19) |
| C9—C8—C13 | 118.4 (2) | C13'—C8'—C7' | 119.66 (19) |
| C13—C8—C7 | 119.9 (2) | C13'—C8'—C9' | 118.66 (19) |
| C8—C9—H9 | 119.6 | C8'—C9'—H9' | 119.8 |
| C10—C9—C8 | 120.8 (2) | C10'—C9'—C8' | 120.5 (2) |
| C10—C9—H9 | 119.6 | C10'—C9'—H9' | 119.8 |
| C9—C10—C11 | 118.8 (2) | C9'—C10'—C11' | 119.2 (2) |
| C9—C10—H10 | 120.6 | C9'—C10'—H10' | 120.4 |
| C11—C10—H10 | 120.6 | C11'—C10'—H10' | 120.4 |
| C10—C11—O2 | 120.6 (2) | C10'—C11'—O2' | 116.81 (19) |
| C12—C11—O2 | 117.4 (2) | C10'—C11'—C12' | 122.0 (2) |
| C12—C11—C10 | 121.9 (2) | C12'—C11'—O2' | 120.9 (2) |
| C11—C12—C13 | 118.5 (2) | C11'—C12'—C13' | 118.3 (2) |
| C11—C12—H12 | 120.8 | C11'—C12'—H12' | 120.9 |
| C13—C12—H12 | 120.8 | C13'—C12'—H12' | 120.9 |
| C8—C13—H13 | 119.3 | C8'—C13'—H13' | 119.3 |
| C12—C13—C8 | 121.5 (2) | C12'—C13'—C8' | 121.4 (2) |
| C12—C13—H13 | 119.3 | C12'—C13'—H13' | 119.3 |
| O2—C14—C15 | 115.88 (19) | O2'—C14'—C15' | 125.50 (19) |

| | | | |
|-----------------|--------------|---------------------|--------------|
| O2—C14—C19 | 123.40 (19) | O2'—C14'—C19' | 113.92 (19) |
| C15—C14—C19 | 120.7 (2) | C15'—C14'—C19' | 120.5 (2) |
| C14—C15—H15 | 120.0 | C14'—C15'—C16' | 119.8 (2) |
| C16—C15—C14 | 120.1 (2) | C14'—C15'—H15' | 120.1 |
| C16—C15—H15 | 120.0 | C16'—C15'—H15' | 120.1 |
| C15—C16—C17 | 120.4 (2) | C15'—C16'—C17' | 120.5 (2) |
| C15—C16—H16 | 119.8 | C15'—C16'—H16' | 119.7 |
| C17—C16—H16 | 119.8 | C17'—C16'—H16' | 119.7 |
| C16—C17—C18 | 119.0 (2) | C16'—C17'—C18' | 119.0 (2) |
| C16—C17—C20 | 121.3 (2) | C16'—C17'—C20' | 122.2 (2) |
| C18—C17—C20 | 119.7 (2) | C18'—C17'—C20' | 118.8 (2) |
| C19—C18—C17 | 121.0 (2) | C17'—C18'—C21' | 120.8 (2) |
| C17—C18—C21 | 120.0 (2) | C19'—C18'—C17' | 120.43 (19) |
| C19—C18—C21 | 118.97 (19) | C19'—C18'—C21' | 118.6 (2) |
| C14—C19—H19 | 120.6 | C14'—C19'—H19' | 120.2 |
| C18—C19—C14 | 118.72 (19) | C18'—C19'—C14' | 119.6 (2) |
| C18—C19—H19 | 120.6 | C18'—C19'—H19' | 120.2 |
| N2—C20—C17 | 178.4 (3) | N2'—C20'—C17' | 176.1 (3) |
| N3—C21—C18 | 178.8 (3) | N3'—C21'—C18' | 176.3 (3) |
| | | | |
| C14—O2—C11—C10 | -72.6 (3) | C14'—O2'—C11'—C10' | 123.8 (2) |
| C14—O2—C11—C12 | 111.6 (2) | C14'—O2'—C11'—C12' | -62.8 (3) |
| C11—O2—C14—C15 | -176.49 (19) | C11'—O2'—C14'—C15' | -7.5 (3) |
| C11—O2—C14—C19 | 3.3 (3) | C11'—O2'—C14'—C19' | 175.44 (18) |
| C7—N1—C1—C2 | -158.2 (2) | C7'—N1'—C1'—C2' | -179.4 (2) |
| C7—N1—C1—C6 | 26.0 (3) | C7'—N1'—C1'—C6' | -0.9 (3) |
| C1—N1—C7—C8 | -174.19 (19) | C1'—N1'—C7'—C8' | 174.67 (19) |
| N1—C1—C2—O1 | 4.0 (3) | N1'—C1'—C6'—C5' | -176.9 (2) |
| N1—C1—C2—C3 | -177.04 (19) | C2'—C1'—C6'—C5' | 1.5 (3) |
| C6—C1—C2—O1 | -179.83 (19) | O1'—C2'—C1'—N1' | -2.7 (3) |
| C6—C1—C2—C3 | -0.9 (3) | O1'—C2'—C1'—C6' | 178.7 (2) |
| N1—C1—C6—C5 | 176.8 (2) | C3'—C2'—C1'—N1' | 177.1 (2) |
| C2—C1—C6—C5 | 1.0 (3) | C3'—C2'—C1'—C6' | -1.5 (3) |
| C4—C3—C2—O1 | 179.47 (19) | C4'—C3'—C2'—O1' | 179.7 (2) |
| C4—C3—C2—C1 | 0.5 (3) | C4'—C3'—C2'—C1' | -0.1 (4) |
| C5—C4—C3—C2 | -0.2 (3) | C5'—C4'—C3'—C2' | 1.7 (4) |
| C6—C5—C4—C3 | 0.4 (3) | C3'—C4'—C5'—C6' | -1.7 (4) |
| C1—C6—C5—C4 | -0.8 (3) | C4'—C5'—C6'—C1' | 0.1 (4) |
| C9—C8—C7—N1 | -0.2 (3) | N1'—C7'—C8'—C9' | -7.0 (3) |
| C13—C8—C7—N1 | 177.8 (2) | N1'—C7'—C8'—C13' | 176.9 (2) |
| C7—C8—C9—C10 | 176.8 (2) | C7'—C8'—C9'—C10' | -177.02 (19) |
| C13—C8—C9—C10 | -1.2 (3) | C13'—C8'—C9'—C10' | -0.9 (3) |
| C8—C9—C10—C11 | 1.4 (3) | C7'—C8'—C13'—C12' | 176.5 (2) |
| O2—C11—C10—C9 | -176.21 (19) | C9'—C8'—C13'—C12' | 0.3 (3) |
| C12—C11—C10—C9 | -0.5 (3) | C8'—C9'—C10'—C11' | 1.2 (3) |
| O2—C11—C12—C13 | 175.25 (19) | C9'—C10'—C11'—O2' | 172.43 (18) |
| C10—C11—C12—C13 | -0.6 (3) | C9'—C10'—C11'—C12' | -0.9 (3) |
| C11—C12—C13—C8 | 0.8 (3) | O2'—C11'—C12'—C13' | -172.77 (19) |
| C12—C13—C8—C7 | -178.0 (2) | C10'—C11'—C12'—C13' | 0.3 (3) |

| | | | |
|-----------------|-------------|---------------------|--------------|
| C12—C13—C8—C9 | 0.1 (3) | C8'—C13'—C12'—C11' | 0.0 (3) |
| O2—C14—C15—C16 | -179.2 (2) | O2'—C14'—C15'—C16' | -177.6 (2) |
| C19—C14—C15—C16 | 1.0 (3) | C19'—C14'—C15'—C16' | -0.8 (3) |
| C14—C15—C16—C17 | -0.5 (3) | O2'—C14'—C19'—C18' | 176.48 (18) |
| C18—C17—C16—C15 | -0.5 (3) | C15'—C14'—C19'—C18' | -0.7 (3) |
| C20—C17—C16—C15 | -179.3 (2) | C14'—C15'—C16'—C17' | 1.4 (3) |
| C19—C18—C17—C16 | 1.0 (3) | C15'—C16'—C17'—C18' | -0.6 (3) |
| C19—C18—C17—C20 | 179.9 (2) | C15'—C16'—C17'—C20' | 177.1 (2) |
| C21—C18—C17—C16 | -178.7 (2) | C16'—C17'—C18'—C19' | -0.9 (3) |
| C21—C18—C17—C20 | 0.1 (3) | C16'—C17'—C18'—C21' | 174.4 (2) |
| C17—C18—C19—C14 | -0.6 (3) | C20'—C17'—C18'—C19' | -178.65 (19) |
| C21—C18—C19—C14 | 179.2 (2) | C20'—C17'—C18'—C21' | -3.3 (3) |
| C18—C19—C14—O2 | 179.77 (19) | C17'—C18'—C19'—C14' | 1.6 (3) |
| C18—C19—C14—C15 | -0.4 (3) | C21'—C18'—C19'—C14' | -173.8 (2) |

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C8-ring.

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| O1—H1...N1 | 0.84 | 2.24 | 2.713 (3) | 116 |
| O1—H1...N2 ⁱ | 0.84 | 2.50 | 2.993 (3) | 119 |
| O1'—H1'...N1' | 0.84 | 2.18 | 2.659 (3) | 116 |
| O1'—H1'...N3 ⁱ | 0.84 | 2.39 | 2.948 (3) | 125 |
| C3'—H3'...N3 ⁱⁱ | 0.95 | 2.52 | 3.344 (4) | 145 |
| C5—H5...O1 ⁱⁱⁱ | 0.95 | 2.40 | 3.180 (3) | 139 |
| C12—H12...O1 ^{iv} | 0.95 | 2.35 | 3.214 (3) | 151 |
| C6'—H6'...Cg ^v | 0.95 | 2.93 | 3.785 (3) | 151 |

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