Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,5-Bis[1-(2,4-dihydroxyphenyl)ethylidene]carbonohydrazide dimethylformamide disolvate

Qing-Peng He,[a]* Bo Tan[a] and Ze-Hua Lu[b]

[a]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China, and [b]Liaocheng International Peace Hospital, Shandong 252059, People's Republic of China
Correspondence e-mail: heqp2008@163.com

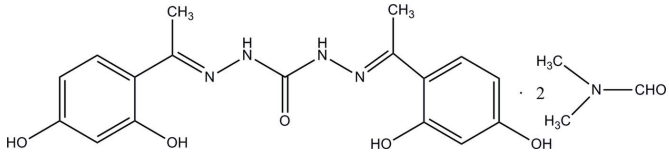
Received 15 October 2010; accepted 22 October 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.152; data-to-parameter ratio = 13.5.

In the title compound, $C_{17}H_{18}N_4O_5\cdot 2C_3H_7NO$, two solvent molecules are linked to the main molecule *via* N—H···O and O—H···O hydrogen bonds, forming a hydrogen-bonded trimer. Intramolecular O—H···N hydrogen bonds influence the molecular conformation of the main molecule, and the two benzene rings form a dihedral angle of 10.55 (18)°. In the crystal, intermolecular O—H···O hydrogen bonds link hydrogen-bonded trimers into ribbons extending along the *b* axis.

Related literature

For the biological activity of carbonohydrazide derivatives, see: Loncle *et al.* (2004); Li *et al.* (2004). For a related structure, see: Zukerman-Schpector *et al.* (2009).



Experimental

Crystal data

$C_{17}H_{18}N_4O_5\cdot 2C_3H_7NO$
M_r = 504.55
Monoclinic, $P2_1/n$
a = 11.3506 (11) Å
b = 9.0160 (7) Å
c = 24.953 (3) Å
β = 97.546 (1)°
V = 2531.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.50 × 0.37 × 0.35 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.952, T_{max} = 0.966
12361 measured reflections
4466 independent reflections
2158 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.152
S = 1.03
4466 reflections
331 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.83	2.549 (3)	145
O3—H3···N4	0.82	1.84	2.562 (3)	146
O2—H2···O7	0.82	1.90	2.704 (4)	168
N2—H2′···O6	0.86	2.13	2.918 (3)	153
N3—H3′···O6	0.86	2.16	2.932 (3)	149
O4—H4···O5^{i}	0.82	1.86	2.680 (3)	173

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

Data collection: *SMART* (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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This project was supported by the University Student Science and Technology Culture Foundation of Liaocheng University (grant No. SRT10056HX2) and the Foundation of Liaocheng University (grant No. X09010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2779).

References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Li, M. X., Cai, P., Duan, C. Y., Lu, F., Xie, J. & Meng, Q. J. (2004). *Inorg. Chem.* **43**, 5174–5176.
Loncle, C., Brunel, J. M., Vidal, N., Dherbomez, M. & Letourneux, Y. (2004). *Eur. J. Med. Chem.* **39**, 1067–1071.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zukerman-Schpector, J., Affan, M. A., Foo, S. W. & Tiekink, E. R. T. (2009). *Acta Cryst.* E**65**, o2951.

supporting information

Acta Cryst. (2010). E**66**, o2968 [https://doi.org/10.1107/S1600536810043151]

1,5-Bis[1-(2,4-dihydroxyphenyl)ethylidene]carbonohydrazide dimethylformamide disolvate

Qing-Peng He, Bo Tan and Ze-Hua Lu

S1. Comment

Carbonohydrazide Schiff base derivatives are known to exhibit a wide range of interesting biological activities, including antibacterial antifungal, anticonvulsant, anticancer activities as well as herbicidal and fungicidal activity (Loncle *et al.*, 2004; Li *et al.*, 2004). Herewith we present the crystal structure of the title compound (I) - a new carbonohydrazide derivative.

In (I) (Fig. 1), the bond lengths and angles of the main molecule are normal and correspond to those observed in *N*′′,*N*′′′-bis (1-(2-hydroxyphenyl)ethylidene)carbonohydrazide dimethyl sulfoxide solvate (Zukerman-Schpector *et al.*, 2009). The intramolecular O—H···N hydrogen bonds (Table 1) influence the molecular conformation. Two DMF solvent molecules are linked to the main molecule *via* N—H···O and O—H···O hydrogen bonds (Table 1) forming a hydrogen-bonded trimer (Fig. 1). Intermolecular O—H···O hydrogen bonds (Table 1) link hydrogen-bonded trimers into ribbons extended along the *b* axis.

S2. Experimental

2, 4-Dihydroxylacetophenone (10.0 mmol) and carbohydrazide (5.0 mmol) were mixed in 50 ml flash. After 3h stirring at 373 K, the resulting mixture was cooled to room temperature, and recrystalized from DMF, and afforded the title compound as a crystalline solid.

S3. Refinement

All H atoms were placed in idealized positions (C—H 0.93–0.96 Å, N—H 0.86 Å, O—H 0.82 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2–1.5 U_{eq}(parent atom).

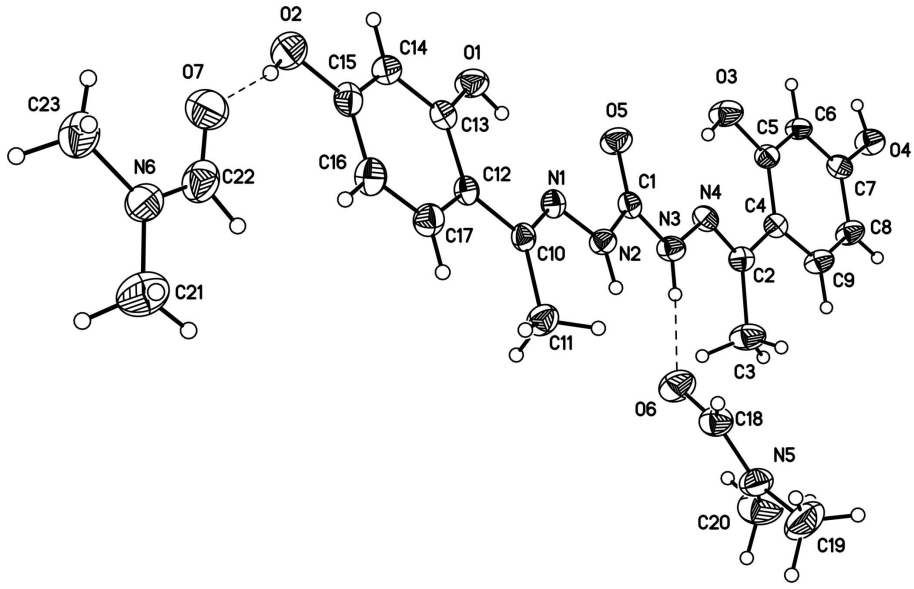


Figure 1

The content of asymmetric unit of the title compound showing the atomic numbering scheme and 30% probability displacement ellipsoids. Dashed lines denote intermolecular hydrogen bonds.

1,5-Bis[1-(2,4-dihydroxyphenyl)ethylidene]carbonohydrazide dimethylformamide disolvate

Crystal data

$C_{17}H_{18}N_4O_5\cdot 2C_3H_7NO$
$M_r = 504.55$
Monoclinic, $P2_1/n$
$a = 11.3506\ (11)$ Å
$b = 9.0160\ (7)$ Å
$c = 24.953\ (3)$ Å
$\beta = 97.546\ (1)°$
$V = 2531.5\ (4)$ Å^3
$Z = 4$
$F(000) = 1072$
$D_x = 1.324$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2127 reflections
$\theta = 2.9–23.9°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colourless
0.50 × 0.37 × 0.35 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.952$, $T_{max} = 0.966$
12361 measured reflections
4466 independent reflections
2158 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -11\rightarrow13$
$k = -10\rightarrow10$
$l = -29\rightarrow27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.152$
$S = 1.03$
4466 reflections
331 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2 + 0.4683P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.009$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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}
N3	0.5482 (2)	1.0132 (3)	0.38574 (9)	0.0413 (7)
H3′	0.6233	1.0203	0.3961	0.050*
N4	0.4960 (2)	1.0910 (3)	0.34129 (9)	0.0379 (7)
N1	0.4829 (2)	0.7684 (3)	0.48746 (9)	0.0362 (7)
N2	0.5404 (2)	0.8673 (3)	0.45843 (9)	0.0375 (7)
H2′	0.6131	0.8921	0.4687	0.045*
C1	0.4790 (3)	0.9250 (4)	0.41282 (12)	0.0352 (8)
C2	0.5629 (3)	1.1733 (4)	0.31528 (12)	0.0371 (8)
O1	0.29729 (18)	0.6107 (3)	0.49012 (9)	0.0542 (7)
H1	0.3414	0.6680	0.4767	0.081*
O4	0.34283 (19)	1.5034 (3)	0.13770 (9)	0.0537 (7)
H4	0.2743	1.4758	0.1286	0.081*
C4	0.5033 (3)	1.2567 (4)	0.26924 (11)	0.0346 (8)
C12	0.4686 (3)	0.6037 (3)	0.55900 (11)	0.0348 (8)
O5	0.37418 (19)	0.8984 (3)	0.39800 (9)	0.0519 (7)
C10	0.5368 (3)	0.7104 (3)	0.53123 (12)	0.0353 (8)
C7	0.3926 (3)	1.4211 (4)	0.18086 (12)	0.0405 (8)
C6	0.3283 (3)	1.3208 (4)	0.20663 (12)	0.0406 (8)
H14	0.2480	1.3068	0.1946	0.049*
O3	0.31113 (19)	1.1458 (3)	0.27370 (9)	0.0607 (7)
H3	0.3505	1.1027	0.2989	0.091*
C14	0.2910 (3)	0.4568 (4)	0.56516 (13)	0.0465 (9)
H16	0.2140	0.4307	0.5509	0.056*
C13	0.3532 (3)	0.5593 (4)	0.53799 (12)	0.0391 (8)
C9	0.5651 (3)	1.3599 (4)	0.24144 (13)	0.0476 (9)
H18	0.6457	1.3738	0.2526	0.057*
C5	0.3820 (3)	1.2408 (4)	0.25034 (12)	0.0378 (8)
C17	0.5158 (3)	0.5373 (4)	0.60781 (13)	0.0472 (9)
H20	0.5923	0.5634	0.6228	0.057*
C15	0.3419 (3)	0.3934 (4)	0.61297 (14)	0.0460 (9)
C16	0.4555 (3)	0.4360 (4)	0.63457 (13)	0.0500 (9)
H22	0.4906	0.3958	0.6671	0.060*

O2	0.2771 (2)	0.2926 (3)	0.63652 (10)	0.0647 (7)
H2	0.3137	0.2667	0.6655	0.097*
C8	0.5119 (3)	1.4409 (4)	0.19856 (13)	0.0482 (9)
H24	0.5560	1.5090	0.1815	0.058*
C11	0.6630 (3)	0.7461 (4)	0.55445 (13)	0.0512 (9)
H26A	0.6754	0.8512	0.5530	0.077*
H26B	0.7168	0.6964	0.5338	0.077*
H26C	0.6771	0.7133	0.5913	0.077*
C3	0.6951 (3)	1.1842 (4)	0.33107 (14)	0.0601 (11)
H32A	0.7117	1.2473	0.3621	0.090*
H32B	0.7310	1.2250	0.3016	0.090*
H32C	0.7271	1.0872	0.3396	0.090*
O6	0.7696 (2)	1.0156 (3)	0.46093 (10)	0.0652 (8)
C18	0.8226 (3)	1.0859 (4)	0.49864 (15)	0.0531 (10)
H18A	0.7916	1.0823	0.5313	0.064*
N5	0.9189 (2)	1.1658 (3)	0.49747 (12)	0.0555 (8)
C20	0.9664 (4)	1.1869 (5)	0.44770 (17)	0.0911 (15)
H20A	0.9235	1.1262	0.4201	0.137*
H20B	1.0488	1.1594	0.4523	0.137*
H20C	0.9587	1.2893	0.4372	0.137*
C19	0.9714 (4)	1.2474 (5)	0.54508 (17)	0.0898 (15)
H19A	0.9311	1.2217	0.5753	0.135*
H19B	0.9636	1.3519	0.5383	0.135*
H19C	1.0540	1.2222	0.5530	0.135*
N6	0.5058 (3)	0.0928 (4)	0.80215 (12)	0.0562 (8)
C23	0.4210 (3)	−0.0012 (4)	0.82410 (14)	0.0664 (11)
H23A	0.3454	0.0059	0.8019	0.100*
H23B	0.4130	0.0302	0.8602	0.100*
H23C	0.4482	−0.1020	0.8247	0.100*
C22	0.4740 (4)	0.1708 (5)	0.75761 (18)	0.0661 (11)
H22A	0.5326	0.2278	0.7448	0.079*
C21	0.6253 (3)	0.0985 (5)	0.83068 (17)	0.0882 (14)
H21A	0.6726	0.1650	0.8123	0.132*
H21B	0.6598	0.0011	0.8318	0.132*
H21C	0.6228	0.1332	0.8669	0.132*
O7	0.3748 (2)	0.1750 (3)	0.73179 (11)	0.0717 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N3	0.0364 (15)	0.0483 (19)	0.0378 (15)	0.0007 (14)	−0.0007 (12)	0.0098 (14)
N4	0.0402 (15)	0.0406 (18)	0.0319 (15)	0.0063 (14)	0.0004 (12)	0.0065 (13)
N1	0.0425 (16)	0.0320 (17)	0.0338 (15)	0.0011 (13)	0.0043 (13)	0.0017 (13)
N2	0.0347 (14)	0.0403 (18)	0.0360 (15)	−0.0025 (13)	−0.0015 (12)	0.0051 (13)
C1	0.040 (2)	0.032 (2)	0.0328 (18)	0.0046 (16)	0.0008 (16)	−0.0022 (16)
C2	0.0377 (18)	0.042 (2)	0.0318 (18)	−0.0001 (17)	0.0061 (15)	−0.0038 (16)
O1	0.0406 (13)	0.0608 (19)	0.0587 (16)	−0.0030 (12)	−0.0026 (12)	0.0149 (13)
O4	0.0482 (14)	0.0626 (18)	0.0477 (14)	0.0000 (13)	−0.0038 (11)	0.0189 (13)

C4	0.0378 (18)	0.037 (2)	0.0282 (17)	0.0016 (16)	0.0029 (14)	−0.0016 (15)
C12	0.0416 (19)	0.030 (2)	0.0327 (18)	0.0023 (16)	0.0054 (15)	−0.0018 (15)
O5	0.0396 (13)	0.0582 (17)	0.0542 (14)	−0.0065 (12)	−0.0077 (11)	0.0107 (12)
C10	0.0405 (18)	0.030 (2)	0.0348 (18)	0.0011 (16)	0.0024 (15)	−0.0051 (16)
C7	0.0394 (19)	0.047 (2)	0.0347 (18)	0.0055 (17)	0.0017 (15)	0.0038 (17)
C6	0.0298 (17)	0.048 (2)	0.0434 (19)	−0.0005 (17)	0.0016 (15)	0.0085 (18)
O3	0.0432 (14)	0.072 (2)	0.0669 (18)	−0.0047 (14)	0.0067 (12)	0.0319 (14)
C14	0.042 (2)	0.042 (2)	0.057 (2)	−0.0006 (17)	0.0128 (17)	0.0010 (19)
C13	0.0417 (19)	0.036 (2)	0.0395 (19)	0.0052 (17)	0.0044 (16)	−0.0005 (16)
C9	0.0382 (19)	0.059 (3)	0.044 (2)	−0.0081 (18)	−0.0004 (16)	0.0053 (19)
C5	0.0373 (19)	0.041 (2)	0.0373 (18)	0.0001 (17)	0.0119 (15)	0.0050 (16)
C17	0.051 (2)	0.045 (2)	0.045 (2)	−0.0019 (18)	0.0012 (17)	−0.0013 (18)
C15	0.056 (2)	0.038 (2)	0.049 (2)	0.0041 (19)	0.0249 (19)	0.0009 (18)
C16	0.065 (2)	0.047 (2)	0.039 (2)	0.000 (2)	0.0053 (18)	0.0057 (18)
O2	0.0669 (17)	0.0618 (19)	0.0703 (19)	−0.0031 (15)	0.0271 (13)	0.0148 (15)
C8	0.042 (2)	0.054 (3)	0.047 (2)	−0.0096 (18)	0.0022 (16)	0.0161 (19)
C11	0.049 (2)	0.051 (2)	0.050 (2)	−0.0088 (18)	−0.0045 (16)	0.0054 (18)
C3	0.043 (2)	0.080 (3)	0.055 (2)	−0.005 (2)	−0.0022 (17)	0.019 (2)
O6	0.0573 (16)	0.076 (2)	0.0581 (16)	−0.0114 (15)	−0.0095 (13)	−0.0035 (15)
C18	0.047 (2)	0.061 (3)	0.051 (2)	−0.001 (2)	0.0053 (18)	0.008 (2)
N5	0.0405 (17)	0.061 (2)	0.065 (2)	−0.0069 (16)	0.0060 (15)	0.0056 (18)
C20	0.069 (3)	0.113 (4)	0.096 (3)	−0.006 (3)	0.025 (3)	0.036 (3)
C19	0.079 (3)	0.084 (4)	0.099 (3)	−0.032 (3)	−0.016 (3)	−0.016 (3)
N6	0.054 (2)	0.055 (2)	0.060 (2)	−0.0052 (17)	0.0098 (16)	−0.0024 (18)
C23	0.079 (3)	0.063 (3)	0.061 (2)	−0.005 (2)	0.025 (2)	0.005 (2)
C22	0.073 (3)	0.055 (3)	0.076 (3)	−0.007 (2)	0.033 (2)	0.000 (2)
C21	0.072 (3)	0.099 (4)	0.089 (3)	−0.017 (3)	−0.004 (2)	−0.012 (3)
O7	0.0652 (18)	0.078 (2)	0.0736 (19)	0.0075 (16)	0.0137 (15)	0.0123 (16)

Geometric parameters (Å, º)

N3—C1	1.358 (4)	C15—O2	1.352 (4)
N3—N4	1.379 (3)	C15—C16	1.385 (4)
N3—H3′	0.8600	C16—H22	0.9300
N4—C2	1.295 (4)	O2—H2	0.8200
N1—C10	1.291 (3)	C8—H24	0.9300
N1—N2	1.368 (3)	C11—H26A	0.9600
N2—C1	1.358 (3)	C11—H26B	0.9600
N2—H2′	0.8600	C11—H26C	0.9600
C1—O5	1.223 (3)	C3—H32A	0.9600
C2—C4	1.462 (4)	C3—H32B	0.9600
C2—C3	1.504 (4)	C3—H32C	0.9600
O1—C13	1.359 (3)	O6—C18	1.225 (4)
O1—H1	0.8200	C18—N5	1.312 (4)
O4—C7	1.367 (3)	C18—H18A	0.9300
O4—H4	0.8200	N5—C20	1.430 (4)
C4—C9	1.402 (4)	N5—C19	1.456 (4)
C4—C5	1.403 (4)	C20—H20A	0.9600

C12—C17	1.400 (4)	C20—H20B	0.9600
C12—C13	1.403 (4)	C20—H20C	0.9600
C12—C10	1.465 (4)	C19—H19A	0.9600
C10—C11	1.507 (4)	C19—H19B	0.9600
C7—C6	1.374 (4)	C19—H19C	0.9600
C7—C8	1.380 (4)	N6—C22	1.325 (5)
C6—C5	1.381 (4)	N6—C23	1.443 (4)
C6—H14	0.9300	N6—C21	1.447 (4)
O3—C5	1.358 (3)	C23—H23A	0.9600
O3—H3	0.8200	C23—H23B	0.9600
C14—C15	1.380 (4)	C23—H23C	0.9600
C14—C13	1.392 (4)	C22—O7	1.222 (4)
C14—H16	0.9300	C22—H22A	0.9300
C9—C8	1.369 (4)	C21—H21A	0.9600
C9—H18	0.9300	C21—H21B	0.9600
C17—C16	1.367 (4)	C21—H21C	0.9600
C17—H20	0.9300		

C1—N3—N4	118.9 (2)	C15—O2—H2	109.5
C1—N3—H3′	120.6	C9—C8—C7	119.6 (3)
N4—N3—H3′	120.6	C9—C8—H24	120.2
C2—N4—N3	118.5 (3)	C7—C8—H24	120.2
C10—N1—N2	120.4 (2)	C10—C11—H26A	109.5
C1—N2—N1	117.7 (3)	C10—C11—H26B	109.5
C1—N2—H2′	121.1	H26A—C11—H26B	109.5
N1—N2—H2′	121.1	C10—C11—H26C	109.5
O5—C1—N3	124.6 (3)	H26A—C11—H26C	109.5
O5—C1—N2	123.4 (3)	H26B—C11—H26C	109.5
N3—C1—N2	112.0 (3)	C2—C3—H32A	109.5
N4—C2—C4	116.5 (3)	C2—C3—H32B	109.5
N4—C2—C3	122.5 (3)	H32A—C3—H32B	109.5
C4—C2—C3	121.0 (3)	C2—C3—H32C	109.5
C13—O1—H1	109.5	H32A—C3—H32C	109.5
C7—O4—H4	109.5	H32B—C3—H32C	109.5
C9—C4—C5	115.7 (3)	O6—C18—N5	126.4 (4)
C9—C4—C2	121.3 (3)	O6—C18—H18A	116.8
C5—C4—C2	123.0 (3)	N5—C18—H18A	116.8
C17—C12—C13	115.8 (3)	C18—N5—C20	120.1 (3)
C17—C12—C10	121.8 (3)	C18—N5—C19	120.8 (3)
C13—C12—C10	122.4 (3)	C20—N5—C19	118.7 (3)
N1—C10—C12	116.4 (3)	N5—C20—H20A	109.5
N1—C10—C11	124.1 (3)	N5—C20—H20B	109.5
C12—C10—C11	119.6 (3)	H20A—C20—H20B	109.5
C6—C7—O4	122.4 (3)	N5—C20—H20C	109.5
C6—C7—C8	119.7 (3)	H20A—C20—H20C	109.5
O4—C7—C8	117.9 (3)	H20B—C20—H20C	109.5
C7—C6—C5	120.4 (3)	N5—C19—H19A	109.5
C7—C6—H14	119.8	N5—C19—H19B	109.5

C5—C6—H14	119.8	H19A—C19—H19B	109.5
C5—O3—H3	109.5	N5—C19—H19C	109.5
C15—C14—C13	121.0 (3)	H19A—C19—H19C	109.5
C15—C14—H16	119.5	H19B—C19—H19C	109.5
C13—C14—H16	119.5	C22—N6—C23	120.5 (3)
O1—C13—C14	116.5 (3)	C22—N6—C21	121.9 (4)
O1—C13—C12	122.4 (3)	C23—N6—C21	117.6 (3)
C14—C13—C12	121.1 (3)	N6—C23—H23A	109.5
C8—C9—C4	122.9 (3)	N6—C23—H23B	109.5
C8—C9—H18	118.5	H23A—C23—H23B	109.5
C4—C9—H18	118.5	N6—C23—H23C	109.5
O3—C5—C6	116.3 (3)	H23A—C23—H23C	109.5
O3—C5—C4	122.1 (3)	H23B—C23—H23C	109.5
C6—C5—C4	121.6 (3)	O7—C22—N6	126.1 (4)
C16—C17—C12	123.5 (3)	O7—C22—H22A	116.9
C16—C17—H20	118.2	N6—C22—H22A	116.9
C12—C17—H20	118.2	N6—C21—H21A	109.5
O2—C15—C14	117.7 (3)	N6—C21—H21B	109.5
O2—C15—C16	123.3 (3)	H21A—C21—H21B	109.5
C14—C15—C16	119.0 (3)	N6—C21—H21C	109.5
C17—C16—C15	119.7 (3)	H21A—C21—H21C	109.5
C17—C16—H22	120.2	H21B—C21—H21C	109.5
C15—C16—H22	120.2		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.83	2.549 (3)	145
O3—H3···N4	0.82	1.84	2.562 (3)	146
O2—H2···O7	0.82	1.90	2.704 (4)	168
N2—H2′···O6	0.86	2.13	2.918 (3)	153
N3—H3′···O6	0.86	2.16	2.932 (3)	149
O4—H4···O5^{i}	0.82	1.86	2.680 (3)	173

Symmetry code: (i) $-x+1/2, y+1/2, -z+1/2$.