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2-Benzoylpyridine semicarbazone

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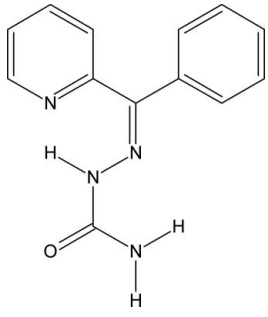
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.150; data-to-parameter ratio = 14.1.

The title compound, $C_{13}H_{12}N_4O$, crystallizes with two independent molecules in the asymmetric unit. The compound crystallizes as the ZE isomer, where Z and E refer to the configuration around the C=N and N—C bonds, respectively, with an N—H···N_{py} (py is pyridine) intramolecular hydrogen bond. The dihedral angles between the least-squares planes through the semicarbazone group and the pyridyl ring are 22.70 (9) and 27.26 (9)° for the two molecules. There are intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Beraldo & Gambino (2004); Beraldo *et al.* (2002); Teixeira *et al.* (2003); Farrell (2002); Pérez-Rebolledo *et al.* (2006).



Experimental

Crystal data

$C_{13}H_{12}N_4O$
M_r = 240.27
Monoclinic, $C2/c$
a = 22.9281 (7) Å
b = 9.1868 (2) Å
c = 23.1869 (7) Å
β = 93.049 (1)°
V = 4877.1 (2) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 K
0.18 × 0.14 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
16551 measured reflections
4588 independent reflections
3011 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.150
S = 1.07
4588 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11A···O1^{i}	0.86	2.17	3.029 (2)	178
N11—H11B···O2^{ii}	0.86	2.33	2.917 (2)	126
N21—H21B···O1^{ii}	0.86	2.27	2.883 (2)	128
N21—H21A···O2^{iii}	0.86	2.15	3.005 (2)	173
N12—H12···N14	0.86	2.06	2.683 (2)	129
N22—H22···N24	0.86	2.10	2.712 (2)	128

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

Data collection: *COLLECT* (Enraf–Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2110).

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2-Benzoylpyridine semicarbazone

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S1. Comment

Semicarbazones present a wide range of biological applications as antitumoral, anticonvulsant, anti-trypanosomal, herbicidal and biocidal agents (Beraldo & Gambino, 2004; Beraldo *et al.*, 2002; Teixeira *et al.*, 2003). In some cases complexation to metal ions can improve properties of these ligands, such as lipophilicity and pharmacological activity. Moreover, mechanisms of action of bioactive compounds can involve coordination to metal-containing enzymes (Farrell, 2002). As part of our research aiming to understand the molecular and biological properties of semicarbazones we previously prepared 2-Benzoylpyridine semicarbazone (H2Bz4PS) and its Cu(II) and Zn(II) complexes (Pérez-Rebolledo *et al.*, 2006). Here we describe the synthesis and crystal structure of H2Bz4PS (Fig. 1).

The molecular conformation can be described using three planar groups, the phenyl ring, the pyridyl ring and the semicarbazone group. The dihedral angles between the least-square planes through the semicarbazone group and the pyridyl ring are 22.70° and 27.26°, for molecule I and II respectively. The angle between the least-square planes through the semicarbazone group and phenyl ring are almost the same, 32.96° and 32.49°, for molecule I and II respectively. The dihedral angles between the phenyl and the pyridyl rings are 53.12° and 53.99° for molecule I and II respectively. The molecular conformation is fixed by an intramolecular interactions of the N—H···N type, N12—H12···N14 for molecule I and N22—H22···N24 for molecule II. The crystal packing is stabilized by N—H···O intermolecular interactions that form centrosymmetric dimers (Fig. 2). Another N—H···O hydrogen bond gives rise to the formation of infinite chains along the *b* axis.

S2. Experimental

2-Benzoylpyridine semicarbazone (H2Bz4PS) was prepared by adding portion-wise an aqueous solution containing equimolar amounts (2 mmol) of semicarbazide hydrochloride and sodium acetate to 2-Benzoylpyridine (2 mmol) in ethanol at room temperature. The reaction mixture was kept under stirring for 20 h. The resulting solid was filtered off and washed with distilled water and ether and then dried. H2Bz4PS: Yield: 69.4%. Melting point: 181.5–182.7 °C. Anal. Calc: C, 64.99; H, 5.03; N, 23.32%. Found: C, 64.02; H, 4.95; N, 23.05%.

S3. Refinement

The model was refined by full-matrix least squares on F^2 with *SHELXL97* (Sheldrick, 1997). All the hydrogen atoms were stereochemically positioned and refined with the riding model. Hydrogen atoms of the CH, NH and NH_2 groups were set isotropic with a thermal parameter 20% greater than the equivalent isotropic displacement parameter of the atom to which each one was bonded.

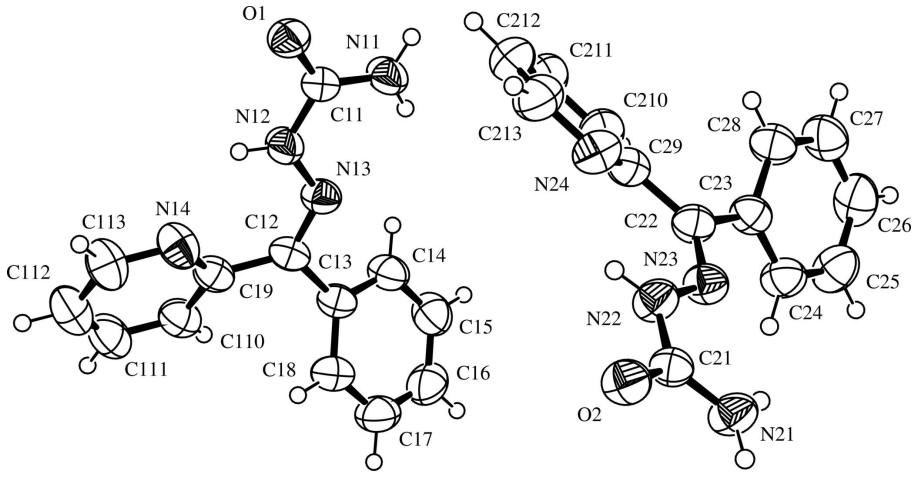

Figure 1

The molecular structure of the title. Displacement ellipsoids are drawn at the 50% probability level.

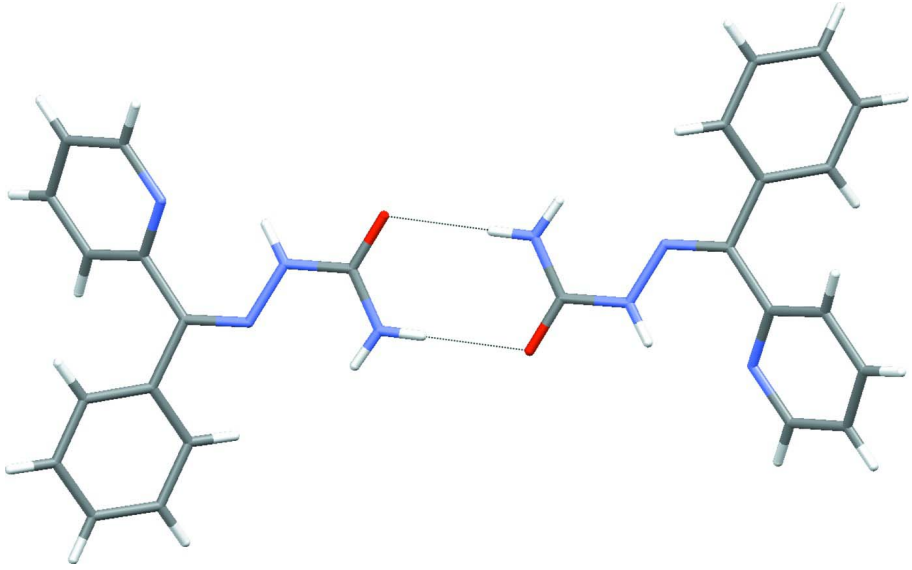

Figure 2

Centrosymmetric dimers linking two molecules of H2Bz4PS in the crystal packing. The dotted lines represent the hydrogen bonds of the type N—H··· O.

2-Benzoylpyridine semicarbazone

Crystal data

$C_{13}H_{12}N_4O$
$M_r = 240.27$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 22.9281\ (7)$ Å
$b = 9.1868\ (2)$ Å
$c = 23.1869\ (7)$ Å
$\beta = 93.049\ (1)°$
$V = 4877.1\ (2)$ Å^3
$Z = 16$

$F(000) = 2016$
$D_x = 1.309$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 23344 reflections
$\theta = 2.9–25.7°$
$\mu = 0.09$ mm^{-1}
$T = 294$ K
Prism, colourless
0.18 × 0.14 × 0.04 mm

Data collection

KappaCCD diffractometer
φ scans and ω scans with κ offsets
16551 measured reflections
4588 independent reflections
3011 reflections with $I > 2\sigma(I)$

$R_{int} = 0.066$
$\theta_{max} = 25.7°$, $\theta_{min} = 3.5°$
$h = -27 \rightarrow 27$
$k = -10 \rightarrow 11$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.150$
$S = 1.07$
4588 reflections
325 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0842P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.32552 (5)	0.15282 (12)	0.00628 (6)	0.0579 (4)
N11	0.30310 (7)	0.38523 (15)	0.02708 (7)	0.0638 (5)
H11A	0.2668	0.3735	0.0168	0.077*
H11B	0.3154	0.4685	0.0396	0.077*
N12	0.39721 (7)	0.30226 (14)	0.03898 (7)	0.0560 (4)
H12	0.4234	0.2373	0.0338	0.067*
N13	0.41230 (6)	0.43452 (15)	0.06270 (6)	0.0518 (4)
N14	0.50663 (7)	0.22107 (17)	0.07080 (8)	0.0646 (5)
C11	0.33995 (8)	0.27542 (18)	0.02374 (8)	0.0472 (4)
C12	0.46602 (8)	0.46234 (18)	0.07889 (7)	0.0503 (4)
C13	0.47417 (8)	0.60980 (18)	0.10515 (8)	0.0507 (5)
C14	0.43912 (9)	0.7256 (2)	0.08574 (9)	0.0615 (5)
H14	0.4120	0.7117	0.0550	0.074*
C15	0.44422 (10)	0.8602 (2)	0.11153 (11)	0.0717 (6)
H15	0.4210	0.9369	0.0977	0.086*
C16	0.48359 (10)	0.8818 (2)	0.15773 (11)	0.0752 (6)
H16	0.4864	0.9723	0.1756	0.090*
C17	0.51862 (10)	0.7691 (2)	0.17715 (10)	0.0728 (6)
H17	0.5458	0.7840	0.2078	0.087*
C18	0.51390 (9)	0.6347 (2)	0.15160 (9)	0.0612 (5)
H18	0.5376	0.5590	0.1655	0.073*
C19	0.51699 (8)	0.36475 (18)	0.07344 (8)	0.0526 (5)
C110	0.57304 (9)	0.4197 (2)	0.07022 (8)	0.0625 (5)
H110	0.5795	0.5196	0.0709	0.075*

C111	0.61896 (9)	0.3247 (3)	0.06597 (10)	0.0745 (6)
H111	0.6568	0.3601	0.0642	0.089*
C112	0.60892 (10)	0.1782 (3)	0.06428 (10)	0.0746 (6)
H112	0.6395	0.1124	0.0620	0.090*
C113	0.55268 (10)	0.1312 (2)	0.06610 (10)	0.0732 (6)
H113	0.5456	0.0316	0.0640	0.088*
O2	0.24288 (6)	0.15322 (12)	0.42544 (5)	0.0583 (4)
N21	0.21621 (7)	0.38036 (15)	0.44999 (7)	0.0600 (4)
H21A	0.2252	0.3660	0.4860	0.072*
H21B	0.2025	0.4632	0.4386	0.072*
N22	0.20957 (7)	0.30602 (15)	0.35554 (6)	0.0568 (4)
H22	0.2161	0.2435	0.3291	0.068*
N23	0.18510 (7)	0.43784 (15)	0.34154 (6)	0.0529 (4)
N24	0.17683 (8)	0.22916 (17)	0.24561 (7)	0.0621 (4)
C21	0.22340 (8)	0.27519 (17)	0.41217 (7)	0.0468 (4)
C22	0.17017 (8)	0.46887 (18)	0.28832 (7)	0.0507 (4)
C23	0.14314 (8)	0.61504 (18)	0.28004 (8)	0.0517 (5)
C24	0.16044 (9)	0.7306 (2)	0.31577 (9)	0.0618 (5)
H24	0.1901	0.7173	0.3442	0.074*
C25	0.13392 (11)	0.8647 (2)	0.30944 (9)	0.0726 (6)
H25	0.1458	0.9412	0.3336	0.087*
C26	0.09007 (11)	0.8860 (2)	0.26773 (10)	0.0758 (7)
H26	0.0722	0.9765	0.2637	0.091*
C27	0.07268 (10)	0.7732 (2)	0.23192 (10)	0.0720 (6)
H27	0.0430	0.7876	0.2035	0.086*
C28	0.09885 (9)	0.6396 (2)	0.23788 (9)	0.0620 (5)
H28	0.0868	0.5641	0.2133	0.074*
C29	0.17786 (8)	0.37337 (19)	0.23733 (8)	0.0532 (5)
C210	0.18628 (9)	0.4333 (2)	0.18346 (8)	0.0666 (6)
H210	0.1890	0.5336	0.1790	0.080*
C211	0.19057 (11)	0.3423 (3)	0.13692 (10)	0.0781 (6)
H211	0.1953	0.3808	0.1004	0.094*
C212	0.18792 (10)	0.1954 (3)	0.14452 (10)	0.0742 (6)
H212	0.1901	0.1324	0.1133	0.089*
C213	0.18198 (10)	0.1423 (2)	0.19957 (10)	0.0717 (6)
H213	0.1815	0.0420	0.2050	0.086*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0576 (8)	0.0475 (7)	0.0680 (9)	−0.0063 (6)	−0.0032 (6)	−0.0060 (6)
N11	0.0486 (10)	0.0495 (9)	0.0915 (13)	0.0005 (7)	−0.0132 (9)	−0.0110 (8)
N12	0.0465 (10)	0.0483 (9)	0.0721 (11)	0.0010 (6)	−0.0058 (8)	−0.0077 (7)
N13	0.0498 (10)	0.0488 (8)	0.0559 (10)	−0.0047 (6)	−0.0052 (7)	0.0005 (6)
N14	0.0537 (11)	0.0583 (10)	0.0818 (13)	0.0034 (8)	0.0039 (9)	0.0122 (8)
C11	0.0461 (11)	0.0498 (10)	0.0451 (10)	−0.0030 (8)	−0.0023 (8)	−0.0002 (8)
C12	0.0466 (11)	0.0546 (11)	0.0489 (11)	−0.0046 (8)	−0.0059 (8)	0.0086 (8)
C13	0.0464 (11)	0.0526 (10)	0.0524 (11)	−0.0071 (8)	−0.0034 (8)	0.0037 (8)

C14	0.0532 (12)	0.0604 (12)	0.0695 (14)	−0.0044 (9)	−0.0093 (10)	−0.0010 (9)
C15	0.0604 (14)	0.0597 (12)	0.0945 (18)	0.0003 (9)	0.0013 (12)	−0.0048 (11)
C16	0.0682 (16)	0.0723 (14)	0.0859 (17)	−0.0156 (11)	0.0104 (12)	−0.0246 (12)
C17	0.0649 (15)	0.0865 (15)	0.0660 (14)	−0.0142 (12)	−0.0055 (11)	−0.0133 (11)
C18	0.0572 (13)	0.0693 (13)	0.0558 (12)	−0.0072 (9)	−0.0076 (10)	−0.0003 (9)
C19	0.0492 (12)	0.0595 (11)	0.0486 (11)	−0.0013 (8)	−0.0026 (8)	0.0096 (8)
C110	0.0531 (13)	0.0725 (12)	0.0616 (13)	−0.0041 (10)	0.0008 (9)	0.0043 (10)
C111	0.0470 (13)	0.0974 (17)	0.0794 (16)	0.0036 (11)	0.0073 (11)	0.0075 (12)
C112	0.0556 (14)	0.0909 (17)	0.0780 (16)	0.0163 (11)	0.0093 (11)	0.0196 (12)
C113	0.0645 (15)	0.0662 (13)	0.0893 (17)	0.0127 (10)	0.0092 (12)	0.0157 (11)
O2	0.0712 (10)	0.0462 (7)	0.0562 (8)	0.0068 (6)	−0.0069 (7)	0.0044 (6)
N21	0.0811 (12)	0.0497 (9)	0.0476 (9)	0.0128 (7)	−0.0106 (8)	0.0001 (7)
N22	0.0737 (11)	0.0499 (9)	0.0458 (9)	0.0109 (7)	−0.0049 (8)	0.0016 (6)
N23	0.0589 (10)	0.0485 (9)	0.0504 (9)	0.0032 (7)	−0.0049 (7)	0.0065 (7)
N24	0.0722 (12)	0.0599 (10)	0.0539 (10)	−0.0070 (8)	0.0013 (8)	−0.0043 (7)
C21	0.0481 (11)	0.0459 (10)	0.0456 (11)	−0.0006 (8)	−0.0034 (8)	0.0045 (8)
C22	0.0531 (11)	0.0530 (10)	0.0454 (11)	−0.0011 (8)	−0.0022 (8)	0.0062 (8)
C23	0.0523 (12)	0.0555 (11)	0.0469 (11)	0.0013 (8)	−0.0012 (9)	0.0085 (8)
C24	0.0688 (14)	0.0627 (12)	0.0528 (12)	0.0030 (10)	−0.0063 (10)	0.0011 (9)
C25	0.0964 (18)	0.0580 (13)	0.0632 (14)	0.0093 (11)	0.0034 (12)	−0.0002 (9)
C26	0.0908 (18)	0.0693 (14)	0.0678 (15)	0.0263 (12)	0.0102 (12)	0.0162 (11)
C27	0.0681 (15)	0.0846 (15)	0.0623 (14)	0.0175 (11)	−0.0046 (11)	0.0153 (11)
C28	0.0623 (13)	0.0638 (12)	0.0587 (13)	0.0021 (9)	−0.0074 (10)	0.0078 (9)
C29	0.0502 (12)	0.0589 (12)	0.0500 (11)	−0.0016 (8)	−0.0030 (8)	0.0028 (8)
C210	0.0732 (15)	0.0745 (13)	0.0524 (13)	0.0056 (10)	0.0058 (10)	0.0077 (10)
C211	0.0852 (18)	0.0993 (18)	0.0504 (13)	0.0141 (13)	0.0088 (11)	0.0019 (11)
C212	0.0694 (15)	0.0977 (18)	0.0557 (14)	0.0032 (12)	0.0037 (11)	−0.0171 (11)
C213	0.0772 (16)	0.0686 (13)	0.0690 (15)	−0.0080 (10)	0.0019 (12)	−0.0112 (11)

Geometric parameters (Å, º)

O1—C11	1.2360 (19)	O2—C21	1.2390 (19)
N11—C11	1.321 (2)	N21—C21	1.321 (2)
N11—H11A	0.8600	N21—H21A	0.8600
N11—H11B	0.8600	N21—H21B	0.8600
N12—C11	1.364 (2)	N22—C21	1.364 (2)
N12—N13	1.3705 (19)	N22—N23	1.3665 (18)
N12—H12	0.8600	N22—H22	0.8600
N13—C12	1.294 (2)	N23—C22	1.295 (2)
N14—C19	1.342 (2)	N24—C29	1.339 (2)
N14—C113	1.349 (3)	N24—C213	1.343 (3)
C12—C19	1.484 (2)	C22—C23	1.487 (2)
C12—C13	1.493 (2)	C22—C29	1.490 (2)
C13—C18	1.392 (2)	C23—C28	1.390 (2)
C13—C14	1.393 (3)	C23—C24	1.392 (3)
C14—C15	1.376 (3)	C24—C25	1.378 (3)
C14—H14	0.9300	C24—H24	0.9300
C15—C16	1.378 (3)	C25—C26	1.371 (3)

C15—H15	0.9300	C25—H25	0.9300
C16—C17	1.371 (3)	C26—C27	1.374 (3)
C16—H16	0.9300	C26—H26	0.9300
C17—C18	1.371 (3)	C27—C28	1.370 (3)
C17—H17	0.9300	C27—H27	0.9300
C18—H18	0.9300	C28—H28	0.9300
C19—C110	1.386 (3)	C29—C210	1.388 (3)
C110—C111	1.375 (3)	C210—C211	1.372 (3)
C110—H110	0.9300	C210—H210	0.9300
C111—C112	1.366 (3)	C211—C212	1.363 (3)
C111—H111	0.9300	C211—H211	0.9300
C112—C113	1.362 (3)	C212—C213	1.380 (3)
C112—H112	0.9300	C212—H212	0.9300
C113—H113	0.9300	C213—H213	0.9300
C11—N11—H11A	120.0	C21—N21—H21A	120.0
C11—N11—H11B	120.0	C21—N21—H21B	120.0
H11A—N11—H11B	120.0	H21A—N21—H21B	120.0
C11—N12—N13	118.90 (14)	C21—N22—N23	118.96 (14)
C11—N12—H12	120.6	C21—N22—H22	120.5
N13—N12—H12	120.6	N23—N22—H22	120.5
C12—N13—N12	120.51 (15)	C22—N23—N22	120.40 (14)
C19—N14—C113	117.91 (17)	C29—N24—C213	118.09 (17)
O1—C11—N11	123.66 (17)	O2—C21—N21	123.56 (16)
O1—C11—N12	119.14 (15)	O2—C21—N22	119.28 (15)
N11—C11—N12	117.18 (15)	N21—C21—N22	117.14 (14)
N13—C12—C19	126.72 (16)	N23—C22—C23	114.15 (15)
N13—C12—C13	113.21 (15)	N23—C22—C29	126.16 (15)
C19—C12—C13	120.07 (15)	C23—C22—C29	119.68 (15)
C18—C13—C14	117.82 (16)	C28—C23—C24	117.99 (16)
C18—C13—C12	121.83 (16)	C28—C23—C22	121.42 (16)
C14—C13—C12	120.23 (16)	C24—C23—C22	120.56 (16)
C15—C14—C13	120.76 (19)	C25—C24—C23	120.56 (19)
C15—C14—H14	119.6	C25—C24—H24	119.7
C13—C14—H14	119.6	C23—C24—H24	119.7
C14—C15—C16	120.3 (2)	C26—C25—C24	120.4 (2)
C14—C15—H15	119.8	C26—C25—H25	119.8
C16—C15—H15	119.8	C24—C25—H25	119.8
C17—C16—C15	119.63 (19)	C25—C26—C27	119.81 (19)
C17—C16—H16	120.2	C25—C26—H26	120.1
C15—C16—H16	120.2	C27—C26—H26	120.1
C16—C17—C18	120.4 (2)	C28—C27—C26	120.2 (2)
C16—C17—H17	119.8	C28—C27—H27	119.9
C18—C17—H17	119.8	C26—C27—H27	119.9
C17—C18—C13	121.05 (19)	C27—C28—C23	121.07 (19)
C17—C18—H18	119.5	C27—C28—H28	119.5
C13—C18—H18	119.5	C23—C28—H28	119.5
N14—C19—C110	121.19 (17)	N24—C29—C210	121.71 (17)

N14—C19—C12	117.39 (16)	N24—C29—C22	117.71 (16)
C110—C19—C12	121.42 (16)	C210—C29—C22	120.57 (17)
C111—C110—C19	119.2 (2)	C211—C210—C29	119.1 (2)
C111—C110—H110	120.4	C211—C210—H210	120.5
C19—C110—H110	120.4	C29—C210—H210	120.5
C112—C111—C110	119.9 (2)	C212—C211—C210	119.7 (2)
C112—C111—H111	120.0	C212—C211—H211	120.1
C110—C111—H111	120.0	C210—C211—H211	120.1
C113—C112—C111	118.0 (2)	C211—C212—C213	118.48 (19)
C113—C112—H112	121.0	C211—C212—H212	120.8
C111—C112—H112	121.0	C213—C212—H212	120.8
N14—C113—C112	123.7 (2)	N24—C213—C212	122.8 (2)
N14—C113—H113	118.1	N24—C213—H213	118.6
C112—C113—H113	118.1	C212—C213—H213	118.6

C11—N12—N13—C12	178.38 (16)	C21—N22—N23—C22	−178.29 (16)
N13—N12—C11—O1	−174.77 (15)	N23—N22—C21—O2	176.43 (15)
N13—N12—C11—N11	7.2 (2)	N23—N22—C21—N21	−5.0 (2)
N12—N13—C12—C19	1.8 (3)	N22—N23—C22—C23	178.90 (15)
N12—N13—C12—C13	−178.45 (15)	N22—N23—C22—C29	−1.2 (3)
N13—C12—C13—C18	142.89 (18)	N23—C22—C23—C28	−145.14 (19)
C19—C12—C13—C18	−37.3 (3)	C29—C22—C23—C28	34.9 (3)
N13—C12—C13—C14	−33.1 (2)	N23—C22—C23—C24	32.8 (3)
C19—C12—C13—C14	146.70 (18)	C29—C22—C23—C24	−147.07 (18)
C18—C13—C14—C15	0.6 (3)	C28—C23—C24—C25	0.4 (3)
C12—C13—C14—C15	176.71 (19)	C22—C23—C24—C25	−177.65 (18)
C13—C14—C15—C16	−1.1 (3)	C23—C24—C25—C26	0.0 (3)
C14—C15—C16—C17	1.4 (3)	C24—C25—C26—C27	−0.3 (3)
C15—C16—C17—C18	−1.2 (3)	C25—C26—C27—C28	0.2 (3)
C16—C17—C18—C13	0.8 (3)	C26—C27—C28—C23	0.2 (3)
C14—C13—C18—C17	−0.4 (3)	C24—C23—C28—C27	−0.5 (3)
C12—C13—C18—C17	−176.51 (18)	C22—C23—C28—C27	177.56 (19)
C113—N14—C19—C110	1.3 (3)	C213—N24—C29—C210	−2.5 (3)
C113—N14—C19—C12	−179.70 (17)	C213—N24—C29—C22	178.06 (18)
N13—C12—C19—N14	−24.8 (3)	N23—C22—C29—N24	29.3 (3)
C13—C12—C19—N14	155.40 (16)	C23—C22—C29—N24	−150.77 (17)
N13—C12—C19—C110	154.13 (19)	N23—C22—C29—C210	−150.11 (19)
C13—C12—C19—C110	−25.6 (3)	C23—C22—C29—C210	29.8 (3)
N14—C19—C110—C111	−1.9 (3)	N24—C29—C210—C211	3.5 (3)
C12—C19—C110—C111	179.14 (18)	C22—C29—C210—C211	−177.08 (19)
C19—C110—C111—C112	0.8 (3)	C29—C210—C211—C212	−1.6 (3)
C110—C111—C112—C113	0.9 (3)	C210—C211—C212—C213	−1.2 (3)
C19—N14—C113—C112	0.4 (3)	C29—N24—C213—C212	−0.4 (3)
C111—C112—C113—N14	−1.6 (3)	C211—C212—C213—N24	2.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11*A*···O1^{i}	0.86	2.17	3.029 (2)	178
N11—H11*B*···O2^{ii}	0.86	2.33	2.917 (2)	126
N21—H21*B*···O1^{ii}	0.86	2.27	2.883 (2)	128
N21—H21*A*···O2^{iii}	0.86	2.15	3.005 (2)	173
N12—H12···N14	0.86	2.06	2.683 (2)	129
N22—H22···N24	0.86	2.10	2.712 (2)	128

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