Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*,*N*′,*N*′-Tetraisobutylpyridine-2,6-dicarboxamide

Michaela Pojarová,[a]* Michal Dušek,[a] Emanuel Makrlík,[b] Vasily A. Babain[c] and Petr Vaňura[d]

[a]Institute of Physics, AS CR, v.v.i., Na Slovance 2, 182 21 Praha 8, Czech Republic, [b]Faculty of Environmental Sciences, Czech University of Life Sciences, Prague, Kamýcká 129, 165 21 Prague 6, Czech Republic, [c]Khlopin Radium Institute, Research and Production Association, 2nd Murinskiy Prospect b. 28, 194021 St Petersburg, Russian Federation, and [d]Department of Analytical Chemistry, Institute of Chemical Technology, Prague, Technická 5, 166 28 Prague 6, Czech Republic
Correspondence e-mail: pojarova@fzu.cz

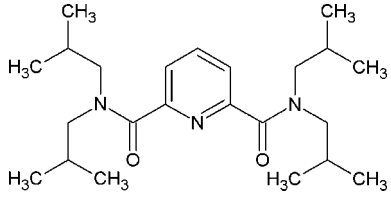
Received 26 September 2011; accepted 3 October 2011

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.112; data-to-parameter ratio = 16.4.

In the title compound, $C_{23}H_{39}N_3O_2$, the amide O atoms are displaced by 1.020 (1) and 1.211 (1) Å from the mean plane of the central pyridine ring. In the crystal, molecules are connected by weak C—H···O hydrogen bonds between methylene groups in the isobutyl substituents and the amide O atoms.

Related literature

The title compound has been investigated for its extractive properties towards trivalent metals in a synergistic mixture with chlorinated cobalt dicarbollide. For further information, see: Alyapyshev *et al.* (2004, 2006); Romanovskiy *et al.* (2006); Babain *et al.* (2007); Makrlík *et al.* (2009, 2011). For further synthetic details, see: Nikitskaya *et al.* (1958); Shimada *et al.* (2004).



Experimental

Crystal data

$C_{23}H_{39}N_3O_2$
M_r = 389.57
Monoclinic, $P2_1/c$
a = 10.5247 (2) Å
b = 17.7765 (3) Å
c = 12.8773 (2) Å
β = 96.877 (2)°
V = 2391.91 (7) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 120 K
0.49 × 0.42 × 0.23 mm

Data collection

Agilent Xcalibur Atlas Gemini ultra diffractometer
Absorption correction: analytical (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.929, T_{max} = 0.962
31214 measured reflections
4272 independent reflections
3867 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.112
S = 1.05
4272 reflections
261 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O2^{i}	0.97	2.57	3.5226 (15)	166
C11—H11A···O1^{ii}	0.97	2.55	3.4790 (15)	160

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

Data collection: *CrysAlis PRO* (Agilent, 2011); 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: *Mercury* (Macrae *et al.*, 2006) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This study was supported financially by the Institutional Research Plan No. AVOZ10100521 of the Institute of Physics, the project Praemium Academiae of the Academy of Science of the Czech Republic and by the Grant Agency of Faculty of Environmental Sciences, Czech University of Life Sciences, Prague (project No. 42900/1312/3114 "Environmental Aspects of Sustainable Developement of Society") and by the Czech Ministry of Education, Youth and Sports (project MSM 6046137307).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6423).

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Alyapyshev, M. Y., Babain, V. A. & Smirnov, I. V. (2004). *Radiochemistry*, **46**, 270–271.
Alyapyshev, M. Y., Babain, V. A., Smirnov, I. V. & Shadrin, A. Y. (2006). *Radiochemistry*, **48**, 369–373.
Babain, V. A., Alyapyshev, M. Y. & Kiseleva, R. N. (2007). *Radiochim. Acta*, **95**, 217–223.
Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Makrlík, E., Vaňura, P., Selucký, P., Babain, V. A. & Smirnov, I. V. (2009). *J. Radioanal. Nucl. Chem.* **279**, 743–747.
Makrlík, E., Vaňura, P., Selucký, P., Babain, V. A. & Smirnov, I. V. (2011). *J. Radioanal. Nucl. Chem.* **288**, 233–238.

Nikitskaya, E. S., Usovskaya, V. S. & Rubtzov, M. V. (1958). *Zh. Obsch. Khim.* **28**, 161–166.
Romanovskiy, V. N., Babain, V. A., Alyapyshev, M. Y., Smirbov, V. A., Herbst, R. S., Lan, J. D. & Todd, T. A. (2006). *Separ. Sci. Technol.* **41**, 2111–2127.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shimada, A., Yaita, T., Narita, H., Tachimori, S. & Okuno, K. (2004). *Solvent Extr. Ion Exch.* **22**, 147–161.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, o2896–o2897 [doi:10.1107/S1600536811040608]

N,*N*,*N*′,*N*′-Tetraisobutylpyridine-2,6-dicarboxamide

Michaela Pojarová, Michal Dušek, Emanuel Makrlík, Vasily A. Babain and Petr Vaňura

S1. Comment

The title compound, (I), shown in Figure 1 and Scheme 1, has been investigated in a synergistic mixtures with the dicarbollylcobaltate anion and its halogen derivatives for significant extraction properties towards trivalent metal cations (Alyapyshev *et al.*,2004). It consists of pyridine ring with a di-isobutylamide groups in position 2 and 6. This molecule lacks of crystallographic symmetry and the asymmetric unit contains one molecule. While at first impression, the amide groups seem to be related by a mirror plane, closer look reveales their differences. The carbon atoms of carbonyl groups do not lay in a plane of the pyridine ring and they differ in the distance to this plane (0.062 Å for C6 and 0.234 Å for C15). The molecules form bands along the *c* axis (Fig. 2) *via* system of hydrogen bonds (Table 1).

S2. Experimental

The title compound was synthesized as described in Shimada *et al.* (2004), and Nikitskaya *et al.* (1958). Colourless prisms were prepared by slow evaporation from an acetonitrile solution.

S3. Refinement

The hydrogen atoms were localized from the difference Fourier map. Despite of that, all hydrogen atoms connected to C were constrained to ideal positions. The isotropic temperature parameters of hydrogen atoms were calculated as 1.2*U_{eq} of the parent atom.

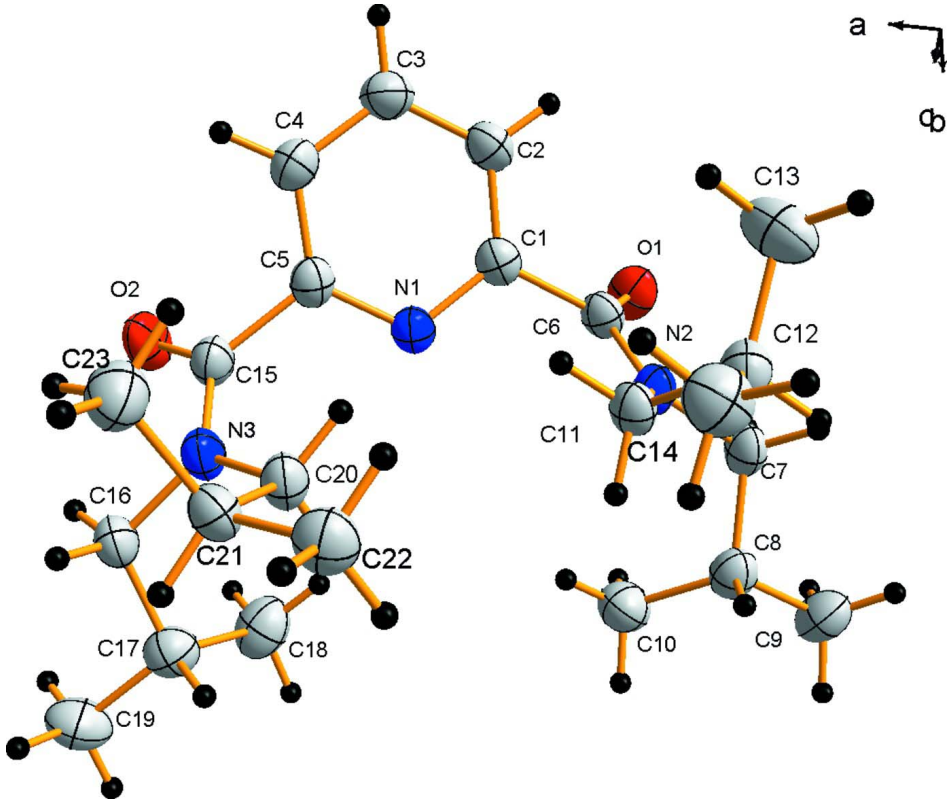


Figure 1

View of the *N*,*N*,*N*′,*N*′-tetraisobutyl-2,6-dipicolinamide, together with atom-labelling scheme. Displacement ellipsoids are shown at the 50% probability level.

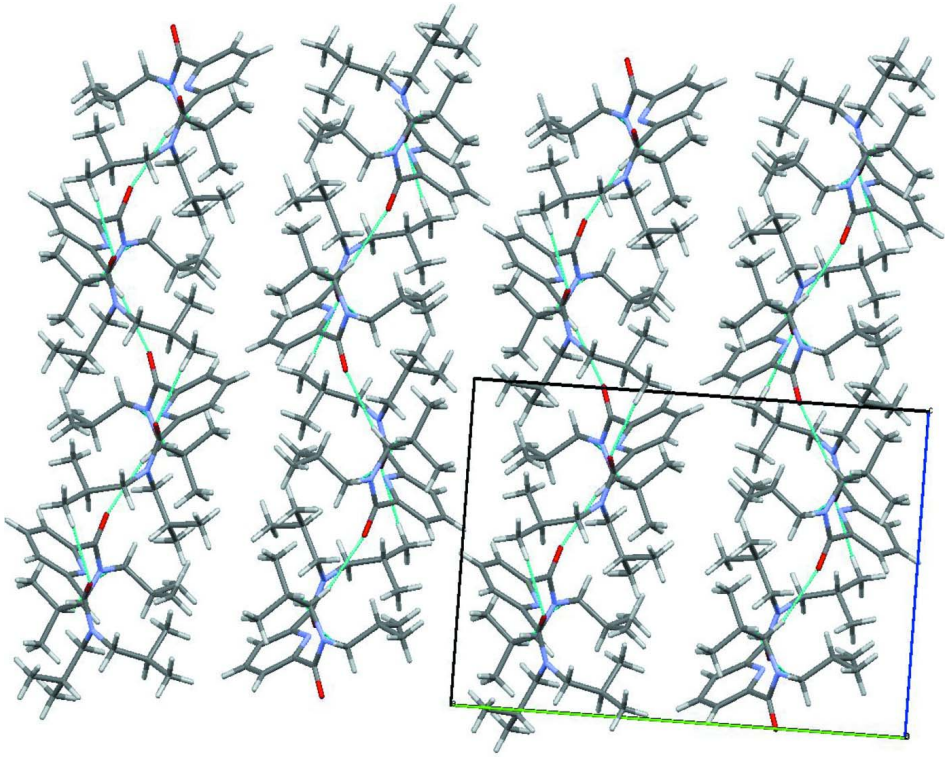


Figure 2

Projection along the *b* axis with highlighted hydrogen bonds between the molecules in the bands in direction of *c* axis.

N,N,N′,N′-Tetraisobutylpyridine-2,6-dicarboxamide

Crystal data

$C_{23}H_{39}N_3O_2$
$M_r = 389.57$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.5247\ (2)$ Å
$b = 17.7765\ (3)$ Å
$c = 12.8773\ (2)$ Å
$\beta = 96.877\ (2)°$
$V = 2391.91\ (7)$ Å^3
$Z = 4$
$F(000) = 856$
$D_x = 1.082$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 15197 reflections
$\theta = 3.5–67.0°$
$\mu = 0.54$ mm^{-1}
$T = 120$ K
Prism, colourless
0.49 × 0.42 × 0.23 mm

Data collection

Agilent Xcalibur Atlas Gemini ultra diffractometer
Radiation source: Enhance Ultra (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.3784 pixels mm^{-1}
Rotation method data acquisition using ω scans
Absorption correction: analytical (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.929$, $T_{max} = 0.962$
31214 measured reflections
4272 independent reflections
3867 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 67.1°$, $\theta_{min} = 4.2°$
$h = -12\rightarrow12$
$k = -20\rightarrow21$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.112$
$S = 1.05$
4272 reflections
261 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.5367P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ 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. The hydrogen atoms were localized from the difference Fourier map. Despite of that, all hydrogen atoms connected to C were constrained to ideal positions. The isotropic temperature parameters of hydrogen atoms were calculated as $1.2*U_{eq}$ of the parent atom.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.59347 (11)	0.14933 (7)	0.60811 (8)	0.0311 (3)
C2	0.60691 (12)	0.08382 (7)	0.55206 (9)	0.0371 (3)
H2	0.5408	0.0668	0.5033	0.044*
C3	0.72048 (12)	0.04424 (7)	0.57014 (10)	0.0402 (3)
H3	0.7308	−0.0011	0.5361	0.048*
C4	0.81870 (12)	0.07328 (7)	0.63991 (10)	0.0371 (3)
H4	0.8965	0.0482	0.6529	0.045*
C5	0.79847 (11)	0.14055 (7)	0.68995 (9)	0.0319 (3)
C6	0.47213 (11)	0.19491 (7)	0.58800 (9)	0.0329 (3)
N2	0.40863 (9)	0.21191 (6)	0.66956 (7)	0.0332 (2)
C7	0.30023 (11)	0.26406 (7)	0.65316 (9)	0.0363 (3)
H7A	0.2221	0.2366	0.6604	0.044*
H7B	0.2939	0.2832	0.5822	0.044*
C8	0.31001 (12)	0.33034 (8)	0.72858 (10)	0.0396 (3)
H8	0.3019	0.3115	0.7990	0.048*
C9	0.19691 (14)	0.38209 (9)	0.69475 (12)	0.0509 (4)
H9A	0.2051	0.4023	0.6267	0.061*
H9B	0.1958	0.4225	0.7441	0.061*
H9C	0.1187	0.3540	0.6922	0.061*
C10	0.43658 (14)	0.37205 (8)	0.73123 (12)	0.0492 (3)
H10A	0.5058	0.3383	0.7532	0.059*
H10B	0.4381	0.4133	0.7795	0.059*

H10C	0.4457	0.3909	0.6627	0.059*
C11	0.43174 (11)	0.17506 (7)	0.77252 (9)	0.0337 (3)
H11A	0.4472	0.2134	0.8261	0.040*
H11B	0.5083	0.1444	0.7748	0.040*
C12	0.32074 (12)	0.12556 (7)	0.79723 (10)	0.0383 (3)
H12	0.2446	0.1573	0.7971	0.046*
C13	0.29120 (17)	0.06398 (9)	0.71727 (12)	0.0577 (4)
H13A	0.3641	0.0315	0.7176	0.069*
H13B	0.2715	0.0859	0.6491	0.069*
H13C	0.2191	0.0353	0.7342	0.069*
C14	0.35334 (15)	0.09285 (8)	0.90645 (11)	0.0492 (3)
H14A	0.2806	0.0662	0.9261	0.059*
H14B	0.3756	0.1328	0.9553	0.059*
H14C	0.4244	0.0589	0.9068	0.059*
C15	0.90910 (11)	0.17978 (7)	0.75374 (10)	0.0352 (3)
N3	0.89638 (9)	0.20256 (6)	0.85171 (8)	0.0351 (2)
C16	0.99475 (11)	0.25225 (7)	0.90474 (10)	0.0375 (3)
H16A	1.0630	0.2581	0.8610	0.045*
H16B	1.0309	0.2288	0.9696	0.045*
C17	0.94382 (13)	0.32978 (7)	0.92891 (10)	0.0407 (3)
H17	0.8868	0.3241	0.9833	0.049*
C18	0.86814 (15)	0.36539 (9)	0.83386 (12)	0.0528 (4)
H18A	0.9224	0.3715	0.7796	0.063*
H18B	0.8369	0.4137	0.8526	0.063*
H18C	0.7972	0.3336	0.8092	0.063*
C19	1.05650 (15)	0.37855 (8)	0.97250 (11)	0.0505 (4)
H19A	1.1168	0.3817	0.9223	0.061*
H19B	1.0973	0.3567	1.0361	0.061*
H19C	1.0265	0.4281	0.9867	0.061*
C20	0.78661 (11)	0.18394 (7)	0.90704 (9)	0.0357 (3)
H20A	0.7305	0.1502	0.8638	0.043*
H20B	0.7390	0.2296	0.9166	0.043*
C21	0.82297 (11)	0.14717 (7)	1.01368 (9)	0.0355 (3)
H21	0.8725	0.1832	1.0598	0.043*
C22	0.69990 (13)	0.12864 (8)	1.05952 (10)	0.0417 (3)
H22A	0.6509	0.1738	1.0644	0.050*
H22B	0.7204	0.1073	1.1280	0.050*
H22C	0.6508	0.0932	1.0151	0.050*
C23	0.90338 (13)	0.07718 (8)	1.00455 (12)	0.0479 (3)
H23A	0.8561	0.0417	0.9589	0.057*
H23B	0.9241	0.0550	1.0725	0.057*
H23C	0.9808	0.0905	0.9765	0.057*
N1	0.68718 (9)	0.17810 (6)	0.67644 (7)	0.0313 (2)
O1	0.43906 (9)	0.21594 (6)	0.49754 (6)	0.0446 (2)
O2	1.00544 (8)	0.19100 (6)	0.71057 (8)	0.0493 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0313 (6)	0.0360 (6)	0.0262 (5)	−0.0027 (5)	0.0038 (4)	0.0022 (4)
C2	0.0380 (6)	0.0393 (6)	0.0333 (6)	−0.0044 (5)	0.0017 (5)	−0.0033 (5)
C3	0.0435 (7)	0.0359 (6)	0.0420 (7)	−0.0001 (5)	0.0077 (5)	−0.0060 (5)
C4	0.0333 (6)	0.0390 (6)	0.0398 (6)	0.0034 (5)	0.0074 (5)	0.0010 (5)
C5	0.0288 (6)	0.0388 (6)	0.0286 (6)	−0.0008 (5)	0.0061 (4)	0.0018 (5)
C6	0.0320 (6)	0.0379 (6)	0.0277 (6)	−0.0019 (5)	−0.0008 (5)	−0.0007 (5)
N2	0.0284 (5)	0.0426 (6)	0.0275 (5)	0.0028 (4)	−0.0008 (4)	0.0013 (4)
C7	0.0281 (6)	0.0455 (7)	0.0340 (6)	0.0033 (5)	−0.0010 (5)	0.0020 (5)
C8	0.0372 (7)	0.0482 (7)	0.0340 (6)	0.0029 (5)	0.0067 (5)	0.0000 (5)
C9	0.0511 (8)	0.0551 (8)	0.0475 (8)	0.0133 (7)	0.0104 (6)	−0.0011 (6)
C10	0.0484 (8)	0.0493 (8)	0.0498 (8)	−0.0065 (6)	0.0057 (6)	−0.0062 (6)
C11	0.0301 (6)	0.0429 (7)	0.0273 (6)	0.0001 (5)	0.0002 (5)	0.0012 (5)
C12	0.0304 (6)	0.0401 (7)	0.0440 (7)	−0.0004 (5)	0.0035 (5)	0.0019 (5)
C13	0.0676 (10)	0.0462 (8)	0.0541 (9)	−0.0115 (7)	−0.0138 (7)	0.0009 (7)
C14	0.0543 (8)	0.0517 (8)	0.0430 (7)	−0.0097 (7)	0.0122 (6)	0.0033 (6)
C15	0.0274 (6)	0.0416 (7)	0.0367 (6)	0.0023 (5)	0.0038 (5)	−0.0011 (5)
N3	0.0262 (5)	0.0459 (6)	0.0329 (5)	−0.0011 (4)	0.0019 (4)	−0.0031 (4)
C16	0.0293 (6)	0.0433 (7)	0.0384 (6)	−0.0012 (5)	−0.0020 (5)	−0.0018 (5)
C17	0.0454 (7)	0.0428 (7)	0.0346 (6)	0.0012 (6)	0.0076 (5)	0.0022 (5)
C18	0.0537 (8)	0.0545 (8)	0.0510 (8)	0.0108 (7)	0.0092 (7)	0.0135 (6)
C19	0.0655 (9)	0.0442 (7)	0.0423 (7)	−0.0099 (7)	0.0081 (7)	−0.0019 (6)
C20	0.0281 (6)	0.0470 (7)	0.0318 (6)	0.0005 (5)	0.0022 (5)	0.0002 (5)
C21	0.0345 (6)	0.0388 (6)	0.0314 (6)	−0.0003 (5)	−0.0027 (5)	−0.0028 (5)
C22	0.0443 (7)	0.0485 (7)	0.0323 (6)	0.0010 (6)	0.0040 (5)	0.0024 (5)
C23	0.0421 (7)	0.0436 (7)	0.0568 (8)	0.0036 (6)	0.0010 (6)	0.0029 (6)
N1	0.0294 (5)	0.0378 (5)	0.0268 (5)	−0.0005 (4)	0.0036 (4)	0.0000 (4)
O1	0.0461 (5)	0.0595 (6)	0.0272 (4)	0.0104 (4)	0.0001 (4)	0.0047 (4)
O2	0.0304 (5)	0.0735 (7)	0.0459 (5)	−0.0086 (4)	0.0117 (4)	−0.0119 (5)

Geometric parameters (Å, º)

C1—N1	1.3419 (15)	C13—H13B	0.9600
C1—C2	1.3862 (17)	C13—H13C	0.9600
C1—C6	1.5084 (16)	C14—H14A	0.9600
C2—C3	1.3825 (18)	C14—H14B	0.9600
C2—H2	0.9300	C14—H14C	0.9600
C3—C4	1.3856 (18)	C15—O2	1.2295 (15)
C3—H3	0.9300	C15—N3	1.3469 (16)
C4—C5	1.3868 (18)	N3—C20	1.4660 (15)
C4—H4	0.9300	N3—C16	1.4660 (16)
C5—N1	1.3412 (15)	C16—C17	1.5242 (18)
C5—C15	1.5125 (17)	C16—H16A	0.9700
C6—O1	1.2332 (14)	C16—H16B	0.9700
C6—N2	1.3450 (16)	C17—C18	1.5165 (19)
N2—C7	1.4655 (15)	C17—C19	1.521 (2)

N2—C11	1.4726 (15)	C17—H17	0.9800
C7—C8	1.5225 (18)	C18—H18A	0.9600
C7—H7A	0.9700	C18—H18B	0.9600
C7—H7B	0.9700	C18—H18C	0.9600
C8—C10	1.5214 (19)	C19—H19A	0.9600
C8—C9	1.5261 (19)	C19—H19B	0.9600
C8—H8	0.9800	C19—H19C	0.9600
C9—H9A	0.9600	C20—C21	1.5276 (17)
C9—H9B	0.9600	C20—H20A	0.9700
C9—H9C	0.9600	C20—H20B	0.9700
C10—H10A	0.9600	C21—C23	1.5172 (18)
C10—H10B	0.9600	C21—C22	1.5225 (18)
C10—H10C	0.9600	C21—H21	0.9800
C11—C12	1.5262 (17)	C22—H22A	0.9600
C11—H11A	0.9700	C22—H22B	0.9600
C11—H11B	0.9700	C22—H22C	0.9600
C12—C13	1.510 (2)	C23—H23A	0.9600
C12—C14	1.5226 (19)	C23—H23B	0.9600
C12—H12	0.9800	C23—H23C	0.9600
C13—H13A	0.9600		

N1—C1—C2	123.28 (11)	H13B—C13—H13C	109.5
N1—C1—C6	116.65 (10)	C12—C14—H14A	109.5
C2—C1—C6	119.93 (10)	C12—C14—H14B	109.5
C3—C2—C1	118.68 (11)	H14A—C14—H14B	109.5
C3—C2—H2	120.7	C12—C14—H14C	109.5
C1—C2—H2	120.7	H14A—C14—H14C	109.5
C2—C3—C4	118.85 (12)	H14B—C14—H14C	109.5
C2—C3—H3	120.6	O2—C15—N3	123.68 (11)
C4—C3—H3	120.6	O2—C15—C5	116.89 (11)
C3—C4—C5	118.58 (11)	N3—C15—C5	119.40 (10)
C3—C4—H4	120.7	C15—N3—C20	124.05 (10)
C5—C4—H4	120.7	C15—N3—C16	118.27 (10)
N1—C5—C4	123.31 (11)	C20—N3—C16	117.60 (10)
N1—C5—C15	116.39 (10)	N3—C16—C17	113.20 (10)
C4—C5—C15	119.92 (10)	N3—C16—H16A	108.9
O1—C6—N2	124.00 (11)	C17—C16—H16A	108.9
O1—C6—C1	117.54 (10)	N3—C16—H16B	108.9
N2—C6—C1	118.44 (10)	C17—C16—H16B	108.9
C6—N2—C7	118.72 (10)	H16A—C16—H16B	107.8
C6—N2—C11	124.00 (10)	C18—C17—C19	111.77 (12)
C7—N2—C11	116.93 (9)	C18—C17—C16	112.09 (11)
N2—C7—C8	113.93 (10)	C19—C17—C16	108.24 (11)
N2—C7—H7A	108.8	C18—C17—H17	108.2
C8—C7—H7A	108.8	C19—C17—H17	108.2
N2—C7—H7B	108.8	C16—C17—H17	108.2
C8—C7—H7B	108.8	C17—C18—H18A	109.5
H7A—C7—H7B	107.7	C17—C18—H18B	109.5

C10—C8—C7	112.56 (10)	H18A—C18—H18B	109.5
C10—C8—C9	111.31 (12)	C17—C18—H18C	109.5
C7—C8—C9	107.08 (11)	H18A—C18—H18C	109.5
C10—C8—H8	108.6	H18B—C18—H18C	109.5
C7—C8—H8	108.6	C17—C19—H19A	109.5
C9—C8—H8	108.6	C17—C19—H19B	109.5
C8—C9—H9A	109.5	H19A—C19—H19B	109.5
C8—C9—H9B	109.5	C17—C19—H19C	109.5
H9A—C9—H9B	109.5	H19A—C19—H19C	109.5
C8—C9—H9C	109.5	H19B—C19—H19C	109.5
H9A—C9—H9C	109.5	N3—C20—C21	113.98 (10)
H9B—C9—H9C	109.5	N3—C20—H20A	108.8
C8—C10—H10A	109.5	C21—C20—H20A	108.8
C8—C10—H10B	109.5	N3—C20—H20B	108.8
H10A—C10—H10B	109.5	C21—C20—H20B	108.8
C8—C10—H10C	109.5	H20A—C20—H20B	107.7
H10A—C10—H10C	109.5	C23—C21—C22	111.16 (11)
H10B—C10—H10C	109.5	C23—C21—C20	111.30 (11)
N2—C11—C12	113.34 (9)	C22—C21—C20	107.93 (10)
N2—C11—H11A	108.9	C23—C21—H21	108.8
C12—C11—H11A	108.9	C22—C21—H21	108.8
N2—C11—H11B	108.9	C20—C21—H21	108.8
C12—C11—H11B	108.9	C21—C22—H22A	109.5
H11A—C11—H11B	107.7	C21—C22—H22B	109.5
C13—C12—C14	111.00 (12)	H22A—C22—H22B	109.5
C13—C12—C11	112.09 (11)	C21—C22—H22C	109.5
C14—C12—C11	108.62 (10)	H22A—C22—H22C	109.5
C13—C12—H12	108.3	H22B—C22—H22C	109.5
C14—C12—H12	108.3	C21—C23—H23A	109.5
C11—C12—H12	108.3	C21—C23—H23B	109.5
C12—C13—H13A	109.5	H23A—C23—H23B	109.5
C12—C13—H13B	109.5	C21—C23—H23C	109.5
H13A—C13—H13B	109.5	H23A—C23—H23C	109.5
C12—C13—H13C	109.5	H23B—C23—H23C	109.5
H13A—C13—H13C	109.5	C5—N1—C1	117.21 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*A*···O2^{i}	0.97	2.57	3.5226 (15)	166
C11—H11*A*···O1^{ii}	0.97	2.55	3.4790 (15)	160

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