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(2*Z*,6*Z*)-N^2,$N^{2'}$-Bis(2,6-diisopropylphenyl)-N^1,$N^{1'}$-bis(2-methoxyethyl)pyridine-2,6-dicarboxamidine

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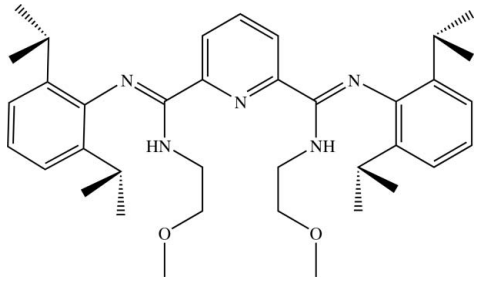
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.062; wR factor = 0.199; data-to-parameter ratio = 14.4.

In the title compound, $C_{37}H_{53}N_5O_2$, the benzene rings make dihedral angles of 84.61 (8) and 67.10 (9)° with the pyridine ring. The crystal structure is stabilized by strong intramolecular interactions. The two (2-methoxyethyl)amine groups are disordered over two positions; the site occupancies are *ca* 0.6 and 0.4.

Related literature

For related literature, see: Archer *et al.* (2006); Bacha *et al.* (1987); Bonnett (1970); Shishkin *et al.* (2004); Sladowska *et al.* (1995).



Experimental

Crystal data

$C_{37}H_{53}N_5O_2$
M_r = 599.84
Monoclinic, $P2_1/c$
a = 9.8343 (6) Å
b = 21.4903 (10) Å
c = 17.8137 (10) Å
β = 105.561 (4)°
V = 3626.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 296 K
0.72 × 0.64 × 0.57 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.960, T_{max} = 0.973
27457 measured reflections
7034 independent reflections
4098 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.199
S = 1.00
7034 reflections
489 parameters
426 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2*A*—H2*A*1···N1	0.86	2.11	2.598 (4)	115
N4*A*—H4*A*1···O2*A*	0.86	2.33	2.735 (5)	110
N4*A*—H4*A*1···N1	0.86	2.29	2.688 (5)	109
C16—H16···N3	0.98	2.40	2.842 (4)	107

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); 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) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2052).

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supporting information

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(2*Z*,6*Z*)-*N*^{2},*N*$^{2'}$-Bis(2,6-diisopropylphenyl)-*N*^{1},*N*$^{1'}$-bis(2-methoxyethyl)-pyridine-2,6-dicarboxamidine

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S1. Comment

Imide functionality is found as a basic structural element in a wide range of naturally occurring compounds such as uracil and thymine. Moreover, many imide-containing unnatural products have been prepared to test the pharmacological properties as well as their structural properties (Bacha *et al.*, 1987; Sladowska *et al.*, 1995). Imidoyl chlorides react with carboxylic acids and their salts, yielding N-substitue imides with regard to Mumm rearrangement reaction (Bonnett, 1970; Shishkin *et al.*, 2004). We describe here the crystal structure of the title compound as determined by an X-ray crystallographic analysis.

The structure of the title compound is shown in Fig. 1. The interatomic distances and angles show no anomalies. In the molecular structure of the title compound, (C10—C15) and (C26—C31) phenyl rings make dihedral angles of 84.61 (8) and 67.10 (9)°, respectively, with the pyridine ring. In the molecule, the two (2-methoxyethyl)amine groups, (N2/O1/C7—C9) and (N4/O2/C23—C25) were disordered over sites N2A/O1A/C7A–C9A; N4A/O2A/C23A—C25A and N2B/O1B/C7B–C9B; N4B/O2B/C23B—C25B, with site occupancy factors 59.7 (3) and 40.3 (3)%, respectively.

There are no significant inter-molecular interactions in the crystal structure of the title compound and the crystal structure is stabilizded by strong intramolecular interactions of the type N—H···N, N—H···O and C—H···N; details of these interactions have been provided in the Table.

S2. Experimental

The title compound was synthesized according to a modification of literature methods (Archer *et al.*, 2006) and X-ray quality crystals were grown from CH_2Cl_2-hexane (1:2 *v*/*v*, 30 ml).

S3. Refinement

H atoms were positioned geometrically and treated using a riding model, fixing the bond lengths at 0.96, 0.97, 0.98, 0.93 and 0.86 Å for CH_3, CH_2, CH, aromatic CH and NH groups, respectively. The displacement parameters of the H atoms were constrained as U_{iso}(H) = 1.2U_{eq} (1.5U_{eq} for methyl) of the parent atom. In the molecule, the two (2-methoxyethyl)-amine groups, (N2/O1/C7—C9) and (N4/O2/C23—C25) show positional disorder and the refined site-occupancy factors of the disordered parts, *viz*. N2A/O1A/C7A–C9A/N4A/O2A/C23A—C25A and N2B/O1B/C7B–C9B/N4B/O2B/C23B—C25B, are 59.7 (3) and 40.3 (3)%, respectively. The disordered atoms were refined using the following restraints: SIMU, DELU and SADI (*SHELXL*; Sheldrick, 1997).

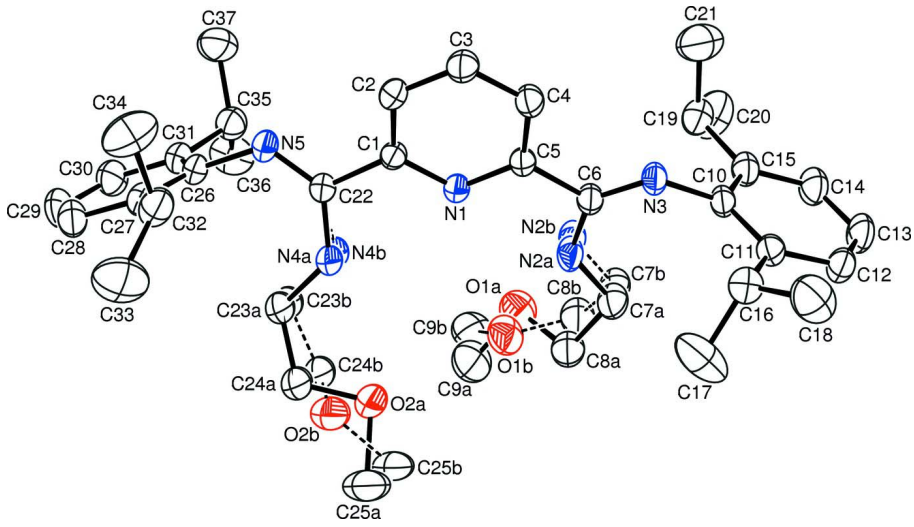

Figure 1

A view of (II), with 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms have been omitted for clarity.

(2*Z*,6*Z*)-*N*^{2},*N*$^{2'}$-Bis(2,6-diisopropylphenyl)- *N*^{1},*N*$^{1'}$-bis(2-methoxyethyl)pyridine-2,6-dicarboxamidine

Crystal data

$C_{37}H_{53}N_5O_2$
$M_r = 599.84$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.8343\ (6)$ Å
$b = 21.4903\ (10)$ Å
$c = 17.8137\ (10)$ Å
$\beta = 105.561\ (4)°$
$V = 3626.8\ (4)$ Å^3
$Z = 4$
$F(000) = 1304$
$D_x = 1.099$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 23890 reflections
$\theta = 1.5–27.2°$
$\mu = 0.07$ mm^{-1}
$T = 296$ K
Prism, light yellow
0.72 × 0.64 × 0.57 mm

Data collection

STOE IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
w scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.960$, $T_{max} = 0.973$
27457 measured reflections
7034 independent reflections
4098 reflections with $I > 2.0\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.5°$
$h = -12\rightarrow12$
$k = -26\rightarrow26$
$l = -21\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.199$
$S = 1.01$
7034 reflections
489 parameters
426 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

$w = 1/[\sigma^2(F_o^2) + (0.1212P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: *SHELXL*,
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0065 (15)

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}	Occ. (<1)
O1A	0.5370 (5)	0.7545 (2)	0.4930 (3)	0.0943 (14)	0.597 (3)
O1B	0.5298 (6)	0.7640 (4)	0.5321 (4)	0.0925 (16)	0.403 (3)
O2A	0.5502 (5)	0.72967 (16)	0.7186 (3)	0.0923 (13)	0.597 (3)
O2B	0.5425 (7)	0.7151 (3)	0.7689 (4)	0.0951 (15)	0.403 (3)
N1	0.2067 (2)	0.64873 (8)	0.54446 (12)	0.0461 (5)	
N2A	0.2482 (4)	0.7518 (2)	0.4776 (4)	0.0654 (14)	0.597 (3)
H2A1	0.3027	0.7290	0.5127	0.078*	0.597 (3)
N2B	0.2535 (5)	0.7427 (4)	0.4586 (6)	0.0632 (15)	0.403 (3)
H2B1	0.3107	0.7130	0.4780	0.076*	0.403 (3)
N3	0.0055 (2)	0.75478 (9)	0.40625 (13)	0.0540 (6)	
N4A	0.4169 (5)	0.6192 (2)	0.6705 (4)	0.0618 (14)	0.597 (3)
H4A1	0.3844	0.6559	0.6572	0.074*	0.597 (3)
N4B	0.4298 (7)	0.6165 (3)	0.6539 (6)	0.0631 (16)	0.403 (3)
H4B1	0.4080	0.6498	0.6264	0.076*	0.403 (3)
N5	0.3329 (2)	0.51445 (9)	0.65512 (13)	0.0552 (6)	
C1	0.1955 (2)	0.59498 (10)	0.58032 (14)	0.0430 (5)	
C2	0.0708 (3)	0.56236 (11)	0.56537 (15)	0.0501 (6)	
H2A	0.0656	0.5249	0.5906	0.060*	
C3	−0.0458 (3)	0.58608 (12)	0.51249 (17)	0.0586 (7)	
H3	−0.1316	0.5652	0.5023	0.070*	
C4	−0.0352 (3)	0.64116 (12)	0.47447 (16)	0.0544 (7)	
H4A	−0.1127	0.6576	0.4378	0.065*	
C5	0.0930 (2)	0.67107 (10)	0.49226 (14)	0.0451 (6)	
C6	0.1146 (3)	0.73043 (11)	0.45166 (16)	0.0517 (6)	
C7A	0.3149 (4)	0.8061 (3)	0.4565 (5)	0.0731 (14)	0.597 (3)
H7A1	0.3125	0.8040	0.4018	0.088*	0.597 (3)
H7A2	0.2635	0.8430	0.4644	0.088*	0.597 (3)
C8A	0.4584 (5)	0.8106 (2)	0.5026 (4)	0.0778 (13)	0.597 (3)
H8A1	0.4608	0.8155	0.5571	0.093*	0.597 (3)
H8A2	0.5025	0.8468	0.4868	0.093*	0.597 (3)
C9A	0.6721 (7)	0.7599 (4)	0.5508 (6)	0.112 (2)	0.597 (3)

H9A1	0.7283	0.7238	0.5485	0.168*	0.597 (3)
H9A2	0.6572	0.7630	0.6018	0.168*	0.597 (3)
H9A3	0.7202	0.7965	0.5405	0.168*	0.597 (3)
C7B	0.3184 (5)	0.7976 (4)	0.4383 (7)	0.0720 (15)	0.403 (3)
H7B1	0.2844	0.8040	0.3825	0.086*	0.403 (3)
H7B2	0.2893	0.8331	0.4638	0.086*	0.403 (3)
C8B	0.4666 (6)	0.7952 (4)	0.4590 (5)	0.0861 (15)	0.403 (3)
H8B1	0.5028	0.8373	0.4621	0.103*	0.403 (3)
H8B2	0.4962	0.7740	0.4179	0.103*	0.403 (3)
C9B	0.6630 (9)	0.7389 (6)	0.5238 (7)	0.104 (3)	0.403 (3)
H9B1	0.7132	0.7193	0.5716	0.155*	0.403 (3)
H9B2	0.7192	0.7722	0.5119	0.155*	0.403 (3)
H9B3	0.6443	0.7090	0.4823	0.155*	0.403 (3)
C10	0.0038 (2)	0.80692 (11)	0.35734 (16)	0.0508 (6)	
C11	−0.0518 (3)	0.86324 (12)	0.37645 (17)	0.0573 (6)	
C12	−0.0666 (3)	0.91245 (13)	0.3238 (2)	0.0662 (8)	
H12	−0.1022	0.9503	0.3354	0.079*	
C13	−0.0297 (3)	0.90611 (14)	0.2554 (2)	0.0741 (9)	
H13	−0.0396	0.9396	0.2213	0.089*	
C14	0.0219 (3)	0.85041 (14)	0.2370 (2)	0.0705 (8)	
H14	0.0455	0.8466	0.1900	0.085*	
C15	0.0398 (3)	0.79974 (12)	0.28689 (17)	0.0588 (7)	
C16	−0.0947 (3)	0.86906 (14)	0.4514 (2)	0.0719 (8)	
H16	−0.1226	0.8273	0.4637	0.086*	
C17	0.0252 (5)	0.8880 (3)	0.5181 (3)	0.1348 (17)	
H17A	−0.0065	0.8909	0.5645	0.202*	
H17B	0.0602	0.9278	0.5072	0.202*	
H17C	0.0992	0.8577	0.5256	0.202*	
C18	−0.2207 (4)	0.9107 (2)	0.4459 (3)	0.1056 (12)	
H18A	−0.2420	0.9119	0.4954	0.158*	
H18B	−0.3005	0.8947	0.4070	0.158*	
H18C	−0.1995	0.9520	0.4317	0.158*	
C19	0.0930 (3)	0.73796 (14)	0.2644 (2)	0.0711 (8)	
H19	0.1530	0.7199	0.3124	0.085*	
C20	0.1838 (5)	0.7434 (2)	0.2081 (3)	0.1138 (14)	
H20A	0.2590	0.7724	0.2283	0.171*	
H20B	0.1272	0.7579	0.1586	0.171*	
H20C	0.2228	0.7034	0.2018	0.171*	
C21	−0.0254 (5)	0.6931 (2)	0.2344 (3)	0.1140 (14)	
H21A	0.0116	0.6546	0.2208	0.171*	
H21B	−0.0909	0.7103	0.1892	0.171*	
H21C	−0.0730	0.6855	0.2741	0.171*	
C22	0.3279 (3)	0.57234 (10)	0.63804 (15)	0.0480 (6)	
C23A	0.5549 (5)	0.6181 (2)	0.7229 (5)	0.0726 (14)	0.597 (3)
H23A	0.5582	0.5861	0.7616	0.087*	0.597 (3)
H23B	0.6221	0.6069	0.6940	0.087*	0.597 (3)
C24A	0.5971 (7)	0.6758 (2)	0.7617 (4)	0.0842 (13)	0.597 (3)
H24A	0.5635	0.6768	0.8082	0.101*	0.597 (3)

H24B	0.6994	0.6768	0.7786	0.101*	0.597 (3)
C25A	0.5939 (11)	0.7803 (3)	0.7842 (5)	0.114 (2)	0.597 (3)
H25A	0.5695	0.8208	0.7619	0.170*	0.597 (3)
H25B	0.6939	0.7783	0.8074	0.170*	0.597 (3)
H25C	0.5452	0.7728	0.8233	0.170*	0.597 (3)
C23B	0.5661 (6)	0.6184 (3)	0.7076 (8)	0.0716 (15)	0.403 (3)
H23C	0.6318	0.5957	0.6858	0.086*	0.403 (3)
H23D	0.5623	0.5975	0.7553	0.086*	0.403 (3)
C24B	0.6177 (7)	0.6806 (3)	0.7259 (5)	0.0820 (13)	0.403 (3)
H24C	0.7161	0.6786	0.7554	0.098*	0.403 (3)
H24D	0.6134	0.7025	0.6777	0.098*	0.403 (3)
C25B	0.5763 (15)	0.7832 (3)	0.7469 (7)	0.103 (3)	0.403 (3)
H25D	0.5296	0.8125	0.7722	0.154*	0.403 (3)
H25E	0.5436	0.7886	0.6915	0.154*	0.403 (3)
H25F	0.6764	0.7901	0.7637	0.154*	0.403 (3)
C26	0.4478 (3)	0.48655 (11)	0.71093 (16)	0.0522 (6)	
C27	0.4385 (3)	0.48101 (12)	0.78807 (17)	0.0607 (7)	
C28	0.5494 (4)	0.45132 (14)	0.84108 (19)	0.0757 (9)	
H28	0.5464	0.4475	0.8926	0.091*	
C29	0.6624 (4)	0.42760 (15)	0.8198 (2)	0.0853 (11)	
H29	0.7357	0.4087	0.8567	0.102*	
C30	0.6674 (3)	0.43182 (14)	0.7434 (2)	0.0727 (9)	
H30	0.7437	0.4148	0.7290	0.087*	
C31	0.5608 (3)	0.46091 (11)	0.68764 (17)	0.0574 (6)	
C32	0.3120 (4)	0.50400 (14)	0.8115 (2)	0.0720 (8)	
H32	0.2695	0.5371	0.7748	0.086*	
C33	0.3440 (6)	0.5318 (2)	0.8925 (3)	0.1256 (16)	
H33A	0.4129	0.5643	0.8973	0.188*	
H33B	0.3803	0.5000	0.9304	0.188*	
H33C	0.2590	0.5488	0.9010	0.188*	
C34	0.2035 (5)	0.45314 (19)	0.8025 (3)	0.1180 (14)	
H34A	0.1230	0.4686	0.8174	0.177*	
H34B	0.2435	0.4186	0.8352	0.177*	
H34C	0.1750	0.4398	0.7491	0.177*	
C35	0.5654 (3)	0.46243 (13)	0.60353 (18)	0.0661 (7)	
H35	0.5049	0.4969	0.5783	0.079*	
C36	0.7109 (4)	0.4741 (2)	0.5927 (3)	0.1046 (12)	
H36A	0.7054	0.4748	0.5381	0.157*	
H36B	0.7737	0.4414	0.6175	0.157*	
H36C	0.7459	0.5133	0.6157	0.157*	
C37	0.5028 (5)	0.40298 (18)	0.5621 (2)	0.0998 (12)	
H37A	0.5055	0.4047	0.5086	0.150*	
H37B	0.4067	0.3988	0.5642	0.150*	
H37C	0.5566	0.3679	0.5871	0.150*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0658 (17)	0.099 (2)	0.109 (3)	0.0041 (16)	0.008 (2)	0.004 (2)
O1B	0.062 (2)	0.099 (3)	0.106 (3)	−0.004 (2)	0.003 (2)	0.015 (3)
O2A	0.099 (2)	0.0544 (16)	0.099 (3)	0.0028 (16)	−0.016 (2)	0.0037 (17)
O2B	0.095 (2)	0.072 (2)	0.099 (3)	−0.001 (2)	−0.008 (3)	−0.015 (2)
N1	0.0457 (11)	0.0400 (10)	0.0484 (13)	0.0014 (8)	0.0054 (9)	0.0052 (8)
N2A	0.0514 (16)	0.0571 (19)	0.077 (3)	−0.0094 (14)	−0.0007 (16)	0.0296 (19)
N2B	0.0511 (18)	0.057 (2)	0.074 (3)	−0.0046 (17)	0.0046 (19)	0.023 (2)
N3	0.0501 (12)	0.0480 (11)	0.0573 (14)	0.0001 (9)	0.0028 (10)	0.0170 (10)
N4A	0.0632 (18)	0.0446 (15)	0.062 (3)	0.0025 (14)	−0.0096 (17)	0.0073 (16)
N4B	0.063 (2)	0.049 (2)	0.062 (3)	−0.0002 (17)	−0.009 (2)	0.010 (2)
N5	0.0582 (13)	0.0428 (11)	0.0592 (15)	0.0043 (9)	0.0064 (10)	0.0108 (10)
C1	0.0516 (13)	0.0373 (11)	0.0402 (14)	0.0020 (9)	0.0122 (10)	0.0013 (9)
C2	0.0563 (15)	0.0415 (12)	0.0524 (16)	−0.0025 (10)	0.0147 (12)	0.0078 (11)
C3	0.0474 (14)	0.0544 (15)	0.0700 (19)	−0.0082 (11)	0.0089 (13)	0.0081 (13)
C4	0.0468 (14)	0.0538 (14)	0.0576 (17)	0.0001 (11)	0.0056 (12)	0.0107 (12)
C5	0.0431 (13)	0.0417 (12)	0.0468 (15)	0.0006 (9)	0.0055 (10)	0.0054 (10)
C6	0.0453 (12)	0.0475 (12)	0.0567 (16)	−0.0024 (10)	0.0041 (11)	0.0128 (11)
C7A	0.0578 (16)	0.064 (2)	0.090 (3)	−0.0137 (15)	0.0061 (17)	0.024 (2)
C8A	0.0589 (17)	0.073 (2)	0.094 (3)	−0.0154 (15)	0.0068 (19)	0.016 (2)
C9A	0.070 (3)	0.118 (5)	0.134 (5)	0.000 (3)	0.002 (3)	0.008 (4)
C7B	0.0578 (18)	0.064 (2)	0.086 (3)	−0.0142 (18)	0.0058 (19)	0.023 (2)
C8B	0.0647 (19)	0.085 (2)	0.101 (3)	−0.0122 (19)	0.009 (2)	0.020 (2)
C9B	0.066 (4)	0.103 (5)	0.127 (6)	−0.001 (3)	0.001 (4)	−0.011 (4)
C10	0.0416 (13)	0.0486 (13)	0.0556 (17)	−0.0012 (10)	0.0015 (11)	0.0161 (11)
C11	0.0503 (14)	0.0513 (13)	0.0623 (16)	−0.0022 (11)	0.0013 (11)	0.0085 (12)
C12	0.0653 (18)	0.0471 (14)	0.080 (2)	0.0028 (12)	0.0078 (15)	0.0143 (14)
C13	0.082 (2)	0.0601 (17)	0.077 (2)	0.0027 (15)	0.0143 (17)	0.0324 (16)
C14	0.0744 (19)	0.0681 (19)	0.067 (2)	0.0023 (15)	0.0164 (15)	0.0235 (15)
C15	0.0530 (14)	0.0589 (14)	0.0616 (18)	0.0010 (11)	0.0101 (12)	0.0171 (12)
C16	0.0779 (18)	0.0651 (16)	0.0686 (18)	0.0024 (13)	0.0126 (14)	0.0033 (14)
C17	0.106 (3)	0.206 (5)	0.076 (3)	0.009 (3)	−0.003 (2)	−0.024 (3)
C18	0.094 (2)	0.128 (3)	0.093 (3)	0.023 (2)	0.022 (2)	−0.008 (2)
C19	0.0732 (17)	0.0620 (15)	0.079 (2)	0.0048 (13)	0.0216 (14)	0.0121 (13)
C20	0.125 (3)	0.100 (3)	0.139 (4)	0.022 (2)	0.074 (3)	0.013 (2)
C21	0.094 (3)	0.092 (2)	0.151 (4)	−0.0075 (19)	0.023 (3)	−0.028 (2)
C22	0.0543 (13)	0.0417 (12)	0.0447 (14)	0.0034 (9)	0.0076 (10)	0.0039 (9)
C23A	0.0672 (18)	0.0554 (16)	0.077 (3)	−0.0006 (16)	−0.0128 (18)	0.0083 (17)
C24A	0.0802 (18)	0.0586 (15)	0.089 (3)	0.0011 (14)	−0.0197 (19)	0.0062 (17)
C25A	0.118 (4)	0.086 (3)	0.118 (5)	−0.010 (3)	0.000 (4)	−0.041 (3)
C23B	0.066 (2)	0.0557 (19)	0.076 (3)	0.0016 (18)	−0.011 (2)	0.0059 (19)
C24B	0.0786 (18)	0.0572 (15)	0.087 (3)	0.0007 (14)	−0.0177 (19)	0.0056 (18)
C25B	0.109 (5)	0.069 (3)	0.104 (6)	−0.007 (3)	−0.017 (5)	−0.028 (4)
C26	0.0591 (15)	0.0381 (12)	0.0544 (17)	0.0035 (11)	0.0063 (12)	0.0089 (11)
C27	0.0772 (17)	0.0425 (12)	0.0599 (18)	0.0056 (12)	0.0142 (13)	0.0072 (11)
C28	0.103 (3)	0.0622 (17)	0.055 (2)	0.0127 (17)	0.0093 (17)	0.0108 (14)

C29	0.092 (2)	0.074 (2)	0.073 (3)	0.0310 (18)	−0.0061 (19)	0.0139 (17)
C30	0.073 (2)	0.0632 (18)	0.076 (2)	0.0209 (14)	0.0089 (16)	0.0038 (15)
C31	0.0628 (15)	0.0470 (13)	0.0585 (15)	0.0074 (11)	0.0096 (12)	0.0048 (11)
C32	0.0908 (19)	0.0578 (15)	0.0726 (19)	0.0042 (13)	0.0312 (16)	0.0072 (13)
C33	0.140 (4)	0.128 (3)	0.117 (3)	0.007 (3)	0.048 (3)	−0.042 (3)
C34	0.110 (3)	0.086 (2)	0.172 (4)	−0.017 (2)	0.064 (3)	−0.014 (2)
C35	0.0743 (17)	0.0610 (15)	0.0634 (17)	0.0057 (13)	0.0194 (14)	0.0022 (13)
C36	0.094 (2)	0.132 (3)	0.096 (3)	−0.015 (2)	0.041 (2)	−0.012 (2)
C37	0.128 (3)	0.091 (2)	0.076 (2)	−0.021 (2)	0.020 (2)	−0.0139 (18)

Geometric parameters (Å, º)

O1A—C9A	1.452 (7)	C16—C18	1.510 (5)
O1A—C8A	1.465 (5)	C16—H16	0.9800
O1B—C8B	1.449 (6)	C17—H17A	0.9600
O1B—C9B	1.461 (7)	C17—H17B	0.9600
O2A—C24A	1.398 (5)	C17—H17C	0.9600
O2A—C25A	1.570 (6)	C18—H18A	0.9600
O2B—C24B	1.410 (6)	C18—H18B	0.9600
O2B—C25B	1.574 (7)	C18—H18C	0.9600
N1—C5	1.337 (3)	C19—C21	1.496 (5)
N1—C1	1.339 (3)	C19—C20	1.515 (5)
N2A—C6	1.350 (4)	C19—H19	0.9800
N2A—C7A	1.438 (4)	C20—H20A	0.9600
N2A—H2A1	0.8600	C20—H20B	0.9600
N2B—C6	1.363 (4)	C20—H20C	0.9600
N2B—C7B	1.433 (5)	C21—H21A	0.9600
N2B—H2B1	0.8600	C21—H21B	0.9600
N3—C6	1.271 (3)	C21—H21C	0.9600
N3—C10	1.417 (3)	C23A—C24A	1.426 (5)
N4A—C22	1.358 (4)	C23A—H23A	0.9700
N4A—C23A	1.426 (4)	C23A—H23B	0.9700
N4A—H4A1	0.8600	C24A—H24A	0.9700
N4B—C22	1.354 (5)	C24A—H24B	0.9700
N4B—C23B	1.423 (5)	C25A—H25A	0.9600
N4B—H4B1	0.8600	C25A—H25B	0.9600
N5—C22	1.279 (3)	C25A—H25C	0.9600
N5—C26	1.422 (3)	C23B—C24B	1.437 (6)
C1—C2	1.375 (3)	C23B—H23C	0.9700
C1—C22	1.507 (3)	C23B—H23D	0.9700
C2—C3	1.372 (4)	C24B—H24C	0.9700
C2—H2A	0.9300	C24B—H24D	0.9700
C3—C4	1.381 (4)	C25B—H25D	0.9600
C3—H3	0.9300	C25B—H25E	0.9600
C4—C5	1.375 (3)	C25B—H25F	0.9600
C4—H4A	0.9300	C26—C31	1.399 (4)
C5—C6	1.509 (3)	C26—C27	1.406 (4)
C7A—C8A	1.433 (6)	C27—C28	1.391 (4)

C7A—H7A1	0.9700	C27—C32	1.498 (4)
C7A—H7A2	0.9700	C28—C29	1.366 (5)
C8A—H8A1	0.9700	C28—H28	0.9300
C8A—H8A2	0.9700	C29—C30	1.378 (5)
C9A—H9A1	0.9600	C29—H29	0.9300
C9A—H9A2	0.9600	C30—C31	1.384 (4)
C9A—H9A3	0.9600	C30—H30	0.9300
C7B—C8B	1.405 (6)	C31—C35	1.512 (4)
C7B—H7B1	0.9700	C32—C34	1.506 (5)
C7B—H7B2	0.9700	C32—C33	1.515 (5)
C8B—H8B1	0.9700	C32—H32	0.9800
C8B—H8B2	0.9700	C33—H33A	0.9600
C9B—H9B1	0.9600	C33—H33B	0.9600
C9B—H9B2	0.9600	C33—H33C	0.9600
C9B—H9B3	0.9600	C34—H34A	0.9600
C10—C15	1.401 (4)	C34—H34B	0.9600
C10—C11	1.407 (4)	C34—H34C	0.9600
C11—C12	1.395 (4)	C35—C36	1.515 (5)
C11—C16	1.510 (5)	C35—C37	1.521 (5)
C12—C13	1.367 (5)	C35—H35	0.9800
C12—H12	0.9300	C36—H36A	0.9600
C13—C14	1.374 (5)	C36—H36B	0.9600
C13—H13	0.9300	C36—H36C	0.9600
C14—C15	1.386 (4)	C37—H37A	0.9600
C14—H14	0.9300	C37—H37B	0.9600
C15—C19	1.520 (4)	C37—H37C	0.9600
C16—C17	1.488 (5)		

C9A—O1A—C8A	105.2 (5)	C21—C19—C15	111.6 (3)
C8B—O1B—C9B	105.0 (5)	C20—C19—C15	114.4 (3)
C24A—O2A—C25A	100.4 (4)	C21—C19—H19	106.5
C24B—O2B—C25B	100.2 (5)	C20—C19—H19	106.5
C5—N1—C1	118.8 (2)	C15—C19—H19	106.5
C6—N2A—C7A	131.1 (4)	C19—C20—H20A	109.5
C6—N2A—H2A1	114.5	C19—C20—H20B	109.5
C7A—N2A—H2A1	114.5	H20A—C20—H20B	109.5
C6—N2B—C7B	129.7 (5)	C19—C20—H20C	109.5
C6—N2B—H2B1	115.1	H20A—C20—H20C	109.5
C7B—N2B—H2B1	115.1	H20B—C20—H20C	109.5
C6—N3—C10	125.9 (2)	C19—C21—H21A	109.5
C22—N4A—C23A	131.1 (4)	C19—C21—H21B	109.5
C22—N4A—H4A1	114.4	H21A—C21—H21B	109.5
C23A—N4A—H4A1	114.4	C19—C21—H21C	109.5
C22—N4B—C23B	132.1 (5)	H21A—C21—H21C	109.5
C22—N4B—H4B1	114.0	H21B—C21—H21C	109.5
C23B—N4B—H4B1	114.0	N5—C22—N4B	130.9 (4)
C22—N5—C26	123.3 (2)	N5—C22—N4A	129.9 (3)
N1—C1—C2	122.1 (2)	N5—C22—C1	116.5 (2)

N1—C1—C22	115.9 (2)	N4B—C22—C1	111.8 (4)
C2—C1—C22	122.0 (2)	N4A—C22—C1	113.0 (3)
C3—C2—C1	118.8 (2)	C24A—C23A—N4A	113.9 (3)
C3—C2—H2A	120.6	C24A—C23A—H23A	108.8
C1—C2—H2A	120.6	N4A—C23A—H23A	108.8
C2—C3—C4	119.7 (2)	C24A—C23A—H23B	108.8
C2—C3—H3	120.1	N4A—C23A—H23B	108.8
C4—C3—H3	120.1	H23A—C23A—H23B	107.7
C5—C4—C3	118.2 (2)	O2A—C24A—C23A	116.3 (5)
C5—C4—H4A	120.9	O2A—C24A—H24A	108.2
C3—C4—H4A	120.9	C23A—C24A—H24A	108.2
N1—C5—C4	122.5 (2)	O2A—C24A—H24B	108.2
N1—C5—C6	116.0 (2)	C23A—C24A—H24B	108.2
C4—C5—C6	121.5 (2)	H24A—C24A—H24B	107.4
N3—C6—N2A	131.0 (3)	O2A—C25A—H25A	109.5
N3—C6—N2B	129.2 (4)	O2A—C25A—H25B	109.5
N3—C6—C5	116.7 (2)	H25A—C25A—H25B	109.5
N2A—C6—C5	111.8 (3)	O2A—C25A—H25C	109.5
N2B—C6—C5	112.7 (3)	H25A—C25A—H25C	109.5
C8A—C7A—N2A	110.7 (3)	H25B—C25A—H25C	109.5
C8A—C7A—H7A1	109.5	N4B—C23B—C24B	113.0 (4)
N2A—C7A—H7A1	109.5	N4B—C23B—H23C	109.0
C8A—C7A—H7A2	109.5	C24B—C23B—H23C	109.0
N2A—C7A—H7A2	109.5	N4B—C23B—H23D	109.0
H7A1—C7A—H7A2	108.1	C24B—C23B—H23D	109.0
C7A—C8A—O1A	110.3 (4)	H23C—C23B—H23D	107.8
C7A—C8A—H8A1	109.6	O2B—C24B—C23B	114.1 (6)
O1A—C8A—H8A1	109.6	O2B—C24B—H24C	108.7
C7A—C8A—H8A2	109.6	C23B—C24B—H24C	108.7
O1A—C8A—H8A2	109.6	O2B—C24B—H24D	108.7
H8A1—C8A—H8A2	108.1	C23B—C24B—H24D	108.7
O1A—C9A—H9A1	109.5	H24C—C24B—H24D	107.6
O1A—C9A—H9A2	109.5	O2B—C25B—H25D	109.5
H9A1—C9A—H9A2	109.5	O2B—C25B—H25E	109.5
O1A—C9A—H9A3	109.5	H25D—C25B—H25E	109.5
H9A1—C9A—H9A3	109.5	O2B—C25B—H25F	109.5
H9A2—C9A—H9A3	109.5	H25D—C25B—H25F	109.5
C8B—C7B—N2B	113.8 (4)	H25E—C25B—H25F	109.5
C8B—C7B—H7B1	108.8	C31—C26—C27	121.4 (2)
N2B—C7B—H7B1	108.8	C31—C26—N5	120.3 (2)
C8B—C7B—H7B2	108.8	C27—C26—N5	118.1 (2)
N2B—C7B—H7B2	108.8	C28—C27—C26	117.3 (3)
H7B1—C7B—H7B2	107.7	C28—C27—C32	121.4 (3)
C7B—C8B—O1B	114.7 (5)	C26—C27—C32	121.3 (3)
C7B—C8B—H8B1	108.6	C29—C28—C27	122.0 (3)
O1B—C8B—H8B1	108.6	C29—C28—H28	119.0
C7B—C8B—H8B2	108.6	C27—C28—H28	119.0
O1B—C8B—H8B2	108.6	C28—C29—C30	119.8 (3)

H8B1—C8B—H8B2	107.6	C28—C29—H29	120.1
O1B—C9B—H9B1	109.5	C30—C29—H29	120.1
O1B—C9B—H9B2	109.5	C29—C30—C31	121.1 (3)
H9B1—C9B—H9B2	109.5	C29—C30—H30	119.4
O1B—C9B—H9B3	109.5	C31—C30—H30	119.4
H9B1—C9B—H9B3	109.5	C30—C31—C26	118.3 (3)
H9B2—C9B—H9B3	109.5	C30—C31—C35	120.1 (3)
C15—C10—C11	121.3 (2)	C26—C31—C35	121.5 (2)
C15—C10—N3	120.0 (2)	C27—C32—C34	110.4 (3)
C11—C10—N3	118.2 (2)	C27—C32—C33	114.8 (3)
C12—C11—C10	117.8 (3)	C34—C32—C33	110.3 (4)
C12—C11—C16	121.9 (3)	C27—C32—H32	107.0
C10—C11—C16	120.3 (2)	C34—C32—H32	107.0
C13—C12—C11	121.2 (3)	C33—C32—H32	107.0
C13—C12—H12	119.4	C32—C33—H33A	109.5
C11—C12—H12	119.4	C32—C33—H33B	109.5
C12—C13—C14	120.2 (3)	H33A—C33—H33B	109.5
C12—C13—H13	119.9	C32—C33—H33C	109.5
C14—C13—H13	119.9	H33A—C33—H33C	109.5
C13—C14—C15	121.5 (3)	H33B—C33—H33C	109.5
C13—C14—H14	119.2	C32—C34—H34A	109.5
C15—C14—H14	119.2	C32—C34—H34B	109.5
C14—C15—C10	117.9 (3)	H34A—C34—H34B	109.5
C14—C15—C19	120.7 (3)	C32—C34—H34C	109.5
C10—C15—C19	121.4 (2)	H34A—C34—H34C	109.5
C17—C16—C11	112.3 (3)	H34B—C34—H34C	109.5
C17—C16—C18	110.5 (3)	C31—C35—C36	114.2 (3)
C11—C16—C18	114.2 (3)	C31—C35—C37	110.3 (3)
C17—C16—H16	106.4	C36—C35—C37	110.5 (3)
C11—C16—H16	106.4	C31—C35—H35	107.1
C18—C16—H16	106.4	C36—C35—H35	107.1
C16—C17—H17A	109.5	C37—C35—H35	107.1
C16—C17—H17B	109.5	C35—C36—H36A	109.5
H17A—C17—H17B	109.5	C35—C36—H36B	109.5
C16—C17—H17C	109.5	H36A—C36—H36B	109.5
H17A—C17—H17C	109.5	C35—C36—H36C	109.5
H17B—C17—H17C	109.5	H36A—C36—H36C	109.5
C16—C18—H18A	109.5	H36B—C36—H36C	109.5
C16—C18—H18B	109.5	C35—C37—H37A	109.5
H18A—C18—H18B	109.5	C35—C37—H37B	109.5
C16—C18—H18C	109.5	H37A—C37—H37B	109.5
H18A—C18—H18C	109.5	C35—C37—H37C	109.5
H18B—C18—H18C	109.5	H37A—C37—H37C	109.5
C21—C19—C20	110.8 (4)	H37B—C37—H37C	109.5

C5—N1—C1—C2	−0.3 (4)	C10—C11—C16—C18	−145.9 (3)
C5—N1—C1—C22	179.6 (2)	C14—C15—C19—C21	−99.9 (4)
N1—C1—C2—C3	−0.5 (4)	C10—C15—C19—C21	78.3 (4)

C22—C1—C2—C3	179.5 (2)	C14—C15—C19—C20	26.8 (5)
C1—C2—C3—C4	1.2 (4)	C10—C15—C19—C20	−155.0 (3)
C2—C3—C4—C5	−1.0 (4)	C26—N5—C22—N4B	13.8 (8)
C1—N1—C5—C4	0.5 (4)	C26—N5—C22—N4A	−6.0 (6)
C1—N1—C5—C6	−177.6 (2)	C26—N5—C22—C1	−177.3 (2)
C3—C4—C5—N1	0.2 (4)	C23B—N4B—C22—N5	−15.7 (16)
C3—C4—C5—C6	178.2 (3)	C23B—N4B—C22—N4A	77.2 (18)
C10—N3—C6—N2A	14.4 (6)	C23B—N4B—C22—C1	175.0 (11)
C10—N3—C6—N2B	−8.1 (8)	C23A—N4A—C22—N5	13.1 (11)
C10—N3—C6—C5	−173.9 (2)	C23A—N4A—C22—N4B	−87 (2)
C7A—N2A—C6—N3	−7.2 (10)	C23A—N4A—C22—C1	−175.3 (7)
C7A—N2A—C6—N2B	84.3 (16)	N1—C1—C22—N5	−159.8 (2)
C7A—N2A—C6—C5	−179.3 (6)	C2—C1—C22—N5	20.2 (4)
C7B—N2B—C6—N3	23.4 (14)	N1—C1—C22—N4B	11.2 (6)
C7B—N2B—C6—N2A	−79.6 (16)	C2—C1—C22—N4B	−168.8 (6)
C7B—N2B—C6—C5	−170.3 (9)	N1—C1—C22—N4A	27.5 (5)
N1—C5—C6—N3	−174.9 (2)	C2—C1—C22—N4A	−152.6 (4)
C4—C5—C6—N3	7.0 (4)	C22—N4A—C23A—C24A	−162.2 (8)
N1—C5—C6—N2A	−1.6 (5)	C25A—O2A—C24A—C23A	170.5 (7)
C4—C5—C6—N2A	−179.7 (4)	N4A—C23A—C24A—O2A	−35.4 (11)
N1—C5—C6—N2B	17.0 (6)	C22—N4B—C23B—C24B	−158.4 (11)
C4—C5—C6—N2B	−161.1 (6)	C25B—O2B—C24B—C23B	−156.3 (7)
C6—N2A—C7A—C8A	177.6 (7)	N4B—C23B—C24B—O2B	67.9 (12)
N2A—C7A—C8A—O1A	57.8 (8)	C22—N5—C26—C31	−91.5 (3)
C9A—O1A—C8A—C7A	−171.3 (7)	C22—N5—C26—C27	93.7 (3)
C6—N2B—C7B—C8B	175.6 (11)	C31—C26—C27—C28	2.7 (4)
N2B—C7B—C8B—O1B	−37.0 (14)	N5—C26—C27—C28	177.4 (2)
C9B—O1B—C8B—C7B	152.0 (10)	C31—C26—C27—C32	−175.1 (3)
C6—N3—C10—C15	78.4 (4)	N5—C26—C27—C32	−0.3 (4)
C6—N3—C10—C11	−109.6 (3)	C26—C27—C28—C29	−0.8 (5)
C15—C10—C11—C12	−1.6 (4)	C32—C27—C28—C29	177.0 (3)
N3—C10—C11—C12	−173.5 (2)	C27—C28—C29—C30	−1.2 (5)
C15—C10—C11—C16	177.8 (2)	C28—C29—C30—C31	1.3 (5)
N3—C10—C11—C16	5.9 (4)	C29—C30—C31—C26	0.6 (5)
C10—C11—C12—C13	0.6 (4)	C29—C30—C31—C35	−177.3 (3)
C16—C11—C12—C13	−178.8 (3)	C27—C26—C31—C30	−2.6 (4)
C11—C12—C13—C14	0.6 (5)	N5—C26—C31—C30	−177.2 (2)
C12—C13—C14—C15	−0.8 (5)	C27—C26—C31—C35	175.2 (2)
C13—C14—C15—C10	−0.2 (4)	N5—C26—C31—C35	0.6 (4)
C13—C14—C15—C19	178.2 (3)	C28—C27—C32—C34	−87.2 (4)
C11—C10—C15—C14	1.4 (4)	C26—C27—C32—C34	90.4 (4)
N3—C10—C15—C14	173.1 (2)	C28—C27—C32—C33	38.3 (4)
C11—C10—C15—C19	−176.9 (2)	C26—C27—C32—C33	−144.1 (3)
N3—C10—C15—C19	−5.2 (4)	C30—C31—C35—C36	−40.5 (4)
C12—C11—C16—C17	−93.3 (4)	C26—C31—C35—C36	141.7 (3)
C10—C11—C16—C17	87.2 (4)	C30—C31—C35—C37	84.7 (4)
C12—C11—C16—C18	33.5 (4)	C26—C31—C35—C37	−93.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H2*A*1···N1	0.86	2.11	2.598 (4)	115
N4*A*—H4*A*1···O2*A*	0.86	2.33	2.735 (5)	110
N4*A*—H4*A*1···N1	0.86	2.29	2.688 (5)	109
C16—H16···N3	0.98	2.40	2.842 (4)	107