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N^2,N^2,N^6,N^6-Tetraphenylpyridine-2,6-diamine

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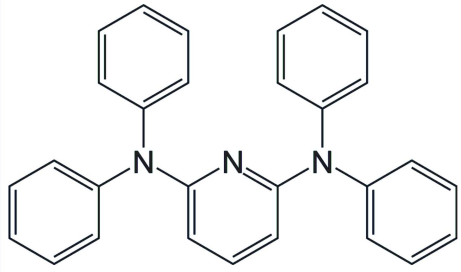
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{29}H_{23}N_3$, the molecule has an unsymmetrical structure, although it can possess *Cs* symmetry. The NC_3 units around the amino N atoms are approximately planar and make dihedral angles of 13.41 (5) and 31.05 (5)° with the pyridine ring. In the crystal, C—H···N interactions between the phenyl and pyridyl rings lead to a columnar stack along the *b* axis.

3D view

Chemical scheme



Structure description

Aryl-substituted 2,6-diaminopyridines are used as blue luminous materials (Chen *et al.*, 2001) and as part of molecular receptors (Yao *et al.*, 2009; Fa *et al.*, 2014). For related structures, see: Chen *et al.* (2001), Klinga *et al.* (1994), Berry *et al.* (2003) and Wang *et al.* (2007).

The title molecule has an unsymmetrical structure (Fig. 1), although it can possess *Cs* symmetry. The N2/C1/C6/C12 (r.m.s. deviation = 0.023 Å) and N3/C5/C18/C24 (r.m.s. deviation = 0.008 Å) units around the amino N atoms are approximately planar and subtend dihedral angles of 13.41 (5) and 31.05 (5)°, respectively, to the N1/C1–C5 pyridyl ring, indicating some conjugation between them. As a result of steric repulsion, the four phenyl rings exhibit large dihedral angles to the pyridyl ring plane, *viz*. 67.17 (5)° for the C6–C11 ring, 42.64 (5)° for the C12–C17 ring, 59.26 (5)° for the C18–C23 ring and 85.25 (5)° for the C24–C29 ring. The C12–C17 and C24-C29 phenyl rings make a dihedral angle of 52.51 (5)° and are oriented *syn* to the diaminopyridine moiety.

In the crystal, C—H···N hydrogen bonds between the phenyl and pyridyl rings makes a columnar stack along the *b* axis and C—H···π interactions are also observed (Table 1 and Fig. 2). These interactions are thought to be one of the reasons for lowering molecular symmetry.

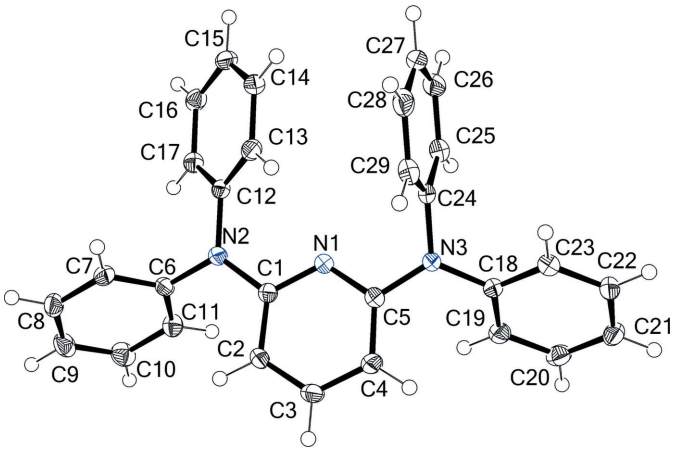


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level and H atoms are shown as small spheres.

Synthesis and crystallization

The title compound was obtained as a minor product by the reaction of *N*,*N*′-(pyridine-2,6-diyl)diacetamide with bromobenzene in the presence of CuI.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

This work was supported by Research for Promoting Technological Seeds from Japan Science and Technology Agency (JST).

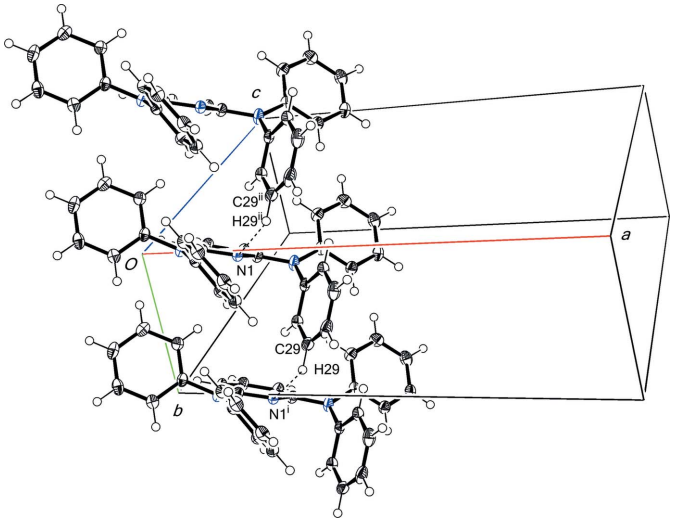


Figure 2
A view of the intermolecular interactions in the title compound. [Symmetry codes:(i) x, $y+1$, z; (ii) x, $y-1$, z.]

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

*Cg*3 and *Cg*4 are the centriods of the C12–C17 and C18–C23 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C29—H29···N1^{i}	0.95	2.71	3.4649 (18)	137
C15—H15···*Cg*4^{ii}	0.95	3.00	3.8133 (17)	145
C28—H28···*Cg*3^{i}	0.95	2.80	3.5831 (17)	140

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{29}H_{23}N_3$
M_r	413.52
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	93
a, b, c (Å)	19.949 (4), 5.6952 (10), 20.921 (4)
β (°)	113.152 (2)
V (Å^3)	2185.5 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.12 × 0.10 × 0.06
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Numerical (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.992, 0.996
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	16972, 4997, 4014
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.115, 1.08
No. of reflections	4997
No. of parameters	289
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.21

Computer programs: *CrystalClear* (Rigaku, 2008), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *CrystalStructure* (Rigaku, 2014).

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full crystallographic data

IUCrData (2017). **2**, x170521 [https://doi.org/10.1107/S2414314617005211]

N^2,N^2,N^6,N^6-Tetraphenylpyridine-2,6-diamine

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N^2,N^2,N^6,N^6-Tetraphenylpyridine-2,6-diamine

Crystal data

$C_{29}H_{23}N_3$
M_r = 413.52
Monoclinic, $P2_1/c$
a = 19.949 (4) Å
b = 5.6952 (10) Å
c = 20.921 (4) Å
β = 113.152 (2)°
V = 2185.5 (7) Å^3
Z = 4
$F(000)$ = 872.00
D_x = 1.257 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 6510 reflections
θ = 2.0–31.1°
μ = 0.07 mm^{-1}
T = 93 K
Block, colorless
0.12 × 0.10 × 0.06 mm

Data collection

Rigaku Saturn724+ diffractometer
Detector resolution: 7.111 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Rigaku, 1999)
T_{min} = 0.992, T_{max} = 0.996
16972 measured reflections
4997 independent reflections
4014 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.027
θ_{max} = 27.5°, θ_{min} = 3.2°
h = −25→22
k = −6→7
l = −26→26

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 1.08
4997 reflections
289 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
$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2 + 0.3246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.22089 (5)	0.05699 (18)	0.02057 (5)	0.0183 (2)
N2	0.13310 (5)	−0.10586 (18)	−0.07967 (5)	0.0192 (2)
N3	0.31284 (6)	0.2296 (2)	0.11341 (5)	0.0237 (2)
C1	0.15290 (6)	−0.0247 (2)	−0.01159 (6)	0.0179 (2)
C2	0.10344 (6)	−0.0310 (2)	0.02107 (6)	0.0210 (3)
C3	0.12642 (7)	0.0567 (2)	0.08790 (7)	0.0240 (3)
C4	0.19604 (7)	0.1464 (2)	0.12166 (7)	0.0245 (3)
C5	0.24170 (6)	0.1413 (2)	0.08529 (6)	0.0204 (3)
C6	0.06996 (6)	−0.2532 (2)	−0.10914 (6)	0.0196 (2)
C7	0.01295 (7)	−0.1862 (2)	−0.17059 (6)	0.0218 (3)
C8	−0.04818 (7)	−0.3288 (3)	−0.19904 (7)	0.0262 (3)
C9	−0.05299 (7)	−0.5353 (3)	−0.16599 (7)	0.0294 (3)
C10	0.00375 (7)	−0.6018 (2)	−0.10515 (7)	0.0292 (3)
C11	0.06585 (7)	−0.4628 (2)	−0.07697 (7)	0.0238 (3)
C12	0.17718 (6)	−0.0741 (2)	−0.11891 (6)	0.0183 (2)
C13	0.21613 (7)	0.1330 (2)	−0.11500 (6)	0.0209 (3)
C14	0.25942 (7)	0.1554 (2)	−0.15304 (6)	0.0235 (3)
C15	0.26401 (7)	−0.0251 (2)	−0.19596 (7)	0.0248 (3)
C16	0.22393 (7)	−0.2281 (2)	−0.20109 (7)	0.0244 (3)
C17	0.18107 (7)	−0.2534 (2)	−0.16269 (6)	0.0210 (3)
C18	0.35806 (6)	0.2183 (2)	0.18519 (6)	0.0200 (3)
C19	0.35523 (7)	0.0266 (2)	0.22566 (7)	0.0238 (3)
C20	0.40196 (7)	0.0158 (3)	0.29523 (7)	0.0272 (3)
C21	0.45213 (7)	0.1935 (3)	0.32528 (7)	0.0273 (3)
C22	0.45537 (7)	0.3831 (2)	0.28495 (7)	0.0251 (3)
C23	0.40846 (7)	0.3967 (2)	0.21551 (6)	0.0228 (3)
C24	0.34234 (6)	0.3263 (2)	0.06662 (6)	0.0195 (2)
C25	0.39688 (7)	0.2069 (2)	0.05433 (7)	0.0235 (3)
C26	0.42474 (7)	0.3004 (3)	0.00875 (7)	0.0309 (3)
C27	0.39866 (8)	0.5121 (3)	−0.02417 (7)	0.0329 (3)
C28	0.34452 (8)	0.6312 (3)	−0.01182 (7)	0.0305 (3)
C29	0.31614 (7)	0.5382 (2)	0.03378 (7)	0.0248 (3)
H2	0.05578	−0.09348	−0.002	0.0252*
H3	0.09391	0.05535	0.11106	0.0288*
H4	0.21202	0.20849	0.1674	0.0294*
H7	0.01587	−0.04361	−0.19293	0.0262*
H8	−0.08681	−0.28475	−0.24128	0.0314*
H9	−0.09524	−0.63103	−0.18513	0.0353*
H10	0.00031	−0.74309	−0.0825	0.0350*
H11	0.10531	−0.51116	−0.03587	0.0286*
H13	0.21306	0.25848	−0.08637	0.0251*
H14	0.28622	0.29604	−0.14967	0.0282*
H15	0.29416	−0.00949	−0.22134	0.0298*
H16	0.22571	−0.35106	−0.23107	0.0292*
H17	0.15421	−0.39404	−0.16635	0.0252*

H19	0.3213	−0.09649	0.20555	0.0286*
H20	0.39959	−0.11459	0.32259	0.0327*
H21	0.48393	0.18543	0.37298	0.0327*
H22	0.48998	0.50438	0.30504	0.0301*
H23	0.41067	0.52825	0.18848	0.0274*
H25	0.41495	0.06202	0.07707	0.0281*
H26	0.46187	0.21904	0.00005	0.0371*
H27	0.418	0.5757	−0.05533	0.0395*
H28	0.32672	0.77647	−0.03445	0.0366*
H29	0.27894	0.61958	0.04235	0.0298*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0165 (5)	0.0207 (5)	0.0176 (5)	−0.0013 (4)	0.0066 (4)	−0.0004 (4)
N2	0.0183 (5)	0.0224 (5)	0.0177 (5)	−0.0051 (4)	0.0078 (4)	−0.0031 (4)
N3	0.0184 (5)	0.0362 (6)	0.0155 (5)	−0.0090 (5)	0.0056 (4)	0.0007 (4)
C1	0.0178 (6)	0.0182 (6)	0.0176 (6)	−0.0009 (5)	0.0070 (5)	−0.0009 (4)
C2	0.0160 (6)	0.0258 (6)	0.0213 (6)	−0.0042 (5)	0.0074 (5)	−0.0035 (5)
C3	0.0226 (6)	0.0295 (7)	0.0247 (6)	−0.0051 (5)	0.0145 (5)	−0.0039 (5)
C4	0.0248 (6)	0.0313 (7)	0.0200 (6)	−0.0072 (5)	0.0116 (5)	−0.0074 (5)
C5	0.0186 (6)	0.0231 (6)	0.0193 (6)	−0.0041 (5)	0.0071 (5)	−0.0009 (5)
C6	0.0167 (6)	0.0240 (6)	0.0193 (6)	−0.0033 (5)	0.0083 (5)	−0.0046 (5)
C7	0.0219 (6)	0.0268 (7)	0.0179 (6)	0.0008 (5)	0.0090 (5)	−0.0024 (5)
C8	0.0199 (6)	0.0363 (8)	0.0197 (6)	0.0010 (5)	0.0051 (5)	−0.0070 (5)
C9	0.0224 (6)	0.0335 (8)	0.0316 (7)	−0.0086 (6)	0.0098 (6)	−0.0127 (6)
C10	0.0297 (7)	0.0241 (7)	0.0343 (7)	−0.0073 (6)	0.0131 (6)	−0.0031 (6)
C11	0.0231 (6)	0.0236 (6)	0.0225 (6)	−0.0015 (5)	0.0066 (5)	−0.0015 (5)
C12	0.0164 (5)	0.0224 (6)	0.0156 (5)	0.0012 (5)	0.0056 (4)	0.0018 (5)
C13	0.0224 (6)	0.0216 (6)	0.0180 (6)	−0.0009 (5)	0.0073 (5)	0.0002 (5)
C14	0.0212 (6)	0.0284 (7)	0.0203 (6)	−0.0035 (5)	0.0075 (5)	0.0040 (5)
C15	0.0209 (6)	0.0355 (7)	0.0202 (6)	0.0032 (5)	0.0103 (5)	0.0056 (5)
C16	0.0231 (6)	0.0302 (7)	0.0199 (6)	0.0044 (5)	0.0086 (5)	−0.0015 (5)
C17	0.0198 (6)	0.0230 (6)	0.0198 (6)	0.0003 (5)	0.0073 (5)	−0.0002 (5)
C18	0.0176 (6)	0.0262 (6)	0.0167 (6)	−0.0012 (5)	0.0073 (5)	−0.0016 (5)
C19	0.0257 (6)	0.0248 (6)	0.0225 (6)	−0.0049 (5)	0.0113 (5)	−0.0029 (5)
C20	0.0307 (7)	0.0312 (7)	0.0227 (6)	0.0012 (6)	0.0135 (6)	0.0040 (5)
C21	0.0236 (6)	0.0393 (8)	0.0174 (6)	0.0021 (6)	0.0063 (5)	−0.0011 (5)
C22	0.0206 (6)	0.0317 (7)	0.0219 (6)	−0.0045 (5)	0.0073 (5)	−0.0060 (5)
C23	0.0211 (6)	0.0255 (7)	0.0224 (6)	−0.0025 (5)	0.0091 (5)	−0.0004 (5)
C24	0.0166 (5)	0.0258 (6)	0.0148 (5)	−0.0057 (5)	0.0045 (5)	−0.0019 (5)
C25	0.0183 (6)	0.0276 (7)	0.0220 (6)	−0.0011 (5)	0.0053 (5)	−0.0002 (5)
C26	0.0223 (7)	0.0461 (9)	0.0268 (7)	−0.0060 (6)	0.0123 (6)	−0.0078 (6)
C27	0.0282 (7)	0.0505 (9)	0.0189 (6)	−0.0193 (7)	0.0081 (6)	−0.0002 (6)
C28	0.0290 (7)	0.0293 (7)	0.0241 (7)	−0.0105 (6)	0.0007 (6)	0.0061 (6)
C29	0.0196 (6)	0.0252 (7)	0.0255 (6)	−0.0022 (5)	0.0043 (5)	−0.0011 (5)

Geometric parameters (Å, º)

N1—C1	1.3384 (14)	C24—C25	1.390 (2)
N1—C5	1.3394 (16)	C24—C29	1.3850 (18)
N2—C1	1.3985 (16)	C25—C26	1.385 (2)
N2—C6	1.4354 (15)	C26—C27	1.384 (2)
N2—C12	1.4309 (19)	C27—C28	1.383 (2)
N3—C5	1.3988 (16)	C28—C29	1.392 (2)
N3—C18	1.4170 (14)	C2—H2	0.950
N3—C24	1.4357 (19)	C3—H3	0.950
C1—C2	1.404 (2)	C4—H4	0.950
C2—C3	1.3822 (18)	C7—H7	0.950
C3—C4	1.3847 (18)	C8—H8	0.950
C4—C5	1.398 (2)	C9—H9	0.950
C6—C7	1.3937 (15)	C10—H10	0.950
C6—C11	1.3886 (19)	C11—H11	0.950
C7—C8	1.3895 (18)	C13—H13	0.950
C8—C9	1.386 (2)	C14—H14	0.950
C9—C10	1.3827 (16)	C15—H15	0.950
C10—C11	1.3908 (18)	C16—H16	0.950
C12—C13	1.3971 (18)	C17—H17	0.950
C12—C17	1.3937 (19)	C19—H19	0.950
C13—C14	1.391 (2)	C20—H20	0.950
C14—C15	1.392 (2)	C21—H21	0.950
C15—C16	1.385 (2)	C22—H22	0.950
C16—C17	1.392 (2)	C23—H23	0.950
C18—C19	1.3963 (19)	C25—H25	0.950
C18—C23	1.3945 (17)	C26—H26	0.950
C19—C20	1.3872 (17)	C27—H27	0.950
C20—C21	1.3881 (19)	C28—H28	0.950
C21—C22	1.387 (2)	C29—H29	0.950
C22—C23	1.3868 (16)		
N1···C3	2.761 (2)	C20···H27^{xi}	3.0597
N1···C12	2.7986 (17)	C21···H14^{xi}	3.5492
N1···C13	2.8335 (18)	C21···H15^{xi}	3.4211
N1···C18	3.5752 (14)	C21···H22^{xii}	3.5219
N1···C24	2.7047 (15)	C21···H23^{xii}	3.0133
N1···C25	3.4065 (19)	C21···H25^{xiii}	3.3689
N1···C29	3.2838 (18)	C21···H27^{xi}	3.2235
N2···C5	3.5645 (15)	C22···H15^{xi}	3.2474
N3···C1	3.5433 (15)	C22···H20^{ii}	3.2761
C1···C4	2.7522 (19)	C22···H22^{xii}	3.3164
C1···C7	3.5218 (15)	C22···H23^{xii}	3.2196
C1···C11	3.0406 (17)	C22···H25^{xiii}	3.1925
C1···C13	3.037 (2)	C23···H15^{xi}	3.1187
C2···C5	2.7316 (16)	C23···H19^{ii}	3.3335
C2···C6	2.8351 (18)	C23···H22^{xii}	3.1572

C2···C11	3.0997 (18)	C25···H21^{xiii}	3.5425
C4···C18	3.0005 (18)	C25···H22^{xii}	3.1400
C4···C19	3.1387 (17)	C25···H28^{i}	3.0618
C5···C19	2.9917 (16)	C26···H21^{xiii}	3.2718
C5···C25	3.423 (2)	C26···H21^{ix}	3.4794
C5···C29	3.120 (2)	C26···H27^{iii}	2.9808
C6···C9	2.7781 (18)	C26···H28^{i}	3.4865
C6···C17	2.850 (2)	C27···H20^{ix}	3.2659
C7···C10	2.776 (2)	C27···H21^{xiii}	3.2619
C7···C12	3.0862 (19)	C27···H21^{ix}	3.4158
C7···C17	3.315 (2)	C27···H26^{iii}	3.0392
C8···C11	2.7769 (17)	C27···H27^{iii}	3.4074
C11···C12	3.484 (2)	C28···H21^{xiii}	3.5253
C12···C15	2.806 (2)	C28···H25^{ii}	3.0656
C13···C16	2.778 (2)	C29···H25^{ii}	3.4934
C14···C17	2.7668 (19)	H2···C2^{iv}	3.1232
C18···C21	2.7940 (17)	H2···C3^{iv}	3.3688
C18···C25	3.125 (2)	H2···C10^{ii}	3.4371
C18···C29	3.4597 (19)	H2···C10^{v}	3.3971
C19···C22	2.7754 (18)	H2···H2^{iv}	2.4980
C20···C23	2.770 (2)	H2···H3^{iv}	2.9686
C23···C24	2.8935 (17)	H2···H10^{ii}	2.5647
C23···C25	3.461 (2)	H2···H10^{v}	2.6075
C24···C27	2.769 (2)	H3···C6^{iv}	3.4432
C25···C28	2.7764 (19)	H3···C7^{iv}	2.9561
C26···C29	2.774 (2)	H3···C8^{iv}	2.8226
N1···C29^{i}	3.4649 (18)	H3···C9^{v}	3.3906
C2···C10^{ii}	3.5741 (17)	H3···C9^{iv}	3.1933
C10···C2^{i}	3.5741 (17)	H3···C10^{v}	3.2083
C17···C28^{i}	3.5964 (17)	H3···H2^{iv}	2.9686
C25···C28^{i}	3.553 (2)	H3···H7^{iv}	3.2687
C26···C27^{iii}	3.572 (2)	H3···H8^{iv}	3.0745
C27···C26^{iii}	3.572 (2)	H3···H9^{v}	2.8652
C28···C17^{ii}	3.5964 (17)	H3···H10^{v}	2.4838
C28···C25^{ii}	3.553 (2)	H3···H16^{vi}	3.5138
C29···N1^{ii}	3.4649 (18)	H4···C14^{xi}	3.5796
N1···H2	3.2532	H4···C15^{xi}	3.1888
N1···H4	3.2618	H4···H8^{iv}	3.4428
N1···H13	2.4641	H4···H9^{iv}	3.4692
N1···H25	3.5759	H4···H14^{xi}	3.5191
N1···H29	3.3764	H4···H15^{xi}	2.8359
N2···H2	2.6449	H4···H16^{vi}	2.8765
N2···H7	2.6176	H7···C7^{viii}	3.3669
N2···H11	2.6219	H7···C8^{viii}	2.8575
N2···H13	2.6543	H7···C9^{ii}	3.3457
N2···H17	2.6000	H7···C9^{viii}	3.3138
N3···H4	2.6687	H7···C10^{ii}	3.1798
N3···H19	2.6338	H7···H3^{iv}	3.2687

N3···H23	2.5998	H7···H8^{viii}	2.7573
N3···H25	2.6183	H7···H9^{ii}	3.2780
N3···H29	2.6098	H7···H9^{viii}	3.5270
C1···H3	3.2483	H7···H10^{ii}	2.9878
C1···H11	2.9078	H8···C7^{vii}	3.5964
C1···H13	2.8223	H8···C12^{vii}	3.2211
C2···H4	3.2727	H8···C13^{vii}	3.1331
C2···H11	2.9887	H8···C14^{vii}	3.2977
C4···H2	3.2705	H8···C15^{vii}	3.5277
C4···H19	2.7909	H8···C16^{vii}	3.5663
C5···H3	3.2361	H8···C17^{vii}	3.4240
C5···H13	3.4722	H8···H3^{iv}	3.0745
C5···H19	2.7466	H8···H4^{iv}	3.4428
C5···H25	3.5561	H8···H7^{vii}	2.7573
C5···H29	3.0503	H8···H13^{vii}	3.5020
C6···H2	2.5359	H8···H16^{viii}	3.5851
C6···H8	3.2645	H8···H17^{viii}	2.9070
C6···H10	3.2609	H9···C3^{v}	3.3757
C6···H17	2.5461	H9···C15^{vii}	3.3618
C7···H2	3.3286	H9···C16^{vii}	2.7852
C7···H9	3.2639	H9···C17^{vii}	3.0441
C7···H11	3.2681	H9···H3^{v}	2.8652
C7···H17	3.0255	H9···H4^{iv}	3.4692
C8···H10	3.2544	H9···H7^{i}	3.2780
C9···H7	3.2643	H9···H7^{vii}	3.5270
C9···H11	3.2622	H9···H16^{vii}	2.7982
C10···H2	3.5149	H9···H17^{vii}	3.2261
C10···H8	3.2542	H10···N2^{i}	3.3416
C11···H2	2.6783	H10···C1^{i}	3.2386
C11···H7	3.2678	H10···C2^{i}	2.8481
C11···H9	3.2630	H10···C2^{v}	3.1116
C11···H17	3.0577	H10···C3^{v}	3.0609
C12···H7	2.9775	H10···C6^{i}	3.3602
C12···H14	3.2698	H10···C7^{i}	3.1928
C12···H16	3.2737	H10···H2^{i}	2.5647
C13···H15	3.2793	H10···H2^{v}	2.6075
C13···H17	3.2626	H10···H3^{v}	2.4838
C14···H16	3.2518	H10···H7^{i}	2.9878
C15···H13	3.2759	H11···N1^{i}	3.2586
C15···H17	3.2654	H11···C1^{i}	3.0552
C16···H14	3.2498	H11···C2^{i}	3.1971
C17···H7	3.3240	H11···C3^{i}	3.4761
C17···H13	3.2638	H11···C5^{i}	3.5105
C17···H15	3.2713	H11···H13^{i}	3.0404
C18···H4	2.7887	H11···H29^{i}	3.2822
C18···H20	3.2666	H13···C11^{ii}	3.4112
C18···H22	3.2679	H13···C17^{ii}	3.1441
C18···H25	3.0357	H13···H8^{viii}	3.5020

C18···H29	3.5967	H13···H11^{ii}	3.0404
C19···H4	2.8254	H13···H17^{ii}	2.5592
C19···H21	3.2691	H13···H28^{i}	3.4526
C19···H23	3.2662	H14···C16^{ii}	2.9992
C20···H22	3.2535	H14···C17^{ii}	3.2575
C21···H19	3.2670	H14···C19^{ix}	3.5415
C21···H23	3.2631	H14···C20^{ix}	3.1467
C22···H20	3.2527	H14···C21^{ix}	3.5492
C23···H19	3.2668	H14···H4^{ix}	3.5191
C23···H21	3.2662	H14···H16^{ii}	2.6039
C23···H25	3.5120	H14···H17^{ii}	3.0741
C24···H13	3.2487	H14···H20^{ix}	3.1266
C24···H23	2.6358	H15···C18^{ix}	3.1875
C24···H26	3.2574	H15···C19^{x}	3.5282
C24···H28	3.2592	H15···C19^{ix}	3.3675
C25···H23	3.2702	H15···C20^{x}	3.5317
C25···H27	3.2576	H15···C20^{ix}	3.4734
C25···H29	3.2647	H15···C21^{ix}	3.4211
C26···H14	3.3793	H15···C22^{ix}	3.2474
C26···H28	3.2559	H15···C23^{ix}	3.1187
C27···H14	2.9679	H15···H4^{ix}	2.8359
C27···H25	3.2590	H15···H19^{x}	2.8844
C27···H29	3.2603	H15···H20^{x}	2.8865
C28···H13	3.2558	H15···H23^{ix}	3.5244
C28···H14	3.2674	H16···C4^{x}	3.3523
C28···H26	3.2550	H16···C14^{i}	3.1865
C29···H13	3.0032	H16···C19^{x}	3.2147
C29···H23	3.0389	H16···C20^{x}	3.4676
C29···H25	3.2642	H16···H3^{x}	3.5138
C29···H27	3.2603	H16···H4^{x}	2.8765
H2···H3	2.3403	H16···H8^{vii}	3.5851
H2···H11	2.7726	H16···H9^{viii}	2.7982
H3···H4	2.3490	H16···H14^{i}	2.6039
H4···H19	2.6530	H16···H19^{x}	2.7335
H7···H8	2.3401	H16···H20^{x}	3.2045
H7···H17	3.2714	H17···C13^{i}	2.9821
H8···H9	2.3351	H17···C14^{i}	3.2569
H9···H10	2.3308	H17···H8^{vii}	2.9070
H10···H11	2.3403	H17···H9^{viii}	3.2261
H11···H17	3.3079	H17···H13^{i}	2.5592
H13···H14	2.3344	H17···H14^{i}	3.0741
H13···H29	3.2289	H17···H28^{i}	3.5963
H14···H15	2.3426	H19···C15^{vi}	3.4709
H14···H27	3.0436	H19···C16^{vi}	3.4014
H14···H28	3.5240	H19···C23^{i}	3.3335
H15···H16	2.3392	H19···H15^{vi}	2.8844
H16···H17	2.3338	H19···H16^{vi}	2.7335
H19···H20	2.3320	H19···H23^{i}	2.8939

H20···H21	2.3382	H19···H29^{i}	3.5662
H21···H22	2.3387	H20···C15^{vi}	3.2940
H22···H23	2.3312	H20···C16^{vi}	3.4588
H23···H25	3.5563	H20···C22^{i}	3.2761
H23···H29	3.1946	H20···C27^{xi}	3.2659
H25···H26	2.3363	H20···H14^{xi}	3.1266
H26···H27	2.3317	H20···H15^{vi}	2.8865
H27···H28	2.3323	H20···H16^{vi}	3.2045
H28···H29	2.3437	H20···H22^{i}	2.9353
N1···H11^{ii}	3.2586	H20···H23^{i}	3.5421
N1···H28^{i}	3.2009	H20···H27^{xi}	2.4433
N1···H29^{i}	2.7092	H21···C25^{xii}	3.5425
N2···H10^{ii}	3.3416	H21···C26^{xii}	3.2718
N2···H29^{i}	3.4038	H21···C26^{xi}	3.4794
C1···H10^{ii}	3.2386	H21···C27^{xii}	3.2619
C1···H11^{ii}	3.0552	H21···C27^{xi}	3.4158
C1···H29^{i}	3.0771	H21···C28^{xii}	3.5253
C2···H2^{iv}	3.1232	H21···H23^{xii}	3.0003
C2···H10^{ii}	2.8481	H21···H25^{xiii}	2.8467
C2···H10^{v}	3.1116	H21···H26^{xi}	2.9115
C2···H11^{ii}	3.1971	H21···H27^{xii}	3.5921
C3···H2^{iv}	3.3688	H21···H27^{xi}	2.7825
C3···H9^{v}	3.3757	H22···C18^{xiii}	3.1982
C3···H10^{v}	3.0609	H22···C19^{xiii}	3.3946
C3···H11^{ii}	3.4761	H22···C20^{ii}	3.3652
C4···H16^{vi}	3.3523	H22···C20^{xiii}	3.5508
C5···H11^{ii}	3.5105	H22···C21^{xiii}	3.5219
C5···H29^{i}	3.2728	H22···C22^{xiii}	3.3164
C6···H3^{iv}	3.4432	H22···C23^{xiii}	3.1572
C6···H10^{ii}	3.3602	H22···C25^{xiii}	3.1400
C7···H3^{iv}	2.9561	H22···H20^{ii}	2.9353
C7···H7^{vii}	3.3669	H22···H23^{xii}	3.3299
C7···H8^{viii}	3.5964	H22···H23^{xiii}	3.5548
C7···H10^{ii}	3.1928	H22···H25^{xiii}	2.4717
C8···H3^{iv}	2.8226	H23···C19^{ii}	3.2495
C8···H7^{vii}	2.8575	H23···C21^{xiii}	3.0133
C9···H3^{v}	3.3906	H23···C22^{xiii}	3.2196
C9···H3^{iv}	3.1933	H23···H15^{xi}	3.5244
C9···H7^{i}	3.3457	H23···H19^{ii}	2.8939
C9···H7^{vii}	3.3138	H23···H20^{ii}	3.5421
C10···H2^{i}	3.4371	H23···H21^{xiii}	3.0003
C10···H2^{v}	3.3971	H23···H22^{xii}	3.5548
C10···H3^{v}	3.2083	H23···H22^{xiii}	3.3299
C10···H7^{i}	3.1798	H25···C21^{xii}	3.3689
C11···H13^{i}	3.4112	H25···C22^{xii}	3.1925
C12···H8^{viii}	3.2211	H25···C28^{i}	3.0656
C12···H28^{i}	2.9327	H25···C29^{i}	3.4934
C13···H8^{viii}	3.1331	H25···H21^{xii}	2.8467

C13···H17^{ii}	2.9821	H25···H22^{xii}	2.4717
C13···H28^{i}	2.9842	H25···H28^{i}	2.8208
C14···H4^{ix}	3.5796	H25···H29^{i}	3.5622
C14···H8^{viii}	3.2977	H26···C27^{iii}	3.0392
C14···H16^{ii}	3.1865	H26···H21^{ix}	2.9115
C14···H17^{ii}	3.2569	H26···H26^{xiv}	2.9226
C14···H28^{i}	3.1617	H26···H26^{iii}	3.5438
C15···H4^{ix}	3.1888	H26···H27^{iii}	2.5036
C15···H8^{viii}	3.5277	H26···H28^{i}	3.5515
C15···H9^{viii}	3.3618	H27···C20^{ix}	3.0597
C15···H19^{x}	3.4709	H27···C21^{ix}	3.2235
C15···H20^{x}	3.2940	H27···C26^{iii}	2.9808
C15···H28^{i}	3.3068	H27···C27^{iii}	3.4074
C16···H8^{viii}	3.5663	H27···H20^{ix}	2.4433
C16···H9^{viii}	2.7852	H27···H21^{xiii}	3.5921
C16···H14^{i}	2.9992	H27···H21^{ix}	2.7825
C16···H19^{x}	3.4014	H27···H26^{iii}	2.5036
C16···H20^{x}	3.4588	H27···H27^{iii}	3.2941
C16···H28^{i}	3.2769	H28···N1^{ii}	3.2009
C17···H8^{viii}	3.4240	H28···C12^{ii}	2.9327
C17···H9^{viii}	3.0441	H28···C13^{ii}	2.9842
C17···H13^{i}	3.1441	H28···C14^{ii}	3.1617
C17···H14^{i}	3.2575	H28···C15^{ii}	3.3068
C17···H28^{i}	3.0886	H28···C16^{ii}	3.2769
C18···H15^{xi}	3.1875	H28···C17^{ii}	3.0886
C18···H22^{xii}	3.1982	H28···C25^{ii}	3.0618
C19···H14^{xi}	3.5415	H28···C26^{ii}	3.4865
C19···H15^{vi}	3.5282	H28···H13^{ii}	3.4526
C19···H15^{xi}	3.3675	H28···H17^{ii}	3.5963
C19···H16^{vi}	3.2147	H28···H25^{ii}	2.8208
C19···H22^{xii}	3.3946	H28···H26^{ii}	3.5515
C19···H23^{i}	3.2495	H29···N1^{ii}	2.7092
C20···H14^{xi}	3.1467	H29···N2^{ii}	3.4038
C20···H15^{vi}	3.5317	H29···C1^{ii}	3.0771
C20···H15^{xi}	3.4734	H29···C5^{ii}	3.2728
C20···H16^{vi}	3.4676	H29···H11^{ii}	3.2822
C20···H22^{i}	3.3652	H29···H19^{ii}	3.5662
C20···H22^{xii}	3.5508	H29···H25^{ii}	3.5622

C1—N1—C5	118.87 (12)	C24—C29—C28	119.73 (14)
C1—N2—C6	118.65 (11)	C1—C2—H2	121.112
C1—N2—C12	123.46 (9)	C3—C2—H2	121.119
C6—N2—C12	117.44 (10)	C2—C3—H3	119.450
C5—N3—C18	123.18 (12)	C4—C3—H3	119.452
C5—N3—C24	118.12 (9)	C3—C4—H4	121.547
C18—N3—C24	118.63 (10)	C5—C4—H4	121.569
N1—C1—N2	116.84 (12)	C6—C7—H7	120.153
N1—C1—C2	122.10 (11)	C8—C7—H7	120.150

N2—C1—C2	121.06 (10)	C7—C8—H8	119.883
C1—C2—C3	117.77 (11)	C9—C8—H8	119.887
C2—C3—C4	121.10 (15)	C8—C9—H9	120.023
C3—C4—C5	116.88 (13)	C10—C9—H9	120.027
N1—C5—N3	114.45 (12)	C9—C10—H10	119.846
N1—C5—C4	123.25 (10)	C11—C10—H10	119.840
N3—C5—C4	122.28 (11)	C6—C11—H11	120.123
N2—C6—C7	119.74 (11)	C10—C11—H11	120.125
N2—C6—C11	120.24 (9)	C12—C13—H13	120.001
C7—C6—C11	120.02 (11)	C14—C13—H13	119.990
C6—C7—C8	119.70 (12)	C13—C14—H14	119.524
C7—C8—C9	120.23 (11)	C15—C14—H14	119.533
C8—C9—C10	119.95 (12)	C14—C15—H15	120.523
C9—C10—C11	120.31 (13)	C16—C15—H15	120.524
C6—C11—C10	119.75 (11)	C15—C16—H16	119.727
N2—C12—C13	121.74 (12)	C17—C16—H16	119.723
N2—C12—C17	119.35 (11)	C12—C17—H17	119.679
C13—C12—C17	118.90 (13)	C16—C17—H17	119.708
C12—C13—C14	120.01 (12)	C18—C19—H19	119.997
C13—C14—C15	120.94 (13)	C20—C19—H19	119.992
C14—C15—C16	118.95 (15)	C19—C20—H20	119.651
C15—C16—C17	120.55 (14)	C21—C20—H20	119.664
C12—C17—C16	120.61 (12)	C20—C21—H21	120.340
N3—C18—C19	121.16 (11)	C22—C21—H21	120.337
N3—C18—C23	119.59 (12)	C21—C22—H22	119.764
C19—C18—C23	119.20 (10)	C23—C22—H22	119.757
C18—C19—C20	120.01 (12)	C18—C23—H23	119.855
C19—C20—C21	120.69 (13)	C22—C23—H23	119.850
C20—C21—C22	119.32 (11)	C24—C25—H25	120.185
C21—C22—C23	120.48 (12)	C26—C25—H25	120.183
C18—C23—C22	120.30 (12)	C25—C26—H26	119.895
N3—C24—C25	119.92 (11)	C27—C26—H26	119.891
N3—C24—C29	119.78 (13)	C26—C27—H27	119.916
C25—C24—C29	120.30 (14)	C28—C27—H27	119.919
C24—C25—C26	119.63 (12)	C27—C28—H28	120.024
C25—C26—C27	120.21 (15)	C29—C28—H28	120.017
C26—C27—C28	120.17 (16)	C24—C29—H29	120.133
C27—C28—C29	119.96 (13)	C28—C29—H29	120.135

C1—N1—C5—N3	−177.95 (9)	C3—C4—C5—N3	179.10 (10)
C1—N1—C5—C4	0.67 (17)	N2—C6—C7—C8	−179.94 (11)
C5—N1—C1—N2	178.55 (9)	N2—C6—C11—C10	178.61 (11)
C5—N1—C1—C2	−1.86 (16)	C7—C6—C11—C10	−2.0 (2)
C1—N2—C6—C7	122.77 (12)	C11—C6—C7—C8	0.6 (2)
C1—N2—C6—C11	−57.80 (15)	C6—C7—C8—C9	0.9 (2)
C6—N2—C1—N1	162.66 (9)	C7—C8—C9—C10	−1.1 (2)
C6—N2—C1—C2	−16.93 (15)	C8—C9—C10—C11	−0.2 (2)
C1—N2—C12—C13	−38.32 (14)	C9—C10—C11—C6	1.7 (2)

C1—N2—C12—C17	142.21 (9)	N2—C12—C13—C14	178.86 (8)
C12—N2—C1—N1	−9.43 (15)	N2—C12—C17—C16	−179.52 (8)
C12—N2—C1—C2	170.98 (9)	C13—C12—C17—C16	0.99 (15)
C6—N2—C12—C13	149.50 (9)	C17—C12—C13—C14	−1.67 (15)
C6—N2—C12—C17	−29.97 (13)	C12—C13—C14—C15	0.78 (15)
C12—N2—C6—C7	−64.67 (14)	C13—C14—C15—C16	0.80 (16)
C12—N2—C6—C11	114.77 (12)	C14—C15—C16—C17	−1.49 (16)
C5—N3—C18—C19	35.16 (18)	C15—C16—C17—C12	0.60 (16)
C5—N3—C18—C23	−147.51 (11)	N3—C18—C19—C20	177.64 (12)
C18—N3—C5—N1	−147.66 (11)	N3—C18—C23—C22	−177.09 (11)
C18—N3—C5—C4	33.71 (18)	C19—C18—C23—C22	0.3 (2)
C5—N3—C24—C25	−109.07 (11)	C23—C18—C19—C20	0.3 (2)
C5—N3—C24—C29	70.77 (14)	C18—C19—C20—C21	−0.4 (2)
C24—N3—C5—N1	29.38 (15)	C19—C20—C21—C22	−0.2 (2)
C24—N3—C5—C4	−149.25 (11)	C20—C21—C22—C23	0.8 (2)
C18—N3—C24—C25	68.10 (14)	C21—C22—C23—C18	−0.8 (2)
C18—N3—C24—C29	−112.06 (11)	N3—C24—C25—C26	179.54 (9)
C24—N3—C18—C19	−141.86 (11)	N3—C24—C29—C28	−179.69 (8)
C24—N3—C18—C23	35.46 (17)	C25—C24—C29—C28	0.15 (16)
N1—C1—C2—C3	1.73 (16)	C29—C24—C25—C26	−0.29 (16)
N2—C1—C2—C3	−178.70 (9)	C24—C25—C26—C27	0.28 (17)
C1—C2—C3—C4	−0.40 (17)	C25—C26—C27—C28	−0.12 (18)
C2—C3—C4—C5	−0.69 (18)	C26—C27—C28—C29	−0.02 (18)
C3—C4—C5—N1	0.59 (18)	C27—C28—C29—C24	0.01 (17)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, *y*+1, *z*; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*, −*y*, −*z*; (v) −*x*, −*y*−1, −*z*; (vi) *x*, −*y*−1/2, *z*+1/2; (vii) −*x*, *y*−1/2, −*z*−1/2; (viii) −*x*, *y*+1/2, −*z*−1/2; (ix) *x*, −*y*+1/2, *z*−1/2; (x) *x*, −*y*−1/2, *z*−1/2; (xi) *x*, −*y*+1/2, *z*+1/2; (xii) −*x*+1, *y*−1/2, −*z*+1/2; (xiii) −*x*+1, *y*+1/2, −*z*+1/2; (xiv) −*x*+1, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centriods of the C12–C17 and C18–C23 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C29—H29···N1^{ii}	0.95	2.71	3.4649 (18)	137
C15—H15···*Cg*4^{ix}	0.95	3.00	3.8133 (17)	145
C28—H28···*Cg*3^{ii}	0.95	2.80	3.5831 (17)	140

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