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2-(Pyridin-2-yl)-1,8-naphthyridine

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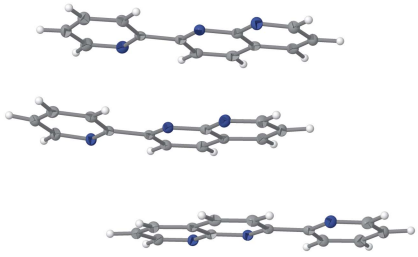
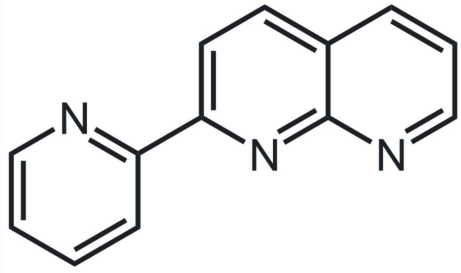
The title compound, $C_{13}H_9N_3$, has three symmetry-independent molecules in the asymmetric unit. The dihedral angles between the naphthyridine ring system and the pyridine group are in the range 3.927 (4)–7.362 (4)°. In the crystal, C—H···N interactions and aromatic π–π stacking [centroid–centroid distances = 3.5755 (7) and 3.6544 (7) Å] generate a three-dimensional network.

3D view



Chemical scheme



Structure description

1,8-Naphthyridines are key components of several antibacterial agents (Stanforth, 1996). In addition to medicinal applications, 1,8-naphthyridine and its derivatives have been employed in coordination chemistry. For example, the title compound is utilized not only as a bidendate ligand (Oyama & Hamada, 2008), but also as a bridging ligand for binuclear complexes (Campos-Fernández *et al.*, 2002). Although numerous crystal structures of metal complexes containing the title compound have been described (Oyama & Hamada, 2008; Oyama *et al.*, 2011, 2017), no structural characterization of the title compound has been reported so far.

The title compound crystallizes with three molecules in the asymmetric unit (Fig. 1), which exhibit comparable bond lengths and angles. As expected, the naphthyridine ring system is almost planar. Additionally, the two aromatic groups tend to be coplanar in the related compounds with 1,8-naphthyridyl and aromatic ring systems (Sinha *et al.*, 2009). The pyridine rings make dihedral angles of 3.927 (4)–7.362 (4)° with the naphthyridine ring systems in the title compound. All H atoms attached to C atoms are clearly visible in the difference map and the assignment of N atoms in aromatic rings is unambiguous. Although the title compound exists in a *cis* conformation on coordinating to metals (Oyama & Hamada, 2008; Oyama *et al.*, 2011, 2017), the pyridine N atom exists in a *trans* conformation with respect to the naphthyridine N atoms in the present case. The bond

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N4^{i}	1.008 (15)	2.529 (17)	3.4161 (16)	146.6 (14)
C7—H7···N1	0.962 (16)	2.462 (17)	2.8037 (16)	100.6 (12)
C12—H12···N1^{ii}	0.967 (15)	2.616 (17)	3.4845 (16)	149.6 (14)
C15—H15···N8^{iii}	0.949 (15)	2.507 (17)	3.3470 (16)	147.6 (14)
C17—H17···N5	0.940 (16)	2.453 (16)	2.7856 (15)	100.7 (12)
C20—H20···N4	0.985 (16)	2.460 (17)	2.8036 (15)	100.0 (12)
C33—H33···N7	0.948 (16)	2.456 (16)	2.7944 (16)	100.9 (13)
C38—H38···N2^{i}	0.991 (16)	2.511 (17)	3.4016 (16)	149.5 (14)

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

lengths and angles are within normal ranges [C—N = 1.3188 (16)–1.3665 (15) Å, C—C = 1.3591 (17)–1.4224 (18) Å and C—N—C = 116.74 (12)–118.15 (11)°]. These values are similar to those of a related aryl-substituted 1,8-naphthyridine (Xiong *et al.*, 2016).

In the crystal packing, supramolecular layers in the *ab* plane are stabilized by C—H···N and π–π interactions [$Cg\cdots Cg$ = 3.5755 (7) and 3.6544 (7) Å] (Table 1 and Fig. 2). These effects lead to small dihedral angles between the naphthyridine ring system and the pyridine group. Meanwhile, the interplanar distance between rings *Cg*1 and *Cg*7^{iv} [symmetry code: (iv) $-x+1, y+\frac{1}{2}, -z+1$; *Cg*1 and *Cg*7 are the centroids of the N2/C6–C10 and N6/C22–C26 rings, respectively] is longer [3.8082 (7) Å], suggesting that one unit consists of three molecules.

Synthesis and crystallization

The precursor (2-aminonicotinaldehyde) and the title compound were synthesized according to the method of Campos-Fernández *et al.* (2002). A direct condensation reaction using 2-aminonicotinaldehyde (696 mg, 5.70 mmol), 2-acetylpyridine (1.0 ml, 8.92 mmol) and potassium hydroxide (25 mg, 0.45 mmol) in methanol (5 ml) afforded a light-brown solid in 80% yield. The crude product was recrystallized from an acetone–diethyl ether mixture (1:30 *v*/*v*) at room

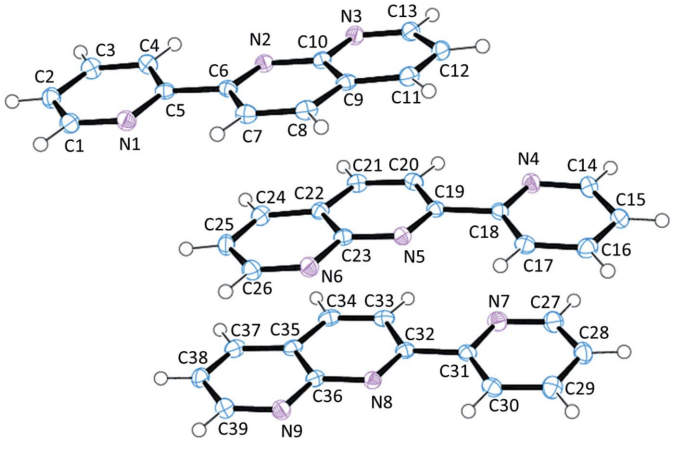


Figure 1
The three independent molecules of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_9N_3$
M_r	207.23
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	93
a, b, c (Å)	6.1708 (2), 16.9596 (7), 14.2882 (6)
β (°)	99.9699 (19)
V (Å^3)	1472.74 (10)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.45 × 0.20 × 0.10
Data collection	
Diffractometer	Rigaku Saturn724
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)
T_{min}, T_{max}	0.928, 0.991
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	14789, 6626, 6058
R_{int}	0.014
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.093, 1.04
No. of reflections	6626
No. of parameters	515
No. of restraints	1
H-atom treatment	Only H-atom coordinates refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.19

Computer programs: *CrystalClear* (Rigaku, 2008), *SIR97* (Altomare *et al.*, 1999), *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *CrystalStructure* (Rigaku, 2010), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

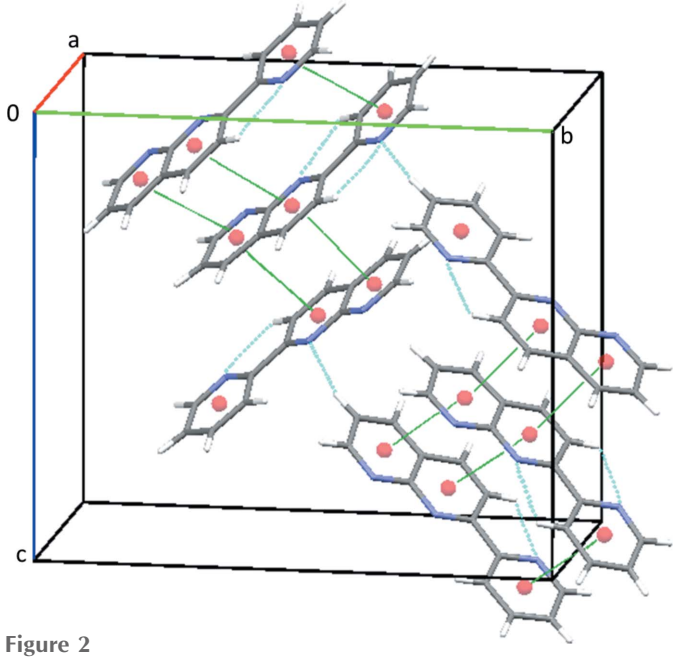


Figure 2
A view along the *a* axis, showing weak C—H···N hydrogen bonds (blue) and π–π contacts (green). Ring centroids are shown as coloured spheres.

temperature to give good-quality crystals suitable for X-ray diffraction.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was an inversion twin, with twin fractions of 0.7 (11) and 0.3 (11).

Funding information

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full crystallographic data

IUCrData (2017). **2**, x171221 [https://doi.org/10.1107/S2414314617012214]

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Crystal data

$C_{13}H_9N_3$
M_r = 207.23
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 6.1708 (2) Å
b = 16.9596 (7) Å
c = 14.2882 (6) Å
β = 99.9699 (19)°
V = 1472.74 (10) Å^3
Z = 6
$F(000)$ = 648.00
D_x = 1.402 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 4248 reflections
θ = 3.1–27.5°
μ = 0.09 mm^{-1}
T = 93 K
Prism, yellow
0.45 × 0.20 × 0.10 mm

Data collection

Rigaku Saturn724 diffractometer
Detector resolution: 28.944 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
T_{min} = 0.928, T_{max} = 0.991
14789 measured reflections
6626 independent reflections
6058 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.014
θ_{max} = 27.5°
h = −8→8
k = −22→22
l = −18→18

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.093
S = 1.04
6626 reflections
515 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 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). All H atoms were identified in a difference Fourier map and their positions refined freely with U_{iso}(H) = 1.2U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.87594 (17)	0.28801 (6)	0.69204 (7)	0.0204 (3)
N2	0.66559 (16)	0.46716 (6)	0.57649 (7)	0.0172 (2)
N3	0.57101 (16)	0.58104 (6)	0.49070 (7)	0.0195 (2)
N4	0.70483 (16)	0.59955 (6)	0.12837 (7)	0.0207 (3)
N5	0.92194 (17)	0.42608 (6)	0.25484 (7)	0.0177 (2)
N6	1.01665 (17)	0.31352 (6)	0.34193 (7)	0.0209 (3)
N7	0.53827 (17)	0.42723 (6)	−0.01887 (7)	0.0233 (3)
N8	0.75468 (17)	0.25164 (6)	0.10279 (7)	0.0179 (2)
N9	0.85512 (17)	0.14117 (6)	0.19418 (7)	0.0209 (3)
C1	0.8171 (3)	0.23280 (7)	0.74938 (9)	0.0218 (3)
C2	0.6213 (2)	0.23424 (7)	0.78485 (9)	0.0221 (3)
C3	0.4808 (2)	0.29730 (8)	0.76089 (9)	0.0221 (3)
C4	0.5402 (2)	0.35602 (7)	0.70257 (9)	0.0195 (3)
C5	0.73813 (19)	0.34860 (6)	0.66848 (8)	0.0168 (3)
C6	0.80663 (19)	0.40977 (7)	0.60424 (8)	0.0162 (3)
C7	1.01571 (19)	0.40401 (7)	0.57595 (8)	0.0192 (3)
C8	1.07842 (18)	0.46107 (7)	0.51931 (8)	0.0189 (3)
C9	0.93315 (19)	0.52367 (7)	0.48811 (8)	0.0170 (3)
C10	0.72520 (19)	0.52397 (7)	0.51823 (8)	0.0163 (3)
C11	0.9799 (2)	0.58520 (7)	0.42822 (8)	0.0196 (3)
C12	0.8255 (2)	0.64204 (7)	0.40108 (8)	0.0212 (3)
C13	0.6239 (2)	0.63686 (7)	0.43447 (8)	0.0203 (3)
C14	0.7579 (3)	0.64916 (7)	0.06284 (9)	0.0230 (3)
C15	0.9466 (2)	0.64282 (7)	0.02335 (9)	0.0224 (3)
C16	1.0919 (2)	0.58223 (8)	0.05402 (9)	0.0222 (3)
C17	1.03995 (19)	0.52957 (7)	0.12084 (8)	0.0189 (3)
C18	0.84483 (19)	0.54007 (7)	0.15603 (8)	0.0168 (3)
C19	0.77970 (19)	0.48275 (7)	0.22518 (8)	0.0162 (3)
C20	0.5714 (2)	0.48967 (7)	0.25356 (8)	0.0182 (3)
C21	0.50999 (19)	0.43385 (7)	0.31242 (8)	0.0191 (3)
C22	0.65624 (18)	0.37180 (7)	0.34473 (8)	0.0171 (3)
C23	0.86361 (19)	0.37057 (7)	0.31452 (8)	0.0169 (3)
C24	0.6076 (2)	0.31011 (7)	0.40441 (8)	0.0208 (3)
C25	0.7604 (2)	0.25285 (7)	0.43064 (8)	0.0218 (3)
C26	0.9624 (3)	0.25739 (7)	0.39766 (9)	0.0221 (3)
C27	0.5951 (3)	0.48079 (8)	−0.07890 (9)	0.0257 (3)
C28	0.7876 (3)	0.47778 (8)	−0.11602 (9)	0.0245 (3)
C29	0.9295 (3)	0.41530 (8)	−0.09078 (9)	0.0238 (3)
C30	0.8740 (2)	0.35895 (7)	−0.02897 (9)	0.0206 (3)
C31	0.6778 (2)	0.36714 (7)	0.00599 (8)	0.0179 (3)
C32	0.61384 (19)	0.30907 (7)	0.07453 (8)	0.0173 (3)
C33	0.4090 (2)	0.31726 (7)	0.10632 (8)	0.0200 (3)
C34	0.3500 (2)	0.26294 (7)	0.16728 (9)	0.0214 (3)
C35	0.49601 (19)	0.20031 (7)	0.19869 (8)	0.0185 (3)
C36	0.70007 (19)	0.19762 (7)	0.16541 (8)	0.0175 (3)

C37	0.4553 (2)	0.14189 (7)	0.26402 (9)	0.0219 (3)
C38	0.6114 (2)	0.08649 (7)	0.29344 (9)	0.0231 (3)
C39	0.8090 (3)	0.08885 (7)	0.25631 (9)	0.0226 (3)
H1	0.918 (3)	0.1879 (9)	0.7651 (10)	0.0261*
H2	0.588 (3)	0.1882 (9)	0.8247 (10)	0.0265*
H3	0.338 (3)	0.3016 (9)	0.7824 (10)	0.0266*
H4	0.450 (3)	0.4017 (9)	0.6859 (10)	0.0233*
H7	1.110 (3)	0.3603 (9)	0.5981 (10)	0.0230*
H8	1.222 (3)	0.4602 (9)	0.5002 (10)	0.0227*
H11	1.126 (3)	0.5869 (9)	0.4105 (10)	0.0235*
H12	0.852 (3)	0.6858 (9)	0.3612 (10)	0.0254*
H13	0.515 (3)	0.6776 (9)	0.4162 (10)	0.0244*
H14	0.650 (3)	0.6926 (9)	0.0445 (10)	0.0276*
H15	0.972 (3)	0.6769 (9)	−0.0263 (10)	0.0268*
H16	1.231 (3)	0.5731 (9)	0.0279 (10)	0.0267*
H17	1.131 (3)	0.4865 (9)	0.1423 (10)	0.0226*
H20	0.477 (3)	0.5351 (9)	0.2313 (10)	0.0218*
H21	0.366 (3)	0.4350 (9)	0.3317 (10)	0.0229*
H24	0.458 (3)	0.3102 (9)	0.4236 (10)	0.0250*
H25	0.737 (3)	0.2052 (10)	0.4710 (10)	0.0261*
H26	1.076 (3)	0.2168 (9)	0.4170 (10)	0.0265*
H27	0.489 (3)	0.5225 (10)	−0.0949 (11)	0.0309*
H28	0.826 (3)	0.5167 (10)	−0.1569 (11)	0.0293*
H29	1.073 (3)	0.4118 (9)	−0.1160 (10)	0.0286*
H30	0.970 (3)	0.3149 (9)	−0.0107 (10)	0.0247*
H33	0.317 (3)	0.3607 (9)	0.0848 (10)	0.0240*
H34	0.210 (3)	0.2664 (9)	0.1898 (10)	0.0257*
H37	0.314 (3)	0.1435 (9)	0.2909 (10)	0.0263*
H38	0.589 (3)	0.0444 (9)	0.3389 (11)	0.0278*
H39	0.926 (3)	0.0485 (9)	0.2772 (10)	0.0271*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0203 (6)	0.0204 (5)	0.0210 (5)	0.0033 (5)	0.0048 (4)	0.0011 (4)
N2	0.0162 (5)	0.0183 (5)	0.0176 (5)	−0.0002 (4)	0.0040 (4)	−0.0010 (4)
N3	0.0200 (5)	0.0199 (5)	0.0191 (5)	0.0020 (4)	0.0047 (4)	0.0008 (4)
N4	0.0219 (5)	0.0185 (5)	0.0221 (5)	0.0016 (4)	0.0049 (4)	0.0023 (4)
N5	0.0195 (5)	0.0167 (5)	0.0171 (5)	0.0017 (4)	0.0033 (4)	0.0006 (4)
N6	0.0230 (6)	0.0206 (5)	0.0194 (5)	0.0053 (4)	0.0046 (4)	0.0024 (4)
N7	0.0246 (6)	0.0228 (6)	0.0219 (5)	0.0041 (5)	0.0022 (4)	0.0012 (5)
N8	0.0189 (5)	0.0176 (5)	0.0174 (5)	−0.0010 (4)	0.0037 (4)	−0.0010 (4)
N9	0.0208 (5)	0.0201 (5)	0.0227 (5)	0.0013 (4)	0.0062 (4)	0.0014 (4)
C1	0.0236 (7)	0.0211 (6)	0.0205 (6)	0.0051 (5)	0.0035 (5)	0.0005 (5)
C2	0.0243 (7)	0.0210 (6)	0.0206 (6)	−0.0032 (5)	0.0029 (5)	0.0012 (5)
C3	0.0182 (6)	0.0241 (6)	0.0244 (6)	−0.0025 (5)	0.0043 (5)	0.0002 (5)
C4	0.0158 (6)	0.0192 (6)	0.0230 (6)	0.0016 (5)	0.0023 (5)	0.0000 (5)
C5	0.0157 (6)	0.0178 (6)	0.0161 (5)	−0.0014 (5)	0.0005 (5)	−0.0033 (5)

C6	0.0157 (6)	0.0164 (6)	0.0155 (5)	−0.0006 (5)	0.0001 (5)	−0.0026 (5)
C7	0.0158 (6)	0.0199 (6)	0.0212 (6)	0.0022 (5)	0.0009 (5)	−0.0021 (5)
C8	0.0127 (6)	0.0232 (6)	0.0212 (6)	−0.0019 (5)	0.0039 (5)	−0.0040 (5)
C9	0.0153 (6)	0.0191 (6)	0.0166 (6)	−0.0039 (5)	0.0028 (5)	−0.0051 (5)
C10	0.0151 (6)	0.0183 (6)	0.0152 (5)	−0.0000 (5)	0.0022 (5)	−0.0020 (5)
C11	0.0175 (6)	0.0223 (6)	0.0199 (6)	−0.0043 (5)	0.0060 (5)	−0.0026 (5)
C12	0.0252 (7)	0.0199 (6)	0.0191 (6)	−0.0052 (5)	0.0056 (5)	−0.0005 (5)
C13	0.0222 (6)	0.0194 (6)	0.0194 (6)	0.0028 (5)	0.0036 (5)	0.0006 (5)
C14	0.0274 (7)	0.0185 (6)	0.0235 (6)	0.0013 (5)	0.0052 (5)	0.0035 (5)
C15	0.0293 (7)	0.0178 (6)	0.0207 (6)	−0.0053 (5)	0.0062 (5)	−0.0002 (5)
C16	0.0218 (7)	0.0246 (7)	0.0210 (6)	−0.0039 (5)	0.0061 (5)	−0.0032 (5)
C17	0.0176 (6)	0.0183 (6)	0.0200 (6)	−0.0005 (5)	0.0011 (5)	−0.0022 (5)
C18	0.0194 (6)	0.0148 (6)	0.0157 (5)	−0.0015 (5)	0.0013 (5)	−0.0012 (5)
C19	0.0164 (6)	0.0163 (6)	0.0155 (6)	−0.0022 (5)	0.0018 (5)	−0.0026 (5)
C20	0.0166 (6)	0.0170 (6)	0.0202 (6)	0.0009 (5)	0.0010 (5)	−0.0018 (5)
C21	0.0139 (6)	0.0219 (6)	0.0212 (6)	−0.0017 (5)	0.0027 (5)	−0.0029 (5)
C22	0.0165 (6)	0.0186 (6)	0.0156 (5)	−0.0032 (5)	0.0012 (5)	−0.0023 (5)
C23	0.0161 (6)	0.0184 (6)	0.0160 (6)	−0.0007 (5)	0.0017 (5)	−0.0028 (5)
C24	0.0192 (6)	0.0236 (7)	0.0196 (6)	−0.0043 (5)	0.0035 (5)	−0.0014 (5)
C25	0.0281 (7)	0.0194 (6)	0.0171 (6)	−0.0037 (5)	0.0018 (5)	0.0026 (5)
C26	0.0255 (7)	0.0193 (6)	0.0207 (6)	0.0033 (5)	0.0020 (5)	0.0011 (5)
C27	0.0298 (7)	0.0246 (7)	0.0218 (6)	0.0063 (6)	0.0015 (6)	0.0037 (5)
C28	0.0303 (7)	0.0211 (6)	0.0209 (6)	−0.0019 (6)	0.0016 (5)	0.0037 (5)
C29	0.0222 (7)	0.0257 (7)	0.0232 (6)	−0.0037 (5)	0.0030 (5)	0.0008 (5)
C30	0.0200 (6)	0.0181 (6)	0.0227 (6)	0.0016 (5)	0.0011 (5)	−0.0009 (5)
C31	0.0205 (6)	0.0167 (6)	0.0153 (5)	−0.0017 (5)	−0.0001 (5)	−0.0031 (5)
C32	0.0164 (6)	0.0181 (6)	0.0167 (6)	−0.0022 (5)	0.0015 (5)	−0.0039 (5)
C33	0.0179 (6)	0.0219 (6)	0.0196 (6)	0.0030 (5)	0.0017 (5)	−0.0047 (5)
C34	0.0163 (6)	0.0267 (7)	0.0221 (6)	−0.0008 (5)	0.0053 (5)	−0.0067 (5)
C35	0.0181 (6)	0.0206 (6)	0.0173 (6)	−0.0034 (5)	0.0043 (5)	−0.0058 (5)
C36	0.0169 (6)	0.0191 (6)	0.0173 (6)	−0.0022 (5)	0.0045 (5)	−0.0030 (5)
C37	0.0225 (7)	0.0234 (6)	0.0214 (6)	−0.0073 (5)	0.0079 (5)	−0.0052 (5)
C38	0.0309 (7)	0.0201 (6)	0.0198 (6)	−0.0068 (5)	0.0082 (5)	−0.0007 (5)
C39	0.0259 (7)	0.0201 (6)	0.0221 (6)	−0.0008 (5)	0.0050 (5)	0.0007 (5)

Geometric parameters (Å, º)

N1—C1	1.3353 (17)	C25—C26	1.409 (2)
N1—C5	1.3391 (15)	C27—C28	1.383 (2)
N2—C6	1.3200 (15)	C28—C29	1.3823 (19)
N2—C10	1.3648 (16)	C29—C30	1.3839 (19)
N3—C10	1.3665 (15)	C30—C31	1.3944 (19)
N3—C13	1.3188 (16)	C31—C32	1.4896 (18)
N4—C14	1.3408 (17)	C32—C33	1.4219 (18)
N4—C18	1.3423 (16)	C33—C34	1.3601 (18)
N5—C19	1.3210 (16)	C34—C35	1.4148 (17)
N5—C23	1.3599 (16)	C35—C36	1.4217 (18)
N6—C23	1.3614 (16)	C35—C37	1.4133 (18)

N6—C26	1.3209 (17)	C37—C38	1.3591 (17)
N7—C27	1.3371 (18)	C38—C39	1.412 (2)
N7—C31	1.3418 (16)	C1—H1	0.986 (15)
N8—C32	1.3212 (16)	C2—H2	1.009 (15)
N8—C36	1.3630 (16)	C3—H3	0.985 (16)
N9—C36	1.3656 (16)	C4—H4	0.960 (15)
N9—C39	1.3205 (17)	C7—H7	0.963 (15)
C1—C2	1.389 (2)	C8—H8	0.972 (15)
C2—C3	1.3818 (18)	C11—H11	0.978 (16)
C3—C4	1.3878 (19)	C12—H12	0.968 (16)
C4—C5	1.3967 (19)	C13—H13	0.967 (15)
C5—C6	1.4939 (17)	C14—H14	0.998 (15)
C6—C7	1.4206 (18)	C15—H15	0.949 (16)
C7—C8	1.3600 (17)	C16—H16	1.004 (15)
C8—C9	1.4111 (16)	C17—H17	0.941 (15)
C9—C10	1.4224 (18)	C20—H20	0.984 (15)
C9—C11	1.4107 (17)	C21—H21	0.973 (15)
C11—C12	1.3640 (17)	C24—H24	1.008 (16)
C12—C13	1.4097 (19)	C25—H25	1.017 (16)
C14—C15	1.383 (2)	C26—H26	0.986 (15)
C15—C16	1.3840 (18)	C27—H27	0.965 (16)
C16—C17	1.3848 (19)	C28—H28	0.938 (17)
C17—C18	1.3942 (18)	C29—H29	1.013 (16)
C18—C19	1.4901 (17)	C30—H30	0.961 (15)
C19—C20	1.4178 (18)	C33—H33	0.949 (15)
C20—C21	1.3630 (18)	C34—H34	0.976 (16)
C21—C22	1.4109 (16)	C37—H37	1.011 (16)
C22—C23	1.4197 (18)	C38—H38	0.992 (16)
C22—C24	1.4144 (17)	C39—H39	1.003 (15)
C24—C25	1.3602 (17)		

N1···N2	3.5917 (14)	C23···H34^{iv}	3.490 (16)
N1···C3	2.7870 (18)	C24···H13^{vi}	3.588 (15)
N1···C7	2.8037 (16)	C24···H37	3.589 (15)
N2···C4	2.8070 (17)	C25···H7	3.453 (14)
N2···C8	2.8087 (16)	C25···H13^{vi}	3.256 (15)
N2···C13	3.5052 (16)	C26···H7	3.344 (14)
N3···C6	3.5166 (16)	C26···H24^{iv}	3.146 (15)
N3···C11	2.8196 (17)	C26···H34^{iv}	3.570 (16)
N4···N5	3.5885 (14)	C26···H37^{iv}	3.453 (16)
N4···C16	2.7925 (18)	C27···H4^{xi}	3.585 (14)
N4···C20	2.8035 (16)	C27···H16^{ii}	3.320 (15)
N5···C17	2.7856 (16)	C27···H29^{ii}	3.382 (15)
N5···C21	2.8072 (17)	C28···H4^{xi}	3.460 (14)
N5···C26	3.4979 (16)	C28···H16	3.518 (14)
N6···C19	3.5090 (16)	C28···H39^{ix}	3.357 (16)
N6···C24	2.8199 (18)	C29···H16	3.522 (14)
N7···N8	3.5874 (14)	C29···H17	3.559 (14)

N7···C29	2.7901 (18)	C29···H33^{iv}	3.284 (13)
N7···C33	2.7943 (17)	C30···H15^{v}	3.286 (16)
N8···C30	2.8070 (17)	C30···H17	3.441 (14)
N8···C34	2.8141 (18)	C30···H33^{iv}	2.927 (13)
N8···C39	3.5059 (16)	C31···H14^{xii}	3.587 (15)
N9···C32	3.5166 (16)	C32···H14^{xii}	2.912 (15)
N9···C37	2.8172 (18)	C32···H15^{v}	3.555 (16)
C1···C4	2.7088 (17)	C33···H14^{xii}	2.995 (15)
C2···C5	2.7315 (17)	C33···H15^{xii}	3.402 (15)
C6···C9	2.7464 (18)	C33···H17^{ii}	3.427 (15)
C7···C10	2.7424 (17)	C33···H30^{ii}	2.928 (14)
C9···C13	2.7216 (17)	C34···H14^{xii}	3.252 (15)
C10···C12	2.7482 (17)	C34···H15^{xii}	2.958 (14)
C14···C17	2.7075 (17)	C34···H30^{ii}	3.268 (14)
C15···C18	2.7272 (18)	C35···H14^{xii}	3.438 (14)
C19···C22	2.7367 (17)	C35···H15^{xii}	3.479 (14)
C20···C23	2.7469 (17)	C35···H27^{xii}	3.368 (16)
C22···C26	2.7222 (17)	C36···H14^{xii}	3.380 (14)
C23···C25	2.7405 (18)	C36···H15^{v}	3.092 (16)
C27···C30	2.7050 (18)	C36···H16^{v}	3.560 (15)
C28···C31	2.7254 (19)	C36···H27^{xii}	3.284 (16)
C32···C35	2.7431 (17)	C36···H34^{iv}	3.315 (15)
C33···C36	2.7442 (17)	C37···H25	3.338 (14)
C35···C39	2.7260 (17)	C37···H27^{xii}	3.217 (16)
C36···C38	2.7468 (18)	C37···H28^{xii}	2.991 (15)
N1···C12^{i}	3.4847 (17)	C38···H4^{vi}	3.176 (16)
N2···C8^{ii}	3.5751 (15)	C38···H25	3.226 (15)
N2···C38^{iii}	3.4016 (17)	C38···H27^{xii}	3.000 (15)
N3···C21	3.5398 (16)	C38···H28^{xii}	3.266 (15)
N3···C38^{iii}	3.4626 (18)	C39···H26	3.373 (14)
N4···C2^{iii}	3.4160 (17)	C39···H27^{xii}	2.915 (14)
N4···C27	3.5484 (17)	C39···H28^{v}	3.114 (17)
N5···C21^{iv}	3.5817 (16)	C39···H37^{iv}	3.208 (15)
N5···C32	3.5347 (15)	H1···N4^{i}	2.957 (14)
N6···C8	3.5350 (16)	H1···C11^{i}	3.414 (15)
N6···C36	3.5121 (15)	H1···C12^{i}	3.169 (16)
N7···C18	3.4422 (15)	H1···C14^{i}	2.961 (13)
N8···C15^{v}	3.3470 (18)	H1···C15^{i}	3.089 (14)
N9···C15^{v}	3.5319 (18)	H1···C16^{i}	3.155 (15)
N9···C26	3.4799 (16)	H1···C17^{i}	3.129 (15)
C2···N4^{vi}	3.4160 (17)	H1···C18^{i}	3.020 (15)
C2···C30^{vii}	3.5420 (17)	H1···H3^{iv}	3.20 (2)
C4···C7^{ii}	3.5190 (16)	H1···H11^{i}	3.01 (2)
C4···C28^{vii}	3.4559 (18)	H1···H12^{i}	2.48 (3)
C6···C24	3.3620 (16)	H1···H13^{vi}	3.390 (18)
C7···C4^{iv}	3.5190 (16)	H1···H14^{i}	3.464 (19)
C7···C24	3.5704 (16)	H1···H20^{vi}	3.57 (2)
C7···C25	3.4974 (16)	H2···N4^{vi}	2.528 (16)

C7···C26	3.5342 (17)	H2···C14^{vi}	2.959 (16)
C8···N2^{iv}	3.5751 (15)	H2···C15^{i}	3.376 (14)
C8···N6	3.5350 (16)	H2···C16^{i}	2.992 (14)
C8···C23	3.3663 (16)	H2···C17^{i}	3.536 (15)
C9···C22	3.5410 (16)	H2···H12^{vi}	3.455 (19)
C9···C23	3.5650 (17)	H2···H13^{vi}	3.395 (19)
C10···C21	3.3756 (16)	H2···H14^{vi}	2.57 (3)
C10···C22	3.5527 (17)	H2···H16^{i}	2.95 (2)
C11···C19	3.4236 (16)	H2···H20^{vi}	2.73 (2)
C12···N1^{viii}	3.4847 (17)	H3···N1^{ii}	2.929 (14)
C12···C20	3.5261 (16)	H3···N7^{vii}	3.593 (14)
C12···C26^{viii}	3.5365 (17)	H3···C1^{ii}	3.376 (15)
C13···C20	3.5676 (17)	H3···C14^{vi}	3.519 (16)
C14···C27	3.5440 (18)	H3···H1^{ii}	3.20 (2)
C15···N8^{ix}	3.3470 (18)	H3···H7^{ii}	2.935 (19)
C15···N9^{ix}	3.5319 (18)	H3···H12^{vi}	2.93 (2)
C15···C28	3.4765 (18)	H3···H14^{vi}	3.08 (2)
C16···C28	3.3146 (18)	H3···H29^{xiii}	3.02 (3)
C16···C29	3.5470 (19)	H4···C7^{ii}	2.862 (14)
C17···C20^{iv}	3.5577 (16)	H4···C8^{ii}	3.169 (14)
C17···C28	3.5812 (17)	H4···C27^{vii}	3.585 (14)
C17···C29	3.5566 (18)	H4···C28^{vii}	3.460 (14)
C18···N7	3.4422 (15)	H4···C38^{iii}	3.176 (16)
C18···C27	3.5864 (17)	H4···H7^{ii}	2.355 (19)
C19···C11	3.4236 (16)	H4···H8^{ii}	2.950 (19)
C20···C12	3.5261 (16)	H4···H28^{vii}	3.52 (2)
C20···C13	3.5676 (17)	H4···H38^{iii}	2.45 (3)
C20···C17^{ii}	3.5577 (16)	H4···H39^{iii}	3.50 (3)
C21···N3	3.5398 (16)	H7···C3^{iv}	3.152 (14)
C21···N5^{ii}	3.5817 (16)	H7···C4^{iv}	2.809 (14)
C21···C10	3.3756 (16)	H7···C25	3.453 (14)
C21···C33	3.5121 (17)	H7···C26	3.344 (14)
C22···C9	3.5410 (16)	H7···H3^{iv}	2.935 (19)
C22···C10	3.5527 (17)	H7···H4^{iv}	2.355 (19)
C22···C34	3.4277 (16)	H7···H12^{i}	3.02 (3)
C23···C8	3.3663 (16)	H7···H26	3.53 (2)
C23···C9	3.5650 (17)	H8···N2^{iv}	2.767 (14)
C24···C6	3.3620 (16)	H8···N3^{iv}	2.993 (15)
C24···C7	3.5704 (16)	H8···N6	3.452 (14)
C24···C34	3.5752 (17)	H8···C10^{iv}	3.255 (15)
C24···C35	3.4469 (16)	H8···C21^{iv}	3.493 (15)
C24···C37	3.5205 (17)	H8···C23	3.495 (13)
C25···C7	3.4974 (16)	H8···H4^{iv}	2.950 (19)
C25···C35	3.5450 (16)	H8···H21^{iv}	2.74 (2)
C25···C37	3.3470 (17)	H8···H24^{iv}	3.21 (2)
C25···C38	3.4677 (17)	H8···H38^{viii}	2.78 (2)
C26···N9	3.4799 (16)	H11···N3^{iv}	2.788 (14)
C26···C7	3.5342 (17)	H11···C1^{viii}	3.426 (15)

C26···C12^{i}	3.5365 (17)	H11···C13^{iv}	3.148 (15)
C26···C36	3.5776 (17)	H11···C19	3.569 (14)
C26···C39	3.5331 (17)	H11···H1^{viii}	3.01 (2)
C27···N4	3.5484 (17)	H11···H13^{iv}	2.84 (2)
C27···C14	3.5440 (18)	H11···H21^{iv}	3.27 (2)
C27···C18	3.5864 (17)	H11···H25^{viii}	2.67 (2)
C27···C38^{x}	3.5890 (18)	H12···N1^{viii}	2.614 (16)
C28···C4^{xi}	3.4559 (18)	H12···C1^{viii}	2.899 (16)
C28···C15	3.4765 (18)	H12···C2^{iii}	3.385 (14)
C28···C16	3.3146 (18)	H12···C3^{iii}	3.099 (14)
C28···C17	3.5812 (17)	H12···H1^{viii}	2.48 (3)
C29···C16	3.5470 (19)	H12···H2^{iii}	3.455 (19)
C29···C17	3.5566 (18)	H12···H3^{iii}	2.93 (2)
C30···C2^{xi}	3.5420 (17)	H12···H7^{viii}	3.02 (3)
C30···C33^{iv}	3.5951 (17)	H12···H25^{viii}	3.189 (19)
C32···N5	3.5347 (15)	H12···H26^{viii}	3.17 (2)
C33···C21	3.5121 (17)	H13···N1^{iii}	3.230 (14)
C33···C30^{ii}	3.5951 (17)	H13···C1^{iii}	2.999 (13)
C34···C22	3.4277 (16)	H13···C2^{iii}	3.007 (14)
C34···C24	3.5752 (17)	H13···C3^{iii}	3.247 (15)
C35···C24	3.4469 (16)	H13···C4^{iii}	3.457 (15)
C35···C25	3.5450 (16)	H13···C5^{iii}	3.415 (15)
C36···N6	3.5121 (15)	H13···C24^{iii}	3.588 (15)
C36···C26	3.5776 (17)	H13···C25^{iii}	3.256 (15)
C37···C24	3.5205 (17)	H13···H1^{iii}	3.390 (18)
C37···C25	3.3470 (17)	H13···H2^{iii}	3.395 (19)
C38···N2^{vi}	3.4016 (17)	H13···H11^{ii}	2.84 (2)
C38···N3^{vi}	3.4626 (18)	H13···H20	3.56 (2)
C38···C25	3.4677 (17)	H13···H24^{iii}	3.19 (2)
C38···C27^{xii}	3.5890 (18)	H13···H25^{iii}	2.47 (3)
C39···C26	3.5331 (17)	H13···H26^{viii}	3.228 (18)
N1···H2	3.284 (16)	H14···N8^{x}	3.138 (14)
N1···H4	3.249 (15)	H14···C2^{iii}	3.265 (16)
N1···H7	2.464 (16)	H14···C3^{iii}	3.509 (16)
N2···H4	2.483 (16)	H14···C31^{x}	3.587 (15)
N2···H7	3.259 (15)	H14···C32^{x}	2.912 (15)
N3···H12	3.273 (16)	H14···C33^{x}	2.995 (15)
N4···H15	3.254 (16)	H14···C34^{x}	3.252 (15)
N4···H17	3.234 (15)	H14···C35^{x}	3.438 (14)
N4···H20	2.458 (15)	H14···C36^{x}	3.380 (14)
N5···H17	2.453 (15)	H14···H1^{viii}	3.464 (19)
N5···H20	3.277 (14)	H14···H2^{iii}	2.57 (3)
N6···H25	3.294 (16)	H14···H3^{iii}	3.08 (2)
N7···H28	3.248 (17)	H14···H16^{ii}	3.26 (2)
N7···H30	3.261 (15)	H14···H27	3.55 (3)
N7···H33	2.457 (16)	H14···H30^{ix}	3.23 (3)
N8···H30	2.508 (16)	H14···H33^{x}	3.42 (3)
N8···H33	3.248 (15)	H15···N8^{ix}	2.506 (16)

N9···H38	3.294 (16)	H15···N9^{ix}	2.854 (16)
C1···H3	3.287 (15)	H15···C30^{ix}	3.286 (16)
C2···H4	3.266 (15)	H15···C32^{ix}	3.555 (16)
C3···H1	3.268 (15)	H15···C33^{x}	3.402 (15)
C4···H2	3.325 (15)	H15···C34^{x}	2.958 (14)
C5···H1	3.168 (15)	H15···C35^{x}	3.479 (14)
C5···H3	3.282 (16)	H15···C36^{ix}	3.092 (16)
C5···H7	2.670 (16)	H15···H28	3.33 (3)
C6···H4	2.667 (16)	H15···H30^{ix}	2.41 (3)
C6···H8	3.292 (15)	H15···H34^{x}	2.85 (2)
C8···H11	2.687 (15)	H16···N4^{iv}	3.060 (14)
C9···H7	3.279 (15)	H16···N7^{iv}	3.257 (15)
C9···H12	3.285 (15)	H16···N8^{ix}	3.566 (15)
C10···H8	3.304 (15)	H16···N9^{ix}	3.331 (14)
C10···H11	3.309 (16)	H16···C14^{iv}	3.454 (14)
C10···H13	3.153 (15)	H16···C27^{iv}	3.320 (15)
C11···H8	2.694 (14)	H16···C28	3.518 (14)
C11···H13	3.246 (15)	H16···C29	3.522 (14)
C13···H11	3.287 (15)	H16···C36^{ix}	3.560 (15)
C14···H16	3.307 (15)	H16···H2^{viii}	2.95 (2)
C15···H17	3.248 (15)	H16···H14^{iv}	3.26 (2)
C16···H14	3.291 (15)	H16···H20^{iv}	3.106 (19)
C17···H15	3.246 (15)	H16···H27^{iv}	2.70 (3)
C18···H14	3.165 (15)	H16···H28	3.442 (19)
C18···H16	3.294 (16)	H16···H29	3.46 (2)
C18···H20	2.674 (15)	H17···C20^{iv}	2.901 (14)
C19···H17	2.645 (16)	H17···C21^{iv}	3.194 (13)
C19···H21	3.290 (15)	H17···C29	3.559 (14)
C21···H24	2.684 (15)	H17···C30	3.441 (14)
C22···H20	3.301 (15)	H17···C33^{iv}	3.427 (15)
C22···H25	3.343 (16)	H17···H20^{iv}	2.433 (19)
C23···H21	3.306 (15)	H17···H21^{iv}	2.972 (19)
C23···H24	3.331 (16)	H17···H33^{iv}	2.62 (3)
C23···H26	3.161 (15)	H20···C2^{iii}	3.432 (15)
C24···H21	2.692 (14)	H20···C12	3.462 (13)
C24···H26	3.270 (15)	H20···C13	3.364 (14)
C26···H24	3.321 (16)	H20···C16^{ii}	3.260 (13)
C27···H29	3.299 (16)	H20···C17^{ii}	2.883 (13)
C28···H30	3.252 (15)	H20···H1^{iii}	3.57 (2)
C29···H27	3.264 (16)	H20···H2^{iii}	2.73 (2)
C30···H28	3.224 (16)	H20···H13	3.56 (2)
C31···H27	3.131 (16)	H20···H16^{ii}	3.106 (19)
C31···H29	3.321 (16)	H20···H17^{ii}	2.433 (19)
C31···H33	2.668 (16)	H21···N3	3.450 (14)
C32···H30	2.692 (16)	H21···N5^{ii}	2.776 (14)
C32···H34	3.298 (16)	H21···N6^{ii}	3.005 (15)
C34···H37	2.722 (15)	H21···C8^{ii}	3.491 (15)
C35···H33	3.263 (15)	H21···C10	3.499 (13)

C35···H38	3.307 (15)	H21···C23^{ii}	3.257 (15)
C36···H34	3.317 (15)	H21···H8^{ii}	2.74 (2)
C36···H37	3.347 (16)	H21···H11^{ii}	3.27 (2)
C36···H39	3.182 (15)	H21···H17^{ii}	2.972 (19)
C37···H34	2.707 (14)	H21···H34	3.54 (2)
C37···H39	3.286 (15)	H24···N2	3.540 (15)
C39···H37	3.308 (15)	H24···N6^{ii}	2.770 (14)
H1···H2	2.34 (3)	H24···C6	3.496 (14)
H2···H3	2.47 (2)	H24···C26^{ii}	3.146 (15)
H3···H4	2.36 (3)	H24···H8^{ii}	3.21 (2)
H7···H8	2.37 (2)	H24···H13^{vi}	3.19 (2)
H8···H11	2.52 (2)	H24···H26^{ii}	2.83 (2)
H11···H12	2.40 (2)	H24···H34	3.505 (19)
H12···H13	2.35 (3)	H24···H37	3.43 (2)
H14···H15	2.40 (3)	H25···N1	3.427 (14)
H15···H16	2.41 (2)	H25···N3^{vi}	2.952 (16)
H16···H17	2.36 (2)	H25···C11^{i}	2.897 (15)
H20···H21	2.40 (2)	H25···C12^{i}	3.172 (14)
H21···H24	2.50 (2)	H25···C13^{vi}	3.030 (16)
H24···H25	2.49 (2)	H25···C37	3.338 (14)
H25···H26	2.36 (3)	H25···C38	3.226 (15)
H27···H28	2.40 (3)	H25···H11^{i}	2.67 (2)
H28···H29	2.35 (2)	H25···H12^{i}	3.189 (19)
H29···H30	2.39 (3)	H25···H13^{vi}	2.47 (3)
H33···H34	2.36 (3)	H25···H37	3.493 (19)
H34···H37	2.56 (2)	H25···H38	3.35 (2)
H37···H38	2.40 (2)	H26···N3^{i}	3.286 (15)
H38···H39	2.40 (3)	H26···N9	3.483 (14)
N1···H3^{iv}	2.929 (14)	H26···C9^{i}	3.548 (15)
N1···H12^{i}	2.614 (16)	H26···C10^{i}	3.559 (15)
N1···H13^{vi}	3.230 (14)	H26···C11^{i}	3.202 (15)
N1···H25	3.427 (14)	H26···C12^{i}	2.861 (14)
N1···H29^{vii}	3.500 (14)	H26···C13^{i}	2.901 (14)
N2···H8^{ii}	2.767 (14)	H26···C39	3.373 (14)
N2···H24	3.540 (15)	H26···H7	3.53 (2)
N2···H37^{iii}	3.530 (15)	H26···H12^{i}	3.17 (2)
N2···H38^{iii}	2.509 (16)	H26···H13^{i}	3.228 (18)
N2···H39^{viii}	3.285 (14)	H26···H24^{iv}	2.83 (2)
N3···H8^{ii}	2.993 (15)	H26···H34^{iv}	3.59 (2)
N3···H11^{ii}	2.788 (14)	H26···H37^{iv}	2.81 (3)
N3···H21	3.450 (14)	H26···H39	3.51 (2)
N3···H25^{iii}	2.952 (16)	H27···N4	3.490 (15)
N3···H26^{viii}	3.286 (15)	H27···N9^{x}	3.086 (15)
N3···H37^{iii}	3.255 (14)	H27···C14	3.339 (15)
N3···H38^{iii}	2.849 (16)	H27···C35^{x}	3.368 (16)
N4···H1^{viii}	2.957 (14)	H27···C36^{x}	3.284 (16)
N4···H2^{iii}	2.528 (16)	H27···C37^{x}	3.217 (16)
N4···H16^{ii}	3.060 (14)	H27···C38^{x}	3.000 (15)

N4···H27	3.490 (15)	H27···C39^{x}	2.915 (14)
N5···H21^{iv}	2.776 (14)	H27···H14	3.55 (3)
N5···H34^{iv}	3.453 (15)	H27···H16^{ii}	2.70 (3)
N6···H8	3.452 (14)	H27···H29^{ii}	3.15 (3)
N6···H21^{iv}	3.005 (15)	H27···H38^{x}	3.46 (2)
N6···H24^{iv}	2.770 (14)	H27···H39^{x}	3.351 (19)
N6···H34^{iv}	2.772 (16)	H28···N9^{ix}	2.997 (17)
N6···H37^{iv}	3.562 (15)	H28···C15	3.332 (16)
N7···H3^{xi}	3.593 (14)	H28···C16	3.361 (15)
N7···H16^{ii}	3.257 (15)	H28···C37^{x}	2.991 (15)
N7···H29^{ii}	2.977 (14)	H28···C38^{x}	3.266 (15)
N8···H14^{xii}	3.138 (14)	H28···C39^{ix}	3.114 (17)
N8···H15^{v}	2.506 (16)	H28···H4^{xi}	3.52 (2)
N8···H16^{v}	3.566 (15)	H28···H15	3.33 (3)
N8···H34^{iv}	2.878 (14)	H28···H16	3.442 (19)
N9···H15^{v}	2.854 (16)	H28···H37^{x}	2.91 (2)
N9···H16^{v}	3.331 (14)	H28···H38^{x}	3.35 (2)
N9···H26	3.483 (14)	H28···H39^{ix}	2.55 (3)
N9···H27^{xii}	3.086 (15)	H29···N1^{xi}	3.500 (14)
N9···H28^{v}	2.997 (17)	H29···N7^{iv}	2.977 (14)
N9···H34^{iv}	3.058 (15)	H29···C5^{xi}	3.563 (14)
N9···H37^{iv}	2.930 (14)	H29···C27^{iv}	3.382 (15)
C1···H3^{iv}	3.376 (15)	H29···H3^{xiv}	3.02 (3)
C1···H11^{i}	3.426 (15)	H29···H16	3.46 (2)
C1···H12^{i}	2.899 (16)	H29···H27^{iv}	3.15 (3)
C1···H13^{vi}	2.999 (13)	H29···H33^{iv}	3.123 (19)
C2···H12^{vi}	3.385 (14)	H29···H39^{ix}	3.27 (2)
C2···H13^{vi}	3.007 (14)	H30···C2^{xi}	3.585 (14)
C2···H14^{vi}	3.265 (16)	H30···C14^{v}	3.422 (16)
C2···H20^{vi}	3.432 (15)	H30···C15^{v}	2.974 (15)
C2···H30^{vii}	3.585 (14)	H30···C33^{iv}	2.928 (14)
C3···H7^{ii}	3.152 (14)	H30···C34^{iv}	3.268 (14)
C3···H12^{vi}	3.099 (14)	H30···H14^{v}	3.23 (3)
C3···H13^{vi}	3.247 (15)	H30···H15^{v}	2.41 (3)
C3···H14^{vi}	3.509 (16)	H30···H33^{iv}	2.457 (19)
C4···H7^{ii}	2.809 (14)	H30···H34^{iv}	3.099 (19)
C4···H13^{vi}	3.457 (15)	H33···C17^{ii}	3.419 (16)
C4···H38^{iii}	3.321 (16)	H33···C20	3.429 (14)
C5···H13^{vi}	3.415 (15)	H33···C21	3.492 (14)
C5···H29^{vii}	3.563 (14)	H33···C29^{ii}	3.284 (13)
C6···H24	3.496 (14)	H33···C30^{ii}	2.927 (13)
C6···H38^{iii}	3.537 (16)	H33···H14^{xii}	3.42 (3)
C6···H39^{viii}	3.186 (15)	H33···H17^{ii}	2.62 (3)
C7···H4^{iv}	2.862 (14)	H33···H29^{ii}	3.123 (19)
C7···H38^{viii}	3.475 (15)	H33···H30^{ii}	2.457 (19)
C7···H39^{viii}	3.205 (15)	H34···N5^{ii}	3.453 (15)
C8···H4^{iv}	3.169 (14)	H34···N6^{ii}	2.772 (16)
C8···H21^{iv}	3.491 (15)	H34···N8^{ii}	2.878 (14)

C8···H38^{viii}	2.979 (14)	H34···N9^{ii}	3.058 (15)
C8···H39^{viii}	3.268 (15)	H34···C23^{ii}	3.490 (16)
C9···H26^{viii}	3.548 (15)	H34···C26^{ii}	3.570 (16)
C9···H38^{viii}	3.522 (13)	H34···C36^{ii}	3.315 (15)
C9···H39^{viii}	3.341 (14)	H34···H15^{xii}	2.85 (2)
C10···H8^{ii}	3.255 (15)	H34···H21	3.54 (2)
C10···H21	3.499 (13)	H34···H24	3.505 (19)
C10···H26^{viii}	3.559 (15)	H34···H26^{ii}	3.59 (2)
C10···H37^{iii}	3.440 (15)	H34···H30^{ii}	3.099 (19)
C10···H38^{iii}	3.067 (16)	H37···N2^{vi}	3.530 (15)
C10···H39^{viii}	3.342 (14)	H37···N3^{vi}	3.255 (14)
C11···H1^{viii}	3.414 (15)	H37···N6^{ii}	3.562 (15)
C11···H25^{viii}	2.897 (15)	H37···N9^{ii}	2.930 (14)
C11···H26^{viii}	3.202 (15)	H37···C10^{vi}	3.440 (15)
C12···H1^{viii}	3.169 (16)	H37···C24	3.589 (15)
C12···H20	3.462 (13)	H37···C26^{ii}	3.453 (16)
C12···H25^{viii}	3.172 (14)	H37···C39^{ii}	3.208 (15)
C12···H26^{viii}	2.861 (14)	H37···H24	3.43 (2)
C13···H11^{ii}	3.148 (15)	H37···H25	3.493 (19)
C13···H20	3.364 (14)	H37···H26^{ii}	2.81 (3)
C13···H25^{iii}	3.030 (16)	H37···H28^{xii}	2.91 (2)
C13···H26^{viii}	2.901 (14)	H37···H39^{ii}	2.86 (2)
C14···H1^{viii}	2.961 (13)	H38···N2^{vi}	2.509 (16)
C14···H2^{iii}	2.959 (16)	H38···N3^{vi}	2.849 (16)
C14···H3^{iii}	3.519 (16)	H38···C4^{vi}	3.321 (16)
C14···H16^{ii}	3.454 (14)	H38···C6^{vi}	3.537 (16)
C14···H27	3.339 (15)	H38···C7^{i}	3.475 (15)
C14···H30^{ix}	3.422 (16)	H38···C8^{i}	2.979 (14)
C15···H1^{viii}	3.089 (14)	H38···C9^{i}	3.522 (13)
C15···H2^{viii}	3.376 (14)	H38···C10^{vi}	3.067 (16)
C15···H28	3.332 (16)	H38···H4^{vi}	2.45 (3)
C15···H30^{ix}	2.974 (15)	H38···H8^{i}	2.78 (2)
C16···H1^{viii}	3.155 (15)	H38···H25	3.35 (2)
C16···H2^{viii}	2.992 (14)	H38···H27^{xii}	3.46 (2)
C16···H20^{iv}	3.260 (13)	H38···H28^{xii}	3.35 (2)
C16···H28	3.361 (15)	H39···N2^{i}	3.285 (14)
C17···H1^{viii}	3.129 (15)	H39···C6^{i}	3.186 (15)
C17···H2^{viii}	3.536 (15)	H39···C7^{i}	3.205 (15)
C17···H20^{iv}	2.883 (13)	H39···C8^{i}	3.268 (15)
C17···H33^{iv}	3.419 (16)	H39···C9^{i}	3.341 (14)
C18···H1^{viii}	3.020 (15)	H39···C10^{i}	3.342 (14)
C19···H11	3.569 (14)	H39···C28^{v}	3.357 (16)
C20···H17^{ii}	2.901 (14)	H39···H4^{vi}	3.50 (3)
C20···H33	3.429 (14)	H39···H26	3.51 (2)
C21···H8^{ii}	3.493 (15)	H39···H27^{xii}	3.351 (19)
C21···H17^{ii}	3.194 (13)	H39···H28^{v}	2.55 (3)
C21···H33	3.492 (14)	H39···H29^{v}	3.27 (2)
C23···H8	3.495 (13)	H39···H37^{iv}	2.86 (2)

C23···H21^{iv}	3.257 (15)		
C1—N1—C5	117.64 (12)	C34—C35—C36	118.06 (11)
C6—N2—C10	118.06 (11)	C34—C35—C37	124.02 (12)
C10—N3—C13	116.77 (11)	C36—C35—C37	117.88 (11)
C14—N4—C18	117.04 (11)	N8—C36—N9	115.40 (11)
C19—N5—C23	118.14 (11)	N8—C36—C35	122.14 (11)
C23—N6—C26	116.74 (12)	N9—C36—C35	122.47 (11)
C27—N7—C31	117.27 (12)	C35—C37—C38	119.43 (13)
C32—N8—C36	118.15 (11)	C37—C38—C39	118.43 (12)
C36—N9—C39	116.88 (12)	N9—C39—C38	124.90 (12)
N1—C1—C2	123.91 (12)	N1—C1—H1	116.9 (9)
C1—C2—C3	118.10 (12)	C2—C1—H1	119.2 (9)
C2—C3—C4	119.00 (13)	C1—C2—H2	118.0 (9)
C3—C4—C5	118.84 (11)	C3—C2—H2	123.9 (9)
N1—C5—C4	122.48 (11)	C2—C3—H3	122.5 (9)
N1—C5—C6	116.90 (11)	C4—C3—H3	118.5 (9)
C4—C5—C6	120.61 (10)	C3—C4—H4	121.8 (10)
N2—C6—C5	117.04 (11)	C5—C4—H4	119.4 (10)
N2—C6—C7	123.32 (11)	C6—C7—H7	119.3 (10)
C5—C6—C7	119.64 (10)	C8—C7—H7	121.6 (10)
C6—C7—C8	119.10 (11)	C7—C8—H8	121.5 (9)
C7—C8—C9	119.52 (11)	C9—C8—H8	119.0 (9)
C8—C9—C10	117.66 (11)	C9—C11—H11	118.3 (9)
C8—C9—C11	124.24 (12)	C12—C11—H11	122.4 (9)
C10—C9—C11	118.10 (11)	C11—C12—H12	121.8 (9)
N2—C10—N3	115.33 (11)	C13—C12—H12	119.9 (9)
N2—C10—C9	122.32 (11)	N3—C13—H13	116.4 (9)
N3—C10—C9	122.35 (11)	C12—C13—H13	118.4 (9)
C9—C11—C12	119.26 (12)	N4—C14—H14	114.5 (10)
C11—C12—C13	118.29 (12)	C15—C14—H14	121.4 (9)
N3—C13—C12	125.23 (11)	C14—C15—H15	121.1 (10)
N4—C14—C15	124.10 (12)	C16—C15—H15	120.5 (10)
C14—C15—C16	118.26 (12)	C15—C16—H16	123.0 (9)
C15—C16—C17	118.86 (13)	C17—C16—H16	118.1 (9)
C16—C17—C18	118.92 (11)	C16—C17—H17	122.0 (10)
N4—C18—C17	122.80 (11)	C18—C17—H17	119.1 (10)
N4—C18—C19	116.86 (11)	C19—C20—H20	119.0 (9)
C17—C18—C19	120.31 (11)	C21—C20—H20	122.1 (9)
N5—C19—C18	116.54 (11)	C20—C21—H21	121.7 (9)
N5—C19—C20	123.59 (12)	C22—C21—H21	119.0 (9)
C18—C19—C20	119.84 (11)	C22—C24—H24	117.6 (9)
C19—C20—C21	118.80 (11)	C25—C24—H24	123.4 (9)
C20—C21—C22	119.30 (12)	C24—C25—H25	124.4 (9)
C21—C22—C23	118.07 (11)	C26—C25—H25	116.9 (9)
C21—C22—C24	123.95 (12)	N6—C26—H26	115.5 (9)
C23—C22—C24	117.97 (11)	C25—C26—H26	119.5 (9)
N5—C23—N6	115.26 (11)	N7—C27—H27	114.0 (10)

N5—C23—C22	122.06 (11)	C28—C27—H27	122.0 (10)
N6—C23—C22	122.67 (11)	C27—C28—H28	122.6 (10)
C22—C24—C25	119.01 (12)	C29—C28—H28	119.0 (10)
C24—C25—C26	118.69 (12)	C28—C29—H29	120.3 (9)
N6—C26—C25	124.92 (12)	C30—C29—H29	121.0 (9)
N7—C27—C28	123.98 (13)	C29—C30—H30	120.1 (10)
C27—C28—C29	118.41 (13)	C31—C30—H30	120.8 (10)
C28—C29—C30	118.70 (13)	C32—C33—H33	119.3 (10)
C29—C30—C31	119.07 (12)	C34—C33—H33	121.4 (10)
N7—C31—C30	122.56 (12)	C33—C34—H34	121.4 (9)
N7—C31—C32	116.43 (11)	C35—C34—H34	119.6 (9)
C30—C31—C32	121.01 (11)	C35—C37—H37	119.7 (9)
N8—C32—C31	116.94 (11)	C38—C37—H37	120.8 (9)
N8—C32—C33	123.26 (12)	C37—C38—H38	121.9 (9)
C31—C32—C33	119.80 (11)	C39—C38—H38	119.7 (9)
C32—C33—C34	119.33 (11)	N9—C39—H39	115.5 (9)
C33—C34—C35	119.02 (12)	C38—C39—H39	119.6 (9)

C1—N1—C5—C4	0.89 (16)	C11—C9—C10—N2	−179.70 (10)
C1—N1—C5—C6	−179.97 (9)	C11—C9—C10—N3	0.45 (16)
C5—N1—C1—C2	0.73 (17)	C9—C11—C12—C13	0.09 (16)
C6—N2—C10—N3	178.97 (9)	C11—C12—C13—N3	0.13 (17)
C6—N2—C10—C9	−0.89 (16)	N4—C14—C15—C16	−0.90 (18)
C10—N2—C6—C5	179.62 (9)	C14—C15—C16—C17	1.59 (17)
C10—N2—C6—C7	−0.49 (16)	C15—C16—C17—C18	−0.98 (17)
C10—N3—C13—C12	−0.06 (16)	C16—C17—C18—N4	−0.44 (17)
C13—N3—C10—N2	179.90 (9)	C16—C17—C18—C19	177.64 (10)
C13—N3—C10—C9	−0.24 (15)	N4—C18—C19—N5	−177.53 (9)
C14—N4—C18—C17	1.15 (16)	N4—C18—C19—C20	4.20 (15)
C14—N4—C18—C19	−176.99 (9)	C17—C18—C19—N5	4.28 (15)
C18—N4—C14—C15	−0.47 (17)	C17—C18—C19—C20	−173.98 (9)
C19—N5—C23—N6	179.55 (9)	N5—C19—C20—C21	−2.03 (17)
C19—N5—C23—C22	0.40 (16)	C18—C19—C20—C21	176.11 (9)
C23—N5—C19—C18	−176.97 (9)	C19—C20—C21—C22	1.14 (16)
C23—N5—C19—C20	1.22 (16)	C20—C21—C22—C23	0.34 (16)
C23—N6—C26—C25	−0.39 (17)	C20—C21—C22—C24	−178.77 (10)
C26—N6—C23—N5	−178.05 (9)	C21—C22—C23—N5	−1.17 (16)
C26—N6—C23—C22	1.10 (16)	C21—C22—C23—N6	179.73 (10)
C27—N7—C31—C30	−0.64 (16)	C21—C22—C24—C25	179.46 (10)
C27—N7—C31—C32	178.72 (9)	C23—C22—C24—C25	0.34 (16)
C31—N7—C27—C28	−0.21 (17)	C24—C22—C23—N5	177.99 (10)
C32—N8—C36—N9	−178.06 (9)	C24—C22—C23—N6	−1.10 (16)
C32—N8—C36—C35	1.63 (16)	C22—C24—C25—C26	0.32 (16)
C36—N8—C32—C31	−179.91 (9)	C24—C25—C26—N6	−0.32 (18)
C36—N8—C32—C33	0.11 (16)	N7—C27—C28—C29	0.81 (19)
C36—N9—C39—C38	1.07 (17)	C27—C28—C29—C30	−0.56 (18)
C39—N9—C36—N8	178.70 (9)	C28—C29—C30—C31	−0.22 (17)
C39—N9—C36—C35	−0.98 (16)	C29—C30—C31—N7	0.86 (17)

N1—C1—C2—C3	−1.29 (18)	C29—C30—C31—C32	−178.48 (10)
C1—C2—C3—C4	0.22 (17)	N7—C31—C32—N8	−177.05 (9)
C2—C3—C4—C5	1.26 (17)	N7—C31—C32—C33	2.93 (15)
C3—C4—C5—N1	−1.89 (17)	C30—C31—C32—N8	2.33 (16)
C3—C4—C5—C6	179.00 (10)	C30—C31—C32—C33	−177.69 (10)
N1—C5—C6—N2	176.21 (9)	N8—C32—C33—C34	−1.46 (17)
N1—C5—C6—C7	−3.69 (15)	C31—C32—C33—C34	178.56 (9)
C4—C5—C6—N2	−4.63 (15)	C32—C33—C34—C35	1.02 (16)
C4—C5—C6—C7	175.47 (10)	C33—C34—C35—C36	0.60 (16)
N2—C6—C7—C8	1.67 (17)	C33—C34—C35—C37	178.06 (10)
C5—C6—C7—C8	−178.43 (9)	C34—C35—C36—N8	−2.00 (16)
C6—C7—C8—C9	−1.43 (16)	C34—C35—C36—N9	177.67 (10)
C7—C8—C9—C10	0.15 (16)	C34—C35—C37—C38	−176.60 (10)
C7—C8—C9—C11	−179.04 (10)	C36—C35—C37—C38	0.86 (16)
C8—C9—C10—N2	1.06 (16)	C37—C35—C36—N8	−179.62 (10)
C8—C9—C10—N3	−178.79 (9)	C37—C35—C36—N9	0.05 (16)
C8—C9—C11—C12	178.83 (10)	C35—C37—C38—C39	−0.81 (17)
C10—C9—C11—C12	−0.36 (16)	C37—C38—C39—N9	−0.19 (18)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N4^{vi}	1.008 (15)	2.529 (17)	3.4161 (16)	146.6 (14)
C7—H7···N1	0.962 (16)	2.462 (17)	2.8037 (16)	100.6 (12)
C12—H12···N1^{viii}	0.967 (15)	2.616 (17)	3.4845 (16)	149.6 (14)
C15—H15···N8^{ix}	0.949 (15)	2.507 (17)	3.3470 (16)	147.6 (14)
C17—H17···N5	0.940 (16)	2.453 (16)	2.7856 (15)	100.7 (12)
C20—H20···N4	0.985 (16)	2.460 (17)	2.8036 (15)	100.0 (12)
C33—H33···N7	0.948 (16)	2.456 (16)	2.7944 (16)	100.9 (13)
C38—H38···N2^{vi}	0.991 (16)	2.511 (17)	3.4016 (16)	149.5 (14)

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