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4-[4-(Azidomethyl)phenyl]-2,6-diphenylpyridine

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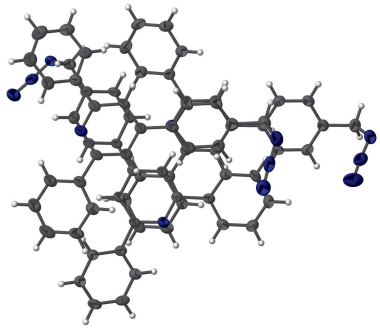
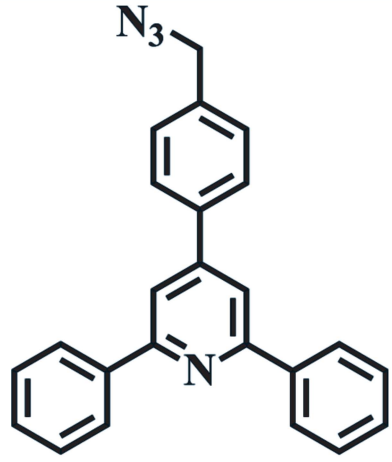
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{24}H_{18}N_4$, crystallizes with three molecules in the asymmetric unit. In the crystal, weak C—H$\cdots\pi$ interactions link the molecules.

3D view



Chemical scheme



Structure description

Derivatives of the title compound can be used as coordinating ligands in metal complexes (Ai *et al.*, 2016; Fernandez-Cestau *et al.*, 2017). Herein we report the crystal structure of the title compound (Fig. 1), which crystallizes with three molecules, *A* (containing N1), *B* (containing N4) and *C* (containing N9), in the asymmetric unit. In molecule *A*, the dihedral angles between the pyridine ring and its *ortho* phenyl substituents are 14.0 (2) and 22.86 (18)°; the dihedral angle between the pyridine ring and the *para*-substituent phenyl ring is 9.17 (18)° and the C13—C24—N2—N3 torsion angle for the linkage of the azide group to the aromatic ring is 47.0 (4)°. Equivalent data for molecule B are 5.75 (19), 22.37 (18), 23.39 (17) and 65.5 (4)°, respectively. The equivalent angles for molecule C are 7.5 (2), 22.57 (19), 27.31 (18) and 57.3 (5)°, respectively. In the crystal, weak C—H$\cdots\pi$ interactions link the molecules (Table 1, Fig. 2).

Synthesis and crystallization

Sodium azide (0.70 g 100 mmol) was added to a solution of [4-(bromomethyl)phenyl]-2,6-diphenylpyridine (4.00 g, 10 mmol) in DMSO (20 ml). The reaction mixture was stirred for 24 h at room temperature. After completion, the mixture was poured into ice–water and a white solid precipitate appeared. The generated crude product was washed with water and recrystallized from ethanol solution to afford colourless blocks. ^{1}H NMR (400 MHz, DMSO) δ 8.34 (*d*, *J* = 7.5 Hz, 4H), 8.30–8.16 (*m*, 4H), 7.78–7.80 (*d*, *J* = 8, 2H), 7.50–7.60 (*m*, 6H), 4.77 (*s*, 18H), 4.67 (*s*, 2H).

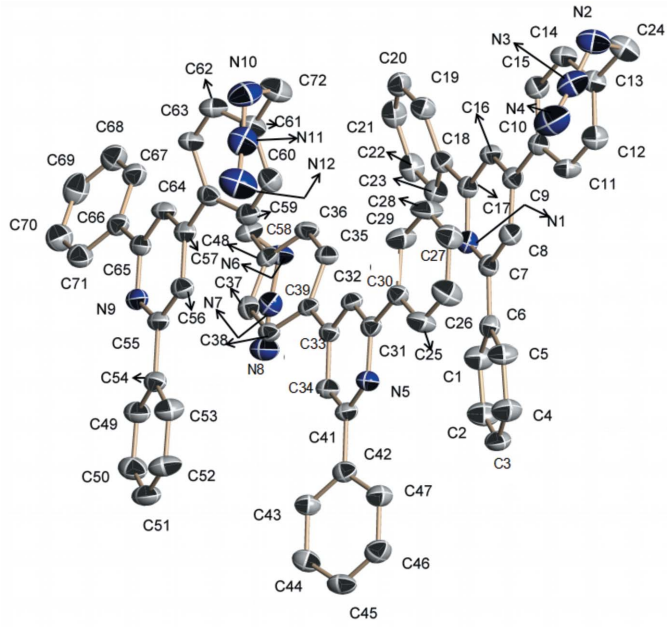


Figure 1
The molecular structure of the title molecule with displacement ellipsoids drawn at the 30% probability level. All H atoms are omitted for clarity.

Refinement

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

Funding information

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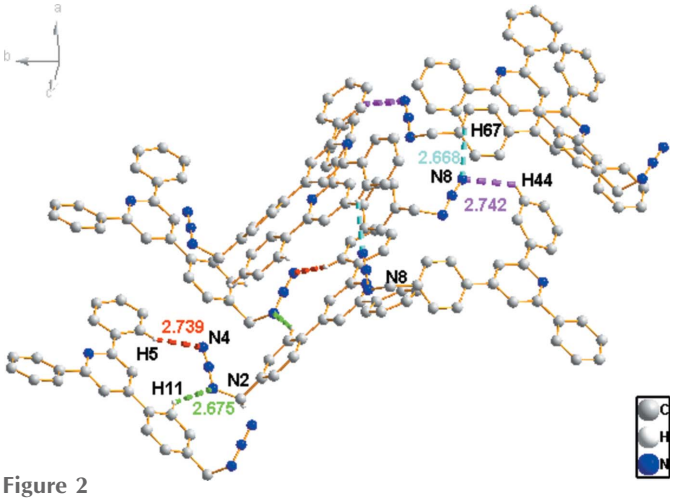

Figure 2
Partial packing diagram of the title compound. Some short C—H···N contacts are indicated by dashed lines.

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

*Cg*4, *Cg*7, *Cg*8 and *Cg*11 are the centroids of the C18–C23, C34–C39, C42–C47 and C58–C63 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···*Cg*8^{i}	0.93	2.92	3.601 (4)	132
C21—H21···*Cg*7^{ii}	0.93	2.78	3.668 (4)	161
C24—H24*B*···*Cg*11^{iii}	0.93	2.84	3.443 (5)	121
C36—H36···*Cg*4	0.93	2.82	3.601 (4)	142

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{18}N_4$
M_r	362.42
Crystal system, space group	Monoclinic, *Pc*
Temperature (K)	298
a, *b*, *c* (Å)	12.8109 (13), 19.708 (2), 11.4152 (12)
β (°)	108.649 (1)
V (Å^3)	2730.8 (5)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker SMART CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19076, 9342, 8030
R_{int}	0.029
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.105, 1.05
No. of reflections	9342
No. of parameters	757
No. of restraints	8
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.19

Computer programs: *SMART* and *SAINT* (Bruker, 1997), *SHELXS97* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

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full crystallographic data

IUCrData (2019). **4**, x190295 [https://doi.org/10.1107/S2414314619002955]

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Crystal data

$C_{24}H_{18}N_4$
M_r = 362.42
Monoclinic, *Pc*
a = 12.8109 (13) Å
b = 19.708 (2) Å
c = 11.4152 (12) Å
β = 108.649 (1)°
V = 2730.8 (5) Å^3
Z = 6
F(000) = 1140
D_x = 1.322 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 6582 reflections
θ = 2.3–26.0°
μ = 0.08 mm^{-1}
T = 298 K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
19076 measured reflections
9342 independent reflections
8030 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°, θ_{min} = 1.0°
h = −15→15
k = −23→23
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.105
S = 1.05
9342 reflections
757 parameters
8 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.3774P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2172 (4)	0.14940 (19)	0.1061 (4)	0.0420 (10)
H1	0.2426	0.1130	0.1594	0.050*
C2	0.2083 (4)	0.1427 (2)	−0.0169 (4)	0.0481 (11)
H2	0.2269	0.1017	−0.0454	0.058*
C3	0.1721 (3)	0.1959 (2)	−0.0979 (4)	0.0398 (9)
H3	0.1648	0.1911	−0.1812	0.048*
C4	0.1470 (4)	0.2561 (2)	−0.0532 (4)	0.0452 (10)
H4	0.1242	0.2929	−0.1064	0.054*
C5	0.1549 (4)	0.26297 (19)	0.0691 (4)	0.0394 (9)
H5	0.1371	0.3043	0.0970	0.047*
C6	0.1891 (3)	0.20950 (17)	0.1521 (3)	0.0295 (8)
C7	0.1918 (3)	0.21537 (16)	0.2831 (3)	0.0282 (8)
C8	0.1415 (3)	0.26991 (17)	0.3216 (3)	0.0302 (8)
H8	0.1103	0.3046	0.2663	0.036*
C9	0.1373 (3)	0.27298 (17)	0.4408 (3)	0.0285 (8)
C10	0.0784 (3)	0.32896 (16)	0.4812 (3)	0.0281 (8)
C11	0.0137 (3)	0.37504 (17)	0.3968 (4)	0.0332 (9)
H11	0.0115	0.3729	0.3147	0.040*
C12	−0.0475 (3)	0.42398 (18)	0.4320 (4)	0.0365 (9)
H12	−0.0915	0.4532	0.3727	0.044*
C13	−0.0447 (3)	0.43036 (17)	0.5531 (4)	0.0330 (9)
C14	0.0220 (3)	0.38596 (18)	0.6395 (4)	0.0354 (9)
H14	0.0266	0.3898	0.7222	0.043*
C15	0.0818 (3)	0.33614 (18)	0.6041 (3)	0.0336 (9)
H15	0.1253	0.3067	0.6635	0.040*
C16	0.1883 (3)	0.22085 (16)	0.5201 (3)	0.0290 (8)
H16	0.1869	0.2206	0.6011	0.035*
C17	0.2414 (3)	0.16893 (16)	0.4790 (3)	0.0280 (8)
C18	0.3011 (3)	0.11430 (17)	0.5659 (3)	0.0298 (8)
C19	0.3390 (3)	0.12554 (18)	0.6924 (3)	0.0350 (9)
H19	0.3276	0.1675	0.7234	0.042*
C20	0.3938 (3)	0.07480 (19)	0.7735 (4)	0.0385 (9)
H20	0.4185	0.0830	0.8582	0.046*
C21	0.4117 (3)	0.01249 (19)	0.7287 (4)	0.0408 (10)
H21	0.4473	−0.0217	0.7830	0.049*
C22	0.3763 (3)	0.00117 (18)	0.6028 (4)	0.0401 (10)
H22	0.3896	−0.0406	0.5723	0.048*
C23	0.3213 (3)	0.05130 (17)	0.5216 (4)	0.0347 (9)
H23	0.2977	0.0430	0.4370	0.042*
C24	−0.1127 (4)	0.48394 (17)	0.5891 (4)	0.0449 (11)
H24A	−0.1833	0.4876	0.5246	0.054*
H24B	−0.1264	0.4699	0.6644	0.054*
C25	0.2984 (3)	0.43191 (19)	0.1563 (4)	0.0417 (10)
H25	0.3011	0.4290	0.0760	0.050*
C26	0.2404 (4)	0.4843 (2)	0.1881 (4)	0.0469 (11)

H26	0.2041	0.5159	0.1286	0.056*
C27	0.2359 (3)	0.49014 (19)	0.3063 (4)	0.0408 (10)
H27	0.1979	0.5258	0.3274	0.049*
C28	0.2883 (4)	0.4427 (2)	0.3926 (4)	0.0465 (11)
H28	0.2851	0.4458	0.4726	0.056*
C29	0.3462 (4)	0.3899 (2)	0.3618 (4)	0.0418 (10)
H29	0.3812	0.3582	0.4218	0.050*
C30	0.3528 (3)	0.38354 (17)	0.2436 (3)	0.0291 (8)
C31	0.4136 (3)	0.32597 (17)	0.2091 (3)	0.0281 (8)
C32	0.4599 (3)	0.27377 (16)	0.2895 (3)	0.0276 (8)
H32	0.4563	0.2748	0.3696	0.033*
C33	0.5118 (3)	0.21960 (16)	0.2524 (3)	0.0266 (8)
C34	0.5617 (3)	0.16276 (16)	0.3367 (3)	0.0255 (7)
C35	0.5280 (3)	0.14773 (17)	0.4389 (3)	0.0303 (8)
H35	0.4726	0.1735	0.4532	0.036*
C36	0.5752 (3)	0.09545 (17)	0.5191 (3)	0.0313 (8)
H36	0.5509	0.0865	0.5861	0.038*
C37	0.6585 (3)	0.05612 (16)	0.5004 (3)	0.0297 (8)
C38	0.6941 (3)	0.07155 (16)	0.4004 (3)	0.0314 (8)
H38	0.7511	0.0466	0.3876	0.038*
C39	0.6457 (3)	0.12352 (16)	0.3199 (3)	0.0275 (8)
H39	0.6700	0.1323	0.2529	0.033*
C40	0.5136 (3)	0.22171 (18)	0.1312 (3)	0.0304 (8)
H40	0.5455	0.1862	0.1011	0.036*
C41	0.4683 (3)	0.27611 (17)	0.0548 (3)	0.0284 (8)
C42	0.4702 (3)	0.28054 (17)	−0.0749 (3)	0.0314 (8)
C43	0.5484 (3)	0.24521 (17)	−0.1117 (3)	0.0330 (8)
H43	0.6002	0.2184	−0.0549	0.040*
C44	0.5495 (3)	0.24965 (17)	−0.2323 (4)	0.0375 (9)
H44	0.6027	0.2262	−0.2557	0.045*
C45	0.4726 (3)	0.28851 (18)	−0.3180 (4)	0.0395 (9)
H45	0.4728	0.2906	−0.3993	0.047*
C46	0.3953 (3)	0.32442 (19)	−0.2822 (4)	0.0395 (10)
H46	0.3439	0.3513	−0.3393	0.047*
C47	0.3941 (3)	0.32042 (19)	−0.1620 (3)	0.0370 (9)
H47	0.3416	0.3447	−0.1388	0.044*
C48	0.7046 (3)	−0.00393 (18)	0.5824 (4)	0.0361 (9)
H48A	0.7833	−0.0069	0.5966	0.043*
H48B	0.6935	0.0027	0.6618	0.043*
C49	0.9052 (3)	0.1648 (2)	0.2320 (4)	0.0387 (9)
H49	0.9288	0.1282	0.2855	0.046*
C50	0.9134 (4)	0.1616 (2)	0.1147 (4)	0.0445 (10)
H50	0.9431	0.1230	0.0903	0.053*
C51	0.8786 (4)	0.2142 (2)	0.0336 (4)	0.0476 (11)
H51	0.8849	0.2117	−0.0453	0.057*
C52	0.8342 (4)	0.2709 (2)	0.0696 (4)	0.0491 (11)
H52	0.8094	0.3068	0.0148	0.059*
C53	0.8264 (4)	0.2744 (2)	0.1876 (4)	0.0444 (10)

H53	0.7963	0.3129	0.2111	0.053*
C54	0.8622 (3)	0.22190 (17)	0.2714 (3)	0.0319 (8)
C55	0.8566 (3)	0.22446 (17)	0.3994 (3)	0.0293 (8)
C56	0.8022 (3)	0.27609 (18)	0.4407 (3)	0.0317 (8)
H56	0.7687	0.3112	0.3876	0.038*
C57	0.7978 (3)	0.27529 (17)	0.5605 (3)	0.0293 (8)
C58	0.7436 (3)	0.33115 (17)	0.6084 (3)	0.0315 (8)
C59	0.6588 (3)	0.36879 (18)	0.5300 (4)	0.0349 (9)
H59	0.6351	0.3595	0.4457	0.042*
C60	0.6084 (3)	0.42047 (18)	0.5757 (4)	0.0374 (9)
H60	0.5511	0.4451	0.5216	0.045*
C61	0.6424 (3)	0.43557 (19)	0.7004 (4)	0.0380 (9)
C62	0.7273 (3)	0.39818 (19)	0.7786 (4)	0.0387 (9)
H62	0.7508	0.4076	0.8628	0.046*
C63	0.7779 (3)	0.34714 (18)	0.7345 (3)	0.0346 (9)
H63	0.8354	0.3230	0.7891	0.042*
C64	0.8480 (3)	0.22099 (18)	0.6349 (3)	0.0318 (9)
H64	0.8460	0.2180	0.7155	0.038*
C65	0.9012 (3)	0.17099 (17)	0.5890 (3)	0.0307 (8)
C66	0.9547 (3)	0.11118 (17)	0.6645 (3)	0.0323 (8)
C67	0.9254 (3)	0.08887 (19)	0.7661 (4)	0.0364 (9)
H67	0.8723	0.1124	0.7895	0.044*
C68	0.9745 (3)	0.0323 (2)	0.8316 (4)	0.0433 (10)
H68	0.9534	0.0177	0.8981	0.052*
C69	1.0544 (4)	−0.0027 (2)	0.8002 (4)	0.0507 (12)
H69	1.0873	−0.0408	0.8449	0.061*
C70	1.0847 (4)	0.0194 (2)	0.7014 (4)	0.0484 (11)
H70	1.1392	−0.0037	0.6800	0.058*
C71	1.0355 (3)	0.07546 (19)	0.6336 (4)	0.0404 (10)
H71	1.0566	0.0894	0.5667	0.048*
C72	0.5887 (4)	0.4925 (2)	0.7489 (4)	0.0516 (11)
H72A	0.5116	0.4954	0.6993	0.062*
H72B	0.5922	0.4823	0.8333	0.062*
N1	0.2418 (2)	0.16545 (14)	0.3615 (3)	0.0303 (7)
N2	−0.0585 (3)	0.55181 (17)	0.6094 (3)	0.0498 (9)
N3	−0.0203 (3)	0.57001 (16)	0.5287 (3)	0.0466 (9)
N4	0.0178 (4)	0.5914 (2)	0.4591 (4)	0.0671 (12)
N5	0.4189 (2)	0.32805 (14)	0.0933 (3)	0.0309 (7)
N6	0.6509 (3)	−0.06933 (14)	0.5263 (3)	0.0352 (7)
N7	0.6711 (3)	−0.08424 (14)	0.4303 (3)	0.0345 (7)
N8	0.6842 (3)	−0.10260 (16)	0.3418 (3)	0.0436 (8)
N9	0.9067 (2)	0.17328 (15)	0.4743 (3)	0.0318 (7)
N10	0.6430 (3)	0.55916 (18)	0.7462 (4)	0.0554 (10)
N11	0.6441 (3)	0.57498 (17)	0.6416 (4)	0.0494 (9)
N12	0.6505 (4)	0.59316 (19)	0.5491 (4)	0.0660 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.057 (3)	0.032 (2)	0.039 (3)	0.0068 (19)	0.019 (2)	0.0018 (18)
C2	0.068 (3)	0.037 (2)	0.043 (3)	0.004 (2)	0.023 (2)	−0.0092 (19)
C3	0.045 (2)	0.047 (2)	0.028 (2)	−0.0054 (19)	0.0125 (19)	−0.0090 (18)
C4	0.058 (3)	0.045 (2)	0.033 (3)	0.007 (2)	0.016 (2)	0.0044 (19)
C5	0.057 (3)	0.032 (2)	0.030 (2)	0.0045 (18)	0.016 (2)	−0.0025 (17)
C6	0.0280 (19)	0.0269 (17)	0.032 (2)	−0.0027 (14)	0.0077 (16)	−0.0016 (15)
C7	0.0273 (19)	0.0264 (17)	0.030 (2)	−0.0031 (14)	0.0082 (16)	0.0004 (15)
C8	0.033 (2)	0.0265 (17)	0.030 (2)	0.0022 (15)	0.0085 (17)	0.0046 (15)
C9	0.029 (2)	0.0256 (17)	0.030 (2)	−0.0039 (14)	0.0086 (17)	−0.0002 (15)
C10	0.0297 (19)	0.0245 (17)	0.030 (2)	−0.0035 (14)	0.0100 (16)	−0.0010 (15)
C11	0.048 (2)	0.0289 (17)	0.025 (2)	0.0019 (16)	0.0159 (18)	0.0029 (15)
C12	0.044 (2)	0.0291 (19)	0.036 (2)	0.0043 (16)	0.0124 (19)	0.0053 (17)
C13	0.042 (2)	0.0254 (17)	0.035 (2)	−0.0045 (16)	0.0169 (18)	−0.0022 (16)
C14	0.047 (2)	0.0317 (19)	0.030 (2)	−0.0041 (17)	0.0171 (19)	−0.0015 (16)
C15	0.037 (2)	0.0302 (19)	0.032 (2)	0.0015 (16)	0.0098 (18)	0.0045 (16)
C16	0.033 (2)	0.0305 (18)	0.024 (2)	−0.0016 (15)	0.0093 (16)	0.0004 (15)
C17	0.028 (2)	0.0257 (17)	0.030 (2)	−0.0020 (14)	0.0092 (17)	0.0014 (15)
C18	0.031 (2)	0.0280 (17)	0.031 (2)	0.0000 (15)	0.0111 (17)	0.0026 (15)
C19	0.040 (2)	0.0326 (19)	0.035 (2)	0.0005 (16)	0.0148 (19)	0.0033 (17)
C20	0.035 (2)	0.045 (2)	0.033 (2)	0.0008 (17)	0.0075 (18)	0.0102 (18)
C21	0.039 (2)	0.036 (2)	0.045 (3)	0.0025 (17)	0.012 (2)	0.0166 (19)
C22	0.040 (2)	0.0289 (19)	0.051 (3)	0.0025 (17)	0.015 (2)	0.0057 (18)
C23	0.036 (2)	0.0313 (19)	0.036 (2)	−0.0008 (16)	0.0110 (18)	0.0022 (16)
C24	0.061 (3)	0.0301 (19)	0.055 (3)	0.0033 (19)	0.034 (2)	0.0021 (18)
C25	0.054 (3)	0.044 (2)	0.035 (2)	0.0071 (19)	0.025 (2)	0.0055 (19)
C26	0.059 (3)	0.040 (2)	0.049 (3)	0.016 (2)	0.026 (2)	0.015 (2)
C27	0.047 (2)	0.036 (2)	0.044 (3)	0.0075 (18)	0.021 (2)	−0.0029 (18)
C28	0.067 (3)	0.048 (2)	0.029 (2)	0.014 (2)	0.022 (2)	−0.0037 (19)
C29	0.058 (3)	0.039 (2)	0.028 (2)	0.0107 (19)	0.013 (2)	0.0027 (17)
C30	0.031 (2)	0.0304 (18)	0.026 (2)	−0.0042 (15)	0.0098 (16)	0.0021 (15)
C31	0.029 (2)	0.0280 (18)	0.026 (2)	−0.0040 (14)	0.0075 (16)	−0.0010 (15)
C32	0.031 (2)	0.0305 (17)	0.020 (2)	−0.0032 (15)	0.0068 (15)	−0.0030 (15)
C33	0.028 (2)	0.0277 (17)	0.024 (2)	−0.0055 (14)	0.0090 (16)	−0.0022 (15)
C34	0.0298 (19)	0.0262 (16)	0.0190 (19)	−0.0062 (14)	0.0058 (15)	−0.0025 (14)
C35	0.035 (2)	0.0321 (18)	0.025 (2)	−0.0019 (16)	0.0118 (17)	−0.0028 (15)
C36	0.040 (2)	0.0342 (19)	0.022 (2)	−0.0053 (16)	0.0133 (17)	0.0024 (16)
C37	0.034 (2)	0.0280 (17)	0.024 (2)	−0.0056 (15)	0.0037 (16)	−0.0021 (15)
C38	0.031 (2)	0.0259 (17)	0.037 (2)	−0.0040 (15)	0.0096 (17)	−0.0049 (16)
C39	0.032 (2)	0.0281 (17)	0.024 (2)	−0.0049 (15)	0.0108 (16)	0.0011 (15)
C40	0.036 (2)	0.0305 (19)	0.026 (2)	−0.0023 (15)	0.0129 (17)	−0.0024 (15)
C41	0.034 (2)	0.0299 (18)	0.021 (2)	−0.0034 (15)	0.0087 (16)	−0.0009 (15)
C42	0.038 (2)	0.0283 (18)	0.027 (2)	−0.0036 (16)	0.0099 (17)	0.0014 (16)
C43	0.042 (2)	0.0297 (18)	0.029 (2)	0.0023 (16)	0.0141 (18)	0.0025 (16)
C44	0.051 (2)	0.0297 (19)	0.038 (3)	0.0014 (17)	0.023 (2)	0.0020 (17)
C45	0.057 (3)	0.038 (2)	0.028 (2)	−0.0071 (19)	0.020 (2)	0.0029 (17)

C46	0.046 (2)	0.040 (2)	0.030 (2)	0.0017 (18)	0.0093 (19)	0.0113 (18)
C47	0.044 (2)	0.038 (2)	0.030 (2)	0.0033 (17)	0.0133 (18)	0.0025 (17)
C48	0.047 (2)	0.0342 (19)	0.023 (2)	−0.0016 (17)	0.0063 (18)	−0.0014 (16)
C49	0.047 (2)	0.040 (2)	0.032 (2)	−0.0073 (18)	0.0168 (19)	−0.0054 (18)
C50	0.056 (3)	0.042 (2)	0.041 (3)	−0.0069 (19)	0.023 (2)	−0.0104 (19)
C51	0.057 (3)	0.059 (3)	0.030 (3)	−0.017 (2)	0.018 (2)	−0.010 (2)
C52	0.072 (3)	0.048 (2)	0.026 (2)	−0.002 (2)	0.015 (2)	0.0016 (19)
C53	0.056 (3)	0.045 (2)	0.032 (3)	0.002 (2)	0.014 (2)	−0.0033 (19)
C54	0.035 (2)	0.0339 (19)	0.028 (2)	−0.0106 (16)	0.0114 (17)	−0.0058 (16)
C55	0.033 (2)	0.0321 (18)	0.024 (2)	−0.0128 (15)	0.0111 (17)	−0.0048 (15)
C56	0.036 (2)	0.0314 (18)	0.029 (2)	−0.0071 (15)	0.0115 (17)	−0.0007 (15)
C57	0.033 (2)	0.0271 (18)	0.029 (2)	−0.0095 (15)	0.0112 (17)	−0.0033 (15)
C58	0.036 (2)	0.0312 (18)	0.031 (2)	−0.0071 (16)	0.0161 (18)	−0.0003 (16)
C59	0.039 (2)	0.0355 (19)	0.031 (2)	−0.0091 (17)	0.0128 (18)	−0.0019 (17)
C60	0.039 (2)	0.0345 (19)	0.041 (3)	0.0003 (16)	0.0155 (19)	0.0024 (18)
C61	0.046 (2)	0.037 (2)	0.036 (3)	−0.0018 (18)	0.0202 (19)	0.0006 (18)
C62	0.053 (3)	0.039 (2)	0.027 (2)	−0.0014 (19)	0.0159 (19)	−0.0023 (17)
C63	0.044 (2)	0.038 (2)	0.025 (2)	−0.0015 (17)	0.0148 (18)	−0.0006 (16)
C64	0.042 (2)	0.0336 (19)	0.023 (2)	−0.0089 (16)	0.0149 (17)	−0.0045 (16)
C65	0.031 (2)	0.0333 (18)	0.029 (2)	−0.0104 (15)	0.0118 (17)	−0.0052 (16)
C66	0.033 (2)	0.0334 (18)	0.029 (2)	−0.0065 (16)	0.0074 (17)	−0.0021 (16)
C67	0.038 (2)	0.039 (2)	0.032 (2)	−0.0038 (17)	0.0102 (18)	0.0015 (17)
C68	0.046 (2)	0.043 (2)	0.039 (3)	−0.0049 (19)	0.010 (2)	0.0073 (19)
C69	0.045 (3)	0.044 (2)	0.054 (3)	0.003 (2)	0.004 (2)	0.010 (2)
C70	0.047 (3)	0.051 (2)	0.047 (3)	0.007 (2)	0.014 (2)	−0.001 (2)
C71	0.044 (2)	0.041 (2)	0.038 (3)	−0.0016 (18)	0.014 (2)	−0.0049 (18)
C72	0.065 (3)	0.050 (2)	0.049 (3)	0.012 (2)	0.032 (2)	0.004 (2)
N1	0.0308 (17)	0.0278 (15)	0.0316 (19)	0.0000 (12)	0.0089 (14)	0.0016 (13)
N2	0.074 (3)	0.0356 (18)	0.047 (2)	0.0031 (17)	0.029 (2)	−0.0066 (16)
N3	0.064 (2)	0.0297 (17)	0.041 (2)	−0.0036 (16)	0.009 (2)	−0.0019 (16)
N4	0.089 (3)	0.055 (2)	0.053 (3)	−0.026 (2)	0.017 (2)	0.006 (2)
N5	0.0358 (18)	0.0316 (15)	0.0271 (19)	−0.0011 (13)	0.0127 (14)	−0.0010 (13)
N6	0.051 (2)	0.0309 (15)	0.0275 (19)	−0.0013 (14)	0.0172 (15)	0.0010 (13)
N7	0.0389 (18)	0.0263 (15)	0.036 (2)	−0.0037 (13)	0.0095 (16)	0.0056 (14)
N8	0.056 (2)	0.0419 (18)	0.036 (2)	−0.0070 (16)	0.0195 (18)	−0.0035 (16)
N9	0.0331 (17)	0.0348 (16)	0.0277 (18)	−0.0084 (13)	0.0100 (14)	−0.0018 (14)
N10	0.075 (3)	0.047 (2)	0.041 (3)	0.0088 (19)	0.014 (2)	−0.0124 (18)
N11	0.058 (2)	0.0322 (18)	0.059 (3)	0.0063 (16)	0.019 (2)	−0.0081 (18)
N12	0.093 (3)	0.045 (2)	0.071 (3)	0.005 (2)	0.042 (3)	0.002 (2)

Geometric parameters (Å, º)

C1—C2	1.378 (6)	C38—H38	0.9300
C1—C6	1.389 (5)	C39—H39	0.9300
C1—H1	0.9300	C40—C41	1.387 (5)
C2—C3	1.378 (6)	C40—H40	0.9300
C2—H2	0.9300	C41—N5	1.350 (4)
C3—C4	1.370 (5)	C41—C42	1.491 (5)

C3—H3	0.9300	C42—C47	1.392 (5)
C4—C5	1.373 (6)	C42—C43	1.390 (5)
C4—H4	0.9300	C43—C44	1.384 (5)
C5—C6	1.391 (5)	C43—H43	0.9300
C5—H5	0.9300	C44—C45	1.377 (6)
C6—C7	1.488 (5)	C44—H44	0.9300
C7—N1	1.347 (4)	C45—C46	1.381 (6)
C7—C8	1.395 (5)	C45—H45	0.9300
C8—C9	1.380 (5)	C46—C47	1.379 (5)
C8—H8	0.9300	C46—H46	0.9300
C9—C16	1.387 (5)	C47—H47	0.9300
C9—C10	1.490 (5)	C48—N6	1.505 (5)
C10—C11	1.390 (5)	C48—H48A	0.9700
C10—C15	1.396 (5)	C48—H48B	0.9700
C11—C12	1.381 (5)	C49—C50	1.378 (5)
C11—H11	0.9300	C49—C54	1.390 (5)
C12—C13	1.377 (5)	C49—H49	0.9300
C12—H12	0.9300	C50—C51	1.367 (6)
C13—C14	1.389 (5)	C50—H50	0.9300
C13—C24	1.507 (5)	C51—C52	1.375 (6)
C14—C15	1.383 (5)	C51—H51	0.9300
C14—H14	0.9300	C52—C53	1.383 (6)
C15—H15	0.9300	C52—H52	0.9300
C16—C17	1.391 (5)	C53—C54	1.384 (5)
C16—H16	0.9300	C53—H53	0.9300
C17—N1	1.345 (5)	C54—C55	1.486 (5)
C17—C18	1.497 (5)	C55—N9	1.345 (5)
C18—C19	1.387 (5)	C55—C56	1.398 (5)
C18—C23	1.396 (5)	C56—C57	1.386 (5)
C19—C20	1.391 (5)	C56—H56	0.9300
C19—H19	0.9300	C57—C64	1.389 (5)
C20—C21	1.377 (5)	C57—C58	1.495 (5)
C20—H20	0.9300	C58—C59	1.382 (5)
C21—C22	1.380 (6)	C58—C63	1.400 (5)
C21—H21	0.9300	C59—C60	1.394 (5)
C22—C23	1.384 (5)	C59—H59	0.9300
C22—H22	0.9300	C60—C61	1.381 (6)
C23—H23	0.9300	C60—H60	0.9300
C24—N2	1.490 (5)	C61—C62	1.379 (6)
C24—H24A	0.9700	C61—C72	1.511 (5)
C24—H24B	0.9700	C62—C63	1.376 (5)
C25—C26	1.387 (5)	C62—H62	0.9300
C25—C30	1.393 (5)	C63—H63	0.9300
C25—H25	0.9300	C64—C65	1.392 (5)
C26—C27	1.373 (6)	C64—H64	0.9300
C26—H26	0.9300	C65—N9	1.335 (4)
C27—C28	1.369 (6)	C65—C66	1.491 (5)
C27—H27	0.9300	C66—C71	1.387 (5)

C28—C29	1.385 (5)	C66—C67	1.399 (5)
C28—H28	0.9300	C67—C68	1.377 (5)
C29—C30	1.385 (5)	C67—H67	0.9300
C29—H29	0.9300	C68—C69	1.373 (6)
C30—C31	1.499 (5)	C68—H68	0.9300
C31—N5	1.345 (4)	C69—C70	1.377 (6)
C31—C32	1.380 (5)	C69—H69	0.9300
C32—C33	1.393 (5)	C70—C71	1.380 (6)
C32—H32	0.9300	C70—H70	0.9300
C33—C40	1.392 (5)	C71—H71	0.9300
C33—C34	1.482 (5)	C72—N10	1.492 (6)
C34—C39	1.387 (5)	C72—H72A	0.9700
C34—C35	1.399 (5)	C72—H72B	0.9700
C35—C36	1.383 (5)	N2—N3	1.227 (5)
C35—H35	0.9300	N3—N4	1.139 (5)
C36—C37	1.390 (5)	N6—N7	1.238 (4)
C36—H36	0.9300	N7—N8	1.135 (4)
C37—C38	1.391 (5)	N10—N11	1.238 (5)
C37—C48	1.508 (5)	N11—N12	1.143 (5)
C38—C39	1.383 (5)		

C2—C1—C6	121.3 (4)	C38—C39—C34	121.6 (3)
C2—C1—H1	119.3	C38—C39—H39	119.2
C6—C1—H1	119.3	C34—C39—H39	119.2
C1—C2—C3	120.8 (4)	C41—C40—C33	120.8 (3)
C1—C2—H2	119.6	C41—C40—H40	119.6
C3—C2—H2	119.6	C33—C40—H40	119.6
C4—C3—C2	118.5 (4)	N5—C41—C40	121.8 (3)
C4—C3—H3	120.7	N5—C41—C42	116.0 (3)
C2—C3—H3	120.7	C40—C41—C42	122.3 (3)
C3—C4—C5	120.9 (4)	C47—C42—C43	118.4 (3)
C3—C4—H4	119.5	C47—C42—C41	120.8 (3)
C5—C4—H4	119.5	C43—C42—C41	120.8 (3)
C4—C5—C6	121.5 (4)	C44—C43—C42	120.4 (4)
C4—C5—H5	119.2	C44—C43—H43	119.8
C6—C5—H5	119.2	C42—C43—H43	119.8
C1—C6—C5	116.8 (3)	C45—C44—C43	120.6 (4)
C1—C6—C7	121.4 (3)	C45—C44—H44	119.7
C5—C6—C7	121.8 (3)	C43—C44—H44	119.7
N1—C7—C8	121.5 (3)	C44—C45—C46	119.5 (4)
N1—C7—C6	117.7 (3)	C44—C45—H45	120.2
C8—C7—C6	120.8 (3)	C46—C45—H45	120.2
C9—C8—C7	120.8 (3)	C47—C46—C45	120.1 (4)
C9—C8—H8	119.6	C47—C46—H46	119.9
C7—C8—H8	119.6	C45—C46—H46	119.9
C8—C9—C16	116.9 (3)	C46—C47—C42	121.0 (4)
C8—C9—C10	121.4 (3)	C46—C47—H47	119.5
C16—C9—C10	121.7 (3)	C42—C47—H47	119.5

C11—C10—C15	116.8 (3)	N6—C48—C37	111.9 (3)
C11—C10—C9	121.2 (3)	N6—C48—H48A	109.2
C15—C10—C9	122.0 (3)	C37—C48—H48A	109.2
C12—C11—C10	121.5 (4)	N6—C48—H48B	109.2
C12—C11—H11	119.2	C37—C48—H48B	109.2
C10—C11—H11	119.2	H48A—C48—H48B	107.9
C13—C12—C11	121.4 (4)	C50—C49—C54	120.9 (4)
C13—C12—H12	119.3	C50—C49—H49	119.6
C11—C12—H12	119.3	C54—C49—H49	119.6
C12—C13—C14	117.9 (3)	C51—C50—C49	120.9 (4)
C12—C13—C24	120.4 (4)	C51—C50—H50	119.5
C14—C13—C24	121.7 (4)	C49—C50—H50	119.5
C15—C14—C13	120.8 (4)	C50—C51—C52	119.4 (4)
C15—C14—H14	119.6	C50—C51—H51	120.3
C13—C14—H14	119.6	C52—C51—H51	120.3
C14—C15—C10	121.6 (3)	C51—C52—C53	119.8 (4)
C14—C15—H15	119.2	C51—C52—H52	120.1
C10—C15—H15	119.2	C53—C52—H52	120.1
C9—C16—C17	120.3 (3)	C54—C53—C52	121.6 (4)
C9—C16—H16	119.9	C54—C53—H53	119.2
C17—C16—H16	119.9	C52—C53—H53	119.2
N1—C17—C16	122.2 (3)	C53—C54—C49	117.4 (4)
N1—C17—C18	117.4 (3)	C53—C54—C55	123.0 (3)
C16—C17—C18	120.5 (3)	C49—C54—C55	119.6 (3)
C19—C18—C23	118.4 (3)	N9—C55—C56	121.3 (3)
C19—C18—C17	120.6 (3)	N9—C55—C54	115.9 (3)
C23—C18—C17	121.0 (3)	C56—C55—C54	122.9 (3)
C18—C19—C20	120.9 (4)	C57—C56—C55	120.5 (3)
C18—C19—H19	119.6	C57—C56—H56	119.8
C20—C19—H19	119.6	C55—C56—H56	119.8
C21—C20—C19	120.1 (4)	C56—C57—C64	117.1 (3)
C21—C20—H20	119.9	C56—C57—C58	121.5 (3)
C19—C20—H20	119.9	C64—C57—C58	121.4 (3)
C20—C21—C22	119.5 (4)	C59—C58—C63	117.9 (3)
C20—C21—H21	120.2	C59—C58—C57	121.3 (3)
C22—C21—H21	120.2	C63—C58—C57	120.8 (3)
C21—C22—C23	120.7 (4)	C58—C59—C60	120.8 (4)
C21—C22—H22	119.7	C58—C59—H59	119.6
C23—C22—H22	119.7	C60—C59—H59	119.6
C22—C23—C18	120.4 (4)	C61—C60—C59	120.8 (4)
C22—C23—H23	119.8	C61—C60—H60	119.6
C18—C23—H23	119.8	C59—C60—H60	119.6
N2—C24—C13	113.0 (3)	C60—C61—C62	118.4 (4)
N2—C24—H24A	109.0	C60—C61—C72	120.5 (4)
C13—C24—H24A	109.0	C62—C61—C72	121.1 (4)
N2—C24—H24B	109.0	C63—C62—C61	121.3 (4)
C13—C24—H24B	109.0	C63—C62—H62	119.3
H24A—C24—H24B	107.8	C61—C62—H62	119.3

C26—C25—C30	120.6 (4)	C62—C63—C58	120.8 (4)
C26—C25—H25	119.7	C62—C63—H63	119.6
C30—C25—H25	119.7	C58—C63—H63	119.6
C27—C26—C25	120.9 (4)	C57—C64—C65	120.1 (3)
C27—C26—H26	119.5	C57—C64—H64	119.9
C25—C26—H26	119.5	C65—C64—H64	119.9
C28—C27—C26	119.0 (4)	N9—C65—C64	122.1 (3)
C28—C27—H27	120.5	N9—C65—C66	115.7 (3)
C26—C27—H27	120.5	C64—C65—C66	122.2 (3)
C27—C28—C29	120.6 (4)	C71—C66—C67	118.1 (3)
C27—C28—H28	119.7	C71—C66—C65	119.8 (3)
C29—C28—H28	119.7	C67—C66—C65	122.1 (3)
C30—C29—C28	121.3 (4)	C68—C67—C66	120.5 (4)
C30—C29—H29	119.3	C68—C67—H67	119.8
C28—C29—H29	119.3	C66—C67—H67	119.8
C29—C30—C25	117.5 (3)	C69—C68—C67	120.9 (4)
C29—C30—C31	121.6 (3)	C69—C68—H68	119.5
C25—C30—C31	120.9 (3)	C67—C68—H68	119.5
N5—C31—C32	122.1 (3)	C68—C69—C70	118.9 (4)
N5—C31—C30	115.4 (3)	C68—C69—H69	120.5
C32—C31—C30	122.5 (3)	C70—C69—H69	120.5
C31—C32—C33	120.9 (3)	C69—C70—C71	121.0 (4)
C31—C32—H32	119.5	C69—C70—H70	119.5
C33—C32—H32	119.5	C71—C70—H70	119.5
C40—C33—C32	116.2 (3)	C70—C71—C66	120.6 (4)
C40—C33—C34	121.8 (3)	C70—C71—H71	119.7
C32—C33—C34	122.0 (3)	C66—C71—H71	119.7
C39—C34—C35	117.2 (3)	N10—C72—C61	112.1 (3)
C39—C34—C33	121.6 (3)	N10—C72—H72A	109.2
C35—C34—C33	121.1 (3)	C61—C72—H72A	109.2
C36—C35—C34	121.6 (3)	N10—C72—H72B	109.2
C36—C35—H35	119.2	C61—C72—H72B	109.2
C34—C35—H35	119.2	H72A—C72—H72B	107.9
C35—C36—C37	120.5 (3)	C17—N1—C7	118.3 (3)
C35—C36—H36	119.7	N3—N2—C24	115.0 (3)
C37—C36—H36	119.7	N4—N3—N2	174.6 (4)
C38—C37—C36	118.3 (3)	C31—N5—C41	118.2 (3)
C38—C37—C48	121.0 (3)	N7—N6—C48	112.6 (3)
C36—C37—C48	120.6 (3)	N8—N7—N6	174.2 (4)
C39—C38—C37	120.8 (3)	C65—N9—C55	119.0 (3)
C39—C38—H38	119.6	N11—N10—C72	113.0 (3)
C37—C38—H38	119.6	N12—N11—N10	175.0 (5)

C6—C1—C2—C3	0.7 (7)	C33—C40—C41—N5	−1.5 (5)
C1—C2—C3—C4	1.1 (7)	C33—C40—C41—C42	179.1 (3)
C2—C3—C4—C5	−1.6 (6)	N5—C41—C42—C47	−22.3 (5)
C3—C4—C5—C6	0.3 (7)	C40—C41—C42—C47	157.1 (4)
C2—C1—C6—C5	−1.9 (6)	N5—C41—C42—C43	157.4 (3)

C2—C1—C6—C7	176.0 (4)	C40—C41—C42—C43	−23.2 (5)
C4—C5—C6—C1	1.4 (6)	C47—C42—C43—C44	−0.3 (5)
C4—C5—C6—C7	−176.5 (4)	C41—C42—C43—C44	−180.0 (3)
C1—C6—C7—N1	12.3 (5)	C42—C43—C44—C45	−0.7 (5)
C5—C6—C7—N1	−169.9 (3)	C43—C44—C45—C46	1.4 (6)
C1—C6—C7—C8	−166.0 (4)	C44—C45—C46—C47	−1.1 (6)
C5—C6—C7—C8	11.9 (5)	C45—C46—C47—C42	0.1 (6)
N1—C7—C8—C9	−2.7 (5)	C43—C42—C47—C46	0.6 (6)
C6—C7—C8—C9	175.5 (3)	C41—C42—C47—C46	−179.7 (3)
C7—C8—C9—C16	2.0 (5)	C38—C37—C48—N6	−80.7 (4)
C7—C8—C9—C10	−176.6 (3)	C36—C37—C48—N6	96.0 (4)
C8—C9—C10—C11	8.5 (5)	C54—C49—C50—C51	−0.6 (6)
C16—C9—C10—C11	−170.1 (3)	C49—C50—C51—C52	−0.4 (6)
C8—C9—C10—C15	−174.1 (3)	C50—C51—C52—C53	0.7 (7)
C16—C9—C10—C15	7.3 (5)	C51—C52—C53—C54	−0.1 (7)
C15—C10—C11—C12	−2.3 (5)	C52—C53—C54—C49	−0.9 (6)
C9—C10—C11—C12	175.2 (3)	C52—C53—C54—C55	179.0 (4)
C10—C11—C12—C13	1.7 (6)	C50—C49—C54—C53	1.2 (6)
C11—C12—C13—C14	0.1 (6)	C50—C49—C54—C55	−178.7 (3)
C11—C12—C13—C24	−179.7 (3)	C53—C54—C55—N9	−172.2 (3)
C12—C13—C14—C15	−1.3 (5)	C49—C54—C55—N9	7.7 (5)
C24—C13—C14—C15	178.5 (3)	C53—C54—C55—C56	8.4 (5)
C13—C14—C15—C10	0.7 (5)	C49—C54—C55—C56	−171.8 (3)
C11—C10—C15—C14	1.1 (5)	N9—C55—C56—C57	−0.6 (5)
C9—C10—C15—C14	−176.4 (3)	C54—C55—C56—C57	178.8 (3)
C8—C9—C16—C17	0.6 (5)	C55—C56—C57—C64	−0.9 (5)
C10—C9—C16—C17	179.2 (3)	C55—C56—C57—C58	177.8 (3)
C9—C16—C17—N1	−2.8 (5)	C56—C57—C58—C59	27.8 (5)
C9—C16—C17—C18	177.1 (3)	C64—C57—C58—C59	−153.5 (3)
N1—C17—C18—C19	156.6 (3)	C56—C57—C58—C63	−151.9 (3)
C16—C17—C18—C19	−23.3 (5)	C64—C57—C58—C63	26.8 (5)
N1—C17—C18—C23	−22.5 (5)	C63—C58—C59—C60	−0.8 (5)
C16—C17—C18—C23	157.6 (3)	C57—C58—C59—C60	179.6 (3)
C23—C18—C19—C20	−1.3 (5)	C58—C59—C60—C61	0.4 (5)
C17—C18—C19—C20	179.6 (3)	C59—C60—C61—C62	−0.2 (5)
C18—C19—C20—C21	0.3 (6)	C59—C60—C61—C72	178.9 (4)
C19—C20—C21—C22	1.0 (6)	C60—C61—C62—C63	0.3 (6)
C20—C21—C22—C23	−1.3 (6)	C72—C61—C62—C63	−178.8 (4)
C21—C22—C23—C18	0.3 (6)	C61—C62—C63—C58	−0.7 (6)
C19—C18—C23—C22	1.1 (5)	C59—C58—C63—C62	0.9 (5)
C17—C18—C23—C22	−179.9 (3)	C57—C58—C63—C62	−179.4 (3)
C12—C13—C24—N2	−82.9 (5)	C56—C57—C64—C65	1.0 (5)
C14—C13—C24—N2	97.3 (4)	C58—C57—C64—C65	−177.7 (3)
C30—C25—C26—C27	0.6 (7)	C57—C64—C65—N9	0.4 (5)
C25—C26—C27—C28	−1.0 (6)	C57—C64—C65—C66	−179.0 (3)
C26—C27—C28—C29	0.8 (7)	N9—C65—C66—C71	21.7 (5)
C27—C28—C29—C30	0.0 (7)	C64—C65—C66—C71	−158.8 (4)
C28—C29—C30—C25	−0.4 (6)	N9—C65—C66—C67	−157.6 (3)

C28—C29—C30—C31	−179.0 (4)	C64—C65—C66—C67	21.9 (5)
C26—C25—C30—C29	0.1 (6)	C71—C66—C67—C68	−1.1 (5)
C26—C25—C30—C31	178.7 (4)	C65—C66—C67—C68	178.3 (3)
C29—C30—C31—N5	−176.4 (3)	C66—C67—C68—C69	1.0 (6)
C25—C30—C31—N5	5.1 (5)	C67—C68—C69—C70	−0.1 (6)
C29—C30—C31—C32	4.5 (5)	C68—C69—C70—C71	−0.7 (7)
C25—C30—C31—C32	−174.0 (4)	C69—C70—C71—C66	0.6 (6)
N5—C31—C32—C33	−1.8 (5)	C67—C66—C71—C70	0.3 (6)
C30—C31—C32—C33	177.2 (3)	C65—C66—C71—C70	−179.1 (3)
C31—C32—C33—C40	−0.1 (5)	C60—C61—C72—N10	−88.1 (5)
C31—C32—C33—C34	−179.8 (3)	C62—C61—C72—N10	91.0 (5)
C40—C33—C34—C39	24.7 (5)	C16—C17—N1—C7	2.2 (5)
C32—C33—C34—C39	−155.7 (3)	C18—C17—N1—C7	−177.8 (3)
C40—C33—C34—C35	−157.2 (3)	C8—C7—N1—C17	0.6 (5)
C32—C33—C34—C35	22.5 (5)	C6—C7—N1—C17	−177.7 (3)
C39—C34—C35—C36	−0.8 (5)	C13—C24—N2—N3	47.0 (5)
C33—C34—C35—C36	−179.1 (3)	C32—C31—N5—C41	2.0 (5)
C34—C35—C36—C37	0.2 (5)	C30—C31—N5—C41	−177.1 (3)
C35—C36—C37—C38	1.0 (5)	C40—C41—N5—C31	−0.3 (5)
C35—C36—C37—C48	−175.7 (3)	C42—C41—N5—C31	179.1 (3)
C36—C37—C38—C39	−1.7 (5)	C37—C48—N6—N7	65.5 (4)
C48—C37—C38—C39	175.0 (3)	C64—C65—N9—C55	−2.0 (5)
C37—C38—C39—C34	1.1 (5)	C66—C65—N9—C55	177.5 (3)
C35—C34—C39—C38	0.1 (5)	C56—C55—N9—C65	2.1 (5)
C33—C34—C39—C38	178.4 (3)	C54—C55—N9—C65	−177.4 (3)
C32—C33—C40—C41	1.7 (5)	C61—C72—N10—N11	57.3 (5)
C34—C33—C40—C41	−178.6 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*4, *Cg*7, *Cg*8 and *Cg*11 are the centroids of the C18–C23, C34–C39, C42–C47 and C58–C63 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···*Cg*8^{i}	0.93	2.92	3.601 (4)	132
C21—H21···*Cg*7^{ii}	0.93	2.78	3.668 (4)	161
C24—H24*B*···*Cg*11^{iii}	0.93	2.84	3.443 (5)	121
C36—H36···*Cg*4	0.93	2.82	3.601 (4)	142

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