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(*E*)-*N*-(1*H*-Pyrrol-2-ylmethylidene)-2-{[(*E*)-(1*H*-pyrrol-2-ylmethylidene)amino]methyl}aniline

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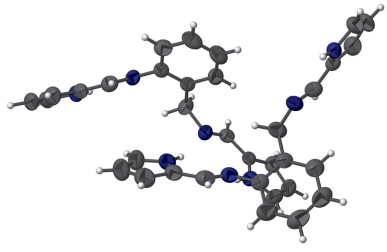
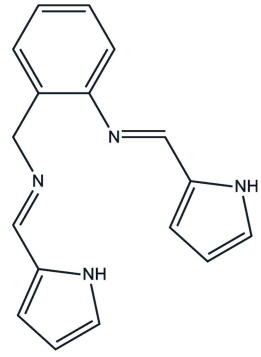
Structural data: full structural data are available from iucrdata.iucr.org

The title salophene-type compound, $C_{17}H_{16}N_4$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. Both (pyrrol-2-yl)methanimine groups have an extended conformation, and an *E* conformation about the C=N bonds. The pyrrole rings are inclined to the aminobenzylamine ring by 43.7 (3) and 78.9 (2)° in molecule *A*, and by 46.8 (3) and 79.3 (3)° in molecule *B*, while the pyrrole rings are inclined to one another by 58.9 (3) and 59.9 (3)° in molecules *A* and *B*, respectively. In the crystal, molecules are linked by N—H···N hydrogen bonds, forming chains propagating along the *a*-axis direction. The chains are linked by C—H···π interactions, forming a three-dimensional supramolecular structure.

3D view



Chemical scheme



Structure description

The title compound was synthesized using Schiff base reactions, which play an important role in coordination chemistry (Ben Guzzi & El Alagi, 2013). Schiff bases have been found to exhibit biological activities such as antimicrobial, antibacterial, antifungal, anti-inflammatory, anti-convulsant, antitumor and anti HIV activities (Liu *et al.* 2007; Arulmurugan *et al.* 2010). Salophene [*N*,*N*′-bis(salicylidene)-1,2-phenylenediamine] ligands are symmetrical and derived from aromatic 1,2–diamino benzene derivatives. They have received great attention due to their synthetic flexibility, rich coordination chemistry and applications in catalysis. Against this background we have synthesized an asymmetric salophene-type compound and report herein on its crystal structure.

The molecular structure of the title compound is shown in Fig. 1. There are two crystallographically independent molecules (*A* and *B*) in the asymmetric unit. The

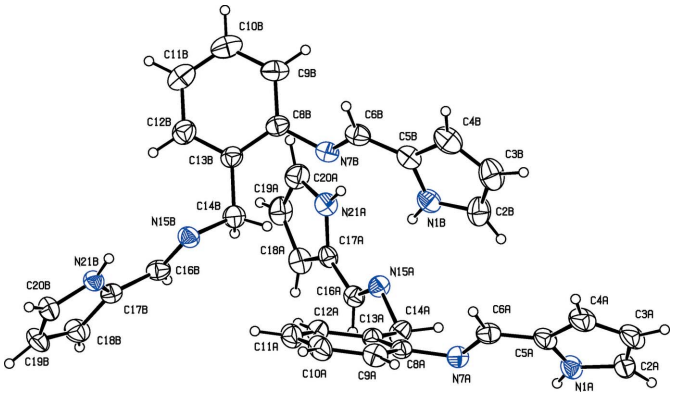


Figure 1
The molecular structure of one of the two independent molecules of the title compound, showing the atomic numbering and displacement ellipsoids drawn at 30% probability level.

pyrrole rings (N1/C2–C5 and N21/C17–C20) are inclined to the aminobenzylamine ring (C8–C13) by 43.7 (3) and 78.9 (2)° in molecule *A*, and by 46.8 (3) and 79.3 (3)° in molecule *B*, while the pyrrole rings are inclined to one another by 58.9 (3) and 59.9 (3)° in molecules *A* and *B*, respectively. The sum of the bond angles at atoms N1 and N21 of the pyrrole rings are

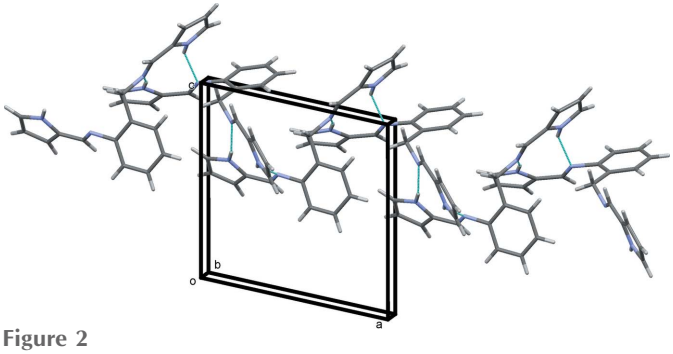


Figure 2
The partial view of the crystal packing of title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines (see Table 1).

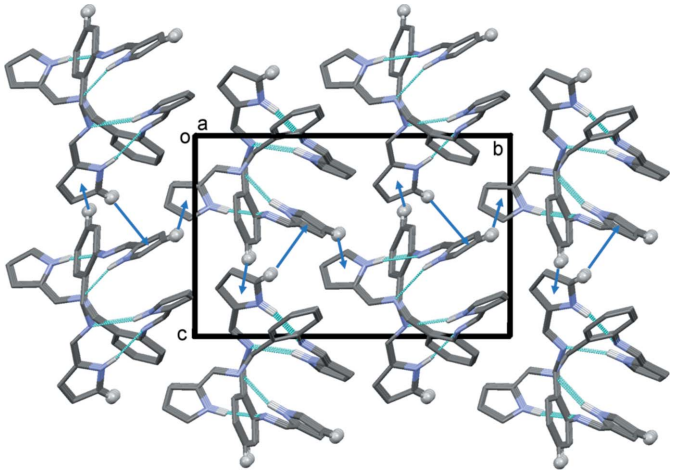


Figure 3
The crystal packing of title compound viewed along the *a* axis. H atoms not involved in hydrogen bonding (dashed lines) and C—H···π interactions (blue arrows) have been omitted for clarity.

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

*Cg*1, *Cg*2 and *Cg*5 are the centroids of rings N1*A*/C2*A*–C5*A*, N21*A*/C17*A*–C20*A* and N21*B*/C17*B*–C20*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···N15*B*^{i}	0.86	2.17	2.990 (5)	160
N1*B*—H1*B*···N15*A*	0.86	2.20	3.028 (5)	162
N21*A*—H21*A*···N7*B*	0.86	2.23	2.984 (5)	146
N21*B*—H21*B*···N7*A*^{ii}	0.86	2.15	2.909 (5)	148
C3*A*—H3*A*···*Cg*5^{iii}	0.93	2.69	3.465 (6)	142
C10*A*—H10*A*···*Cg*2^{iv}	0.93	2.82	3.654 (6)	151
C20*A*—H20*A*···*Cg*1^{v}	0.93	2.97	3.643 (5)	131

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{16}N_4$
M_r	276.34
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	296
a, *b*, *c* (Å)	9.968 (4), 15.529 (6), 10.119 (4)
β (°)	102.558 (9)
V (Å^3)	1528.9 (11)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.25 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker SMART APEXII area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.982, 0.985
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18751, 5057, 3322
R_{int}	0.055
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.583
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.043, 0.092, 0.99
No. of reflections	5057
No. of parameters	380
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.14

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

360.0 and 359.9° in molecule *A*, and 360.1 and 360.0° in molecule *B*, typical for sp^2-hybridized states.

In the crystal, molecules are linked by N—H···N hydrogen bonds, forming chains propagating along the *a*-axis direction (Table 1 and Fig. 2). The chains are linked by C—H···π interactions, forming a three-dimensional supramolecular structure (Table 1 and Fig. 3).

Synthesis and crystallization

To a stirred solution of 2-pyrrolecarboxaldehyde 0.950 g (10 mmol) in 20 ml of ethanol, in a round-bottom flask, was

added 0.610 g (5 mmol) of 2-amino-benzylamine. The mixture was refluxed for 3 h to give a yellow solution. The final reaction mixture was filtered and the filtrate kept in a refrigerator for 12 h. The resulting yellow block-like crystals were filtered off, washed with cold ethanol and dried under vacuum.

Refinement

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

Acknowledgements

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full crystallographic data

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(I)

Crystal data

$C_{17}H_{16}N_4$
M_r = 276.34
Monoclinic, $P2_1$
a = 9.968 (4) Å
b = 15.529 (6) Å
c = 10.119 (4) Å
β = 102.558 (9)°
V = 1528.9 (11) Å^3
Z = 4
$F(000)$ = 584
D_x = 1.201 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3322 reflections
θ = 2.4–24.5°
μ = 0.07 mm^{-1}
T = 296 K
Block, yellow
0.25 × 0.25 × 0.20 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.982, T_{max} = 0.985
18751 measured reflections
5057 independent reflections
3322 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 24.5°, θ_{min} = 2.4°
h = −11→11
k = −18→18
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.092
S = 0.99
5057 reflections
380 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
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0068 (13)

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}
C2A	0.0016 (5)	0.8295 (3)	0.5903 (5)	0.0715 (15)
H2A	−0.0764	0.8156	0.6224	0.086*
C3A	0.0174 (6)	0.9004 (3)	0.5175 (6)	0.0770 (16)
H3A	−0.0471	0.9437	0.4910	0.092*
C4A	0.1469 (5)	0.8965 (3)	0.4897 (5)	0.0717 (14)
H4A	0.1852	0.9369	0.4409	0.086*
C5A	0.2088 (5)	0.8228 (3)	0.5469 (4)	0.0525 (11)
C6A	0.3409 (4)	0.7887 (3)	0.5445 (4)	0.0529 (11)
H6A	0.3999	0.8216	0.5053	0.064*
C8A	0.5163 (4)	0.6869 (2)	0.5839 (4)	0.0439 (10)
C9A	0.5588 (4)	0.6895 (3)	0.4629 (5)	0.0575 (12)
H9A	0.5002	0.7107	0.3854	0.069*
C10A	0.6891 (5)	0.6603 (3)	0.4569 (5)	0.0650 (13)
H10A	0.7183	0.6632	0.3758	0.078*
C11A	0.7745 (5)	0.6275 (3)	0.5696 (6)	0.0635 (13)
H11A	0.8618	0.6081	0.5656	0.076*
C12A	0.7303 (4)	0.6232 (3)	0.6895 (5)	0.0553 (12)
H12A	0.7884	0.6002	0.7658	0.066*
C13A	0.6013 (4)	0.6524 (2)	0.6991 (4)	0.0432 (10)
C14A	0.5551 (4)	0.6468 (3)	0.8314 (4)	0.0541 (12)
H14A	0.4763	0.6841	0.8278	0.065*
H14B	0.5272	0.5883	0.8452	0.065*
C16A	0.7137 (4)	0.6145 (3)	1.0305 (4)	0.0464 (10)
H16A	0.6722	0.5605	1.0208	0.056*
C17A	0.8277 (4)	0.6277 (3)	1.1407 (4)	0.0441 (10)
C18A	0.8902 (4)	0.5727 (3)	1.2417 (4)	0.0572 (12)
H18A	0.8627	0.5166	1.2538	0.069*
C19A	1.0010 (5)	0.6147 (3)	1.3225 (5)	0.0664 (13)
H19A	1.0614	0.5922	1.3977	0.080*
C20A	1.0042 (4)	0.6951 (3)	1.2705 (5)	0.0647 (13)
H20A	1.0679	0.7377	1.3045	0.078*
N1A	0.1186 (3)	0.7820 (2)	0.6087 (4)	0.0561 (10)
H1A	0.1332	0.7342	0.6523	0.067*
N7A	0.3822 (3)	0.7153 (2)	0.5935 (3)	0.0464 (9)
N15A	0.6657 (3)	0.6724 (2)	0.9444 (4)	0.0477 (9)
N21A	0.8989 (3)	0.7029 (2)	1.1607 (3)	0.0522 (9)
H21A	0.8801	0.7483	1.1116	0.063*
C2B	0.5320 (5)	0.8966 (3)	0.8313 (5)	0.0734 (15)
H2B	0.4489	0.8697	0.8322	0.088*

C3B	0.5475 (6)	0.9768 (4)	0.7837 (5)	0.0830 (16)
H3B	0.4772	1.0146	0.7461	0.100*
C4B	0.6876 (6)	0.9924 (3)	0.8013 (5)	0.0773 (15)
H4B	0.7279	1.0425	0.7779	0.093*
C5B	0.7559 (5)	0.9202 (3)	0.8597 (4)	0.0556 (12)
C6B	0.9002 (5)	0.9050 (3)	0.9028 (5)	0.0567 (12)
H6B	0.9605	0.9462	0.8829	0.068*
C8B	1.0951 (4)	0.8292 (3)	1.0099 (4)	0.0504 (11)
C9B	1.1750 (5)	0.8937 (3)	1.0846 (5)	0.0701 (14)
H9B	1.1342	0.9450	1.1024	0.084*
C10B	1.3143 (5)	0.8815 (4)	1.1321 (5)	0.0786 (15)
H10B	1.3671	0.9244	1.1828	0.094*
C11B	1.3744 (5)	0.8068 (4)	1.1049 (5)	0.0731 (15)
H11B	1.4685	0.7990	1.1356	0.088*
C12B	1.2953 (4)	0.7420 (3)	1.0313 (4)	0.0626 (13)
H12B	1.3372	0.6910	1.0138	0.075*
C13B	1.1560 (4)	0.7521 (3)	0.9838 (4)	0.0496 (11)
C14B	1.0713 (4)	0.6807 (3)	0.9077 (5)	0.0609 (13)
H14C	1.0533	0.6379	0.9715	0.073*
H14D	0.9837	0.7036	0.8597	0.073*
C16B	1.1674 (4)	0.5599 (3)	0.8283 (4)	0.0509 (11)
H16B	1.1401	0.5323	0.8997	0.061*
C17B	1.2371 (4)	0.5098 (3)	0.7451 (4)	0.0438 (10)
C18B	1.2663 (5)	0.4240 (3)	0.7486 (5)	0.0645 (13)
H18B	1.2441	0.3841	0.8089	0.077*
C19B	1.3351 (5)	0.4067 (3)	0.6462 (6)	0.0709 (15)
H19B	1.3678	0.3533	0.6260	0.085*
C20B	1.3460 (4)	0.4812 (3)	0.5813 (5)	0.0625 (13)
H20B	1.3878	0.4883	0.5083	0.075*
N1B	0.6582 (4)	0.8626 (2)	0.8772 (4)	0.0571 (10)
H1B	0.6745	0.8121	0.9122	0.068*
N7B	0.9502 (3)	0.8376 (2)	0.9672 (4)	0.0515 (9)
N15B	1.1404 (3)	0.6396 (2)	0.8111 (3)	0.0501 (9)
N21B	1.2854 (3)	0.5437 (2)	0.6407 (3)	0.0467 (8)
H21B	1.2786	0.5969	0.6163	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2A	0.057 (3)	0.067 (4)	0.085 (4)	0.014 (3)	0.002 (3)	−0.021 (3)
C3A	0.083 (4)	0.046 (3)	0.086 (4)	0.024 (3)	−0.015 (3)	−0.007 (3)
C4A	0.083 (4)	0.044 (3)	0.078 (4)	0.007 (3)	−0.005 (3)	0.007 (3)
C5A	0.064 (3)	0.038 (3)	0.051 (3)	0.007 (2)	0.001 (2)	0.003 (2)
C6A	0.061 (3)	0.045 (3)	0.051 (3)	−0.007 (2)	0.009 (2)	0.006 (2)
C8A	0.047 (2)	0.036 (2)	0.049 (3)	−0.005 (2)	0.012 (2)	0.002 (2)
C9A	0.070 (3)	0.055 (3)	0.050 (3)	−0.004 (2)	0.018 (2)	0.003 (2)
C10A	0.078 (3)	0.058 (3)	0.071 (4)	−0.002 (3)	0.043 (3)	−0.005 (3)
C11A	0.062 (3)	0.054 (3)	0.082 (4)	0.001 (2)	0.033 (3)	−0.003 (3)

C12A	0.048 (3)	0.055 (3)	0.062 (3)	0.000 (2)	0.009 (2)	−0.001 (2)
C13A	0.045 (2)	0.039 (2)	0.047 (3)	−0.0040 (19)	0.012 (2)	−0.001 (2)
C14A	0.046 (2)	0.067 (3)	0.047 (3)	−0.003 (2)	0.006 (2)	0.004 (2)
C16A	0.052 (2)	0.047 (3)	0.043 (3)	0.000 (2)	0.018 (2)	−0.001 (2)
C17A	0.049 (2)	0.047 (3)	0.037 (3)	0.008 (2)	0.011 (2)	−0.002 (2)
C18A	0.065 (3)	0.060 (3)	0.047 (3)	0.010 (2)	0.014 (2)	0.011 (3)
C19A	0.064 (3)	0.083 (4)	0.049 (3)	0.016 (3)	0.004 (2)	0.008 (3)
C20A	0.059 (3)	0.083 (4)	0.049 (3)	0.000 (3)	0.005 (3)	−0.009 (3)
N1A	0.059 (2)	0.049 (2)	0.057 (3)	0.011 (2)	0.0046 (19)	0.0025 (19)
N7A	0.050 (2)	0.045 (2)	0.042 (2)	0.0020 (16)	0.0056 (16)	0.0066 (17)
N15A	0.0473 (19)	0.050 (2)	0.044 (2)	0.0010 (17)	0.0059 (17)	0.0038 (19)
N21A	0.058 (2)	0.055 (2)	0.041 (2)	0.0046 (19)	0.0060 (18)	0.0022 (19)
C2B	0.066 (3)	0.083 (4)	0.069 (4)	0.017 (3)	0.011 (3)	0.008 (3)
C3B	0.091 (4)	0.081 (4)	0.075 (4)	0.030 (3)	0.012 (3)	0.017 (3)
C4B	0.103 (4)	0.058 (4)	0.071 (4)	0.008 (3)	0.020 (3)	0.009 (3)
C5B	0.072 (3)	0.049 (3)	0.046 (3)	0.003 (3)	0.015 (2)	0.003 (2)
C6B	0.072 (3)	0.052 (3)	0.049 (3)	−0.008 (3)	0.020 (2)	−0.004 (2)
C8B	0.052 (3)	0.052 (3)	0.048 (3)	−0.010 (2)	0.013 (2)	0.002 (2)
C9B	0.075 (3)	0.055 (3)	0.076 (4)	−0.017 (3)	0.009 (3)	−0.007 (3)
C10B	0.078 (4)	0.083 (4)	0.067 (4)	−0.026 (3)	−0.001 (3)	−0.001 (3)
C11B	0.058 (3)	0.096 (4)	0.064 (4)	−0.016 (3)	0.008 (3)	0.003 (3)
C12B	0.057 (3)	0.074 (4)	0.060 (3)	−0.004 (3)	0.018 (2)	−0.004 (3)
C13B	0.048 (3)	0.056 (3)	0.048 (3)	−0.008 (2)	0.017 (2)	−0.004 (2)
C14B	0.056 (3)	0.064 (3)	0.068 (3)	−0.007 (2)	0.025 (2)	−0.015 (3)
C16B	0.056 (3)	0.051 (3)	0.047 (3)	−0.012 (2)	0.014 (2)	0.000 (2)
C17B	0.045 (2)	0.044 (3)	0.041 (3)	−0.004 (2)	0.005 (2)	0.003 (2)
C18B	0.073 (3)	0.044 (3)	0.073 (4)	0.000 (2)	0.010 (3)	0.011 (3)
C19B	0.074 (3)	0.042 (3)	0.093 (4)	0.016 (2)	0.009 (3)	−0.011 (3)
C20B	0.058 (3)	0.060 (3)	0.071 (3)	0.009 (3)	0.016 (2)	−0.013 (3)
N1B	0.070 (2)	0.048 (2)	0.053 (3)	0.006 (2)	0.012 (2)	0.0033 (19)
N7B	0.059 (2)	0.044 (2)	0.051 (2)	−0.0041 (18)	0.0122 (18)	−0.0031 (19)
N15B	0.055 (2)	0.048 (2)	0.051 (2)	−0.0017 (18)	0.0180 (17)	−0.0071 (19)
N21B	0.0483 (19)	0.040 (2)	0.050 (2)	0.0032 (17)	0.0059 (17)	0.0003 (18)

Geometric parameters (Å, º)

C2A—C3A	1.353 (6)	C2B—N1B	1.351 (5)
C2A—N1A	1.358 (5)	C2B—C3B	1.357 (7)
C2A—H2A	0.9300	C2B—H2B	0.9300
C3A—C4A	1.380 (7)	C3B—C4B	1.389 (7)
C3A—H3A	0.9300	C3B—H3B	0.9300
C4A—C5A	1.368 (5)	C4B—C5B	1.376 (6)
C4A—H4A	0.9300	C4B—H4B	0.9300
C5A—N1A	1.358 (5)	C5B—N1B	1.362 (5)
C5A—C6A	1.424 (6)	C5B—C6B	1.429 (6)
C6A—N7A	1.276 (5)	C6B—N7B	1.276 (5)
C6A—H6A	0.9300	C6B—H6B	0.9300
C8A—C9A	1.380 (5)	C8B—C13B	1.393 (5)

C8A—C13A	1.390 (5)	C8B—C9B	1.395 (5)
C8A—N7A	1.431 (4)	C8B—N7B	1.421 (5)
C9A—C10A	1.389 (6)	C9B—C10B	1.380 (6)
C9A—H9A	0.9300	C9B—H9B	0.9300
C10A—C11A	1.365 (6)	C10B—C11B	1.362 (7)
C10A—H10A	0.9300	C10B—H10B	0.9300
C11A—C12A	1.380 (6)	C11B—C12B	1.390 (6)
C11A—H11A	0.9300	C11B—H11B	0.9300
C12A—C13A	1.387 (5)	C12B—C13B	1.377 (5)
C12A—H12A	0.9300	C12B—H12B	0.9300
C13A—C14A	1.509 (5)	C13B—C14B	1.501 (5)
C14A—N15A	1.461 (5)	C14B—N15B	1.459 (5)
C14A—H14A	0.9700	C14B—H14C	0.9700
C14A—H14B	0.9700	C14B—H14D	0.9700
C16A—N15A	1.272 (4)	C16B—N15B	1.270 (5)
C16A—C17A	1.423 (5)	C16B—C17B	1.433 (6)
C16A—H16A	0.9300	C16B—H16B	0.9300
C17A—N21A	1.359 (5)	C17B—N21B	1.359 (5)
C17A—C18A	1.372 (5)	C17B—C18B	1.362 (5)
C18A—C19A	1.386 (6)	C18B—C19B	1.387 (6)
C18A—H18A	0.9300	C18B—H18B	0.9300
C19A—C20A	1.357 (6)	C19B—C20B	1.346 (6)
C19A—H19A	0.9300	C19B—H19B	0.9300
C20A—N21A	1.358 (5)	C20B—N21B	1.352 (5)
C20A—H20A	0.9300	C20B—H20B	0.9300
N1A—H1A	0.8600	N1B—H1B	0.8600
N21A—H21A	0.8600	N21B—H21B	0.8600

C3A—C2A—N1A	108.5 (4)	N1B—C2B—C3B	108.2 (5)
C3A—C2A—H2A	125.7	N1B—C2B—H2B	125.9
N1A—C2A—H2A	125.7	C3B—C2B—H2B	125.9
C2A—C3A—C4A	107.5 (4)	C2B—C3B—C4B	107.6 (5)
C2A—C3A—H3A	126.2	C2B—C3B—H3B	126.2
C4A—C3A—H3A	126.2	C4B—C3B—H3B	126.2
C5A—C4A—C3A	107.8 (5)	C5B—C4B—C3B	107.7 (5)
C5A—C4A—H4A	126.1	C5B—C4B—H4B	126.2
C3A—C4A—H4A	126.1	C3B—C4B—H4B	126.2
N1A—C5A—C4A	107.5 (4)	N1B—C5B—C4B	106.9 (4)
N1A—C5A—C6A	122.8 (4)	N1B—C5B—C6B	123.5 (4)
C4A—C5A—C6A	129.6 (5)	C4B—C5B—C6B	129.6 (5)
N7A—C6A—C5A	123.2 (4)	N7B—C6B—C5B	123.2 (4)
N7A—C6A—H6A	118.4	N7B—C6B—H6B	118.4
C5A—C6A—H6A	118.4	C5B—C6B—H6B	118.4
C9A—C8A—C13A	120.5 (4)	C13B—C8B—C9B	119.9 (4)
C9A—C8A—N7A	121.5 (4)	C13B—C8B—N7B	118.5 (4)
C13A—C8A—N7A	118.0 (4)	C9B—C8B—N7B	121.4 (4)
C8A—C9A—C10A	119.9 (4)	C10B—C9B—C8B	120.2 (5)
C8A—C9A—H9A	120.0	C10B—C9B—H9B	119.9

C10A—C9A—H9A	120.0	C8B—C9B—H9B	119.9
C11A—C10A—C9A	120.3 (4)	C11B—C10B—C9B	120.0 (5)
C11A—C10A—H10A	119.9	C11B—C10B—H10B	120.0
C9A—C10A—H10A	119.9	C9B—C10B—H10B	120.0
C10A—C11A—C12A	119.5 (4)	C10B—C11B—C12B	120.1 (4)
C10A—C11A—H11A	120.2	C10B—C11B—H11B	119.9
C12A—C11A—H11A	120.2	C12B—C11B—H11B	119.9
C11A—C12A—C13A	121.6 (4)	C13B—C12B—C11B	121.1 (4)
C11A—C12A—H12A	119.2	C13B—C12B—H12B	119.5
C13A—C12A—H12A	119.2	C11B—C12B—H12B	119.5
C12A—C13A—C8A	118.2 (4)	C12B—C13B—C8B	118.7 (4)
C12A—C13A—C14A	120.6 (4)	C12B—C13B—C14B	120.4 (4)
C8A—C13A—C14A	121.2 (3)	C8B—C13B—C14B	120.9 (3)
N15A—C14A—C13A	110.8 (3)	N15B—C14B—C13B	111.8 (3)
N15A—C14A—H14A	109.5	N15B—C14B—H14C	109.3
C13A—C14A—H14A	109.5	C13B—C14B—H14C	109.3
N15A—C14A—H14B	109.5	N15B—C14B—H14D	109.3
C13A—C14A—H14B	109.5	C13B—C14B—H14D	109.3
H14A—C14A—H14B	108.1	H14C—C14B—H14D	107.9
N15A—C16A—C17A	123.5 (4)	N15B—C16B—C17B	124.4 (4)
N15A—C16A—H16A	118.2	N15B—C16B—H16B	117.8
C17A—C16A—H16A	118.2	C17B—C16B—H16B	117.8
N21A—C17A—C18A	106.6 (4)	N21B—C17B—C18B	106.8 (4)
N21A—C17A—C16A	122.8 (4)	N21B—C17B—C16B	123.0 (4)
C18A—C17A—C16A	130.5 (4)	C18B—C17B—C16B	130.2 (5)
C17A—C18A—C19A	108.7 (4)	C17B—C18B—C19B	107.9 (4)
C17A—C18A—H18A	125.6	C17B—C18B—H18B	126.0
C19A—C18A—H18A	125.6	C19B—C18B—H18B	126.0
C20A—C19A—C18A	106.7 (4)	C20B—C19B—C18B	107.7 (4)
C20A—C19A—H19A	126.7	C20B—C19B—H19B	126.2
C18A—C19A—H19A	126.7	C18B—C19B—H19B	126.2
C19A—C20A—N21A	108.7 (4)	C19B—C20B—N21B	108.0 (4)
C19A—C20A—H20A	125.7	C19B—C20B—H20B	126.0
N21A—C20A—H20A	125.7	N21B—C20B—H20B	126.0
C2A—N1A—C5A	108.6 (4)	C2B—N1B—C5B	109.7 (4)
C2A—N1A—H1A	125.7	C2B—N1B—H1B	125.2
C5A—N1A—H1A	125.7	C5B—N1B—H1B	125.2
C6A—N7A—C8A	118.4 (3)	C6B—N7B—C8B	119.3 (4)
C16A—N15A—C14A	116.8 (3)	C16B—N15B—C14B	116.8 (4)
C20A—N21A—C17A	109.3 (4)	C20B—N21B—C17B	109.6 (4)
C20A—N21A—H21A	125.3	C20B—N21B—H21B	125.2
C17A—N21A—H21A	125.3	C17B—N21B—H21B	125.2
N1A—C2A—C3A—C4A	0.2 (6)	N1B—C2B—C3B—C4B	−0.1 (6)
C2A—C3A—C4A—C5A	−0.1 (6)	C2B—C3B—C4B—C5B	0.2 (6)
C3A—C4A—C5A—N1A	0.0 (5)	C3B—C4B—C5B—N1B	−0.2 (5)
C3A—C4A—C5A—C6A	178.5 (4)	C3B—C4B—C5B—C6B	−177.3 (5)
N1A—C5A—C6A—N7A	4.0 (7)	N1B—C5B—C6B—N7B	−3.4 (7)

C4A—C5A—C6A—N7A	−174.4 (4)	C4B—C5B—C6B—N7B	173.3 (5)
C13A—C8A—C9A—C10A	−2.3 (6)	C13B—C8B—C9B—C10B	0.4 (7)
N7A—C8A—C9A—C10A	−179.2 (3)	N7B—C8B—C9B—C10B	175.8 (4)
C8A—C9A—C10A—C11A	1.3 (6)	C8B—C9B—C10B—C11B	0.7 (7)
C9A—C10A—C11A—C12A	0.1 (7)	C9B—C10B—C11B—C12B	−1.1 (8)
C10A—C11A—C12A—C13A	−0.7 (6)	C10B—C11B—C12B—C13B	0.5 (7)
C11A—C12A—C13A—C8A	−0.2 (6)	C11B—C12B—C13B—C8B	0.5 (6)
C11A—C12A—C13A—C14A	179.8 (4)	C11B—C12B—C13B—C14B	−178.3 (4)
C9A—C8A—C13A—C12A	1.7 (6)	C9B—C8B—C13B—C12B	−1.0 (6)
N7A—C8A—C13A—C12A	178.7 (3)	N7B—C8B—C13B—C12B	−176.6 (4)
C9A—C8A—C13A—C14A	−178.3 (4)	C9B—C8B—C13B—C14B	177.9 (4)
N7A—C8A—C13A—C14A	−1.3 (5)	N7B—C8B—C13B—C14B	2.3 (6)
C12A—C13A—C14A—N15A	42.8 (5)	C12B—C13B—C14B—N15B	−42.3 (6)
C8A—C13A—C14A—N15A	−137.2 (4)	C8B—C13B—C14B—N15B	138.9 (4)
N15A—C16A—C17A—N21A	−2.6 (6)	N15B—C16B—C17B—N21B	2.1 (6)
N15A—C16A—C17A—C18A	179.3 (4)	N15B—C16B—C17B—C18B	−176.5 (4)
N21A—C17A—C18A—C19A	−0.7 (5)	N21B—C17B—C18B—C19B	1.0 (5)
C16A—C17A—C18A—C19A	177.6 (4)	C16B—C17B—C18B—C19B	179.8 (4)
C17A—C18A—C19A—C20A	0.5 (5)	C17B—C18B—C19B—C20B	−0.5 (5)
C18A—C19A—C20A—N21A	−0.1 (5)	C18B—C19B—C20B—N21B	−0.2 (5)
C3A—C2A—N1A—C5A	−0.3 (5)	C3B—C2B—N1B—C5B	0.0 (6)
C4A—C5A—N1A—C2A	0.2 (5)	C4B—C5B—N1B—C2B	0.2 (5)
C6A—C5A—N1A—C2A	−178.5 (4)	C6B—C5B—N1B—C2B	177.5 (4)
C5A—C6A—N7A—C8A	179.1 (4)	C5B—C6B—N7B—C8B	−178.0 (4)
C9A—C8A—N7A—C6A	−49.7 (5)	C13B—C8B—N7B—C6B	−132.0 (4)
C13A—C8A—N7A—C6A	133.3 (4)	C9B—C8B—N7B—C6B	52.5 (6)
C17A—C16A—N15A—C14A	175.5 (3)	C17B—C16B—N15B—C14B	−178.7 (3)
C13A—C14A—N15A—C16A	−114.5 (4)	C13B—C14B—N15B—C16B	119.1 (4)
C19A—C20A—N21A—C17A	−0.3 (5)	C19B—C20B—N21B—C17B	0.8 (5)
C18A—C17A—N21A—C20A	0.6 (4)	C18B—C17B—N21B—C20B	−1.1 (4)
C16A—C17A—N21A—C20A	−177.8 (3)	C16B—C17B—N21B—C20B	−180.0 (4)

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg5 are the centroids of rings N1*A*/C2*A*–C5*A*, N21*A*/C17*A*–C20*A* and N21*B*/C17*B*–C20*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···N15*B*^{i}	0.86	2.17	2.990 (5)	160
N1*B*—H1*B*···N15*A*	0.86	2.20	3.028 (5)	162
N21*A*—H21*A*···N7*B*	0.86	2.23	2.984 (5)	146
N21*B*—H21*B*···N7*A*^{ii}	0.86	2.15	2.909 (5)	148
C3*A*—H3*A*···*Cg*5^{iii}	0.93	2.69	3.465 (6)	142
C10*A*—H10*A*···*Cg*2^{iv}	0.93	2.82	3.654 (6)	151
C20*A*—H20*A*···*Cg*1^{v}	0.93	2.97	3.643 (5)	131

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