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Tris[2-(pyrrol-2-ylmethyleneamino)-ethyl]amine

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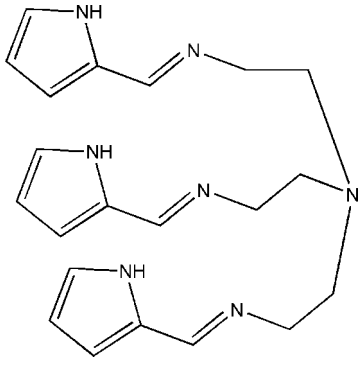
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.049; wR factor = 0.142; data-to-parameter ratio = 19.1.

The title compound, $C_{21}H_{27}N_7$, was synthesized by reaction of tris(2-aminoethyl)amine and pyrrole-2-carbaldehyde in ethanol at room temperature. The structure is stabilized by intra- and intermolecular C—H···N and N—H···N hydrogen-bonding interactions.

Related literature

For the self-assembly of pyrrole Schiff base–metal complexes, see: Wu *et al.* (2003, 2006); Yang, Chen *et al.* (2004); Yang, Shan *et al.* (2004).



Experimental

Crystal data

$C_{21}H_{27}N_7$
M_r = 377.50
Monoclinic, $P2_1/n$
a = 11.494 (2) Å
b = 9.4875 (19) Å
c = 20.232 (4) Å
β = 105.97 (3)°
V = 2121.1 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.80 × 0.08 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.943, T_{max} = 0.995
19300 measured reflections
4832 independent reflections
1905 reflections with $I > 2\sigma(I)$
R_{int} = 0.0685

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.142
S = 1.01
4832 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15B···N2	0.97	2.59	3.246 (4)	125
N3—H3A···N6^{i}	0.86	2.14	2.956 (3)	159
N5—H5A···N4^{ii}	0.86	2.20	3.029 (3)	163
N7—H7A···N2^{i}	0.86	2.13	2.940 (3)	158

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x, -y, -z$.

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1994); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2179).

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Tris[2-(pyrrol-2-ylmethyleneamino)ethyl]amine

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S1. Comment

The chemistry and crystal structure of Schiff base derivatives of pyrrole have been extensively studied for many years as these compounds represent the basic units of porphyrins. More recently, it has been pointed out that pyrrole Schiff bases are ideal building blocks for the self-assembly of metallosupramolecules (Wu *et al.*, 2006; Wu *et al.*, 2003; Yang, Chen *et al.*, 2004; Yang, Shan *et al.*, 2004) due to the presence of many hydrogen bond donors and acceptors. In view of its potential interest in this field, the title compound was synthesized and its crystal structure is reported here.

In the title compound, bond lengths and angles are as expected, with the N2—C3, N4—C10 and N6—C17 bond lengths (mean value 1.270 (3) Å) indicating a remarkable double-bond character. The molecular conformation is stabilized by an intramolecular C—H···N hydrogen bond (Table 1). In the crystal structure, the molecules are linked by intermolecular N—H···N hydrogen bonding interactions (Table 1).

S2. Experimental

The title compound was prepared by reaction of tris(2-aminoethyl)amine, (0.05 mol) and pyrrole-2-carbaldehyde (0.15 mol) in ethanol (40 ml) at room temperature. Single crystals suitable for X-ray measurements were obtained by slow evaporation of an ethanol/acetonitrile solution (1:1 *v*/*v*) at room temperature.

S3. Refinement

All H atoms were fixed geometrically and were treated as riding on the parent atoms, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and with U_{iso}(H) = 1.2 U_{eq}(C, N).

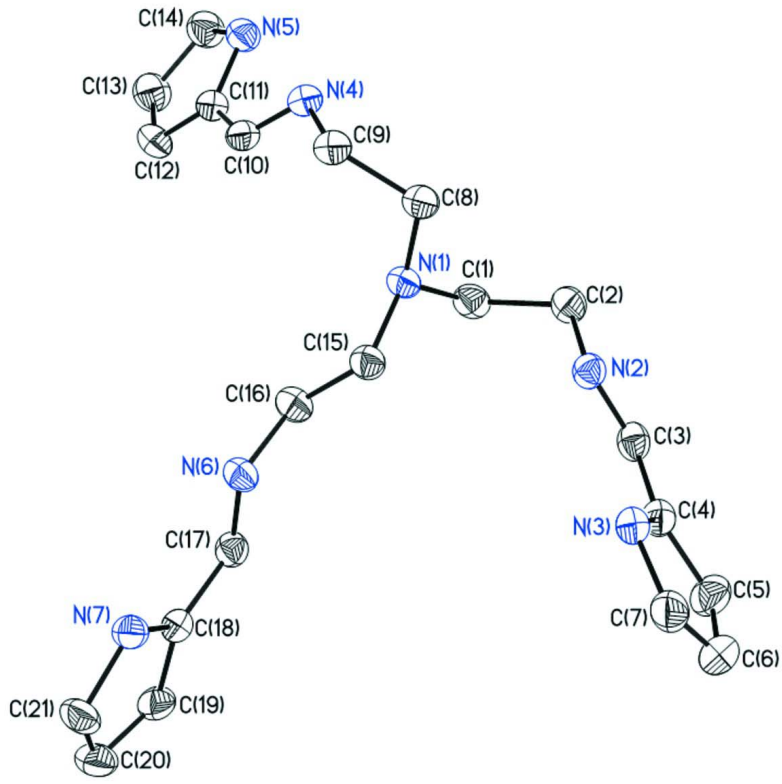

Figure 1

The molecular structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Tris[2-(pyrrol-2-ylmethyleneamino)ethyl]amine

Crystal data

$C_{21}H_{27}N_7$
$M_r = 377.50$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.494\ (2)$ Å
$b = 9.4875\ (19)$ Å
$c = 20.232\ (4)$ Å
$\beta = 105.97\ (3)°$
$V = 2121.1\ (8)$ Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.182$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 19300 reflections
$\theta = 1.9–27.5°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Needle, brown
0.80 × 0.08 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: Rotating Anode
Graphite monochromator
oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.943$, $T_{max} = 0.995$

19300 measured reflections
4832 independent reflections
1905 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -14 \rightarrow 14$
$k = 0 \rightarrow 12$
$l = -13 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.142$
$S = 1.01$
4832 reflections
253 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0318P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.32208 (19)	0.2117 (2)	−0.04712 (11)	0.0456 (6)
N2	0.3346 (2)	0.3634 (2)	−0.17842 (11)	0.0439 (6)
N3	0.47309 (19)	0.6138 (3)	−0.18248 (11)	0.0493 (7)
H3A	0.4361	0.6213	−0.1510	0.059*
N4	0.1461 (2)	0.1199 (3)	0.03356 (12)	0.0477 (6)
N5	0.1051 (2)	−0.1779 (3)	0.05915 (12)	0.0523 (7)
H5A	0.0388	−0.1426	0.0339	0.063*
N6	0.6284 (2)	0.2840 (2)	0.07191 (11)	0.0443 (6)
N7	0.8400 (2)	0.4282 (2)	0.15596 (12)	0.0453 (6)
H7A	0.7761	0.4688	0.1611	0.054*
C1	0.3214 (3)	0.1456 (3)	−0.11191 (15)	0.0520 (8)
H1A	0.2744	0.0595	−0.1159	0.062*
H1B	0.4039	0.1183	−0.1093	0.062*
C2	0.2728 (3)	0.2291 (3)	−0.17799 (14)	0.0503 (8)
H2B	0.2810	0.1726	−0.2164	0.060*
H2C	0.1873	0.2469	−0.1845	0.060*
C3	0.4025 (3)	0.3753 (3)	−0.21867 (14)	0.0470 (8)
H3B	0.4080	0.2990	−0.2465	0.056*
C4	0.4703 (3)	0.4995 (3)	−0.22330 (15)	0.0454 (7)
C5	0.5409 (3)	0.5307 (4)	−0.26616 (17)	0.0646 (10)
H5B	0.5556	0.4714	−0.2996	0.078*

C6	0.5863 (3)	0.6656 (4)	−0.25109 (18)	0.0690 (10)
H6B	0.6366	0.7136	−0.2725	0.083*
C7	0.5439 (3)	0.7142 (4)	−0.19947 (16)	0.0620 (9)
H7B	0.5604	0.8023	−0.1789	0.074*
C8	0.2084 (2)	0.2788 (3)	−0.04489 (15)	0.0553 (8)
H8A	0.1423	0.2371	−0.0799	0.066*
H8B	0.2117	0.3782	−0.0555	0.066*
C9	0.1833 (3)	0.2634 (3)	0.02435 (15)	0.0536 (8)
H9A	0.2556	0.2865	0.0606	0.064*
H9B	0.1199	0.3285	0.0274	0.064*
C10	0.2245 (3)	0.0402 (4)	0.07166 (15)	0.0513 (8)
H10A	0.2993	0.0804	0.0929	0.062*
C11	0.2099 (3)	−0.1055 (3)	0.08539 (15)	0.0483 (8)
C12	0.2924 (3)	−0.2002 (4)	0.12203 (16)	0.0643 (10)
H12A	0.3723	−0.1802	0.1455	0.077*
C13	0.2371 (3)	−0.3313 (4)	0.11832 (18)	0.0688 (10)
H13A	0.2724	−0.4144	0.1388	0.083*
C14	0.1217 (3)	−0.3143 (4)	0.07898 (17)	0.0640 (9)
H14A	0.0634	−0.3849	0.0675	0.077*
C15	0.4299 (2)	0.2945 (3)	−0.01526 (14)	0.0475 (8)
H15A	0.4098	0.3670	0.0135	0.057*
H15B	0.4583	0.3405	−0.0507	0.057*
C16	0.5290 (2)	0.2023 (3)	0.02762 (15)	0.0508 (8)
H16A	0.4952	0.1410	0.0560	0.061*
H16B	0.5606	0.1433	−0.0026	0.061*
C17	0.7349 (3)	0.2535 (3)	0.07048 (14)	0.0448 (7)
H17A	0.7445	0.1841	0.0399	0.054*
C18	0.8415 (2)	0.3190 (3)	0.11291 (13)	0.0422 (7)
C19	0.9607 (3)	0.2851 (4)	0.12042 (15)	0.0558 (9)
H19A	0.9887	0.2142	0.0970	0.067*
C20	1.0321 (3)	0.3751 (4)	0.16917 (17)	0.0640 (10)
H20A	1.1161	0.3751	0.1848	0.077*
C21	0.9557 (3)	0.4631 (4)	0.18960 (16)	0.0587 (9)
H21A	0.9787	0.5355	0.2215	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0367 (14)	0.0511 (15)	0.0462 (14)	−0.0059 (12)	0.0069 (11)	0.0022 (14)
N2	0.0470 (15)	0.0457 (15)	0.0387 (14)	−0.0016 (13)	0.0110 (11)	−0.0027 (13)
N3	0.0465 (15)	0.0601 (17)	0.0389 (14)	−0.0048 (14)	0.0076 (12)	0.0047 (15)
N4	0.0402 (14)	0.0572 (17)	0.0477 (15)	−0.0037 (13)	0.0154 (12)	0.0050 (14)
N5	0.0446 (16)	0.0555 (17)	0.0549 (16)	0.0010 (13)	0.0104 (12)	0.0092 (15)
N6	0.0392 (15)	0.0470 (14)	0.0438 (14)	−0.0015 (12)	0.0066 (11)	−0.0065 (13)
N7	0.0389 (14)	0.0478 (15)	0.0489 (15)	−0.0009 (12)	0.0118 (11)	0.0055 (14)
C1	0.0474 (18)	0.0435 (18)	0.061 (2)	−0.0076 (16)	0.0084 (15)	0.0023 (18)
C2	0.0528 (19)	0.0506 (19)	0.0442 (18)	−0.0093 (16)	0.0080 (15)	−0.0090 (17)
C3	0.0523 (19)	0.0499 (19)	0.0377 (16)	0.0076 (17)	0.0103 (15)	−0.0031 (16)

C4	0.0474 (18)	0.0479 (19)	0.0404 (17)	0.0032 (16)	0.0110 (14)	0.0010 (17)
C5	0.066 (2)	0.076 (3)	0.060 (2)	0.006 (2)	0.0314 (18)	0.007 (2)
C6	0.063 (2)	0.086 (3)	0.061 (2)	−0.011 (2)	0.0206 (18)	0.018 (2)
C7	0.062 (2)	0.060 (2)	0.055 (2)	−0.0187 (19)	0.0002 (17)	0.010 (2)
C8	0.0402 (18)	0.067 (2)	0.0571 (19)	−0.0017 (17)	0.0110 (15)	0.0140 (19)
C9	0.0436 (18)	0.064 (2)	0.0541 (19)	−0.0028 (17)	0.0150 (15)	0.0061 (18)
C10	0.0402 (18)	0.072 (2)	0.0429 (18)	−0.0119 (18)	0.0141 (14)	−0.0050 (19)
C11	0.0395 (18)	0.062 (2)	0.0438 (18)	−0.0033 (17)	0.0114 (14)	0.0017 (18)
C12	0.0400 (19)	0.088 (3)	0.059 (2)	0.004 (2)	0.0024 (16)	0.012 (2)
C13	0.063 (2)	0.067 (2)	0.074 (2)	0.014 (2)	0.0140 (19)	0.018 (2)
C14	0.058 (2)	0.062 (2)	0.070 (2)	−0.0003 (19)	0.0128 (19)	0.009 (2)
C15	0.0443 (18)	0.0481 (18)	0.0476 (17)	−0.0060 (15)	0.0087 (14)	0.0018 (16)
C16	0.0450 (18)	0.0510 (19)	0.0530 (18)	−0.0034 (16)	0.0077 (14)	−0.0060 (17)
C17	0.0464 (19)	0.0486 (18)	0.0404 (16)	0.0026 (16)	0.0134 (14)	−0.0026 (16)
C18	0.0435 (19)	0.0478 (19)	0.0370 (16)	−0.0018 (15)	0.0141 (14)	0.0012 (16)
C19	0.0418 (19)	0.075 (2)	0.056 (2)	0.0056 (18)	0.0231 (15)	0.007 (2)
C20	0.0361 (18)	0.080 (3)	0.073 (2)	−0.004 (2)	0.0112 (17)	0.013 (2)
C21	0.047 (2)	0.058 (2)	0.061 (2)	−0.0204 (18)	−0.0026 (16)	0.0047 (19)

Geometric parameters (Å, º)

N1—C1	1.451 (3)	C6—H6B	0.9300
N1—C15	1.460 (3)	C7—H7B	0.9300
N1—C8	1.465 (3)	C8—C9	1.513 (4)
N2—C3	1.279 (3)	C8—H8A	0.9700
N2—C2	1.459 (3)	C8—H8B	0.9700
N3—C7	1.357 (4)	C9—H9A	0.9700
N3—C4	1.358 (3)	C9—H9B	0.9700
N3—H3A	0.8600	C10—C11	1.429 (4)
N4—C10	1.264 (3)	C10—H10A	0.9300
N4—C9	1.454 (4)	C11—C12	1.368 (4)
N5—C14	1.352 (4)	C12—C13	1.388 (4)
N5—C11	1.362 (3)	C12—H12A	0.9300
N5—H5A	0.8600	C13—C14	1.356 (4)
N6—C17	1.267 (3)	C13—H13A	0.9300
N6—C16	1.464 (3)	C14—H14A	0.9300
N7—C21	1.357 (3)	C15—C16	1.506 (3)
N7—C18	1.357 (3)	C15—H15A	0.9700
N7—H7A	0.8600	C15—H15B	0.9700
C1—C2	1.522 (4)	C16—H16A	0.9700
C1—H1A	0.9700	C16—H16B	0.9700
C1—H1B	0.9700	C17—C18	1.430 (4)
C2—H2B	0.9700	C17—H17A	0.9300
C2—H2C	0.9700	C18—C19	1.374 (4)
C3—C4	1.430 (4)	C19—C20	1.389 (4)
C3—H3B	0.9300	C19—H19A	0.9300
C4—C5	1.373 (4)	C20—C21	1.356 (4)
C5—C6	1.385 (4)	C20—H20A	0.9300

C5—H5B	0.9300	C21—H21A	0.9300
C6—C7	1.350 (4)		
C1—N1—C15	115.1 (2)	N4—C9—C8	110.3 (3)
C1—N1—C8	115.6 (2)	N4—C9—H9A	109.6
C15—N1—C8	114.1 (2)	C8—C9—H9A	109.6
C3—N2—C2	117.7 (2)	N4—C9—H9B	109.6
C7—N3—C4	108.8 (3)	C8—C9—H9B	109.6
C7—N3—H3A	125.6	H9A—C9—H9B	108.1
C4—N3—H3A	125.6	N4—C10—C11	126.5 (3)
C10—N4—C9	117.0 (3)	N4—C10—H10A	116.7
C14—N5—C11	109.3 (3)	C11—C10—H10A	116.7
C14—N5—H5A	125.4	N5—C11—C12	106.6 (3)
C11—N5—H5A	125.4	N5—C11—C10	123.5 (3)
C17—N6—C16	117.5 (2)	C12—C11—C10	129.8 (3)
C21—N7—C18	108.9 (3)	C11—C12—C13	108.7 (3)
C21—N7—H7A	125.5	C11—C12—H12A	125.6
C18—N7—H7A	125.5	C13—C12—H12A	125.6
N1—C1—C2	118.6 (2)	C14—C13—C12	106.5 (3)
N1—C1—H1A	107.7	C14—C13—H13A	126.7
C2—C1—H1A	107.7	C12—C13—H13A	126.7
N1—C1—H1B	107.7	N5—C14—C13	108.8 (3)
C2—C1—H1B	107.7	N5—C14—H14A	125.6
H1A—C1—H1B	107.1	C13—C14—H14A	125.6
N2—C2—C1	113.5 (2)	N1—C15—C16	110.9 (2)
N2—C2—H2B	108.9	N1—C15—H15A	109.5
C1—C2—H2B	108.9	C16—C15—H15A	109.5
N2—C2—H2C	108.9	N1—C15—H15B	109.5
C1—C2—H2C	108.9	C16—C15—H15B	109.5
H2B—C2—H2C	107.7	H15A—C15—H15B	108.0
N2—C3—C4	123.7 (3)	N6—C16—C15	112.6 (2)
N2—C3—H3B	118.2	N6—C16—H16A	109.1
C4—C3—H3B	118.2	C15—C16—H16A	109.1
N3—C4—C5	107.0 (3)	N6—C16—H16B	109.1
N3—C4—C3	122.7 (3)	C15—C16—H16B	109.1
C5—C4—C3	130.3 (3)	H16A—C16—H16B	107.8
C4—C5—C6	108.2 (3)	N6—C17—C18	124.1 (3)
C4—C5—H5B	125.9	N6—C17—H17A	117.9
C6—C5—H5B	125.9	C18—C17—H17A	117.9
C7—C6—C5	106.9 (3)	N7—C18—C19	107.2 (3)
C7—C6—H6B	126.5	N7—C18—C17	123.8 (3)
C5—C6—H6B	126.5	C19—C18—C17	128.9 (3)
C6—C7—N3	109.0 (3)	C18—C19—C20	108.1 (3)
C6—C7—H7B	125.5	C18—C19—H19A	125.9
N3—C7—H7B	125.5	C20—C19—H19A	125.9
N1—C8—C9	112.7 (2)	C21—C20—C19	106.8 (3)
N1—C8—H8A	109.1	C21—C20—H20A	126.6
C9—C8—H8A	109.1	C19—C20—H20A	126.6

N1—C8—H8B	109.1	C20—C21—N7	108.9 (3)
C9—C8—H8B	109.1	C20—C21—H21A	125.5
H8A—C8—H8B	107.8	N7—C21—H21A	125.5
C15—N1—C1—C2	−87.6 (3)	N4—C10—C11—N5	−1.3 (5)
C8—N1—C1—C2	48.9 (3)	N4—C10—C11—C12	175.1 (3)
C3—N2—C2—C1	110.2 (3)	N5—C11—C12—C13	−0.3 (4)
N1—C1—C2—N2	56.6 (3)	C10—C11—C12—C13	−177.2 (3)
C2—N2—C3—C4	−178.6 (3)	C11—C12—C13—C14	0.4 (4)
C7—N3—C4—C5	0.0 (3)	C11—N5—C14—C13	0.1 (4)
C7—N3—C4—C3	−179.5 (2)	C12—C13—C14—N5	−0.3 (4)
N2—C3—C4—N3	3.4 (4)	C1—N1—C15—C16	−85.5 (3)
N2—C3—C4—C5	−175.9 (3)	C8—N1—C15—C16	137.4 (2)
N3—C4—C5—C6	−0.2 (4)	C17—N6—C16—C15	−129.8 (3)
C3—C4—C5—C6	179.2 (3)	N1—C15—C16—N6	−167.7 (2)
C4—C5—C6—C7	0.3 (4)	C16—N6—C17—C18	−177.0 (3)
C5—C6—C7—N3	−0.3 (4)	C21—N7—C18—C19	0.4 (3)
C4—N3—C7—C6	0.2 (3)	C21—N7—C18—C17	178.7 (3)
C1—N1—C8—C9	144.0 (3)	N6—C17—C18—N7	−4.9 (4)
C15—N1—C8—C9	−79.1 (3)	N6—C17—C18—C19	173.0 (3)
C10—N4—C9—C8	102.4 (3)	N7—C18—C19—C20	0.3 (3)
N1—C8—C9—N4	−73.9 (3)	C17—C18—C19—C20	−177.9 (3)
C9—N4—C10—C11	−177.0 (3)	C18—C19—C20—C21	−0.9 (4)
C14—N5—C11—C12	0.1 (3)	C19—C20—C21—N7	1.1 (4)
C14—N5—C11—C10	177.3 (3)	C18—N7—C21—C20	−0.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*B*···N2	0.97	2.59	3.246 (4)	125
N3—H3*A*···N6^{i}	0.86	2.14	2.956 (3)	159
N5—H5*A*···N4^{ii}	0.86	2.20	3.029 (3)	163
N7—H7*A*···N2^{i}	0.86	2.13	2.940 (3)	158

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