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FY4,4′-[(1*E*,1′*E*)-(2-Chloropyrimidine-4,6-diyl)bis(ethene-2,1-diyl)]bis(*N*,*N*-diethylaniline)

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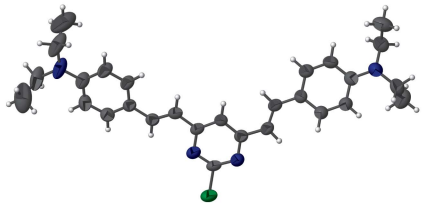
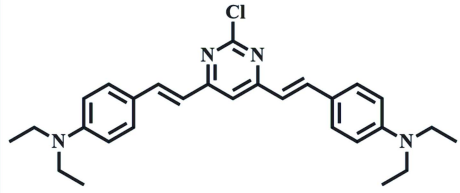
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{28}H_{33}ClN_4$, the central pyrimidine ring is twisted with respect to the two benzene rings, making dihedral angles of 13.56 (19) and 23.1 (2)°. In the crystal, weak C—H···π interactions link the molecules into supramolecular chains propagating along the *c*-axis direction.

3D view



Chemical scheme



Structure description

Pyrimidine derivatives are considered important compounds because of their wide range of biological activities, and also because of their high electron affinity and good planarity, making them suitable building blocks for the construction of chromophores for non-linear optical materials (Wang *et al.*, 2014). The pyrimidine ring also has well known reactivity with an aromatic aldehyde under solvent-free conditions (Li *et al.*, 2009). Moreover, pyrimidine derivatives are excellent candidates for sensor materials with two-photon properties as they involve two N atoms in positions 2 and 4, forming an effective coordinating dentate for metal cations that can be applied to generate various useful materials (Zhang *et al.*, 2016).

In the title compound (Fig. 1), the pyrimidine ring is nearly planar [maximum deviation of 0.008 (4) Å for atom C14) and is twisted with respect to the C5–C10 and C18–C23 benzene rings, making dihedral angles of 13.56 (19) and 23.1 (2)°, respectively.

In the crystal, weak C—H···π interactions (Table 1) link the molecules into supramolecular chains propagating along the *c*-axis direction.

Synthesis and crystallization

A mixture of 4-(diethylamino)benzaldehyde (0.39 g, 2.20 mmol), 2-chloro-4,6-dimethyl pyrimidine (0.14 g, 1 mmol) and ^{t}BuOK (0.56 g, 5 mmol) was milled vigorously for about

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

*Cg*3 is the centroid of the C18–C23 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···*Cg*3^{i}	0.97	2.73	3.606 (8)	151

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

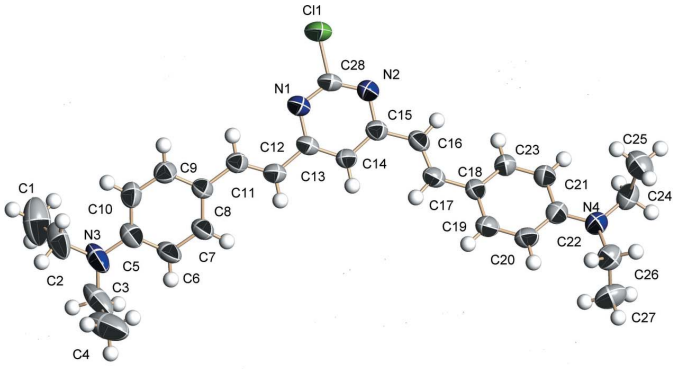


Figure 1
The molecular structure with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

10 min. The reaction was monitored by TLC. After the reaction was completed, the mixture was dispersed in water. The solution was extracted with CH_2Cl_2 several times. The organic layer was washed with water, saturated brine and dried over anhydrous $MgSO_4$. After removing solvent under reduced pressure, the crude product was obtained and purified by flash column chromatography (silica, 8:1 petroleum ether:ethyl acetate) to obtain red crystals. Yield: 60%. ^{1}H NMR (400 MHz, $CDCl_3$-d_6)1.42 (*t*, 12H), 3.41 (*q*, 8H), 6.66 (d, 4H), 7.47 (*d*, 4H),6.68 (*d*, 2H), 7.81 (*d*, 2H), 6.59 (*s*, 1H).

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{33}ClN_4$
M_r	461.03
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	11.791 (5), 15.005 (5), 14.711 (5)
β (°)	92.716 (5)
V (Å^3)	2599.8 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.17
Crystal size (mm)	0.10 × 0.10 × 0.10
Data collection	
Diffractometer	Bruker SMART 1000 CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14693, 4334, 1777
R_{int}	0.087
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.203, 0.91
No. of reflections	4334
No. of parameters	302
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.18

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Zhang, Q., Tian, X.-H., Wang, H., Hu, Z.-J., Wu, J.-Y., Zhou, H.-P., Zhang, S.-Y., Yang, J.-X., Sun, Z.-Q., Tian, Y.-P. & Uvdal, K. (2016). *Sens. Actuators B Chem.* **222**, 574–578.

full crystallographic data

IUCrData (2016). **1**, x161590 [https://doi.org/10.1107/S241431461601590X]

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4,4′-[(1*E*,1′*E*)-(2-Chloropyrimidine-4,6-diyl)bis(ethene-2,1-diyl)]bis(*N*,*N*-diethylaniline)

Crystal data

$C_{28}H_{33}ClN_4$
M_r = 461.03
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.791 (5) Å
b = 15.005 (5) Å
c = 14.711 (5) Å
β = 92.716 (5)°
V = 2599.8 (17) Å^3
Z = 4
$F(000)$ = 984
D_x = 1.178 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1048 reflections
θ = 2.2–17.4°
μ = 0.17 mm^{-1}
T = 296 K
Prism, red
0.1 × 0.1 × 0.1 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
14693 measured reflections
4334 independent reflections
1777 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 25.0°, θ_{min} = 1.9°
h = −14→14
k = −17→17
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.203
S = 0.91
4334 reflections
302 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.23269 (13)	0.36886 (9)	1.30455 (8)	0.0911 (5)
C8	0.1371 (3)	0.5278 (3)	0.8928 (3)	0.0512 (11)
N2	0.2846 (3)	0.2363 (2)	1.2017 (2)	0.0622 (10)
N4	0.4462 (3)	−0.3125 (2)	1.0323 (3)	0.0667 (10)
C17	0.3370 (3)	0.0536 (3)	1.0462 (3)	0.0589 (12)
H17	0.3143	0.0797	0.9910	0.071*
C15	0.2972 (3)	0.1987 (3)	1.1188 (3)	0.0544 (11)
C14	0.2743 (3)	0.2474 (3)	1.0400 (3)	0.0545 (11)
H14	0.2845	0.2221	0.9832	0.065*
C22	0.4249 (4)	−0.2226 (3)	1.0348 (3)	0.0586 (12)
C16	0.3342 (4)	0.1056 (3)	1.1189 (3)	0.0592 (12)
H16	0.3576	0.0809	1.1746	0.071*
C18	0.3711 (4)	−0.0388 (3)	1.0425 (3)	0.0577 (12)
C13	0.2362 (3)	0.3337 (3)	1.0470 (3)	0.0524 (11)
C28	0.2489 (3)	0.3195 (3)	1.1987 (3)	0.0568 (11)
C11	0.1623 (3)	0.4685 (3)	0.9688 (3)	0.0538 (11)
H11	0.1431	0.4892	1.0256	0.065*
N1	0.2235 (3)	0.3717 (2)	1.1294 (3)	0.0576 (9)
C9	0.0828 (3)	0.6091 (3)	0.9065 (3)	0.0609 (12)
H9	0.0591	0.6225	0.9644	0.073*
C23	0.4283 (4)	−0.0820 (3)	1.1142 (3)	0.0632 (12)
H23	0.4492	−0.0496	1.1662	0.076*
N3	0.0790 (4)	0.7150 (3)	0.6822 (3)	0.0945 (14)
C7	0.1674 (4)	0.5118 (3)	0.8045 (3)	0.0622 (12)
H7	0.2020	0.4578	0.7917	0.075*
C20	0.3713 (4)	−0.1784 (3)	0.9612 (3)	0.0661 (13)
H20	0.3519	−0.2100	0.9084	0.079*
C5	0.0961 (4)	0.6541 (3)	0.7508 (3)	0.0686 (13)
C10	0.0631 (4)	0.6696 (3)	0.8384 (3)	0.0679 (13)
H10	0.0265	0.7227	0.8512	0.081*
C12	0.2097 (3)	0.3877 (3)	0.9671 (3)	0.0546 (11)
H12	0.2269	0.3645	0.9108	0.066*
C6	0.1489 (4)	0.5712 (3)	0.7351 (3)	0.0712 (14)
H6	0.1713	0.5572	0.6771	0.085*
C26	0.3941 (4)	−0.3692 (3)	0.9608 (3)	0.0737 (14)
H26A	0.3211	−0.3441	0.9413	0.088*
H26B	0.3806	−0.4278	0.9858	0.088*
C21	0.4554 (4)	−0.1709 (3)	1.1112 (3)	0.0630 (12)
H21	0.4946	−0.1971	1.1607	0.076*
C19	0.3467 (4)	−0.0892 (3)	0.9652 (3)	0.0664 (13)

H19	0.3124	−0.0617	0.9143	0.080*
C24	0.4983 (4)	−0.3591 (3)	1.1105 (3)	0.0738 (14)
H24A	0.5564	−0.3213	1.1391	0.089*
H24B	0.5350	−0.4126	1.0896	0.089*
C27	0.4660 (5)	−0.3787 (3)	0.8790 (3)	0.0968 (17)
H27A	0.4810	−0.3209	0.8545	0.145*
H27B	0.4262	−0.4142	0.8335	0.145*
H27C	0.5364	−0.4072	0.8970	0.145*
C2	0.0210 (5)	0.8003 (4)	0.6974 (4)	0.107 (2)
H2A	−0.0384	0.7908	0.7398	0.128*
H2B	−0.0149	0.8202	0.6402	0.128*
C25	0.4139 (5)	−0.3846 (3)	1.1809 (4)	0.1001 (18)
H25A	0.3784	−0.3319	1.2031	0.150*
H25B	0.4529	−0.4150	1.2306	0.150*
H25C	0.3570	−0.4233	1.1536	0.150*
C3	0.1174 (6)	0.6985 (5)	0.5922 (5)	0.124 (3)
H3A	0.1883	0.6657	0.5970	0.149*
H3B	0.1321	0.7551	0.5631	0.149*
C4	0.0333 (7)	0.6472 (6)	0.5340 (5)	0.165 (3)
H4A	0.0148	0.5928	0.5642	0.248*
H4B	0.0654	0.6337	0.4768	0.248*
H4C	−0.0342	0.6822	0.5236	0.248*
C1	0.0994 (6)	0.8730 (4)	0.7342 (6)	0.157 (3)
H1A	0.1369	0.8534	0.7900	0.235*
H1B	0.0560	0.9257	0.7454	0.235*
H1C	0.1550	0.8861	0.6905	0.235*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1296 (12)	0.0957 (10)	0.0472 (8)	0.0198 (8)	−0.0046 (7)	−0.0099 (7)
C8	0.051 (3)	0.055 (3)	0.047 (3)	−0.006 (2)	0.001 (2)	0.002 (2)
N2	0.075 (3)	0.061 (2)	0.051 (3)	0.0008 (19)	0.000 (2)	0.003 (2)
N4	0.077 (3)	0.059 (2)	0.064 (3)	0.000 (2)	−0.001 (2)	−0.006 (2)
C17	0.069 (3)	0.061 (3)	0.046 (3)	−0.010 (2)	−0.002 (2)	0.004 (2)
C15	0.059 (3)	0.056 (3)	0.048 (3)	−0.009 (2)	0.003 (2)	0.000 (2)
C14	0.068 (3)	0.051 (3)	0.044 (3)	−0.004 (2)	0.003 (2)	−0.002 (2)
C22	0.057 (3)	0.058 (3)	0.062 (3)	−0.004 (2)	0.011 (2)	0.000 (3)
C16	0.073 (3)	0.057 (3)	0.047 (3)	−0.008 (2)	0.000 (2)	0.009 (2)
C18	0.072 (3)	0.050 (3)	0.051 (3)	−0.003 (2)	0.004 (2)	0.004 (2)
C13	0.054 (3)	0.063 (3)	0.040 (3)	−0.008 (2)	−0.001 (2)	0.003 (2)
C28	0.063 (3)	0.071 (3)	0.036 (3)	−0.005 (2)	−0.002 (2)	−0.005 (2)
C11	0.055 (3)	0.056 (3)	0.050 (3)	−0.007 (2)	0.001 (2)	−0.002 (2)
N1	0.061 (2)	0.066 (2)	0.046 (3)	−0.0033 (18)	−0.0008 (19)	0.002 (2)
C9	0.060 (3)	0.063 (3)	0.060 (3)	−0.001 (2)	0.008 (2)	−0.002 (2)
C23	0.077 (3)	0.057 (3)	0.055 (3)	0.002 (2)	−0.003 (2)	−0.002 (2)
N3	0.092 (3)	0.105 (3)	0.089 (4)	0.037 (3)	0.027 (3)	0.051 (3)
C7	0.066 (3)	0.071 (3)	0.050 (3)	0.009 (2)	0.008 (2)	0.011 (2)

C20	0.081 (3)	0.066 (3)	0.051 (3)	−0.006 (3)	0.000 (3)	−0.009 (3)
C5	0.056 (3)	0.080 (3)	0.070 (4)	0.013 (2)	0.013 (3)	0.020 (3)
C10	0.067 (3)	0.057 (3)	0.080 (4)	0.011 (2)	0.008 (3)	0.008 (3)
C12	0.057 (3)	0.062 (3)	0.045 (3)	−0.007 (2)	0.002 (2)	−0.003 (2)
C6	0.074 (3)	0.091 (3)	0.050 (3)	0.016 (3)	0.015 (3)	0.018 (3)
C26	0.069 (3)	0.068 (3)	0.084 (4)	−0.009 (2)	0.003 (3)	−0.007 (3)
C21	0.072 (3)	0.059 (3)	0.057 (3)	0.002 (2)	−0.008 (2)	−0.001 (2)
C19	0.080 (3)	0.068 (3)	0.051 (3)	−0.002 (3)	0.004 (3)	0.001 (3)
C24	0.070 (3)	0.061 (3)	0.090 (4)	0.009 (2)	0.003 (3)	−0.008 (3)
C27	0.099 (4)	0.104 (4)	0.087 (4)	−0.009 (3)	0.003 (3)	−0.034 (3)
C2	0.074 (4)	0.106 (4)	0.141 (5)	0.034 (4)	0.015 (4)	0.058 (4)
C25	0.098 (4)	0.108 (4)	0.095 (4)	0.013 (3)	0.011 (3)	0.026 (3)
C3	0.106 (5)	0.168 (6)	0.100 (6)	0.054 (5)	0.034 (4)	0.078 (5)
C4	0.151 (7)	0.262 (10)	0.084 (6)	0.068 (7)	0.010 (5)	0.029 (6)
C1	0.100 (5)	0.113 (5)	0.257 (10)	0.000 (4)	0.014 (6)	0.061 (6)

Geometric parameters (Å, º)

Cl1—C28	1.743 (4)	C7—H7	0.9300
C8—C7	1.385 (5)	C20—C19	1.371 (5)
C8—C9	1.397 (5)	C20—H20	0.9300
C8—C11	1.448 (5)	C5—C10	1.384 (6)
N2—C28	1.317 (5)	C5—C6	1.414 (6)
N2—C15	1.358 (5)	C10—H10	0.9300
N4—C22	1.373 (5)	C12—H12	0.9300
N4—C24	1.457 (5)	C6—H6	0.9300
N4—C26	1.464 (5)	C26—C27	1.512 (6)
C17—C16	1.325 (5)	C26—H26A	0.9700
C17—C18	1.446 (5)	C26—H26B	0.9700
C17—H17	0.9300	C21—H21	0.9300
C15—C14	1.386 (5)	C19—H19	0.9300
C15—C16	1.463 (5)	C24—C25	1.519 (6)
C14—C13	1.376 (5)	C24—H24A	0.9700
C14—H14	0.9300	C24—H24B	0.9700
C22—C20	1.395 (6)	C27—H27A	0.9600
C22—C21	1.399 (5)	C27—H27B	0.9600
C16—H16	0.9300	C27—H27C	0.9600
C18—C19	1.384 (5)	C2—C1	1.514 (8)
C18—C23	1.387 (5)	C2—H2A	0.9700
C13—N1	1.355 (5)	C2—H2B	0.9700
C13—C12	1.449 (5)	C25—H25A	0.9600
C28—N1	1.309 (5)	C25—H25B	0.9600
C11—C12	1.336 (5)	C25—H25C	0.9600
C11—H11	0.9300	C3—C4	1.492 (9)
C9—C10	1.363 (5)	C3—H3A	0.9700
C9—H9	0.9300	C3—H3B	0.9700
C23—C21	1.373 (5)	C4—H4A	0.9600
C23—H23	0.9300	C4—H4B	0.9600

N3—C5	1.369 (5)	C4—H4C	0.9600
N3—C3	1.442 (7)	C1—H1A	0.9600
N3—C2	1.473 (6)	C1—H1B	0.9600
C7—C6	1.365 (5)	C1—H1C	0.9600
C7—C8—C9	115.3 (4)	C13—C12—H12	117.7
C7—C8—C11	124.4 (4)	C7—C6—C5	120.6 (4)
C9—C8—C11	120.3 (4)	C7—C6—H6	119.7
C28—N2—C15	114.4 (4)	C5—C6—H6	119.7
C22—N4—C24	121.4 (4)	N4—C26—C27	113.3 (4)
C22—N4—C26	121.2 (4)	N4—C26—H26A	108.9
C24—N4—C26	115.9 (4)	C27—C26—H26A	108.9
C16—C17—C18	127.8 (4)	N4—C26—H26B	108.9
C16—C17—H17	116.1	C27—C26—H26B	108.9
C18—C17—H17	116.1	H26A—C26—H26B	107.7
N2—C15—C14	120.4 (4)	C23—C21—C22	120.9 (4)
N2—C15—C16	116.2 (4)	C23—C21—H21	119.6
C14—C15—C16	123.4 (4)	C22—C21—H21	119.6
C13—C14—C15	119.0 (4)	C20—C19—C18	122.1 (4)
C13—C14—H14	120.5	C20—C19—H19	119.0
C15—C14—H14	120.5	C18—C19—H19	119.0
N4—C22—C20	121.6 (4)	N4—C24—C25	113.2 (4)
N4—C22—C21	121.7 (4)	N4—C24—H24A	108.9
C20—C22—C21	116.7 (4)	C25—C24—H24A	108.9
C17—C16—C15	125.5 (4)	N4—C24—H24B	108.9
C17—C16—H16	117.3	C25—C24—H24B	108.9
C15—C16—H16	117.3	H24A—C24—H24B	107.7
C19—C18—C23	116.4 (4)	C26—C27—H27A	109.5
C19—C18—C17	120.5 (4)	C26—C27—H27B	109.5
C23—C18—C17	123.0 (4)	H27A—C27—H27B	109.5
N1—C13—C14	120.9 (4)	C26—C27—H27C	109.5
N1—C13—C12	117.5 (4)	H27A—C27—H27C	109.5
C14—C13—C12	121.6 (4)	H27B—C27—H27C	109.5
N1—C28—N2	130.8 (4)	N3—C2—C1	113.6 (5)
N1—C28—Cl1	114.2 (3)	N3—C2—H2A	108.8
N2—C28—Cl1	114.9 (4)	C1—C2—H2A	108.8
C12—C11—C8	127.9 (4)	N3—C2—H2B	108.8
C12—C11—H11	116.1	C1—C2—H2B	108.8
C8—C11—H11	116.1	H2A—C2—H2B	107.7
C28—N1—C13	114.5 (4)	C24—C25—H25A	109.5
C10—C9—C8	122.5 (4)	C24—C25—H25B	109.5
C10—C9—H9	118.7	H25A—C25—H25B	109.5
C8—C9—H9	118.7	C24—C25—H25C	109.5
C21—C23—C18	122.4 (4)	H25A—C25—H25C	109.5
C21—C23—H23	118.8	H25B—C25—H25C	109.5
C18—C23—H23	118.8	N3—C3—C4	112.7 (6)
C5—N3—C3	121.4 (4)	N3—C3—H3A	109.0
C5—N3—C2	121.5 (5)	C4—C3—H3A	109.0

C3—N3—C2	117.1 (4)	N3—C3—H3B	109.0
C6—C7—C8	123.3 (4)	C4—C3—H3B	109.0
C6—C7—H7	118.4	H3A—C3—H3B	107.8
C8—C7—H7	118.4	C3—C4—H4A	109.5
C19—C20—C22	121.4 (4)	C3—C4—H4B	109.5
C19—C20—H20	119.3	H4A—C4—H4B	109.5
C22—C20—H20	119.3	C3—C4—H4C	109.5
N3—C5—C10	122.4 (4)	H4A—C4—H4C	109.5
N3—C5—C6	121.2 (4)	H4B—C4—H4C	109.5
C10—C5—C6	116.4 (4)	C2—C1—H1A	109.5
C9—C10—C5	121.9 (4)	C2—C1—H1B	109.5
C9—C10—H10	119.1	H1A—C1—H1B	109.5
C5—C10—H10	119.1	C2—C1—H1C	109.5
C11—C12—C13	124.5 (4)	H1A—C1—H1C	109.5
C11—C12—H12	117.7	H1B—C1—H1C	109.5

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C18–C23 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···*Cg*3^{i}	0.97	2.73	3.606 (8)	151

Symmetry code: (i) x, $-y+1/2$, $z-1/2$.