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4,4′-[2,2-Dimethylpropane-1,3-diyl-bis(nitrilomethylidyne)]dibenzonitrile

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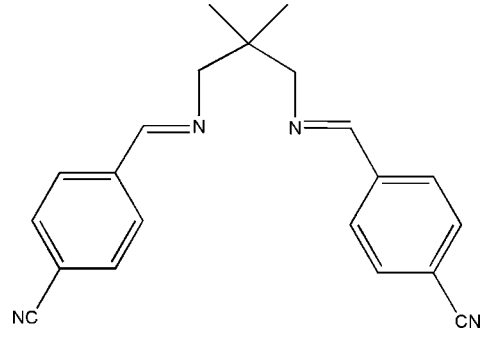
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.057; wR factor = 0.139; data-to-parameter ratio = 23.4.

The title compound, $C_{21}H_{20}N_4$, is a bidentate Schiff base ligand. An intramolecular C—H···N hydrogen bond forms a five-membered ring, producing an S(5) ring motif. The cyano and imino [–C(H$_2$)—N=C–] functional groups are coplanar with the benzene ring in each half of the molecule. The packing of the molecules is controlled by C—H···π and π–π interactions [centroid-to-centroid distance = 3.6944 (8) Å].

Related literature

For related literature on hydrogen-bond motifs, see Bernstein *et al.* (1995). For values of bond lengths, see Allen *et al.* (1987). For related structures, see, for example: Li *et al.* (2005); Bomfim *et al.* (2005); Glidewell *et al.* (2005, 2006); Sun *et al.* (2004); Habibi *et al.* (2007); Fun *et al.* (2008).



Experimental

Crystal data

$C_{21}H_{20}N_4$
M_r = 328.41
Monoclinic, $P2_1/c$
a = 6.3833 (2) Å
b = 34.0679 (8) Å
c = 8.5190 (2) Å
β = 100.654 (2)°
V = 1820.65 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 100.0 (1) K
0.42 × 0.20 × 0.19 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2005)
T_{min} = 0.970, T_{max} = 0.986
21813 measured reflections
5329 independent reflections
3711 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.139
S = 1.04
5329 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

Cg1 is the centroid of the C12–C17 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20B···N2	0.96	2.57	2.923 (2)	102
C21—H21C···Cg1^{i}	0.96	2.95	3.7193 (16)	138

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2578).

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4,4′-[2,2-Dimethylpropane-1,3-diylbis(nitrilomethylidyne)]dibenzonitrile

Hoong-Kun Fun, Hadi Kargar and Reza Kia

S1. Comment

Schiff bases are one of most prevalent mixed-donor ligands in the field of coordination chemistry. They play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism, and supramolecular architectures. Structures of Schiff bases derived from substituted benzaldehydes and closely related to the title compound have been reported (Li *et al.*, 2005; Bomfim *et al.*, 2005; Glidewell *et al.*, 2005, 2006; Sun *et al.*, 2004; Habibi *et al.*, 2007; Fun *et al.*, 2008).

An intramolecular C—H···N hydrogen bond forms a five-membered ring, producing an *S*(5) ring motif (Bernstein *et al.*, 1995). The bond lengths and angles in the molecule (Fig. 1) are within normal ranges (Allen *et al.*, 1987). The cyano and imino (—C(H_2)—N═C—) functional groups are coplanar with the benzene ring in each half of the molcule. The torsion angles of C6—C7—N1—C8 and C12—C11—N2—C10 are -178.95 (13) and -179.43 (12)°, respectively. The packing of the molecule, (Fig. 2), is controlled by C—H···π and π–π interactions [centroid-centroid distance being 3.6944 (8) Å] (Table 1).

S2. Experimental

The synthetic method has been described earlier (Fun *et al.*, 2008). Single crystals suitable for X-ray diffraction were obtained by evaporation of an ethanol solution at room temperature.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å for aromatic H and 0.97 Å for methylene and 0.96 Å for methyl H atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for the methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating-group model was used for the methyl groups.

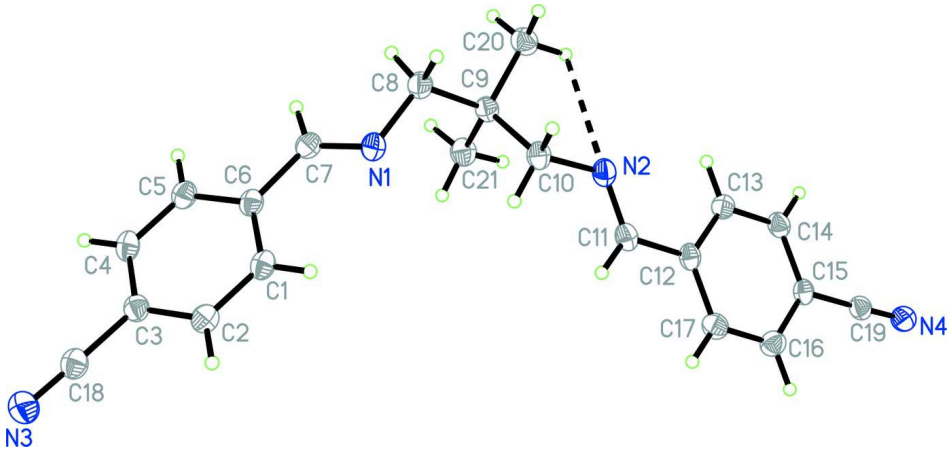

Figure 1

The molecular structure of the title compound with atom labels and 50% probability ellipsoids for non-H atoms. Intramolecular hydrogen bond is shown as a dashed line.

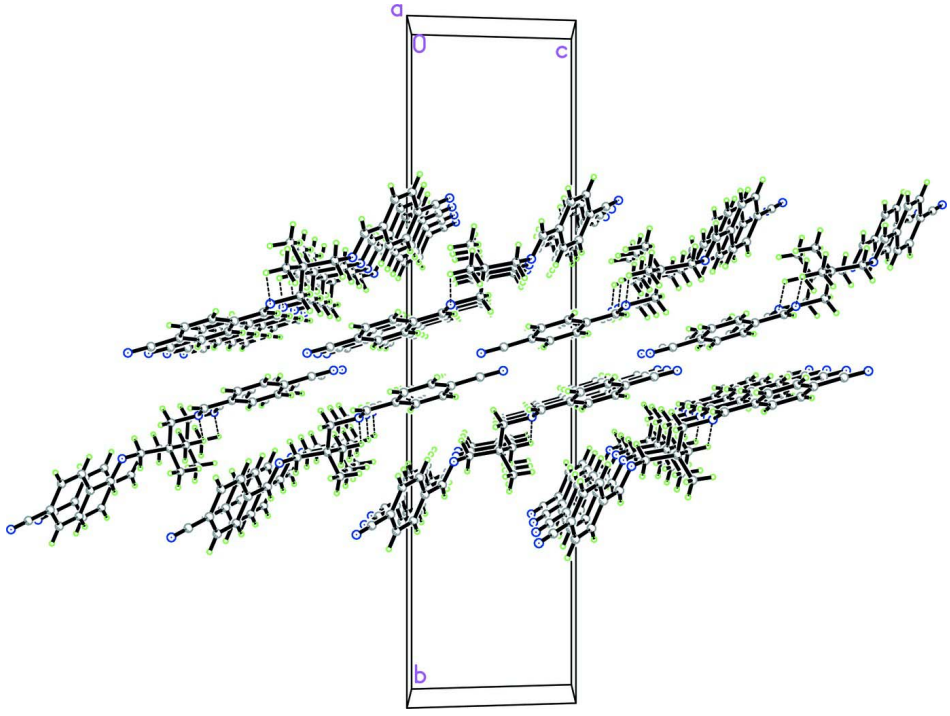

Figure 2

The crystal packing, viewed down the *a* axis, showing stacking of the benzene rings. Intramolecular H bonds are drawn as dashed lines.

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Crystal data

$C_{21}H_{20}N_4$
M_r = 328.41
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 6.3833 (2) Å
b = 34.0679 (8) Å
c = 8.5190 (2) Å
β = 100.654 (2)°

V = 1820.65 (8) Å^3
Z = 4
F(000) = 696
D_x = 1.198 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3870 reflections

θ = 2.4–29.3°
μ = 0.07 mm^{-1}
T = 100 K
Block, colourless
0.42 × 0.20 × 0.19 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker 2005)
T_{min} = 0.970, T_{max} = 0.986

21813 measured reflections
5329 independent reflections
3711 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 30.2°, θ_{min} = 1.2°
h = −9→7
k = −48→48
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.139
S = 1.04
5329 reflections
228 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
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.5007P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Experimental. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.
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	0.8180 (2)	0.14310 (4)	1.22220 (14)	0.0240 (3)
N2	0.7297 (2)	0.07939 (4)	0.76666 (14)	0.0243 (3)
N3	0.1075 (3)	0.23585 (4)	1.75196 (17)	0.0346 (4)
N4	0.2208 (2)	0.01242 (4)	−0.06341 (15)	0.0278 (3)
C1	0.4959 (3)	0.16261 (4)	1.41380 (17)	0.0234 (3)
H1A	0.4844	0.1376	1.3689	0.028*
C2	0.3530 (3)	0.17457 (4)	1.50763 (17)	0.0243 (3)
H2A	0.2462	0.1576	1.5267	0.029*
C3	0.3698 (3)	0.21224 (4)	1.57374 (16)	0.0226 (3)
C4	0.5288 (3)	0.23767 (4)	1.54525 (17)	0.0254 (3)

H4A	0.5386	0.2628	1.5886	0.031*
C5	0.6719 (3)	0.22545 (4)	1.45229 (17)	0.0237 (3)
H5A	0.7789	0.2424	1.4335	0.028*
C6	0.6573 (3)	0.18785 (4)	1.38618 (16)	0.0211 (3)
C7	0.8171 (3)	0.17624 (4)	1.29000 (16)	0.0224 (3)
H7A	0.9230	0.1942	1.2785	0.027*
C8	0.9911 (3)	0.13680 (4)	1.13468 (17)	0.0245 (3)
H8A	1.0761	0.1147	1.1816	0.029*
H8B	1.0823	0.1598	1.1469	0.029*
C9	0.9149 (3)	0.12886 (4)	0.95573 (16)	0.0215 (3)
C10	0.7881 (3)	0.09017 (4)	0.93463 (16)	0.0232 (3)
H10A	0.8736	0.0694	0.9923	0.028*
H10B	0.6600	0.0930	0.9796	0.028*
C11	0.5405 (3)	0.06825 (4)	0.71580 (16)	0.0226 (3)
H11A	0.4445	0.0675	0.7857	0.027*
C12	0.4686 (3)	0.05644 (4)	0.54744 (16)	0.0212 (3)
C13	0.6067 (3)	0.05915 (4)	0.43861 (17)	0.0231 (3)
H13A	0.7442	0.0687	0.4719	0.028*
C14	0.5402 (3)	0.04776 (4)	0.28203 (17)	0.0233 (3)
H14A	0.6322	0.0497	0.2096	0.028*
C15	0.3345 (3)	0.03329 (4)	0.23295 (16)	0.0212 (3)
C16	0.1937 (3)	0.03068 (4)	0.33940 (17)	0.0256 (3)
H16A	0.0561	0.0212	0.3058	0.031*
C17	0.2624 (3)	0.04247 (4)	0.49654 (17)	0.0255 (3)
H17A	0.1694	0.0410	0.5685	0.031*
C18	0.2220 (3)	0.22512 (4)	1.67256 (18)	0.0270 (3)
C19	0.2687 (3)	0.02115 (4)	0.06860 (17)	0.0227 (3)
C20	1.1140 (3)	0.12547 (5)	0.88075 (19)	0.0287 (4)
H20A	1.1895	0.1500	0.8920	0.043*
H20B	1.0729	0.1192	0.7695	0.043*
H20C	1.2046	0.1051	0.9337	0.043*
C21	0.7745 (3)	0.16266 (4)	0.87814 (18)	0.0274 (4)
H21A	0.8507	0.1870	0.8986	0.041*
H21B	0.6466	0.1638	0.9222	0.041*
H21C	0.7381	0.1584	0.7650	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0265 (8)	0.0254 (6)	0.0199 (6)	−0.0005 (5)	0.0037 (5)	−0.0025 (5)
N2	0.0282 (8)	0.0233 (6)	0.0222 (6)	−0.0009 (5)	0.0070 (5)	−0.0030 (5)
N3	0.0335 (10)	0.0336 (8)	0.0379 (8)	0.0006 (6)	0.0099 (7)	−0.0063 (6)
N4	0.0268 (8)	0.0305 (7)	0.0270 (6)	−0.0013 (6)	0.0071 (6)	−0.0028 (5)
C1	0.0282 (9)	0.0186 (7)	0.0219 (7)	−0.0002 (6)	0.0011 (6)	−0.0015 (5)
C2	0.0257 (9)	0.0222 (7)	0.0244 (7)	−0.0010 (6)	0.0028 (6)	0.0011 (5)
C3	0.0230 (9)	0.0247 (7)	0.0193 (6)	0.0030 (6)	0.0015 (6)	−0.0003 (5)
C4	0.0319 (10)	0.0203 (7)	0.0234 (7)	0.0002 (6)	0.0034 (6)	−0.0040 (5)
C5	0.0275 (9)	0.0212 (7)	0.0222 (7)	−0.0033 (6)	0.0037 (6)	−0.0006 (5)

C6	0.0236 (9)	0.0214 (7)	0.0168 (6)	0.0013 (6)	0.0002 (6)	0.0006 (5)
C7	0.0232 (9)	0.0225 (7)	0.0206 (6)	−0.0012 (6)	0.0019 (6)	0.0007 (5)
C8	0.0250 (9)	0.0235 (7)	0.0244 (7)	0.0015 (6)	0.0029 (6)	−0.0025 (5)
C9	0.0232 (9)	0.0200 (7)	0.0220 (6)	0.0002 (6)	0.0059 (6)	−0.0009 (5)
C10	0.0275 (9)	0.0234 (7)	0.0191 (6)	0.0005 (6)	0.0056 (6)	−0.0007 (5)
C11	0.0286 (10)	0.0193 (7)	0.0218 (7)	0.0010 (6)	0.0095 (6)	0.0000 (5)
C12	0.0277 (9)	0.0152 (6)	0.0214 (6)	0.0012 (6)	0.0063 (6)	0.0000 (5)
C13	0.0234 (9)	0.0226 (7)	0.0240 (7)	−0.0016 (6)	0.0058 (6)	−0.0023 (5)
C14	0.0269 (9)	0.0225 (7)	0.0226 (7)	−0.0003 (6)	0.0101 (6)	−0.0013 (5)
C15	0.0266 (9)	0.0161 (6)	0.0211 (6)	0.0020 (6)	0.0051 (6)	−0.0004 (5)
C16	0.0256 (9)	0.0258 (7)	0.0257 (7)	−0.0031 (6)	0.0054 (6)	−0.0004 (6)
C17	0.0274 (10)	0.0289 (8)	0.0227 (7)	−0.0025 (7)	0.0107 (6)	0.0002 (6)
C18	0.0300 (10)	0.0236 (7)	0.0268 (7)	0.0002 (7)	0.0037 (7)	−0.0020 (6)
C19	0.0240 (9)	0.0199 (7)	0.0253 (7)	0.0007 (6)	0.0075 (6)	0.0000 (5)
C20	0.0284 (10)	0.0290 (8)	0.0309 (8)	−0.0013 (7)	0.0112 (7)	−0.0014 (6)
C21	0.0306 (10)	0.0242 (7)	0.0274 (7)	0.0020 (7)	0.0053 (7)	0.0009 (6)

Geometric parameters (Å, º)

N1—C7	1.2687 (18)	C9—C21	1.532 (2)
N1—C8	1.459 (2)	C9—C10	1.539 (2)
N2—C11	1.264 (2)	C10—H10A	0.9700
N2—C10	1.4576 (17)	C10—H10B	0.9700
N3—C18	1.143 (2)	C11—C12	1.4786 (19)
N4—C19	1.1486 (19)	C11—H11A	0.9300
C1—C2	1.380 (2)	C12—C17	1.391 (2)
C1—C6	1.395 (2)	C12—C13	1.396 (2)
C1—H1A	0.9300	C13—C14	1.379 (2)
C2—C3	1.398 (2)	C13—H13A	0.9300
C2—H2A	0.9300	C14—C15	1.392 (2)
C3—C4	1.389 (2)	C14—H14A	0.9300
C3—C18	1.444 (2)	C15—C16	1.392 (2)
C4—C5	1.379 (2)	C15—C19	1.446 (2)
C4—H4A	0.9300	C16—C17	1.389 (2)
C5—C6	1.396 (2)	C16—H16A	0.9300
C5—H5A	0.9300	C17—H17A	0.9300
C6—C7	1.476 (2)	C20—H20A	0.9600
C7—H7A	0.9300	C20—H20B	0.9600
C8—C9	1.536 (2)	C20—H20C	0.9600
C8—H8A	0.9700	C21—H21A	0.9600
C8—H8B	0.9700	C21—H21B	0.9600
C9—C20	1.529 (2)	C21—H21C	0.9600
C7—N1—C8	115.55 (14)	N2—C10—H10B	109.4
C11—N2—C10	117.85 (13)	C9—C10—H10B	109.4
C2—C1—C6	120.21 (13)	H10A—C10—H10B	108.0
C2—C1—H1A	119.9	N2—C11—C12	121.33 (14)
C6—C1—H1A	119.9	N2—C11—H11A	119.3

C1—C2—C3	119.66 (15)	C12—C11—H11A	119.3
C1—C2—H2A	120.2	C17—C12—C13	119.54 (13)
C3—C2—H2A	120.2	C17—C12—C11	120.10 (14)
C4—C3—C2	120.41 (14)	C13—C12—C11	120.36 (15)
C4—C3—C18	119.30 (14)	C14—C13—C12	120.32 (15)
C2—C3—C18	120.29 (15)	C14—C13—H13A	119.8
C5—C4—C3	119.66 (14)	C12—C13—H13A	119.8
C5—C4—H4A	120.2	C13—C14—C15	119.65 (14)
C3—C4—H4A	120.2	C13—C14—H14A	120.2
C4—C5—C6	120.45 (15)	C15—C14—H14A	120.2
C4—C5—H5A	119.8	C16—C15—C14	120.88 (13)
C6—C5—H5A	119.8	C16—C15—C19	120.37 (15)
C1—C6—C5	119.60 (14)	C14—C15—C19	118.75 (14)
C1—C6—C7	122.45 (13)	C17—C16—C15	118.87 (16)
C5—C6—C7	117.95 (14)	C17—C16—H16A	120.6
N1—C7—C6	123.57 (15)	C15—C16—H16A	120.6
N1—C7—H7A	118.2	C16—C17—C12	120.73 (14)
C6—C7—H7A	118.2	C16—C17—H17A	119.6
N1—C8—C9	113.72 (13)	C12—C17—H17A	119.6
N1—C8—H8A	108.8	N3—C18—C3	178.73 (19)
C9—C8—H8A	108.8	N4—C19—C15	177.74 (17)
N1—C8—H8B	108.8	C9—C20—H20A	109.5
C9—C8—H8B	108.8	C9—C20—H20B	109.5
H8A—C8—H8B	107.7	H20A—C20—H20B	109.5
C20—C9—C21	109.99 (12)	C9—C20—H20C	109.5
C20—C9—C8	107.02 (13)	H20A—C20—H20C	109.5
C21—C9—C8	110.40 (12)	H20B—C20—H20C	109.5
C20—C9—C10	110.25 (12)	C9—C21—H21A	109.5
C21—C9—C10	109.88 (13)	C9—C21—H21B	109.5
C8—C9—C10	109.26 (11)	H21A—C21—H21B	109.5
N2—C10—C9	111.35 (11)	C9—C21—H21C	109.5
N2—C10—H10A	109.4	H21A—C21—H21C	109.5
C9—C10—H10A	109.4	H21B—C21—H21C	109.5

C6—C1—C2—C3	0.6 (2)	C21—C9—C10—N2	64.21 (16)
C1—C2—C3—C4	0.2 (2)	C8—C9—C10—N2	−174.52 (13)
C1—C2—C3—C18	−179.80 (14)	C10—N2—C11—C12	−179.43 (12)
C2—C3—C4—C5	−0.6 (2)	N2—C11—C12—C17	176.85 (14)
C18—C3—C4—C5	179.36 (15)	N2—C11—C12—C13	−3.1 (2)
C3—C4—C5—C6	0.3 (2)	C17—C12—C13—C14	−0.6 (2)
C2—C1—C6—C5	−0.8 (2)	C11—C12—C13—C14	179.35 (13)
C2—C1—C6—C7	178.55 (14)	C12—C13—C14—C15	−0.4 (2)
C4—C5—C6—C1	0.4 (2)	C13—C14—C15—C16	0.9 (2)
C4—C5—C6—C7	−179.02 (14)	C13—C14—C15—C19	−179.39 (13)
C8—N1—C7—C6	−178.95 (13)	C14—C15—C16—C17	−0.5 (2)
C1—C6—C7—N1	1.7 (2)	C19—C15—C16—C17	179.79 (14)
C5—C6—C7—N1	−178.92 (14)	C15—C16—C17—C12	−0.4 (2)
C7—N1—C8—C9	−119.58 (14)	C13—C12—C17—C16	1.0 (2)

N1—C8—C9—C20	176.60 (12)	C11—C12—C17—C16	−178.95 (13)
N1—C8—C9—C21	56.91 (17)	C4—C3—C18—N3	−19 (9)
N1—C8—C9—C10	−64.04 (16)	C2—C3—C18—N3	161 (9)
C11—N2—C10—C9	−134.31 (14)	C16—C15—C19—N4	149 (5)
C20—C9—C10—N2	−57.17 (17)	C14—C15—C19—N4	−31 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20*B*···N2	0.96	2.57	2.923 (2)	102
C21—H21*C*···*Cg*1^{i}	0.96	2.95	3.7193 (16)	138

Symmetry code: (i) *x*, *y*, *z*−1.