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(*E*)-*N*-[2-(Biphenyl-4-ylvinyl)phenyl]-furan-2-carboxamide

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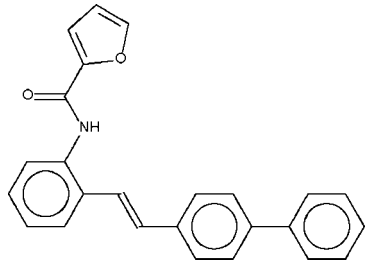
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.106; data-to-parameter ratio = 17.2.

In the title molecule, $C_{25}H_{19}NO_2$, the furyl ring is twisted by 46.3 (1)° with respect to the phenylene ring bearing the amido group. In the stilbene unit, the two phenylene rings (*i.e.* the rings connected through the –CH═CH– fragment) are twisted by 59.2 (1)°; in the biphenylene unit, the two benzene rings are twisted by 35.5 (1)°. In the crystal structure, molecules are linked by an N—H···O_{amido} hydrogen bond into a zigzag chain running along the *c* axis.

Related literature

For the use of radical cations in heterocyclic synthesis, see: Thomas *et al.* (2004, 2008).



Experimental

Crystal data

$C_{25}H_{19}NO_2$ M_r = 365.41
Monoclinic, $P2_1/c$
a = 10.9271 (2) Å
b = 19.7960 (4) Å
c = 8.7969 (1) Å
β = 92.374 (1)°
V = 1901.25 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 (2) K
0.40 × 0.35 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
13179 measured reflections
4356 independent reflections
3681 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.04
4356 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.88	2.05	2.903 (1)	163

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2714).

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supporting information

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(*E*)-*N*-[2-(Biphenyl-4-ylvinyl)phenyl]furan-2-carboxamide

Chin Hui Kee, Noel F. Thomas, Azhar Ariffin, Khalijah Awang and Seik Weng Ng

S1. Comment

In our earlier studies, we reported the synthesis of some stilbene carboxamides whose radical chemistry we investigated (Thomas *et al.*, 2004, 2008). In the present study, we have synthesized a new stilbene carboxamide that incorporates a furan unit (Scheme I, Fig. 1).

S2. Experimental

N-(2-Iodophenyl)furan-2-carboxamide (0.37 g, 1.2 mmol) was dissolved in DMF (20 ml) under a nitrogen atmosphere. The solution was heated to 373 K. Palladium acetate (3.2 mg, 0.014 mmol) was added followed by triethylamine (0.65 ml, 4.7 mmol) and 4-vinylbiphenyl (0.20 g, 1.21 mmol). The mixture was further heated for an hour. The solution was cooled and then mixed with saturated sodium chloride. The organic compound was extracted with ethyl acetate. The ethyl acetate solution was dried with sodium sulfate. The solvent was evaporated and the product purified by column chromatography. Single crystals were obtained by recrystallization from petroleum ether/dichloromethane.

S3. Refinement

Carbon- and nitrogen- bound H-atoms were placed in calculated positions (C—H 0.95, N–H 0.88 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C,N).

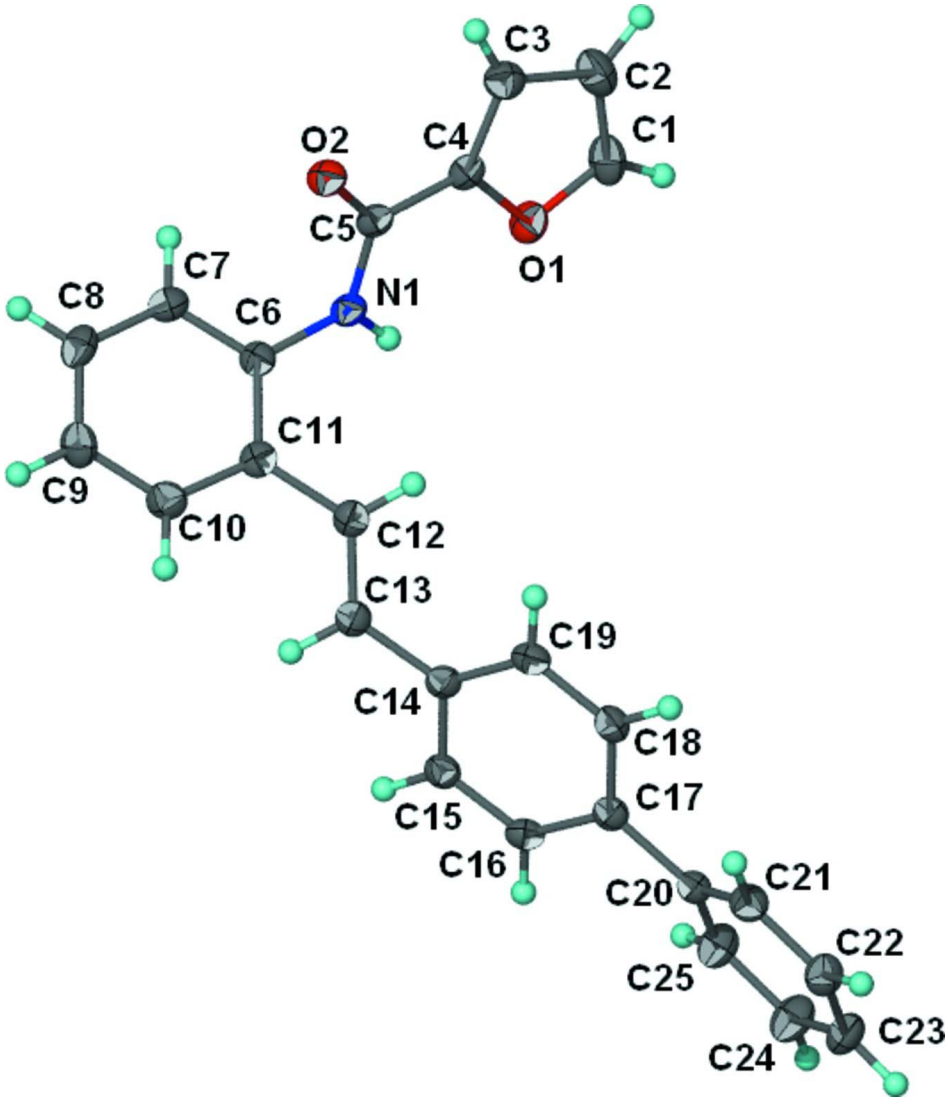

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{25}H_{19}NO_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radiius.

(*E*)-*N*-[2-(Biphenyl-4-ylvinyl)phenyl]furan-2-carboxamide

Crystal data

$C_{25}H_{19}NO_2$
$M_r = 365.41$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.9271\ (2)$ Å
$b = 19.7960\ (4)$ Å
$c = 8.7969\ (1)$ Å
$\beta = 92.374\ (1)°$
$V = 1901.25\ (6)$ Å^3
$Z = 4$

$F(000) = 768$
$D_x = 1.277$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5580 reflections
$\theta = 2.5–28.2°$
$\mu = 0.08$ mm^{-1}
$T = 100$ K
Prism, colorless
0.40 × 0.35 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
13179 measured reflections
4356 independent reflections
3681 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.9°$
$h = -14 \rightarrow 13$
$k = -25 \rightarrow 25$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.106$
$S = 1.04$
4356 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
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.6489P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.69066 (8)	0.17866 (4)	0.88070 (9)	0.0218 (2)
O2	0.56344 (8)	0.18549 (4)	0.50228 (9)	0.01969 (19)
N1	0.52573 (9)	0.25519 (5)	0.70226 (11)	0.0173 (2)
H1	0.5441	0.2651	0.7981	0.021*
C1	0.76833 (12)	0.13051 (7)	0.93850 (15)	0.0263 (3)
H1A	0.8056	0.1316	1.0380	0.032*
C2	0.78542 (12)	0.08127 (7)	0.83672 (16)	0.0274 (3)
H2	0.8347	0.0421	0.8510	0.033*
C3	0.71470 (11)	0.09950 (6)	0.70252 (15)	0.0221 (3)
H3	0.7080	0.0751	0.6096	0.027*
C4	0.65936 (11)	0.15860 (6)	0.73503 (13)	0.0171 (2)
C5	0.57830 (10)	0.20106 (6)	0.63762 (13)	0.0164 (2)
C6	0.44068 (11)	0.29656 (6)	0.61664 (13)	0.0168 (2)
C7	0.34268 (11)	0.26554 (6)	0.53871 (14)	0.0205 (3)
H7	0.3306	0.2183	0.5488	0.025*
C8	0.26273 (11)	0.30299 (7)	0.44657 (14)	0.0228 (3)
H8	0.1971	0.2814	0.3914	0.027*
C9	0.27890 (12)	0.37245 (7)	0.43514 (14)	0.0237 (3)
H9	0.2252	0.3984	0.3707	0.028*
C10	0.37337 (11)	0.40363 (6)	0.51779 (14)	0.0213 (3)
H10	0.3821	0.4513	0.5114	0.026*

C11	0.45663 (11)	0.36676 (6)	0.61073 (13)	0.0172 (2)
C12	0.55685 (11)	0.40039 (6)	0.69725 (13)	0.0176 (2)
H12	0.6298	0.3755	0.7193	0.021*
C13	0.55134 (11)	0.46414 (6)	0.74683 (13)	0.0182 (2)
H13	0.4776	0.4882	0.7240	0.022*
C14	0.64845 (11)	0.50049 (6)	0.83315 (13)	0.0168 (2)
C15	0.61548 (11)	0.55136 (6)	0.93372 (13)	0.0178 (2)
H15	0.5313	0.5613	0.9446	0.021*
C16	0.70291 (11)	0.58746 (6)	1.01760 (13)	0.0179 (2)
H16	0.6778	0.6198	1.0896	0.021*
C17	0.82804 (11)	0.57700 (6)	0.99805 (13)	0.0173 (2)
C18	0.86116 (11)	0.52600 (6)	0.89750 (13)	0.0185 (2)
H18	0.9454	0.5175	0.8830	0.022*
C19	0.77344 (11)	0.48767 (6)	0.81860 (13)	0.0184 (2)
H19	0.7984	0.4523	0.7539	0.022*
C20	0.91995 (11)	0.62106 (6)	1.07784 (13)	0.0177 (2)
C21	1.02722 (11)	0.64044 (6)	1.00799 (14)	0.0204 (3)
H21	1.0433	0.6235	0.9098	0.025*
C22	1.11036 (11)	0.68399 (6)	1.07977 (14)	0.0224 (3)
H22	1.1832	0.6962	1.0312	0.027*
C23	1.08758 (12)	0.70986 (7)	1.22235 (15)	0.0237 (3)
H23	1.1436	0.7405	1.2706	0.028*
C24	0.98214 (13)	0.69059 (7)	1.29408 (15)	0.0274 (3)
H24	0.9665	0.7078	1.3922	0.033*
C25	0.89957 (11)	0.64639 (7)	1.22295 (14)	0.0234 (3)
H25	0.8282	0.6332	1.2735	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0244 (4)	0.0254 (5)	0.0155 (4)	−0.0007 (4)	−0.0020 (3)	0.0003 (3)
O2	0.0252 (4)	0.0194 (4)	0.0144 (4)	0.0002 (3)	−0.0003 (3)	−0.0011 (3)
N1	0.0219 (5)	0.0164 (5)	0.0134 (4)	−0.0005 (4)	−0.0018 (4)	−0.0020 (4)
C1	0.0239 (6)	0.0339 (7)	0.0208 (6)	0.0012 (5)	−0.0029 (5)	0.0074 (5)
C2	0.0232 (6)	0.0279 (7)	0.0311 (7)	0.0034 (5)	0.0011 (5)	0.0086 (6)
C3	0.0225 (6)	0.0205 (6)	0.0236 (6)	−0.0005 (5)	0.0026 (5)	−0.0004 (5)
C4	0.0184 (5)	0.0181 (6)	0.0148 (5)	−0.0039 (4)	0.0013 (4)	0.0001 (4)
C5	0.0177 (5)	0.0147 (5)	0.0168 (5)	−0.0036 (4)	0.0020 (4)	0.0009 (4)
C6	0.0195 (5)	0.0177 (6)	0.0133 (5)	0.0009 (4)	0.0010 (4)	−0.0010 (4)
C7	0.0231 (6)	0.0183 (6)	0.0202 (6)	−0.0015 (5)	0.0011 (5)	−0.0032 (5)
C8	0.0209 (6)	0.0283 (7)	0.0189 (6)	−0.0029 (5)	−0.0021 (5)	−0.0039 (5)
C9	0.0242 (6)	0.0278 (7)	0.0188 (6)	0.0017 (5)	−0.0037 (5)	0.0041 (5)
C10	0.0252 (6)	0.0188 (6)	0.0198 (6)	−0.0007 (5)	0.0005 (5)	0.0030 (5)
C11	0.0199 (5)	0.0188 (6)	0.0131 (5)	−0.0010 (4)	0.0019 (4)	0.0003 (4)
C12	0.0188 (5)	0.0180 (6)	0.0161 (5)	−0.0009 (4)	0.0008 (4)	0.0025 (4)
C13	0.0188 (5)	0.0178 (6)	0.0177 (6)	−0.0010 (4)	0.0002 (4)	0.0016 (4)
C14	0.0202 (6)	0.0132 (5)	0.0170 (5)	−0.0014 (4)	−0.0006 (4)	0.0035 (4)
C15	0.0175 (5)	0.0156 (5)	0.0205 (6)	0.0002 (4)	0.0015 (4)	0.0028 (4)

C16	0.0215 (6)	0.0131 (5)	0.0191 (6)	0.0003 (4)	0.0023 (4)	0.0006 (4)
C17	0.0200 (6)	0.0149 (5)	0.0167 (5)	−0.0002 (4)	−0.0007 (4)	0.0035 (4)
C18	0.0176 (5)	0.0181 (6)	0.0198 (6)	0.0022 (4)	0.0001 (4)	0.0023 (5)
C19	0.0228 (6)	0.0147 (5)	0.0179 (6)	0.0020 (4)	0.0014 (4)	0.0002 (4)
C20	0.0188 (5)	0.0147 (5)	0.0195 (6)	0.0013 (4)	−0.0020 (4)	0.0013 (4)
C21	0.0213 (6)	0.0205 (6)	0.0195 (6)	0.0009 (5)	0.0012 (5)	−0.0007 (5)
C22	0.0194 (6)	0.0239 (6)	0.0240 (6)	−0.0029 (5)	0.0012 (5)	0.0031 (5)
C23	0.0235 (6)	0.0244 (6)	0.0228 (6)	−0.0053 (5)	−0.0039 (5)	−0.0015 (5)
C24	0.0279 (7)	0.0340 (7)	0.0202 (6)	−0.0058 (6)	0.0010 (5)	−0.0061 (5)
C25	0.0216 (6)	0.0280 (7)	0.0208 (6)	−0.0051 (5)	0.0024 (5)	−0.0005 (5)

Geometric parameters (Å, º)

O1—C1	1.3607 (16)	C12—H12	0.9500
O1—C4	1.3714 (14)	C13—C14	1.4676 (16)
O2—C5	1.2340 (14)	C13—H13	0.9500
N1—C5	1.3523 (15)	C14—C15	1.3975 (16)
N1—C6	1.4295 (15)	C14—C19	1.4002 (16)
N1—H1	0.8800	C15—C16	1.3818 (17)
C1—C2	1.342 (2)	C15—H15	0.9500
C1—H1A	0.9500	C16—C17	1.4005 (16)
C2—C3	1.4302 (19)	C16—H16	0.9500
C2—H2	0.9500	C17—C18	1.3996 (17)
C3—C4	1.3528 (17)	C17—C20	1.4845 (16)
C3—H3	0.9500	C18—C19	1.3860 (17)
C4—C5	1.4706 (16)	C18—H18	0.9500
C6—C7	1.3903 (17)	C19—H19	0.9500
C6—C11	1.4019 (16)	C20—C25	1.3979 (17)
C7—C8	1.3825 (18)	C20—C21	1.3994 (16)
C7—H7	0.9500	C21—C22	1.3856 (18)
C8—C9	1.3904 (19)	C21—H21	0.9500
C8—H8	0.9500	C22—C23	1.3869 (18)
C9—C10	1.3832 (18)	C22—H22	0.9500
C9—H9	0.9500	C23—C24	1.3897 (18)
C10—C11	1.4026 (17)	C23—H23	0.9500
C10—H10	0.9500	C24—C25	1.3872 (18)
C11—C12	1.4672 (16)	C24—H24	0.9500
C12—C13	1.3373 (17)	C25—H25	0.9500
C1—O1—C4	105.89 (10)	C12—C13—C14	126.16 (11)
C5—N1—C6	120.70 (10)	C12—C13—H13	116.9
C5—N1—H1	119.6	C14—C13—H13	116.9
C6—N1—H1	119.6	C15—C14—C19	117.80 (11)
C2—C1—O1	111.19 (11)	C15—C14—C13	118.76 (10)
C2—C1—H1A	124.4	C19—C14—C13	123.43 (11)
O1—C1—H1A	124.4	C16—C15—C14	121.34 (11)
C1—C2—C3	106.39 (12)	C16—C15—H15	119.3
C1—C2—H2	126.8	C14—C15—H15	119.3

C3—C2—H2	126.8	C15—C16—C17	120.99 (11)
C4—C3—C2	105.94 (12)	C15—C16—H16	119.5
C4—C3—H3	127.0	C17—C16—H16	119.5
C2—C3—H3	127.0	C18—C17—C16	117.61 (11)
C3—C4—O1	110.59 (11)	C18—C17—C20	122.35 (10)
C3—C4—C5	129.40 (11)	C16—C17—C20	119.99 (10)
O1—C4—C5	119.99 (10)	C19—C18—C17	121.32 (11)
O2—C5—N1	124.22 (11)	C19—C18—H18	119.3
O2—C5—C4	118.13 (10)	C17—C18—H18	119.3
N1—C5—C4	117.65 (10)	C18—C19—C14	120.80 (11)
C7—C6—C11	120.92 (11)	C18—C19—H19	119.6
C7—C6—N1	118.52 (10)	C14—C19—H19	119.6
C11—C6—N1	120.55 (10)	C25—C20—C21	118.08 (11)
C8—C7—C6	120.50 (11)	C25—C20—C17	120.81 (10)
C8—C7—H7	119.8	C21—C20—C17	121.06 (10)
C6—C7—H7	119.8	C22—C21—C20	121.05 (11)
C7—C8—C9	119.57 (12)	C22—C21—H21	119.5
C7—C8—H8	120.2	C20—C21—H21	119.5
C9—C8—H8	120.2	C21—C22—C23	120.20 (11)
C10—C9—C8	119.85 (12)	C21—C22—H22	119.9
C10—C9—H9	120.1	C23—C22—H22	119.9
C8—C9—H9	120.1	C22—C23—C24	119.50 (12)
C9—C10—C11	121.74 (11)	C22—C23—H23	120.2
C9—C10—H10	119.1	C24—C23—H23	120.2
C11—C10—H10	119.1	C25—C24—C23	120.29 (12)
C6—C11—C10	117.32 (11)	C25—C24—H24	119.9
C6—C11—C12	121.45 (11)	C23—C24—H24	119.9
C10—C11—C12	121.22 (11)	C24—C25—C20	120.85 (11)
C13—C12—C11	123.68 (11)	C24—C25—H25	119.6
C13—C12—H12	118.2	C20—C25—H25	119.6
C11—C12—H12	118.2		

C4—O1—C1—C2	−0.80 (14)	C10—C11—C12—C13	28.50 (17)
O1—C1—C2—C3	0.80 (15)	C11—C12—C13—C14	−179.77 (10)
C1—C2—C3—C4	−0.48 (14)	C12—C13—C14—C15	−150.97 (12)
C2—C3—C4—O1	0.00 (14)	C12—C13—C14—C19	30.06 (18)
C2—C3—C4—C5	178.41 (11)	C19—C14—C15—C16	−0.73 (17)
C1—O1—C4—C3	0.47 (13)	C13—C14—C15—C16	−179.76 (10)
C1—O1—C4—C5	−178.11 (10)	C14—C15—C16—C17	3.81 (17)
C6—N1—C5—O2	4.14 (17)	C15—C16—C17—C18	−3.75 (17)
C6—N1—C5—C4	−176.54 (10)	C15—C16—C17—C20	173.84 (10)
C3—C4—C5—O2	−6.48 (18)	C16—C17—C18—C19	0.74 (17)
O1—C4—C5—O2	171.80 (10)	C20—C17—C18—C19	−176.79 (11)
C3—C4—C5—N1	174.16 (12)	C17—C18—C19—C14	2.28 (18)
O1—C4—C5—N1	−7.56 (15)	C15—C14—C19—C18	−2.28 (17)
C5—N1—C6—C7	51.61 (15)	C13—C14—C19—C18	176.70 (11)
C5—N1—C6—C11	−127.90 (12)	C18—C17—C20—C25	−148.23 (12)
C11—C6—C7—C8	3.72 (17)	C16—C17—C20—C25	34.29 (17)

N1—C6—C7—C8	−175.79 (10)	C18—C17—C20—C21	34.12 (17)
C6—C7—C8—C9	−1.66 (18)	C16—C17—C20—C21	−143.35 (12)
C7—C8—C9—C10	−1.08 (18)	C25—C20—C21—C22	−0.62 (18)
C8—C9—C10—C11	1.85 (18)	C17—C20—C21—C22	177.09 (11)
C7—C6—C11—C10	−2.91 (16)	C20—C21—C22—C23	−0.77 (19)
N1—C6—C11—C10	176.59 (10)	C21—C22—C23—C24	1.4 (2)
C7—C6—C11—C12	177.55 (10)	C22—C23—C24—C25	−0.7 (2)
N1—C6—C11—C12	−2.95 (16)	C23—C24—C25—C20	−0.7 (2)
C9—C10—C11—C6	0.14 (17)	C21—C20—C25—C24	1.35 (19)
C9—C10—C11—C12	179.68 (11)	C17—C20—C25—C24	−176.37 (12)
C6—C11—C12—C13	−151.98 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.88	2.05	2.903 (1)	163

Symmetry code: (i) *x*, −*y*+1/2, *z*+1/2.