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Crystal structure of *N*-(2-benzoyl-5-ethynylphenyl)-quinoline-2-carboxamide

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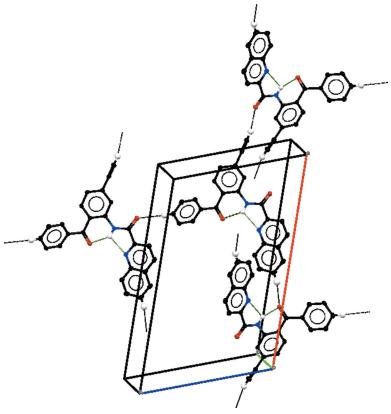
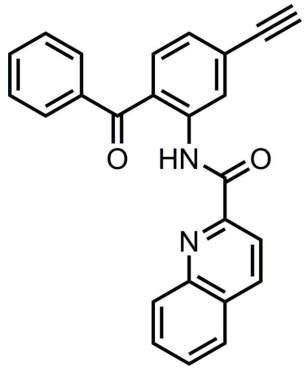
In the title compound, $C_{25}H_{16}N_2O_2$, the quinoline ring system is essentially planar, with a maximum deviation of 0.030 (1) Å, and forms a dihedral angle of 20.9 (1)° with benzoyl benzene ring. The unsubstituted phenyl ring forms dihedral angles of 52.7 (1)° with the quinoline ring system and 54.1 (1)° with the ethynyl-substituted benzene ring. The molecule contains an intramolecular bifurcated N—H···(O,N) hydrogen bond, forming *S*(5) and *S*(6) rings, which may influence the conformation of the molecule. In the crystal, weak C—H···O hydrogen bonds link the molecules into a three-dimensional network. In addition, the three-dimensional structure contains π–π stacking interactions, with centroid–centroid distances of 3.695 (1) and 3.751 (1) Å.

1. Chemical context

Benzophenones are intermediates for the synthesis of pharmaceutical and bioactive materials and are used extensively in the field of medicinal chemistry. The biological activity of these ligands can be attributed to distinct chemical and biochemical advantages: they are chemically more stable than diazo esters, aryl azides and diazirines, and can be manipulated in ambient light and can be activated at 350–360 nm, avoiding protein-damaging wavelengths. These properties produce highly efficient covalent modifications of macromolecules, frequently with remarkable specificity (Dormán & Prestwich, 1994). Several benzophenones are used in industry, cosmetics, medicine and agriculture (Sweetman *et al.*, 2007), and their role as potential anticancer agents and antibiotics has also been examined. In addition, research has been performed on the use of benzophenones as modulators of GABAA receptors (Kopanitsa *et al.*, 2002), COX-1/COX-2 inhibitors (Dannhardt *et al.*, 2002) and EGFR/erbB2 dual inhibitors (Zhang *et al.*, 2004).





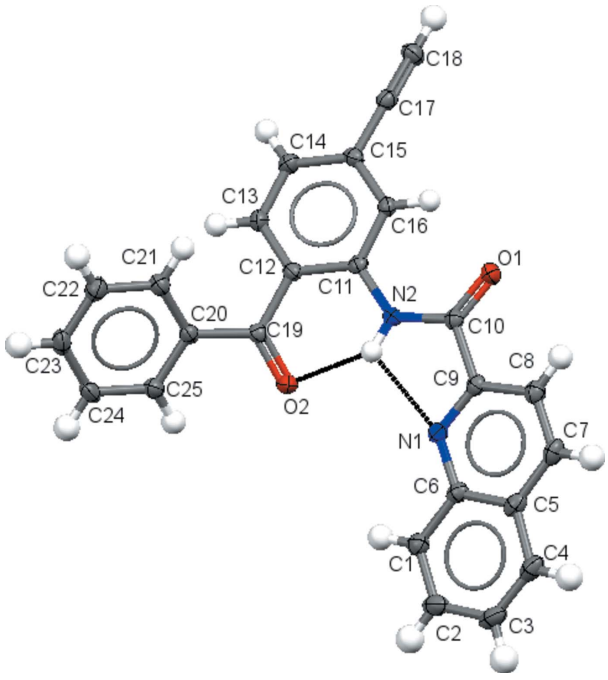


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. Hydrogen bonds are shown as dotted lines.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The quinoline ring system (C1–C9/N1) is essentially planar, with a maximum deviation of 0.030 (1) for C8 and forms a dihedral angle of 20.9 (1)° with ethynyl-substituted benzene ring (C11–C16). The benzoyl ring (C20–C25) forms dihedral angles of 52.7 (1)° with the quinoline ring system and 54.1 (1)° with the ethynyl-substituted benzene ring. The molecule contains an intramolecular bifurcated N—H···(N,O) hydrogen bond (see Table 1), forming *S*(5) and *S*(6) rings, which may influence the conformation of the molecule.

3. Supramolecular features

In the crystal, weak C—H···O hydrogen bonds (Table 1, Fig. 2) link the molecules into a three-dimensional network. In addition, the three-dimensional structure contains π–π stacking interactions with centroid–centroid distances of 3.695 (1) Å for $Cg1\cdots Cg2(x, \frac{3}{2}-y, -\frac{1}{2}+z)$ and 3.751 (1) Å for $Cg3\cdots Cg3(1-x, 1-y, -z)$ where *Cg*1, *Cg*2 and *Cg*3 are the centroids of the C11–C16, C20–C25 and C1–C6 rings, respectively.

4. Database survey

A search of the Cambridge Structural Database (Groom *et al.*, 2016; Version 1.18, April 2016) revealed 12 related structures. There are three reports for (4-ethynylphenyl)(phenyl)-methanone derivatives with different substituents (Szafert *et al.* 2008, 2012; Khera *et al.* 2012). There are two reports where *N*-(2-benzoylphenyl)quinoline-2-carboxamide moieties are reported (Maurizot *et al.* 2004; Hu *et al.* 2009) and seven reports for 3-ethynylaniline derivatives (Li *et al.* 2012; Cummings *et al.* 2010; Khan *et al.* 2003; Dominguez *et al.* 2003; Wang *et al.* 2003; Yi *et al.* 2008; Armitt *et al.* 2008).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2	0.86	2.03	2.701 (12)	135
N2—H2···N1	0.86	2.24	2.658 (13)	110
C3—H3···O2^{i}	0.93	2.47	3.346 (16)	158
C18—H18···O1^{ii}	0.93	2.33	3.242 (15)	167
C23—H23···O1^{iii}	0.93	2.56	3.476 (14)	168

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

5. Synthesis and crystallization

The title compound was prepared using 3-bromoaniline (**1**, Fig. 3) as starting reagent in the presence of boron trichloride (1.1 equiv), $AlCl_3$ (1.1 equiv) and benzonitrile (3 equiv) for 24 h at approximately 353 K. The solution was extracted with DCM, dried and concentrated to obtain (2-amino-4-bromophenyl)(phenyl)methanone (**2**) (petroleum ether:ethyl acetate 9:1, 0.52). Compound **2** (1.8 mmol) was dissolved in triethylamine, $Pd(PPh_3)_2Cl_2$ (0.05 eq), trimethylsilylacetylene (1.5 eq) and copper iodine (0.1 eq) were added and the solution was heated to approximately 343 K overnight. The organic phase

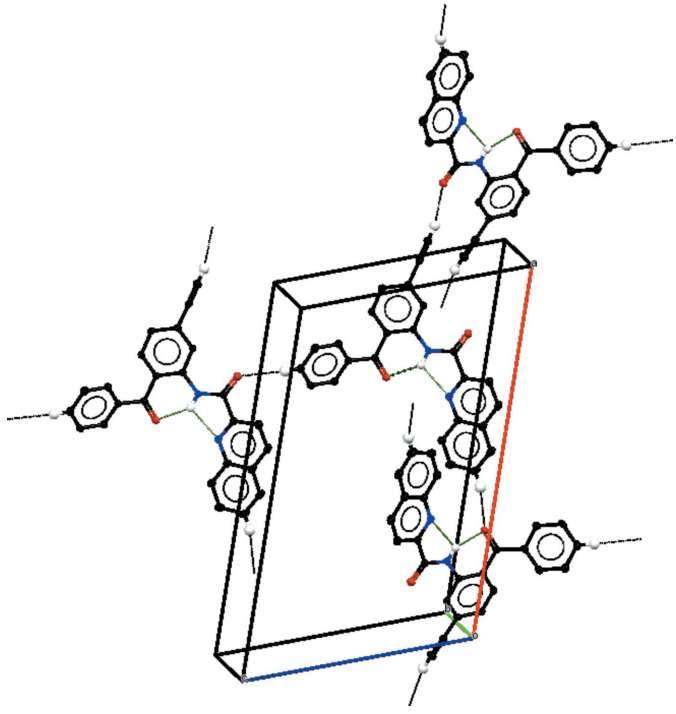


Figure 2
A partial packing diagram of the title compound, viewed approximately along the *b* axis, with intermolecular hydrogen bonds shown as black dotted lines and intramolecular hydrogen bonds shown as green dotted lines.

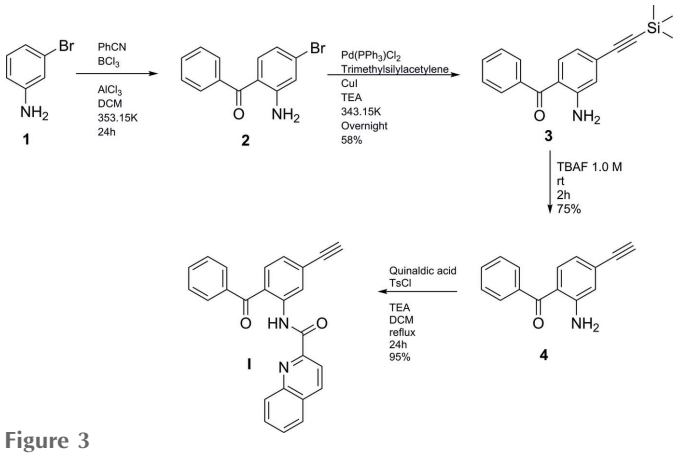


Figure 3
The reaction scheme for the synthesis of the title compound.

was separated and concentrated (petroleum ether:ethyl acetate 7:1, 0.70) and the fraction containing the product (75%) was collected and used for the next step. A solution of compound **3** (0.4 mol, 1 eq) in tetrahydrofurane was stirred and cooled in an ice bath, tetra-*n*-butylammonium fluoride (1.5 eq) was added and the reaction was stirred for two hours. The organic layer was separated and dried over magnesium sulfate to obtain compound **4** (petroleum ether:ethyl acetate 7:1, 0.60). The title compound (I) (Fig. 3) was prepared by refluxing a mixture of quinaldic acid, triethylamine, *p*-toluenesulfonyl chloride and compound **4** for 24 h in dichloromethane. After evaporation of the CH_2Cl_2, the compound was purified by silica column chromatography (petroleum ether:ethyl acetate 7:1, 0.36). Single colourless block-shaped crystals of (I) were obtained by slow evaporation in dichloromethane in a closed flask with petroleum ether.

***N*-(2-benzoyl-5-ethynylphenyl)quinoline-2-carboxamide (I):** Colourless solid (0.323 g, 95%, PE:EA 7:1, R_f = 0.36). **^{1}H NMR (400 MHz, $CDCl_3$)**: δ 9.11 (*d*, ^3J = 1.4 Hz, 1H), 8.41 (*m*, 3H), 7.89 (*d*, ^3J = 8.2 Hz, 1H), 7.84 (*m*, 3H), 7.67 (*m*, 1H), 7.60 (*m*, 2H), 7.50 (*dd*, ^3J = 10.4, ^3J = 4.6 Hz, 2H), 7.28 (*m*, 1H), 3.27 (*s*, 1H, CCH). **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 198.0 (C_{quat}), 163.7 (C_{quat}), 149.6 (C_{quat}), 146.6 (C_{quat}), 139.7 (C_{quat}), 138.6 (C_{quat}), 137.6 (C_{quat}), 133.1 (+), 132.5 (+), 130.5 (+), 130.2 (+), 129.9 (+), 129.4 (+), 128.3 (+), 127.6 (+), 125.8 (+), 124.8 (+), 118.4 (+), 82.8 (C_{quat}), 80.3 (+).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All non-hydrogen atoms were refined anisotropically. Hydrogen-atom positions were calculated geometrically and refined using the riding model: N—H = 0.86 Å and C—H = 0.93 Å with U_{iso}(H) = 1.2U_{eq}(C,N).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{16}N_2O_2$
M_r	376.40
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	123
a, *b*, *c* (Å)	20.2686 (3), 7.58016 (11), 12.6109 (2)
β (°)	107.6002 (17)
V (Å^3)	1846.84 (5)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.70
Crystal size (mm)	0.20 × 0.12 × 0.08
Data collection	
Diffractometer	Rigaku Oxfor Diffraction Super-Nova, Single source at offset, Atlas
Absorption correction	Analytical (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.923, 0.964
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14681, 3484, 3170
R_{int}	0.020
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.612
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.092, 1.05
No. of reflections	3484
No. of parameters	262
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.25

Computer programs: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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Crystal structure of *N*-(2-benzoyl-5-ethynylphenyl)quinoline-2-carboxamide

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Computing details

Data collection: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); cell refinement: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); data reduction: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

N-(2-Benzoyl-5-ethynylphenyl)quinoline-2-carboxamide

Crystal data

$C_{25}H_{16}N_2O_2$
M_r = 376.40
Monoclinic, $P2_1/c$
a = 20.2686 (3) Å
b = 7.58016 (11) Å
c = 12.6109 (2) Å
β = 107.6002 (17)°
V = 1846.84 (5) Å^3
Z = 4
$F(000)$ = 784
D_x = 1.354 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 8847 reflections
θ = 4.6–70.5°
μ = 0.70 mm^{-1}
T = 123 K
Block, colourless
0.20 × 0.12 × 0.08 mm

Data collection

Rigaku Oxfor Diffraction SuperNova, Single source at offset, Atlas diffractometer
Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 5.1773 pixels mm^{-1}
ω scans
Absorption correction: analytical (CrysAlis PRO; Rigaku Oxford Diffraction, 2015)
T_{min} = 0.923, T_{max} = 0.964
14681 measured reflections
3484 independent reflections
3170 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 70.6°, θ_{min} = 4.6°
h = −24→24
k = −9→8
l = −15→15

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.05
3484 reflections
262 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.6041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.80756 (4)	0.44245 (12)	0.17559 (6)	0.0251 (2)
O2	0.71578 (4)	0.59252 (12)	0.48953 (6)	0.0252 (2)
N2	0.77463 (5)	0.50473 (13)	0.33109 (7)	0.0187 (2)
H2	0.7400	0.4943	0.3565	0.022*
N1	0.64362 (5)	0.43688 (13)	0.21772 (8)	0.0204 (2)
C11	0.83488 (5)	0.57608 (14)	0.40482 (9)	0.0176 (2)
C12	0.83608 (5)	0.61666 (15)	0.51504 (9)	0.0185 (2)
C10	0.76382 (6)	0.45000 (15)	0.22485 (9)	0.0192 (2)
C15	0.95056 (5)	0.69688 (15)	0.44286 (9)	0.0196 (2)
C16	0.89330 (5)	0.61127 (15)	0.37169 (9)	0.0188 (2)
H16	0.8940	0.5772	0.3012	0.023*
C20	0.78417 (6)	0.55345 (15)	0.67512 (9)	0.0195 (2)
C9	0.69003 (6)	0.39498 (15)	0.16801 (9)	0.0197 (2)
C19	0.77474 (6)	0.58849 (15)	0.55491 (9)	0.0195 (2)
C6	0.57653 (6)	0.38875 (15)	0.16679 (9)	0.0214 (2)
C13	0.89513 (6)	0.69693 (16)	0.58579 (9)	0.0214 (2)
H13	0.8965	0.7225	0.6585	0.026*
C14	0.95156 (6)	0.73953 (16)	0.55107 (9)	0.0224 (2)
H14	0.9897	0.7959	0.5991	0.027*
C25	0.73004 (6)	0.59635 (16)	0.71778 (10)	0.0234 (3)
H25	0.6904	0.6510	0.6726	0.028*
C5	0.55645 (6)	0.29271 (16)	0.06529 (9)	0.0244 (3)
C21	0.84242 (6)	0.46767 (16)	0.74319 (9)	0.0231 (3)
H21	0.8786	0.4383	0.7154	0.028*
C1	0.52563 (6)	0.43856 (17)	0.21699 (10)	0.0259 (3)
H1	0.5383	0.5024	0.2830	0.031*
C8	0.67500 (6)	0.30330 (16)	0.06614 (10)	0.0244 (3)
H8	0.7096	0.2795	0.0338	0.029*
C23	0.79376 (6)	0.47211 (18)	0.89465 (10)	0.0281 (3)
H23	0.7972	0.4462	0.9682	0.034*
C22	0.84671 (6)	0.42576 (17)	0.85222 (10)	0.0268 (3)
H22	0.8853	0.3664	0.8968	0.032*
C4	0.48571 (6)	0.24644 (17)	0.01817 (11)	0.0302 (3)
H4	0.4719	0.1823	−0.0477	0.036*
C24	0.73547 (6)	0.55729 (18)	0.82745 (10)	0.0276 (3)
H24	0.6999	0.5883	0.8562	0.033*
C7	0.60855 (6)	0.25045 (17)	0.01627 (10)	0.0274 (3)
H7	0.5976	0.1868	−0.0498	0.033*
C2	0.45806 (6)	0.39319 (19)	0.16885 (11)	0.0319 (3)

H2A	0.4250	0.4271	0.2023	0.038*
C3	0.43768 (6)	0.29527 (19)	0.06876 (11)	0.0337 (3)
H3	0.3915	0.2641	0.0373	0.040*
C17	1.00703 (6)	0.75029 (16)	0.40188 (9)	0.0220 (2)
C18	1.05212 (6)	0.80433 (17)	0.37023 (10)	0.0274 (3)
H18	1.0878	0.8471	0.3452	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0219 (4)	0.0344 (5)	0.0207 (4)	−0.0005 (3)	0.0087 (3)	−0.0044 (3)
O2	0.0171 (4)	0.0381 (5)	0.0206 (4)	0.0014 (3)	0.0060 (3)	0.0014 (3)
N2	0.0165 (4)	0.0236 (5)	0.0170 (4)	−0.0014 (4)	0.0064 (3)	−0.0008 (4)
N1	0.0194 (5)	0.0217 (5)	0.0190 (5)	−0.0017 (4)	0.0041 (4)	0.0008 (4)
C11	0.0170 (5)	0.0171 (5)	0.0179 (5)	0.0015 (4)	0.0041 (4)	0.0014 (4)
C12	0.0178 (5)	0.0205 (6)	0.0179 (5)	0.0017 (4)	0.0063 (4)	0.0016 (4)
C10	0.0202 (5)	0.0186 (5)	0.0186 (5)	0.0011 (4)	0.0055 (4)	0.0005 (4)
C15	0.0172 (5)	0.0210 (6)	0.0217 (5)	0.0014 (4)	0.0075 (4)	0.0018 (4)
C16	0.0194 (5)	0.0210 (6)	0.0165 (5)	0.0011 (4)	0.0063 (4)	0.0010 (4)
C20	0.0199 (5)	0.0208 (6)	0.0191 (5)	−0.0039 (4)	0.0077 (4)	−0.0033 (4)
C9	0.0208 (5)	0.0187 (5)	0.0186 (5)	0.0006 (4)	0.0043 (4)	0.0015 (4)
C19	0.0189 (5)	0.0199 (6)	0.0202 (5)	0.0004 (4)	0.0067 (4)	−0.0018 (4)
C6	0.0201 (5)	0.0208 (6)	0.0211 (5)	−0.0016 (4)	0.0029 (4)	0.0042 (4)
C13	0.0214 (5)	0.0263 (6)	0.0167 (5)	−0.0004 (4)	0.0061 (4)	−0.0024 (4)
C14	0.0184 (5)	0.0260 (6)	0.0215 (5)	−0.0028 (4)	0.0042 (4)	−0.0028 (5)
C25	0.0199 (5)	0.0284 (6)	0.0226 (6)	−0.0028 (5)	0.0077 (4)	−0.0042 (5)
C5	0.0252 (6)	0.0218 (6)	0.0219 (6)	−0.0031 (5)	0.0008 (5)	0.0028 (5)
C21	0.0228 (5)	0.0257 (6)	0.0220 (6)	−0.0003 (5)	0.0087 (4)	−0.0013 (5)
C1	0.0232 (6)	0.0305 (7)	0.0229 (6)	−0.0013 (5)	0.0053 (5)	0.0036 (5)
C8	0.0269 (6)	0.0245 (6)	0.0215 (6)	0.0009 (5)	0.0071 (5)	−0.0022 (5)
C23	0.0329 (6)	0.0345 (7)	0.0179 (5)	−0.0118 (5)	0.0093 (5)	−0.0020 (5)
C22	0.0281 (6)	0.0292 (6)	0.0211 (6)	−0.0022 (5)	0.0042 (5)	0.0020 (5)
C4	0.0283 (6)	0.0300 (7)	0.0255 (6)	−0.0077 (5)	−0.0020 (5)	0.0010 (5)
C24	0.0250 (6)	0.0376 (7)	0.0247 (6)	−0.0076 (5)	0.0144 (5)	−0.0079 (5)
C7	0.0321 (6)	0.0253 (6)	0.0210 (6)	−0.0031 (5)	0.0025 (5)	−0.0049 (5)
C2	0.0206 (6)	0.0410 (8)	0.0335 (7)	−0.0012 (5)	0.0073 (5)	0.0082 (6)
C3	0.0212 (6)	0.0391 (8)	0.0341 (7)	−0.0080 (5)	−0.0017 (5)	0.0083 (6)
C17	0.0203 (5)	0.0231 (6)	0.0206 (5)	−0.0006 (4)	0.0034 (4)	−0.0037 (4)
C18	0.0260 (6)	0.0315 (7)	0.0282 (6)	−0.0048 (5)	0.0134 (5)	−0.0042 (5)

Geometric parameters (Å, º)

O1—C10	1.2282 (14)	C14—H14	0.9300
O2—C19	1.2301 (14)	C25—H25	0.9300
N2—H2	0.8600	C25—C24	1.3858 (17)
N2—C11	1.4006 (14)	C5—C4	1.4200 (16)
N2—C10	1.3555 (14)	C5—C7	1.4124 (17)
N1—C9	1.3174 (15)	C21—H21	0.9300

N1—C6	1.3661 (14)	C21—C22	1.3881 (16)
C11—C12	1.4167 (15)	C1—H1	0.9300
C11—C16	1.3952 (15)	C1—C2	1.3637 (17)
C12—C19	1.4907 (15)	C8—H8	0.9300
C12—C13	1.3975 (16)	C8—C7	1.3630 (17)
C10—C9	1.5087 (15)	C23—H23	0.9300
C15—C16	1.3942 (15)	C23—C22	1.3816 (18)
C15—C14	1.3965 (16)	C23—C24	1.3876 (18)
C15—C17	1.4487 (15)	C22—H22	0.9300
C16—H16	0.9300	C4—H4	0.9300
C20—C19	1.4932 (15)	C4—C3	1.367 (2)
C20—C25	1.3984 (15)	C24—H24	0.9300
C20—C21	1.3932 (16)	C7—H7	0.9300
C9—C8	1.4104 (16)	C2—H2A	0.9300
C6—C5	1.4209 (17)	C2—C3	1.414 (2)
C6—C1	1.4152 (17)	C3—H3	0.9300
C13—H13	0.9300	C17—C18	1.1759 (17)
C13—C14	1.3810 (16)	C18—H18	0.9300

C11—N2—H2	115.8	C24—C25—C20	119.96 (11)
C10—N2—H2	115.8	C24—C25—H25	120.0
C10—N2—C11	128.49 (9)	C4—C5—C6	118.79 (11)
C9—N1—C6	117.66 (10)	C7—C5—C6	117.52 (10)
N2—C11—C12	119.21 (9)	C7—C5—C4	123.69 (11)
C16—C11—N2	121.57 (10)	C20—C21—H21	119.8
C16—C11—C12	119.21 (10)	C22—C21—C20	120.31 (11)
C11—C12—C19	122.09 (10)	C22—C21—H21	119.8
C13—C12—C11	118.56 (10)	C6—C1—H1	119.9
C13—C12—C19	119.19 (10)	C2—C1—C6	120.23 (12)
O1—C10—N2	126.05 (10)	C2—C1—H1	119.9
O1—C10—C9	120.68 (10)	C9—C8—H8	120.8
N2—C10—C9	113.27 (9)	C7—C8—C9	118.44 (11)
C16—C15—C14	120.01 (10)	C7—C8—H8	120.8
C16—C15—C17	119.61 (10)	C22—C23—H23	120.0
C14—C15—C17	120.28 (10)	C22—C23—C24	119.96 (11)
C11—C16—H16	119.6	C24—C23—H23	120.0
C15—C16—C11	120.85 (10)	C21—C22—H22	119.9
C15—C16—H16	119.6	C23—C22—C21	120.14 (11)
C25—C20—C19	118.34 (10)	C23—C22—H22	119.9
C21—C20—C19	122.21 (10)	C5—C4—H4	119.7
C21—C20—C25	119.26 (10)	C3—C4—C5	120.62 (12)
N1—C9—C10	117.07 (10)	C3—C4—H4	119.7
N1—C9—C8	124.31 (10)	C25—C24—C23	120.33 (11)
C8—C9—C10	118.62 (10)	C25—C24—H24	119.8
O2—C19—C12	120.71 (10)	C23—C24—H24	119.8
O2—C19—C20	119.02 (10)	C5—C7—H7	120.1
C12—C19—C20	120.27 (9)	C8—C7—C5	119.78 (11)
N1—C6—C5	122.26 (11)	C8—C7—H7	120.1

N1—C6—C1	118.36 (10)	C1—C2—H2A	119.6
C1—C6—C5	119.38 (10)	C1—C2—C3	120.85 (12)
C12—C13—H13	119.0	C3—C2—H2A	119.6
C14—C13—C12	122.08 (10)	C4—C3—C2	120.12 (11)
C14—C13—H13	119.0	C4—C3—H3	119.9
C15—C14—H14	120.4	C2—C3—H3	119.9
C13—C14—C15	119.14 (10)	C18—C17—C15	175.81 (13)
C13—C14—H14	120.4	C17—C18—H18	180.0
C20—C25—H25	120.0		

O1—C10—C9—N1	−167.73 (11)	C19—C12—C13—C14	−174.75 (11)
O1—C10—C9—C8	12.16 (17)	C19—C20—C25—C24	176.64 (11)
N2—C11—C12—C19	−0.98 (16)	C19—C20—C21—C22	−175.07 (11)
N2—C11—C12—C13	−176.45 (10)	C6—N1—C9—C10	179.62 (9)
N2—C11—C16—C15	174.15 (10)	C6—N1—C9—C8	−0.27 (17)
N2—C10—C9—N1	12.51 (15)	C6—C5—C4—C3	0.81 (18)
N2—C10—C9—C8	−167.60 (10)	C6—C5—C7—C8	−0.59 (18)
N1—C9—C8—C7	−1.52 (18)	C6—C1—C2—C3	0.3 (2)
N1—C6—C5—C4	179.47 (11)	C13—C12—C19—O2	148.36 (11)
N1—C6—C5—C7	−1.25 (17)	C13—C12—C19—C20	−32.13 (16)
N1—C6—C1—C2	179.99 (11)	C14—C15—C16—C11	3.68 (17)
C11—N2—C10—O1	5.23 (19)	C25—C20—C19—O2	−25.56 (16)
C11—N2—C10—C9	−175.02 (10)	C25—C20—C19—C12	154.92 (11)
C11—C12—C19—O2	−27.08 (17)	C25—C20—C21—C22	−0.18 (17)
C11—C12—C19—C20	152.43 (11)	C5—C6—C1—C2	0.63 (18)
C11—C12—C13—C14	0.85 (17)	C5—C4—C3—C2	0.2 (2)
C12—C11—C16—C15	−4.60 (16)	C21—C20—C19—O2	149.37 (11)
C12—C13—C14—C15	−1.80 (18)	C21—C20—C19—C12	−30.15 (16)
C10—N2—C11—C12	−176.82 (11)	C21—C20—C25—C24	1.56 (17)
C10—N2—C11—C16	4.43 (18)	C1—C6—C5—C4	−1.20 (17)
C10—C9—C8—C7	178.59 (11)	C1—C6—C5—C7	178.08 (11)
C16—C11—C12—C19	177.81 (10)	C1—C2—C3—C4	−0.7 (2)
C16—C11—C12—C13	2.34 (16)	C22—C23—C24—C25	−0.03 (19)
C16—C15—C14—C13	−0.46 (17)	C4—C5—C7—C8	178.64 (12)
C20—C25—C24—C23	−1.46 (19)	C24—C23—C22—C21	1.41 (19)
C20—C21—C22—C23	−1.30 (19)	C7—C5—C4—C3	−178.42 (12)
C9—N1—C6—C5	1.67 (16)	C17—C15—C16—C11	−172.73 (10)
C9—N1—C6—C1	−177.67 (10)	C17—C15—C14—C13	175.94 (11)
C9—C8—C7—C5	1.89 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2	0.86	2.03	2.701 (12)	135
N2—H2···N1	0.86	2.24	2.658 (13)	110
C3—H3···O2^{i}	0.93	2.47	3.346 (16)	158

C18—H18···O1^{ii}	0.93	2.33	3.242 (15)	167
C23—H23···O1^{iii}	0.93	2.56	3.476 (14)	168

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