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1-[(2-Methyl-8-quinolyl)aminomethylene]naphthalen-2(1*H*)-one

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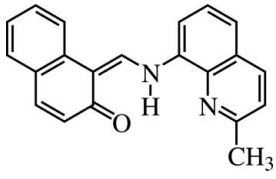
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.127; data-to-parameter ratio = 20.5.

The molecule of the title compound, $C_{21}H_{16}N_2O$, exists in the keto form and the C=O and N—H bonds are mutually *cis* in the crystal structure, although an enol form would be possible through tautomerism. The dihedral angle between the quinoline and the naphthalene systems is 22.04 (2)°. A bifurcated intramolecular N—H···(O,N) hydrogen bond is present.

Related literature

The title compound was prepared and the structure determined, to explore the substituent effects on the fluorescence of metal complexes of 2-hydroxy-1-naphthaldehydene-8-aminoquinoline (II), a fluorescent reagent for molybdenum (Jiang *et al.*, 2001) and beryllium (Jiang & He, 2003). For the structure of (II), see: Sakane *et al.* (2006). For the structures of its metal complexes with technetium, vanadium and tin, see: Tisato *et al.* (1990), Asgedom *et al.* (1996) and Takano & Shibahara (2008), respectively.



Experimental

Crystal data

$C_{21}H_{16}N_2O$ M_r = 312.37
Monoclinic, $P2_1/c$
a = 10.6300 (19) Å
b = 15.0760 (17) Å
c = 10.9853 (17) Å
β = 117.111 (7)°
V = 1567.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 93 K
0.63 × 0.56 × 0.32 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.950, T_{max} = 0.975
17775 measured reflections
4478 independent reflections
4145 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.127
S = 1.01
4478 reflections
218 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H8···O1	0.95	1.86	2.6094 (11)	133
N1—H8···N2	0.95	2.28	2.6714 (14)	104

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*); data reduction: *CrystalStructure* (Rigaku, 2007); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure*; software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2016).

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supporting information

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1-[(2-Methyl-8-quinolyl)aminomethylene]naphthalen-2(1*H*)-one

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S1. Comment

In the present work, the title compound, 2-hydroxy-1-naphthaldehydene-8-amino-2-methylquinoline ($C_{21}H_{16}N_2O$) (I) was prepared and the structure determined, to explore the substituent effects on the fluorescence of metal complexes of 2-hydroxy-1-naphthaldehydene-8-aminoquinoline ($C_{20}H_{14}N_2O$) (II) (Sakane *et al.*, 2006). Compound (II) has been reported as a fluorescent reagent for molybdenum (Jiang *et al.*, 2001) and beryllium (Jiang & He, 2003). The X-ray structures of (II) (Sakane *et al.*, 2006) and its metal complexes with technetium (Tisato *et al.*, 1990), vanadium (Asgedom *et al.*, 1996), and tin (Takano & Shibahara, 2008) have been determined. The molecule of (I) (Fig. 1) exists in the keto form and the C═O and N—H bonds are mutually *cis* which is similar to that found in the structure of (II). In the structure of (I), N—H···$O_{carbonyl}$ and N—H···$N_{pyridine}$ intramolecular hydrogen bonds exist (Table 1) but there is no evidence of formal intermolecular hydrogen-bonding associations (Fig. 2).

S2. Experimental

A suspension of 8-amino-2-methylquinoline (158 mg, 1.0 mmol) and 2-hydroxy-1-naphthaldehyde (172 mg, mmol) in methanol (5 ml) was refluxed at 65°C for three hours. The resultant orange solution was ice-cooled to give an orange powder, which was washed with ice-cooled ethyl acetate: yield 262 mg. For recrystallization, the orange powder was dissolved in toluene (5 ml) at 60°C and kept overnight. Crystals were collected after cooling to room temperature. Yield 205 mg (66%). Anal. found: C, 80.53; H, 5.10; N, 8.95%. Calc. for $C_{21}H_{16}N_2O$: C, 80.75; H, 5.16; N, 8.97%

S3. Refinement

The positions of all H atoms were located from difference maps and refined with restrained distances (N—H, 0.86 Å; C—H, 0.95 Å). The isotropic displacement parameters for these atoms were fixed at $1.2U_{eq}$ of their carrier atoms.

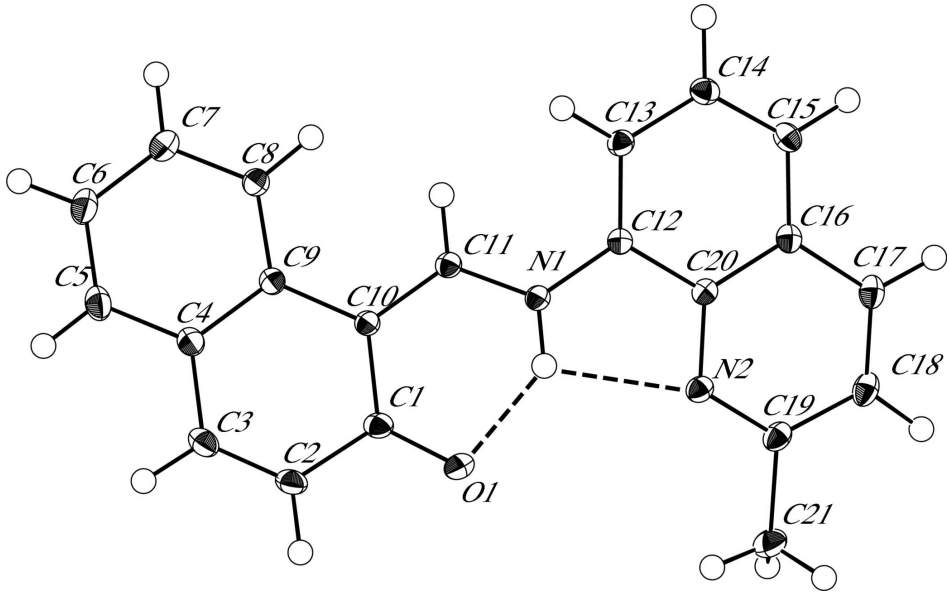

Figure 1

Molecular configuration and atom-numbering scheme for (I) with displacement ellipsoids drawn at the 50% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

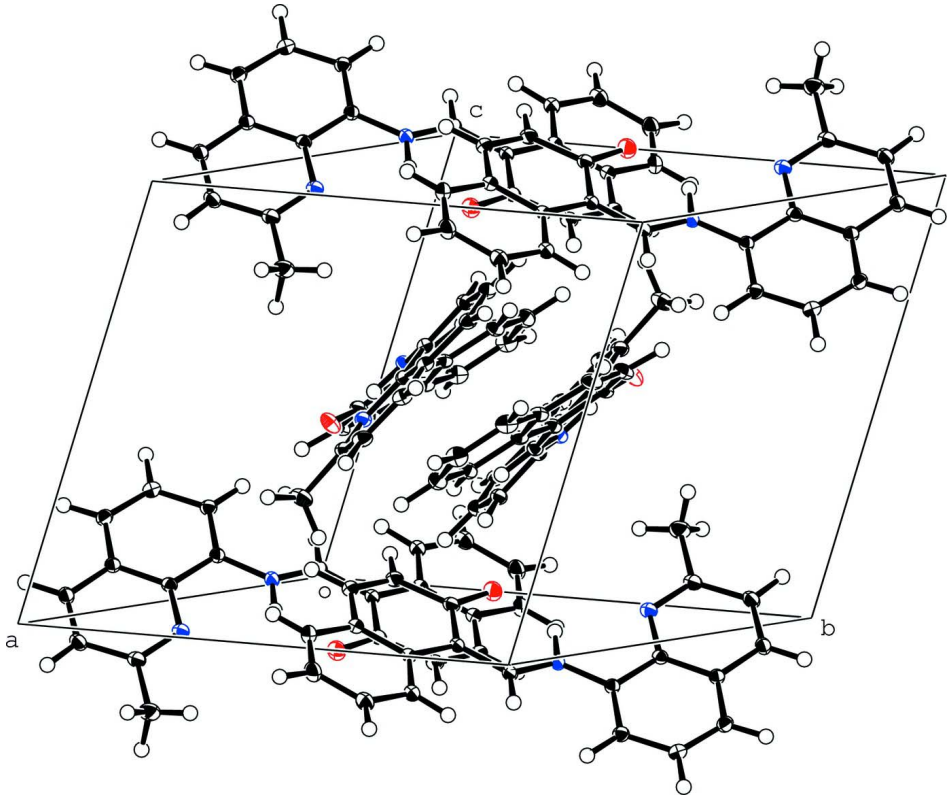

Figure 2

Molecular packing of (I) in the unit cell.

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Crystal data

$C_{21}H_{16}N_2O$
$M_r = 312.37$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.6300\ (19)$ Å
$b = 15.0760\ (17)$ Å
$c = 10.9853\ (17)$ Å
$\beta = 117.111\ (7)°$
$V = 1567.0\ (4)$ Å^3
$Z = 4$
$F(000) = 656.00$
$D_x = 1.324$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 4690 reflections
$\theta = 5.5–30.0°$
$\mu = 0.08$ mm^{-1}
$T = 93$ K
Block, orange
0.63 × 0.56 × 0.32 mm

Data collection

Rigaku Mercury diffractometer
Detector resolution: 7.31 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.950$, $T_{max} = 0.975$
17775 measured reflections
4478 independent reflections
4145 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{int} = 0.038$
$\theta_{max} = 30.0°$
$h = -14\rightarrow14$
$k = -21\rightarrow21$
$l = -14\rightarrow15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.127$
$S = 1.01$
4478 reflections
218 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2 + 0.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. The dihedral angle between the quinoline (C11\simC19, N11) and the naphthalene (C21\simC30) rings is 22.04 (2)°: Mean deviations of the atoms from the former and latter planes are 0.0125 and 0.0186 Å, respectively. The corresponding dihedral angle of (II) is very small (1.67 (4)°).

Refinement. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O(1)	0.43362 (8)	0.17528 (5)	0.40947 (8)	0.02108 (16)
N(1)	0.48710 (8)	0.31627 (5)	0.56290 (8)	0.01363 (15)
N(2)	0.65907 (8)	0.36764 (5)	0.45922 (8)	0.01481 (16)
C(20)	0.65577 (9)	0.42019 (6)	0.55895 (9)	0.01297 (16)
C(13)	0.56130 (9)	0.44289 (6)	0.72100 (9)	0.01487 (17)
C(11)	0.37459 (9)	0.29276 (6)	0.57781 (9)	0.01363 (17)
C(9)	0.15828 (9)	0.20542 (6)	0.52257 (9)	0.01363 (17)
C(12)	0.56770 (9)	0.39321 (6)	0.61849 (9)	0.01290 (16)
C(10)	0.28825 (10)	0.22057 (6)	0.51161 (9)	0.01334 (16)
C(19)	0.73821 (10)	0.39284 (7)	0.40156 (10)	0.01668 (18)

C(16)	0.73327 (9)	0.50023 (6)	0.60430 (9)	0.01425 (17)
C(17)	0.81977 (10)	0.52425 (6)	0.54213 (10)	0.01710 (18)
C(1)	0.32746 (10)	0.16209 (6)	0.42995 (9)	0.01589 (17)
C(18)	0.82189 (10)	0.47128 (7)	0.44228 (10)	0.0181 (2)
C(15)	0.72083 (10)	0.55231 (6)	0.70543 (9)	0.01620 (18)
C(4)	0.07181 (10)	0.13199 (6)	0.45402 (9)	0.01595 (18)
C(8)	0.11163 (10)	0.26091 (6)	0.59766 (9)	0.01582 (17)
C(21)	0.73639 (12)	0.33649 (8)	0.28814 (11)	0.0232 (2)
C(3)	0.11712 (11)	0.07211 (6)	0.37966 (10)	0.0189 (2)
C(6)	−0.09818 (11)	0.17167 (7)	0.53542 (11)	0.0218 (2)
C(5)	−0.05552 (11)	0.11665 (7)	0.46091 (10)	0.0204 (2)
C(7)	−0.01276 (11)	0.24398 (7)	0.60500 (10)	0.0193 (2)
C(14)	0.63655 (10)	0.52346 (6)	0.76214 (9)	0.01640 (18)
C(2)	0.23832 (11)	0.08490 (6)	0.37008 (10)	0.0186 (2)
H(14)	0.6955	0.2786	0.2865	0.031*
H(15)	0.6802	0.3620	0.1945	0.031*
H(16)	0.8329	0.3246	0.2981	0.030*
H(13)	0.8799	0.4859	0.3958	0.022*
H(12)	0.8801	0.5794	0.5735	0.021*
H(11)	0.7731	0.6110	0.7334	0.019*
H(10)	0.6273	0.5617	0.8363	0.020*
H(9)	0.5028	0.4223	0.7652	0.019*
H(7)	0.3521	0.3307	0.6380	0.017*
H(23)	0.2722	0.0414	0.3209	0.024*
H(24)	0.0524	0.0214	0.3345	0.023*
H(27)	−0.1126	0.0658	0.4138	0.026*
H(28)	−0.1878	0.1601	0.5383	0.027*
H(5)	−0.0421	0.2858	0.6598	0.025*
H(6)	0.1698	0.3124	0.6486	0.020*
H(8)	0.5037	0.2828	0.4982	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O(1)	0.0251 (3)	0.0216 (3)	0.0238 (3)	−0.0035 (2)	0.0176 (3)	−0.0051 (2)
N(1)	0.0156 (3)	0.0135 (3)	0.0136 (3)	−0.0013 (2)	0.0082 (2)	−0.0003 (2)
N(2)	0.0144 (3)	0.0174 (3)	0.0131 (3)	0.0008 (2)	0.0066 (2)	0.0003 (2)
C(20)	0.0124 (3)	0.0146 (3)	0.0115 (3)	0.0011 (2)	0.0051 (3)	0.0015 (2)
C(13)	0.0140 (3)	0.0175 (4)	0.0134 (3)	−0.0002 (3)	0.0065 (3)	−0.0007 (3)
C(11)	0.0154 (3)	0.0137 (3)	0.0127 (3)	−0.0002 (2)	0.0072 (3)	0.0008 (2)
C(9)	0.0160 (3)	0.0140 (3)	0.0111 (3)	−0.0016 (3)	0.0064 (3)	0.0014 (2)
C(12)	0.0127 (3)	0.0133 (3)	0.0123 (3)	−0.0000 (2)	0.0053 (3)	0.0006 (2)
C(10)	0.0163 (3)	0.0131 (3)	0.0121 (3)	−0.0018 (2)	0.0078 (3)	−0.0001 (2)
C(19)	0.0144 (3)	0.0226 (4)	0.0134 (4)	0.0011 (3)	0.0066 (3)	0.0017 (3)
C(16)	0.0129 (3)	0.0158 (4)	0.0124 (3)	−0.0006 (2)	0.0043 (3)	0.0017 (2)
C(17)	0.0145 (3)	0.0197 (4)	0.0158 (4)	−0.0024 (3)	0.0058 (3)	0.0033 (3)
C(1)	0.0211 (4)	0.0154 (4)	0.0130 (3)	−0.0009 (3)	0.0094 (3)	−0.0003 (3)
C(18)	0.0150 (4)	0.0248 (4)	0.0153 (4)	−0.0012 (3)	0.0074 (3)	0.0044 (3)

C(15)	0.0165 (4)	0.0151 (4)	0.0142 (4)	−0.0013 (3)	0.0046 (3)	−0.0001 (3)
C(4)	0.0190 (4)	0.0164 (4)	0.0122 (3)	−0.0035 (3)	0.0070 (3)	0.0002 (3)
C(8)	0.0176 (4)	0.0160 (4)	0.0152 (4)	−0.0017 (3)	0.0086 (3)	−0.0001 (3)
C(21)	0.0245 (4)	0.0310 (5)	0.0188 (4)	−0.0020 (4)	0.0138 (3)	−0.0039 (3)
C(3)	0.0254 (4)	0.0166 (4)	0.0142 (4)	−0.0057 (3)	0.0086 (3)	−0.0022 (3)
C(6)	0.0182 (4)	0.0265 (5)	0.0227 (4)	−0.0041 (3)	0.0111 (3)	0.0017 (3)
C(5)	0.0201 (4)	0.0215 (4)	0.0192 (4)	−0.0070 (3)	0.0085 (3)	0.0001 (3)
C(7)	0.0197 (4)	0.0217 (4)	0.0196 (4)	0.0001 (3)	0.0115 (3)	0.0016 (3)
C(14)	0.0163 (4)	0.0174 (4)	0.0141 (4)	0.0003 (3)	0.0057 (3)	−0.0015 (3)
C(2)	0.0269 (4)	0.0164 (4)	0.0148 (4)	−0.0036 (3)	0.0115 (3)	−0.0036 (3)

Geometric parameters (Å, º)

O(1)—C(1)	1.2629 (15)	C(17)—H(12)	1.009
N(1)—C(11)	1.3272 (14)	C(1)—C(2)	1.4549 (12)
N(1)—C(12)	1.4056 (11)	C(18)—H(13)	0.988
N(1)—H(8)	0.951	C(15)—C(14)	1.3743 (17)
N(2)—C(20)	1.3653 (13)	C(15)—H(11)	1.015
N(2)—C(19)	1.3187 (16)	C(4)—C(3)	1.4397 (16)
C(20)—C(12)	1.4240 (16)	C(4)—C(5)	1.4088 (17)
C(20)—C(16)	1.4174 (12)	C(8)—C(7)	1.3846 (17)
C(13)—C(12)	1.3797 (14)	C(8)—H(6)	0.991
C(13)—C(14)	1.4107 (12)	C(21)—H(14)	0.971
C(13)—H(9)	0.997	C(21)—H(15)	1.002
C(11)—C(10)	1.3955 (12)	C(21)—H(16)	0.997
C(11)—H(7)	0.982	C(3)—C(2)	1.3534 (18)
C(9)—C(10)	1.4584 (15)	C(3)—H(24)	0.997
C(9)—C(4)	1.4165 (12)	C(6)—C(5)	1.3791 (18)
C(9)—C(8)	1.4139 (15)	C(6)—C(7)	1.4016 (13)
C(10)—C(1)	1.4479 (15)	C(6)—H(28)	0.983
C(19)—C(18)	1.4238 (14)	C(5)—H(27)	0.969
C(19)—C(21)	1.5008 (17)	C(7)—H(5)	1.014
C(16)—C(17)	1.4196 (17)	C(14)—H(10)	1.038
C(16)—C(15)	1.4149 (15)	C(2)—H(23)	1.015
C(17)—C(18)	1.3653 (16)		
O(1)···C(13)^{i}	3.4444 (14)	H(15)···C(6)^{xii}	3.552
O(1)···C(11)^{i}	3.4375 (13)	H(15)···H(10)^{iv}	3.333
O(1)···H(15)^{ii}	3.084	H(15)···H(23)^{vii}	2.771
O(1)···H(10)^{iii}	3.578	H(15)···H(28)^{xii}	2.687
O(1)···H(9)^{i}	2.505	H(15)···H(8)^{i}	3.042
O(1)···H(7)^{i}	2.701	H(16)···C(8)^{v}	3.413
O(1)···H(6)^{i}	2.964	H(16)···C(6)^{v}	3.303
N(1)···C(16)^{iv}	3.5486 (11)	H(16)···C(6)^{xii}	3.285
N(1)···C(15)^{iv}	3.4002 (10)	H(16)···C(5)^{v}	3.536
N(1)···C(21)^{ii}	3.5316 (12)	H(16)···C(7)^{v}	3.240
N(1)···H(14)^{ii}	2.834	H(16)···C(7)^{xii}	3.381
N(1)···H(15)^{ii}	3.289	H(16)···H(12)^{viii}	3.078

N(1)···H(11)^{iv}	3.353	H(16)···H(23)^{vii}	3.507
N(2)···C(14)^{iv}	3.3939 (10)	H(16)···H(28)^{xii}	2.770
N(2)···H(10)^{iv}	3.454	H(16)···H(5)^{xii}	2.947
N(2)···H(28)^{v}	3.450	H(13)···C(17)^{viii}	2.949
N(2)···H(5)^{v}	3.177	H(13)···C(18)^{viii}	2.914
C(20)···C(13)^{iv}	3.5462 (11)	H(13)···C(3)^{vii}	3.307
C(20)···C(14)^{iv}	3.5818 (10)	H(13)···C(2)^{vii}	2.999
C(20)···H(27)^{vi}	3.543	H(13)···H(13)^{viii}	2.573
C(20)···H(5)^{v}	3.523	H(13)···H(12)^{viii}	2.609
C(13)···O(1)^{ii}	3.4444 (14)	H(13)···H(23)^{vii}	2.339
C(13)···C(20)^{iv}	3.5462 (11)	H(13)···H(24)^{vii}	2.977
C(13)···H(14)^{ii}	3.574	H(13)···H(6)^{iv}	3.088
C(13)···H(27)^{vi}	3.135	H(12)···C(11)^{iv}	3.116
C(11)···O(1)^{ii}	3.4375 (13)	H(12)···C(9)^{iv}	3.379
C(11)···C(17)^{iv}	3.3368 (12)	H(12)···C(10)^{iv}	3.413
C(11)···H(14)^{ii}	3.305	H(12)···C(18)^{viii}	3.339
C(11)···H(12)^{iv}	3.116	H(12)···C(8)^{iv}	3.081
C(11)···H(11)^{iv}	3.371	H(12)···H(16)^{viii}	3.078
C(9)···C(15)^{iii}	3.5225 (12)	H(12)···H(13)^{viii}	2.609
C(9)···H(12)^{iv}	3.379	H(12)···H(7)^{iv}	2.847
C(9)···H(11)^{iii}	2.822	H(12)···H(24)^{vi}	3.016
C(9)···H(10)^{iii}	3.012	H(12)···H(6)^{iv}	2.778
C(9)···H(5)^{i}	3.563	H(11)···N(1)^{iv}	3.353
C(12)···C(16)^{iv}	3.4161 (10)	H(11)···C(11)^{iv}	3.371
C(12)···C(15)^{iv}	3.5772 (10)	H(11)···C(9)^{ix}	2.822
C(12)···H(14)^{ii}	3.111	H(11)···C(10)^{ix}	3.559
C(12)···H(27)^{vi}	3.523	H(11)···C(10)^{iv}	3.538
C(10)···H(12)^{iv}	3.413	H(11)···C(4)^{ix}	3.074
C(10)···H(11)^{iii}	3.559	H(11)···C(8)^{ix}	2.825
C(10)···H(11)^{iv}	3.538	H(11)···C(6)^{ix}	3.351
C(10)···H(10)^{iii}	2.823	H(11)···C(5)^{ix}	3.333
C(19)···C(7)^{v}	3.4127 (13)	H(11)···C(7)^{ix}	3.089
C(19)···H(23)^{vii}	3.279	H(11)···H(24)^{vi}	3.319
C(19)···H(5)^{v}	3.173	H(11)···H(27)^{vi}	3.211
C(16)···N(1)^{iv}	3.5486 (11)	H(11)···H(6)^{ix}	3.248
C(16)···C(12)^{iv}	3.4161 (10)	H(11)···H(8)^{iv}	3.297
C(16)···H(7)^{iv}	3.494	H(10)···O(1)^{ix}	3.578
C(16)···H(24)^{vi}	3.192	H(10)···N(2)^{iv}	3.454
C(16)···H(27)^{vi}	3.187	H(10)···C(9)^{ix}	3.012
C(17)···C(11)^{iv}	3.3368 (12)	H(10)···C(10)^{ix}	2.823
C(17)···H(13)^{viii}	2.949	H(10)···C(1)^{ix}	2.827
C(17)···H(7)^{iv}	2.957	H(10)···C(4)^{ix}	3.154
C(17)···H(24)^{vi}	3.108	H(10)···C(3)^{ix}	3.069
C(17)···H(6)^{iv}	3.268	H(10)···C(2)^{ix}	2.893
C(1)···C(8)^{i}	3.5076 (11)	H(10)···H(15)^{iv}	3.333
C(1)···H(15)^{ii}	3.564	H(10)···H(23)^{ix}	3.428
C(1)···H(10)^{iii}	2.827	H(10)···H(27)^{vi}	3.149
C(1)···H(9)^{i}	3.382	H(9)···O(1)^{ii}	2.505

C(1)···H(7)^{i}	3.336	H(9)···C(1)^{ii}	3.382
C(1)···H(6)^{i}	2.791	H(9)···C(18)^{iv}	3.537
C(18)···C(18)^{viii}	3.5100 (14)	H(9)···C(2)^{ii}	3.492
C(18)···H(13)^{viii}	2.914	H(9)···H(23)^{ii}	2.837
C(18)···H(12)^{viii}	3.339	H(9)···H(28)^{vi}	3.517
C(18)···H(9)^{iv}	3.537	H(7)···O(1)^{ii}	2.701
C(18)···H(7)^{iv}	3.410	H(7)···C(16)^{iv}	3.494
C(18)···H(23)^{vii}	2.800	H(7)···C(17)^{iv}	2.957
C(18)···H(5)^{v}	3.532	H(7)···C(1)^{ii}	3.336
C(18)···H(6)^{iv}	3.424	H(7)···C(18)^{iv}	3.410
C(15)···N(1)^{iv}	3.4002 (10)	H(7)···C(2)^{ii}	3.520
C(15)···C(9)^{ix}	3.5225 (12)	H(7)···H(12)^{iv}	2.847
C(15)···C(12)^{iv}	3.5772 (10)	H(7)···H(23)^{ii}	3.168
C(15)···C(4)^{ix}	3.5751 (11)	H(23)···C(19)^{xiii}	3.279
C(15)···H(24)^{vi}	3.333	H(23)···C(18)^{xiii}	2.800
C(15)···H(27)^{vi}	2.802	H(23)···C(21)^{xiii}	3.299
C(15)···H(8)^{iv}	3.466	H(23)···H(15)^{xiii}	2.771
C(4)···C(15)^{iii}	3.5751 (11)	H(23)···H(16)^{xiii}	3.507
C(4)···H(11)^{iii}	3.074	H(23)···H(13)^{xiii}	2.339
C(4)···H(10)^{iii}	3.154	H(23)···H(10)^{iii}	3.428
C(4)···H(27)^{x}	3.257	H(23)···H(9)^{i}	2.837
C(4)···H(5)^{i}	3.144	H(23)···H(7)^{i}	3.168
C(8)···C(1)^{ii}	3.5076 (11)	H(23)···H(6)^{i}	2.784
C(8)···C(2)^{ii}	3.5355 (13)	H(24)···C(16)^{xv}	3.192
C(8)···H(16)^{xi}	3.413	H(24)···C(17)^{xv}	3.108
C(8)···H(12)^{iv}	3.081	H(24)···C(15)^{xv}	3.333
C(8)···H(11)^{iii}	2.825	H(24)···C(6)^{x}	3.180
C(21)···N(1)^{i}	3.5316 (12)	H(24)···C(5)^{x}	3.052
C(21)···C(6)^{v}	3.5060 (14)	H(24)···H(13)^{xiii}	2.977
C(21)···C(7)^{v}	3.5654 (13)	H(24)···H(12)^{xv}	3.016
C(21)···H(23)^{vii}	3.299	H(24)···H(11)^{xv}	3.319
C(21)···H(28)^{xii}	3.194	H(24)···H(27)^{x}	2.858
C(21)···H(8)^{i}	3.510	H(24)···H(28)^{x}	3.111
C(3)···C(5)^{x}	3.5552 (15)	H(24)···H(5)^{i}	3.375
C(3)···H(13)^{xiii}	3.307	H(27)···C(20)^{xv}	3.543
C(3)···H(10)^{iii}	3.069	H(27)···C(13)^{xv}	3.135
C(3)···H(27)^{x}	3.094	H(27)···C(12)^{xv}	3.523
C(3)···H(5)^{i}	3.092	H(27)···C(16)^{xv}	3.187
C(3)···H(6)^{i}	3.329	H(27)···C(15)^{xv}	2.802
C(6)···C(21)^{xi}	3.5060 (14)	H(27)···C(4)^{x}	3.257
C(6)···H(14)^{xi}	3.070	H(27)···C(3)^{x}	3.094
C(6)···H(15)^{xiv}	3.552	H(27)···C(5)^{x}	3.226
C(6)···H(16)^{xi}	3.303	H(27)···C(14)^{xv}	2.765
C(6)···H(16)^{xiv}	3.285	H(27)···H(11)^{xv}	3.211
C(6)···H(11)^{iii}	3.351	H(27)···H(10)^{xv}	3.149
C(6)···H(24)^{x}	3.180	H(27)···H(24)^{x}	2.858
C(5)···C(3)^{x}	3.5552 (15)	H(27)···H(27)^{x}	3.019
C(5)···H(14)^{xi}	3.467	H(28)···N(2)^{xi}	3.450

C(5)···H(16)^{xi}	3.536	H(28)···C(21)^{xiv}	3.194
C(5)···H(11)^{iii}	3.333	H(28)···H(14)^{xi}	3.042
C(5)···H(24)^{x}	3.052	H(28)···H(14)^{xiv}	3.593
C(5)···H(27)^{x}	3.226	H(28)···H(15)^{xiv}	2.687
C(7)···C(19)^{xi}	3.4127 (13)	H(28)···H(16)^{xiv}	2.770
C(7)···C(21)^{xi}	3.5654 (13)	H(28)···H(9)^{xv}	3.517
C(7)···H(14)^{xi}	3.499	H(28)···H(24)^{x}	3.111
C(7)···H(16)^{xi}	3.240	H(5)···N(2)^{xi}	3.177
C(7)···H(16)^{xiv}	3.381	H(5)···C(20)^{xi}	3.523
C(7)···H(11)^{iii}	3.089	H(5)···C(9)^{ii}	3.563
C(14)···N(2)^{iv}	3.3939 (10)	H(5)···C(19)^{xi}	3.173
C(14)···C(20)^{iv}	3.5818 (10)	H(5)···C(18)^{xi}	3.532
C(14)···H(27)^{vi}	2.765	H(5)···C(4)^{ii}	3.144
C(2)···C(8)^{i}	3.5355 (13)	H(5)···C(3)^{ii}	3.092
C(2)···H(13)^{xiii}	2.999	H(5)···C(2)^{ii}	3.427
C(2)···H(10)^{iii}	2.893	H(5)···H(16)^{xiv}	2.947
C(2)···H(9)^{i}	3.492	H(5)···H(24)^{ii}	3.375
C(2)···H(7)^{i}	3.520	H(6)···O(1)^{ii}	2.964
C(2)···H(5)^{i}	3.427	H(6)···C(17)^{iv}	3.268
C(2)···H(6)^{i}	2.689	H(6)···C(1)^{ii}	2.791
H(14)···N(1)^{i}	2.834	H(6)···C(18)^{iv}	3.424
H(14)···C(13)^{i}	3.574	H(6)···C(3)^{ii}	3.329
H(14)···C(11)^{i}	3.305	H(6)···C(2)^{ii}	2.689
H(14)···C(12)^{i}	3.111	H(6)···H(13)^{iv}	3.088
H(14)···C(6)^{v}	3.070	H(6)···H(12)^{iv}	2.778
H(14)···C(5)^{v}	3.467	H(6)···H(11)^{iii}	3.248
H(14)···C(7)^{v}	3.499	H(6)···H(23)^{ii}	2.784
H(14)···H(28)^{v}	3.042	H(8)···C(15)^{iv}	3.466
H(14)···H(28)^{xii}	3.593	H(8)···C(21)^{ii}	3.510
H(14)···H(8)^{i}	3.027	H(8)···H(14)^{ii}	3.027
H(15)···O(1)^{i}	3.084	H(8)···H(15)^{ii}	3.042
H(15)···N(1)^{i}	3.289	H(8)···H(11)^{iv}	3.297
H(15)···C(1)^{i}	3.564		

C(11)—N(1)—C(12)	124.89 (9)	C(19)—C(18)—H(13)	118.0
C(11)—N(1)—H(8)	115.8	C(17)—C(18)—H(13)	121.9
C(12)—N(1)—H(8)	118.6	C(16)—C(15)—C(14)	119.59 (8)
C(20)—N(2)—C(19)	118.26 (8)	C(16)—C(15)—H(11)	119.1
N(2)—C(20)—C(12)	117.74 (8)	C(14)—C(15)—H(11)	121.3
N(2)—C(20)—C(16)	123.55 (10)	C(9)—C(4)—C(3)	119.20 (10)
C(12)—C(20)—C(16)	118.70 (9)	C(9)—C(4)—C(5)	120.42 (10)
C(12)—C(13)—C(14)	119.82 (10)	C(3)—C(4)—C(5)	120.37 (8)
C(12)—C(13)—H(9)	120.2	C(9)—C(8)—C(7)	121.54 (8)
C(14)—C(13)—H(9)	120.0	C(9)—C(8)—H(6)	119.9
N(1)—C(11)—C(10)	124.03 (10)	C(7)—C(8)—H(6)	118.6
N(1)—C(11)—H(7)	115.9	C(19)—C(21)—H(14)	111.1
C(10)—C(11)—H(7)	120.0	C(19)—C(21)—H(15)	114.3
C(10)—C(9)—C(4)	119.22 (9)	C(19)—C(21)—H(16)	112.8

C(10)—C(9)—C(8)	123.56 (7)	H(14)—C(21)—H(15)	105.9
C(4)—C(9)—C(8)	117.22 (9)	H(14)—C(21)—H(16)	105.7
N(1)—C(12)—C(20)	115.74 (9)	H(15)—C(21)—H(16)	106.5
N(1)—C(12)—C(13)	123.75 (10)	C(4)—C(3)—C(2)	122.09 (8)
C(20)—C(12)—C(13)	120.47 (8)	C(4)—C(3)—H(24)	115.5
C(11)—C(10)—C(9)	120.13 (9)	C(2)—C(3)—H(24)	122.4
C(11)—C(10)—C(1)	119.41 (10)	C(5)—C(6)—C(7)	119.01 (11)
C(9)—C(10)—C(1)	120.45 (7)	C(5)—C(6)—H(28)	119.9
N(2)—C(19)—C(18)	122.17 (10)	C(7)—C(6)—H(28)	121.1
N(2)—C(19)—C(21)	117.77 (9)	C(4)—C(5)—C(6)	121.13 (9)
C(18)—C(19)—C(21)	120.05 (11)	C(4)—C(5)—H(27)	119.0
C(20)—C(16)—C(17)	116.63 (9)	C(6)—C(5)—H(27)	119.9
C(20)—C(16)—C(15)	120.07 (10)	C(8)—C(7)—C(6)	120.67 (11)
C(17)—C(16)—C(15)	123.29 (8)	C(8)—C(7)—H(5)	118.7
C(16)—C(17)—C(18)	119.26 (8)	C(6)—C(7)—H(5)	120.6
C(16)—C(17)—H(12)	119.7	C(13)—C(14)—C(15)	121.26 (9)
C(18)—C(17)—H(12)	121.0	C(13)—C(14)—H(10)	119.1
O(1)—C(1)—C(10)	123.19 (8)	C(15)—C(14)—H(10)	119.6
O(1)—C(1)—C(2)	119.75 (10)	C(1)—C(2)—C(3)	121.72 (10)
C(10)—C(1)—C(2)	117.07 (10)	C(1)—C(2)—H(23)	116.2
C(19)—C(18)—C(17)	120.10 (11)	C(3)—C(2)—H(23)	122.1

C(11)—N(1)—C(12)—C(20)	−161.97 (7)	C(8)—C(9)—C(10)—C(1)	−178.44 (7)
C(11)—N(1)—C(12)—C(13)	15.91 (12)	C(4)—C(9)—C(8)—C(7)	0.50 (12)
C(12)—N(1)—C(11)—C(10)	173.84 (7)	C(8)—C(9)—C(4)—C(3)	−178.14 (7)
C(20)—N(2)—C(19)—C(18)	1.52 (12)	C(8)—C(9)—C(4)—C(5)	0.52 (12)
C(20)—N(2)—C(19)—C(21)	−177.56 (7)	C(11)—C(10)—C(1)—O(1)	−3.56 (12)
C(19)—N(2)—C(20)—C(12)	178.75 (7)	C(11)—C(10)—C(1)—C(2)	176.36 (7)
C(19)—N(2)—C(20)—C(16)	−0.26 (11)	C(9)—C(10)—C(1)—O(1)	175.20 (8)
N(2)—C(20)—C(12)—N(1)	−2.91 (10)	C(9)—C(10)—C(1)—C(2)	−4.88 (11)
N(2)—C(20)—C(12)—C(13)	179.13 (7)	N(2)—C(19)—C(18)—C(17)	−1.38 (13)
N(2)—C(20)—C(16)—C(17)	−1.12 (11)	C(21)—C(19)—C(18)—C(17)	177.69 (8)
N(2)—C(20)—C(16)—C(15)	178.12 (7)	C(20)—C(16)—C(17)—C(18)	1.24 (11)
C(12)—C(20)—C(16)—C(17)	179.88 (7)	C(20)—C(16)—C(15)—C(14)	1.93 (11)
C(12)—C(20)—C(16)—C(15)	−0.89 (11)	C(17)—C(16)—C(15)—C(14)	−178.89 (7)
C(16)—C(20)—C(12)—N(1)	176.15 (6)	C(15)—C(16)—C(17)—C(18)	−177.97 (7)
C(16)—C(20)—C(12)—C(13)	−1.80 (11)	C(16)—C(17)—C(18)—C(19)	−0.10 (12)
C(12)—C(13)—C(14)—C(15)	−2.37 (11)	O(1)—C(1)—C(2)—C(3)	−174.35 (8)
C(14)—C(13)—C(12)—N(1)	−174.36 (7)	C(10)—C(1)—C(2)—C(3)	5.73 (12)
C(14)—C(13)—C(12)—C(20)	3.42 (11)	C(16)—C(15)—C(14)—C(13)	−0.32 (12)
N(1)—C(11)—C(10)—C(9)	−173.35 (7)	C(9)—C(4)—C(3)—C(2)	−1.72 (13)
N(1)—C(11)—C(10)—C(1)	5.42 (12)	C(9)—C(4)—C(5)—C(6)	−0.81 (13)
C(10)—C(9)—C(4)—C(3)	2.44 (12)	C(3)—C(4)—C(5)—C(6)	177.83 (8)
C(10)—C(9)—C(4)—C(5)	−178.90 (8)	C(5)—C(4)—C(3)—C(2)	179.62 (8)
C(4)—C(9)—C(10)—C(11)	179.70 (7)	C(9)—C(8)—C(7)—C(6)	−1.25 (13)
C(4)—C(9)—C(10)—C(1)	0.94 (12)	C(4)—C(3)—C(2)—C(1)	−2.51 (13)

C(10)—C(9)—C(8)—C(7)	179.89 (8)	C(5)—C(6)—C(7)—C(8)	0.94 (14)
C(8)—C(9)—C(10)—C(11)	0.32 (12)	C(7)—C(6)—C(5)—C(4)	0.08 (14)

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+1, *y*−1/2, −*z*+3/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*+1, *y*, *z*; (vi) *x*+1, −*y*+1/2, *z*+1/2; (vii) −*x*+1, *y*+1/2, −*z*+1/2; (viii) −*x*+2, −*y*+1, −*z*+1; (ix) −*x*+1, *y*+1/2, −*z*+3/2; (x) −*x*, −*y*, −*z*+1; (xi) *x*−1, *y*, *z*; (xii) *x*+1, −*y*+1/2, *z*−1/2; (xiii) −*x*+1, *y*−1/2, −*z*+1/2; (xiv) *x*−1, −*y*+1/2, *z*+1/2; (xv) *x*−1, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H8···O1	0.95	1.86	2.6094 (11)	133
N1—H8···N2	0.95	2.28	2.6714 (14)	104