IUCrData

ISSN 2414-3146

(*E*)-2-[(Pyren-1-ylimino)methyl]quinolin-8-ol

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Received 30 March 2016
Accepted 31 March 2016

Edited by P. Bombicz, Hungarian Academy of Sciences, Hungary

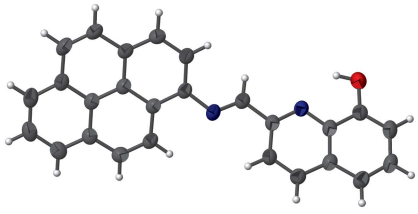
Keywords: crystal structure; pyrene; fluorescence sensor; hydrogen bonding.

CCDC reference: 1471583

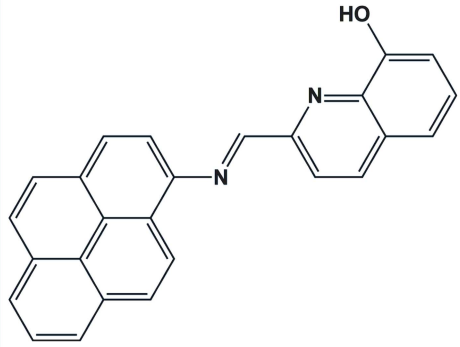
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{26}H_{16}N_2O$, the pyrene ring system (r.m.s. deviation = 0.021 Å) is inclined to the planar quinoline ring system (r.m.s. deviation = 0.017 Å) by 30.62 (5)°, and the conformation about the bridging N=C bond is *E*. There is an intramolecular O—H···N hydrogen bond with an *S*(5) ring motif present. In the crystal, molecules are linked by pairs of C—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(14)$ ring motif, flanked by two $R_2^1(7)$ ring motifs. The dimers stack along the *b* axis with slipped parallel π–π interactions involving neighbouring molecules; the shortest π–π interaction involves aromatic rings of the quinoline ring system [inter-centroid distance = 3.6267 (11) Å].

3D view



Chemical scheme



Structure description

The title compound has recently been shown to act as a reversible pyrene-based turn-on luminescent chemosensor for the selective detection of Fe^{3+} in an aqueous environment (Mukherjee & Talukder, 2016).

In the title compound, Fig. 1, the pyrene ring system (C1–C16) is planar (r.m.s. deviation = 0.021 Å) and it is inclined to the planar quinoline ring system (N2/C18–C26; r.m.s. deviation = 0.017 Å) by 30.62 (5)°. The conformation about the N1=C17 bond is *E* and there is an intramolecular O—H···N hydrogen bond with an *S*(5) ring motif present (Fig. 1 and Table 1).

In the crystal, molecules are linked by pairs of C—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(14)$ ring motif, flanked by two $R_2^1(7)$ ring motifs (Fig. 2 and Table 1). The dimers stack along the *b* axis with slipped parallel π–π interactions involving neighbouring molecules (Fig. 3); the shortest π–π interaction involves aromatic rings (N2/C18–C21/C26) and (C21–C26) of the quinoline ring system [$Cg1\cdots Cg6^{i}$ = 3.6267 (11) Å, interplanar distance = 3.466 (1) Å, slippage = 1.078 Å, symmetry code: (i)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···N2	0.91 (2)	2.03 (2)	2.666 (2)	125 (2)
C2—H2···O1^{i}	0.94	2.52	3.422 (2)	161
C17—H17···O1^{i}	0.94	2.57	3.436 (2)	153

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

$x, y+1, z$; where *Cg*1 and *Cg*6 are the centroids of rings (N2/C18–C21/C26) and (C21–C26), respectively].

Synthesis and crystallization

The title compound was synthesized by a 1:1 condensation of 8-hydroxyquinoline-2-carboxaldehyde and 1-aminopyrene in methanol, and characterized by ^{1}H NMR, ^{13}C NMR, FTIR and UV–Vis spectroscopic studies as reported on recently (Mukherjee & Talukder, 2016). Brown rod-like crystals were obtained by slow evaporation of a solution in methanol.

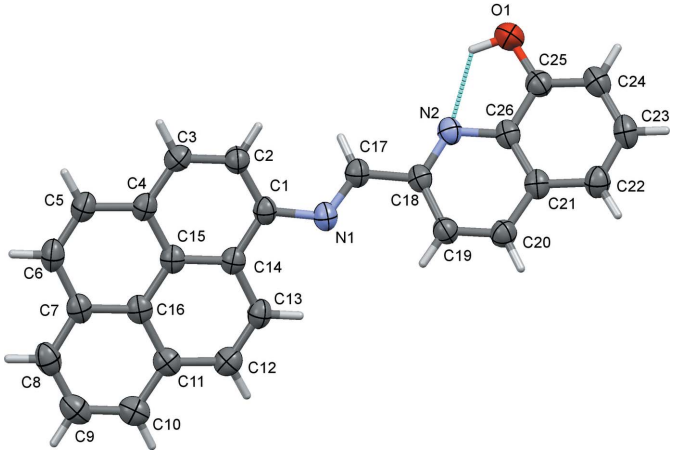


Figure 1
A view of the molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular O—H···N hydrogen bond is shown as a dashed line (see Table 1).

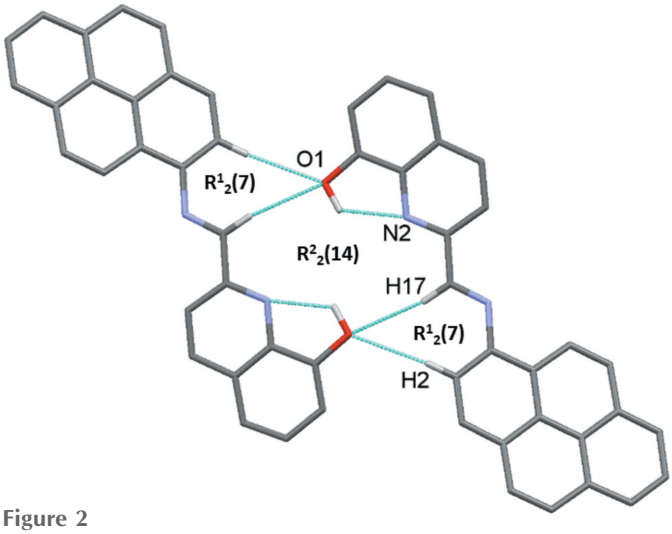


Figure 2
A view of the inversion dimer formed by pairs of C—H···O hydrogen bonds (dashed lines; see Table 1). H atoms not involved in these interactions have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{16}N_2O$
M_r	372.41
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	203
a, b, c (Å)	15.9840 (19), 4.8453 (3), 23.071 (3)
β (°)	93.835 (9)
V (Å^3)	1782.8 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.50 × 0.27 × 0.10
Data collection	
Diffractometer	Stoe *IPDS* 2
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17513, 3558, 2092
R_{int}	0.075
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.623
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.093, 0.88
No. of reflections	3558
No. of parameters	265
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.12

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2009), *SHELXS2014* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

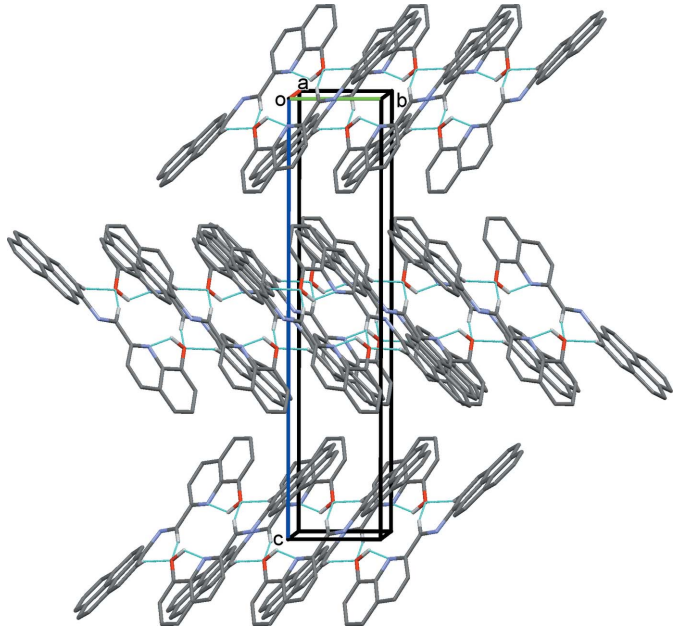


Figure 3
A view along the *a* axis of the crystal packing of the title compound. Hydrogen bonds are shown as a dashed lines (see Table 1), and H atoms not involved in these interactions have been omitted for clarity.

Refinement

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

Acknowledgements

The University of Kalyani, and DST–FIST, DST–PURSE, New Delhi, are gratefully acknowledged for financial support, and instrumental and infrastructural facilities. HSE is grateful to the University of Neuchâtel for continued support.

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full crystallographic data

IUCrData (2016). **1**, x160543 [doi:10.1107/S2414314616005435]

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Crystal data

$C_{26}H_{16}N_2O$
M_r = 372.41
Monoclinic, $P2_1/c$
a = 15.9840 (19) Å
b = 4.8453 (3) Å
c = 23.071 (3) Å
β = 93.835 (9)°
V = 1782.8 (3) Å^3
Z = 4
$F(000)$ = 776
D_x = 1.387 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7937 reflections
θ = 1.3–26.7°
μ = 0.09 mm^{-1}
T = 203 K
Rod, brown
0.50 × 0.27 × 0.10 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: fine-focus sealed tube
Plane graphite monochromator
$\varphi + \omega$ scans
17513 measured reflections
3558 independent reflections
2092 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 26.3°, θ_{min} = 1.3°
h = −19→17
k = −6→5
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.093
S = 0.88
3558 reflections
265 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 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	−0.00534 (9)	−0.8729 (3)	0.43353 (6)	0.0610 (4)
H1O	0.0175 (14)	−0.737 (4)	0.4572 (9)	0.091*
N1	0.24740 (9)	0.0215 (3)	0.50451 (6)	0.0396 (4)
N2	0.11816 (9)	−0.5020 (3)	0.43966 (6)	0.0383 (3)
C1	0.25103 (11)	0.1993 (3)	0.55347 (7)	0.0371 (4)
C2	0.18087 (11)	0.2776 (4)	0.58217 (7)	0.0416 (4)
H2	0.1284	0.1990	0.5712	0.050*
C3	0.18745 (11)	0.4697 (4)	0.62665 (7)	0.0422 (4)
H3	0.1393	0.5183	0.6456	0.051*
C4	0.26386 (11)	0.5926 (3)	0.64404 (7)	0.0385 (4)
C5	0.27221 (12)	0.8001 (4)	0.68850 (7)	0.0449 (5)
H5	0.2248	0.8528	0.7078	0.054*
C6	0.34677 (13)	0.9210 (4)	0.70319 (7)	0.0474 (5)
H6	0.3500	1.0570	0.7323	0.057*
C7	0.42106 (12)	0.8468 (3)	0.67542 (7)	0.0399 (4)
C8	0.49893 (13)	0.9696 (4)	0.68975 (8)	0.0494 (5)
H8	0.5034	1.1074	0.7185	0.059*
C9	0.56911 (13)	0.8912 (4)	0.66230 (8)	0.0509 (5)
H9	0.6210	0.9755	0.6726	0.061*
C10	0.56414 (12)	0.6905 (4)	0.61980 (8)	0.0473 (5)
H10	0.6126	0.6407	0.6014	0.057*
C11	0.48832 (11)	0.5606 (3)	0.60381 (7)	0.0391 (4)
C12	0.47988 (12)	0.3507 (4)	0.56009 (7)	0.0429 (4)
H12	0.5279	0.2912	0.5423	0.051*
C13	0.40516 (11)	0.2356 (4)	0.54364 (7)	0.0408 (4)
H13	0.4022	0.1014	0.5141	0.049*
C14	0.33014 (11)	0.3141 (3)	0.57034 (7)	0.0351 (4)
C15	0.33661 (11)	0.5137 (3)	0.61542 (7)	0.0355 (4)
C16	0.41497 (11)	0.6392 (3)	0.63201 (7)	0.0366 (4)
C17	0.18879 (11)	−0.1557 (3)	0.49708 (7)	0.0403 (4)
H17	0.1504	−0.1802	0.5258	0.048*
C18	0.18104 (11)	−0.3225 (3)	0.44361 (7)	0.0362 (4)
C19	0.23649 (11)	−0.2867 (4)	0.39939 (7)	0.0417 (4)
H19	0.2809	−0.1599	0.4043	0.050*
C20	0.22571 (12)	−0.4362 (4)	0.34949 (7)	0.0436 (4)
H20	0.2624	−0.4121	0.3197	0.052*
C21	0.15907 (11)	−0.6278 (3)	0.34257 (7)	0.0387 (4)
C22	0.14091 (12)	−0.7905 (4)	0.29233 (7)	0.0464 (5)
H22	0.1744	−0.7761	0.2605	0.056*
C23	0.07445 (12)	−0.9689 (4)	0.29029 (8)	0.0474 (5)
H23	0.0625	−1.0744	0.2566	0.057*
C24	0.02363 (12)	−0.9985 (4)	0.33712 (8)	0.0487 (5)
H24	−0.0217	−1.1227	0.3348	0.058*
C25	0.04069 (11)	−0.8446 (4)	0.38630 (8)	0.0430 (4)
C26	0.10779 (11)	−0.6530 (3)	0.38955 (7)	0.0377 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0568 (9)	0.0638 (10)	0.0638 (9)	−0.0192 (8)	0.0142 (7)	−0.0138 (7)
N1	0.0470 (9)	0.0346 (8)	0.0369 (8)	−0.0014 (7)	−0.0005 (7)	−0.0030 (6)
N2	0.0409 (9)	0.0340 (8)	0.0397 (8)	0.0012 (7)	0.0001 (6)	−0.0018 (6)
C1	0.0468 (11)	0.0312 (9)	0.0331 (9)	−0.0013 (8)	0.0009 (8)	0.0000 (7)
C2	0.0454 (11)	0.0398 (10)	0.0396 (9)	−0.0016 (8)	0.0025 (8)	−0.0037 (8)
C3	0.0432 (11)	0.0421 (10)	0.0417 (10)	0.0037 (9)	0.0067 (8)	−0.0007 (8)
C4	0.0491 (11)	0.0332 (9)	0.0335 (9)	0.0016 (8)	0.0050 (8)	0.0010 (7)
C5	0.0566 (12)	0.0414 (10)	0.0374 (9)	0.0035 (9)	0.0071 (8)	−0.0050 (8)
C6	0.0683 (14)	0.0394 (10)	0.0344 (9)	−0.0015 (10)	0.0023 (9)	−0.0049 (8)
C7	0.0522 (11)	0.0339 (10)	0.0328 (9)	−0.0033 (8)	−0.0025 (8)	0.0043 (7)
C8	0.0660 (14)	0.0415 (11)	0.0393 (10)	−0.0100 (10)	−0.0074 (10)	0.0034 (8)
C9	0.0517 (12)	0.0491 (12)	0.0502 (11)	−0.0115 (10)	−0.0092 (9)	0.0093 (9)
C10	0.0460 (11)	0.0452 (11)	0.0498 (10)	0.0009 (9)	−0.0023 (8)	0.0091 (9)
C11	0.0439 (11)	0.0337 (9)	0.0390 (9)	0.0014 (8)	−0.0022 (8)	0.0080 (8)
C12	0.0469 (11)	0.0399 (10)	0.0420 (10)	0.0061 (9)	0.0045 (8)	0.0047 (8)
C13	0.0526 (12)	0.0335 (9)	0.0362 (9)	0.0022 (8)	0.0036 (8)	−0.0020 (7)
C14	0.0448 (11)	0.0287 (9)	0.0318 (8)	0.0016 (8)	0.0025 (7)	0.0039 (7)
C15	0.0462 (11)	0.0280 (9)	0.0319 (8)	0.0022 (8)	−0.0004 (7)	0.0043 (7)
C16	0.0480 (11)	0.0285 (9)	0.0326 (8)	0.0005 (8)	−0.0015 (7)	0.0074 (7)
C17	0.0472 (11)	0.0360 (10)	0.0375 (9)	0.0005 (8)	0.0013 (8)	−0.0014 (8)
C18	0.0390 (10)	0.0308 (9)	0.0381 (9)	0.0023 (8)	−0.0022 (7)	0.0005 (7)
C19	0.0443 (11)	0.0410 (10)	0.0395 (9)	−0.0057 (8)	0.0004 (8)	−0.0014 (8)
C20	0.0498 (11)	0.0431 (10)	0.0382 (10)	−0.0040 (9)	0.0056 (8)	−0.0002 (8)
C21	0.0455 (11)	0.0334 (9)	0.0364 (9)	0.0048 (8)	−0.0038 (8)	0.0008 (7)
C22	0.0602 (13)	0.0410 (10)	0.0377 (10)	−0.0006 (9)	0.0010 (9)	−0.0001 (8)
C23	0.0592 (13)	0.0406 (10)	0.0409 (10)	−0.0005 (9)	−0.0087 (9)	−0.0063 (8)
C24	0.0494 (12)	0.0435 (11)	0.0521 (11)	−0.0056 (9)	−0.0049 (9)	−0.0048 (9)
C25	0.0416 (11)	0.0414 (11)	0.0458 (10)	−0.0001 (9)	0.0016 (8)	−0.0015 (8)
C26	0.0419 (10)	0.0306 (9)	0.0398 (9)	0.0043 (8)	−0.0046 (8)	0.0003 (7)

Geometric parameters (Å, º)

O1—C25	1.362 (2)	C10—H10	0.9400
O1—H1O	0.914 (16)	C11—C16	1.430 (2)
N1—C17	1.274 (2)	C11—C12	1.433 (2)
N1—C1	1.418 (2)	C12—C13	1.349 (2)
N2—C18	1.328 (2)	C12—H12	0.9400
N2—C26	1.369 (2)	C13—C14	1.436 (2)
C1—C2	1.393 (2)	C13—H13	0.9400
C1—C14	1.412 (2)	C14—C15	1.419 (2)
C2—C3	1.384 (2)	C15—C16	1.422 (2)
C2—H2	0.9400	C17—C18	1.473 (2)
C3—C4	1.393 (2)	C17—H17	0.9400
C3—H3	0.9400	C18—C19	1.406 (2)
C4—C15	1.427 (2)	C19—C20	1.361 (2)

C4—C5	1.436 (2)	C19—H19	0.9400
C5—C6	1.351 (3)	C20—C21	1.414 (2)
C5—H5	0.9400	C20—H20	0.9400
C6—C7	1.432 (2)	C21—C26	1.407 (2)
C6—H6	0.9400	C21—C22	1.416 (2)
C7—C8	1.399 (2)	C22—C23	1.368 (3)
C7—C16	1.418 (2)	C22—H22	0.9400
C8—C9	1.378 (3)	C23—C24	1.402 (2)
C8—H8	0.9400	C23—H23	0.9400
C9—C10	1.379 (3)	C24—C25	1.370 (2)
C9—H9	0.9400	C24—H24	0.9400
C10—C11	1.393 (2)	C25—C26	1.416 (2)

C25—O1—H1O	100.9 (15)	C14—C13—H13	119.4
C17—N1—C1	120.46 (15)	C1—C14—C15	119.39 (15)
C18—N2—C26	117.16 (14)	C1—C14—C13	122.38 (15)
C2—C1—C14	119.75 (15)	C15—C14—C13	118.23 (16)
C2—C1—N1	123.56 (16)	C14—C15—C16	120.59 (16)
C14—C1—N1	116.54 (15)	C14—C15—C4	120.00 (16)
C3—C2—C1	120.80 (17)	C16—C15—C4	119.41 (15)
C3—C2—H2	119.6	C7—C16—C15	120.75 (16)
C1—C2—H2	119.6	C7—C16—C11	119.38 (16)
C2—C3—C4	121.51 (17)	C15—C16—C11	119.85 (15)
C2—C3—H3	119.2	N1—C17—C18	120.16 (16)
C4—C3—H3	119.2	N1—C17—H17	119.9
C3—C4—C15	118.53 (15)	C18—C17—H17	119.9
C3—C4—C5	122.87 (16)	N2—C18—C19	122.82 (15)
C15—C4—C5	118.58 (17)	N2—C18—C17	115.95 (15)
C6—C5—C4	121.42 (17)	C19—C18—C17	121.22 (16)
C6—C5—H5	119.3	C20—C19—C18	119.85 (17)
C4—C5—H5	119.3	C20—C19—H19	120.1
C5—C6—C7	121.52 (17)	C18—C19—H19	120.1
C5—C6—H6	119.2	C19—C20—C21	119.79 (16)
C7—C6—H6	119.2	C19—C20—H20	120.1
C8—C7—C16	119.11 (17)	C21—C20—H20	120.1
C8—C7—C6	122.58 (17)	C26—C21—C20	116.30 (15)
C16—C7—C6	118.31 (17)	C26—C21—C22	118.96 (16)
C9—C8—C7	120.85 (18)	C20—C21—C22	124.74 (16)
C9—C8—H8	119.6	C23—C22—C21	119.76 (17)
C7—C8—H8	119.6	C23—C22—H22	120.1
C8—C9—C10	120.73 (18)	C21—C22—H22	120.1
C8—C9—H9	119.6	C22—C23—C24	121.80 (17)
C10—C9—H9	119.6	C22—C23—H23	119.1
C9—C10—C11	120.96 (18)	C24—C23—H23	119.1
C9—C10—H10	119.5	C25—C24—C23	119.28 (18)
C11—C10—H10	119.5	C25—C24—H24	120.4
C10—C11—C16	118.96 (17)	C23—C24—H24	120.4
C10—C11—C12	123.13 (17)	O1—C25—C24	121.29 (17)

C16—C11—C12	117.91 (16)	O1—C25—C26	118.13 (16)
C13—C12—C11	122.10 (17)	C24—C25—C26	120.58 (17)
C13—C12—H12	119.0	N2—C26—C21	124.07 (16)
C11—C12—H12	119.0	N2—C26—C25	116.33 (15)
C12—C13—C14	121.25 (16)	C21—C26—C25	119.60 (16)
C12—C13—H13	119.4		

C17—N1—C1—C2	−26.9 (2)	C8—C7—C16—C11	−0.1 (2)
C17—N1—C1—C14	157.61 (16)	C6—C7—C16—C11	−179.74 (15)
C14—C1—C2—C3	0.8 (3)	C14—C15—C16—C7	177.43 (15)
N1—C1—C2—C3	−174.55 (16)	C4—C15—C16—C7	−1.8 (2)
C1—C2—C3—C4	0.4 (3)	C14—C15—C16—C11	−1.1 (2)
C2—C3—C4—C15	−0.8 (2)	C4—C15—C16—C11	179.69 (14)
C2—C3—C4—C5	177.58 (17)	C10—C11—C16—C7	0.0 (2)
C3—C4—C5—C6	−178.05 (18)	C12—C11—C16—C7	−179.86 (15)
C15—C4—C5—C6	0.4 (3)	C10—C11—C16—C15	178.57 (15)
C4—C5—C6—C7	−0.4 (3)	C12—C11—C16—C15	−1.3 (2)
C5—C6—C7—C8	179.80 (17)	C1—N1—C17—C18	174.56 (15)
C5—C6—C7—C16	−0.6 (3)	C26—N2—C18—C19	−0.9 (2)
C16—C7—C8—C9	0.0 (2)	C26—N2—C18—C17	177.84 (15)
C6—C7—C8—C9	179.57 (17)	N1—C17—C18—N2	179.95 (16)
C7—C8—C9—C10	0.3 (3)	N1—C17—C18—C19	−1.3 (3)
C8—C9—C10—C11	−0.5 (3)	N2—C18—C19—C20	1.3 (3)
C9—C10—C11—C16	0.3 (2)	C17—C18—C19—C20	−177.40 (17)
C9—C10—C11—C12	−179.85 (17)	C18—C19—C20—C21	−0.4 (3)
C10—C11—C12—C13	−177.25 (17)	C19—C20—C21—C26	−0.8 (2)
C16—C11—C12—C13	2.6 (2)	C19—C20—C21—C22	178.81 (18)
C11—C12—C13—C14	−1.5 (3)	C26—C21—C22—C23	−0.2 (3)
C2—C1—C14—C15	−1.6 (2)	C20—C21—C22—C23	−179.72 (18)
N1—C1—C14—C15	174.06 (14)	C21—C22—C23—C24	−0.7 (3)
C2—C1—C14—C13	178.08 (15)	C22—C23—C24—C25	0.2 (3)
N1—C1—C14—C13	−6.2 (2)	C23—C24—C25—O1	−177.90 (17)
C12—C13—C14—C1	179.23 (16)	C23—C24—C25—C26	1.3 (3)
C12—C13—C14—C15	−1.0 (2)	C18—N2—C26—C21	−0.4 (2)
C1—C14—C15—C16	−177.97 (15)	C18—N2—C26—C25	179.63 (15)
C13—C14—C15—C16	2.3 (2)	C20—C21—C26—N2	1.2 (3)
C1—C14—C15—C4	1.2 (2)	C22—C21—C26—N2	−178.43 (16)
C13—C14—C15—C4	−178.51 (15)	C20—C21—C26—C25	−178.82 (16)
C3—C4—C15—C14	0.0 (2)	C22—C21—C26—C25	1.6 (2)
C5—C4—C15—C14	−178.49 (15)	O1—C25—C26—N2	−2.9 (2)
C3—C4—C15—C16	179.21 (15)	C24—C25—C26—N2	177.82 (17)
C5—C4—C15—C16	0.7 (2)	O1—C25—C26—C21	177.05 (16)
C8—C7—C16—C15	−178.69 (15)	C24—C25—C26—C21	−2.2 (3)
C6—C7—C16—C15	1.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N2	0.91 (2)	2.03 (2)	2.666 (2)	125 (2)
C2—H2···O1^{i}	0.94	2.52	3.422 (2)	161
C17—H17···O1^{i}	0.94	2.57	3.436 (2)	153

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