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5-[(*E*)-2-Phenylethen-1-yl]quinolin-8-ol

Jens K. Bjernemose,[a]* Robert J. Less[b] and Paul R. Raithby[b]

[a]Department of Chemistry, University of Southern Denmark, Campusvej 55, DK-5230 Odense M, Denmark, and [b]Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, England

Correspondence e-mail: jkb@chem.sdu.dk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.142
Data-to-parameter ratio = 20.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{17}H_{13}NO$, dimerizes through O—H···N hydrogen bonds with H···N in the range 2.00–2.27 Å. These dimers form an extended structure through π–π stacking and C—H···π interactions.

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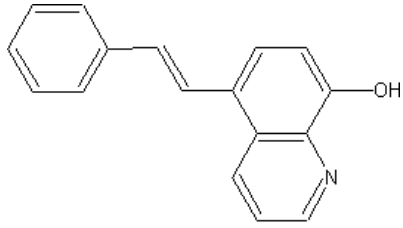
Comment

Due to their luminescence, quinolin-8-olate complexes have been widely used in organic light-emitting diodes and much work has gone into tuning the exact wavelengths produced. In a recent publication, the substituents in the 4′ position of 5-phenylazoquinolin-8-ol, (II), have been varied systematically and the free quinolin-8-ols have been structurally characterized. Their Zn^{II} and Al^{III} complexes [$Zn(II)_2$, $Al(II)_3$] have also been investigated (La Deda *et al.*, 2004). We report here the carbon analogue of La Deda's parent compound, *viz.* 5-[(*E*)-2-phenylethen-1-yl]-quinolin-8-ol, (I).



(I)

Compound (I) crystallizes in the space group $P2_1/c$ with three molecules in the asymmetric unit. They are each essentially planar with modest twists around the ethylene group of 179.51 (12), 177.63 (12) and 176.97 (12)° for molecules *A*, *B* and *C*, respectively, but do show significant twists of the phenylethenyl group relative to the quinoline [8.1 (2), 17.3 (2) and 8.1 (2)°, respectively]. The configuration is *E* and the phenyl group and the pyridine ring in the quinoline take an *anti* conformation in relation to one another. This is the same conformation found in (II) and can be rationalized as the one that ensures minimal interaction between the H atoms on the ethylene and the pyridine.

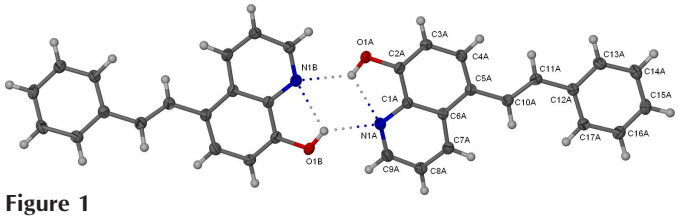


Figure 1
View of molecules *A* and *B* of (I) (50% probability displacement ellipsoids). Dotted lines indicate hydrogen bonds.

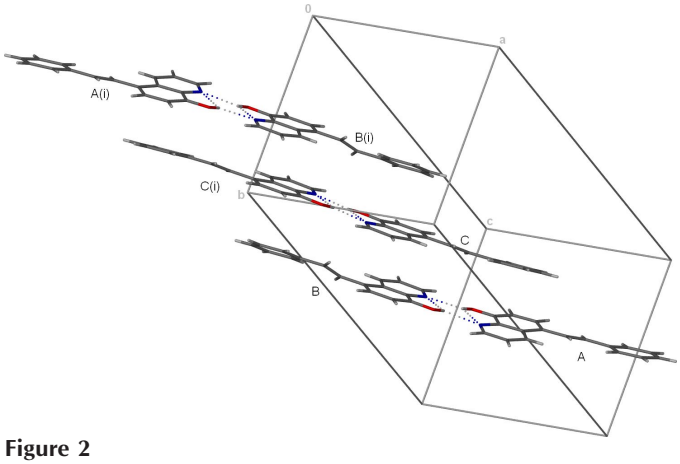


Figure 2
Side view of the π–π stacking along [021] [symmetry code: (i) $1-x$, $2-y$, $-z$].

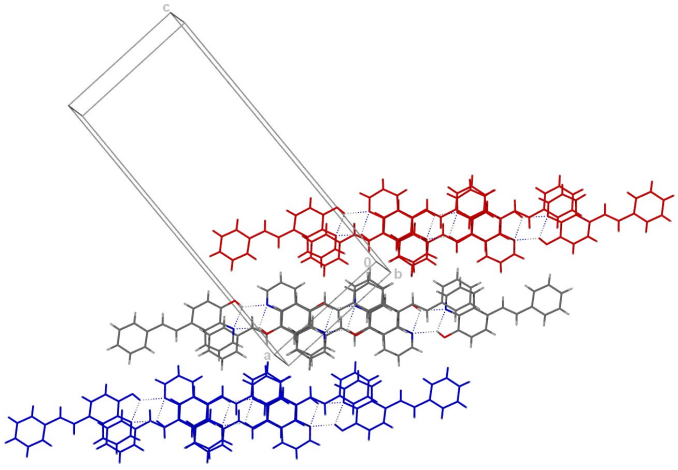


Figure 3
Parallel hexamers viewed along [021].

All three molecules dimerize through O—H···N hydrogen bonds [*A* with *B* and *C* with C^{i}; symmetry code: (i) $1-x$, $2-y$, $-z$; details given in Table 1]. This motif is seen for about 20% of the *ca* 120 quinolin-8-ols in the Cambridge Structural Database (Version 5.25, November 2003 with three updates, the latest being July 2004; Allen, 2002). Half of these, however, are twisted out of planarity compared to (I). The dimers stack through π–π interactions evident in Fig. 2. The quinoline in molecule *C* lies over that in *B* in a head-to-tail fashion (separation 3.49 Å), with the phenylethenyl group above the quinoline in *A* (3.52 Å). Similarly, the phenylethenyl group in *B* is below the quinoline in C^{i} (3.61 Å). This head-to-tail stacking and additional interaction through the phenyl is identical to the packing observed in both substituted examples of (II), but while the stacking continues throughout the structure in both of these, it is finite in (I). Molecules *A*, *B* and *C*, together with their symmetry equivalents [related by symmetry code (i)], form a basic six-molecule building block for the structure. This block then interacts weakly with symmetry-related blocks in a parallel but slightly offset position along *c* (Fig. 3). Furthermore, stronger C—H···π interactions are found to blocks that are tilted and displaced along *b* (Fig. 4). Both these latter interactions are also observed in (II), but again in an infinite form. Finally there are two C—H···O interactions to consider: C16*A*—H16*A*···O1*A*$(1+x, y, z)$ = 2.71 Å and C16*B*—H16*B*···O1*B*$(x-1, y, z)$ = 2.67 Å. The latter is particularly short and this is consistent with the observation that *B* is the molecule with the largest deviation from planarity of the phenylethenyl and quinoline groups.

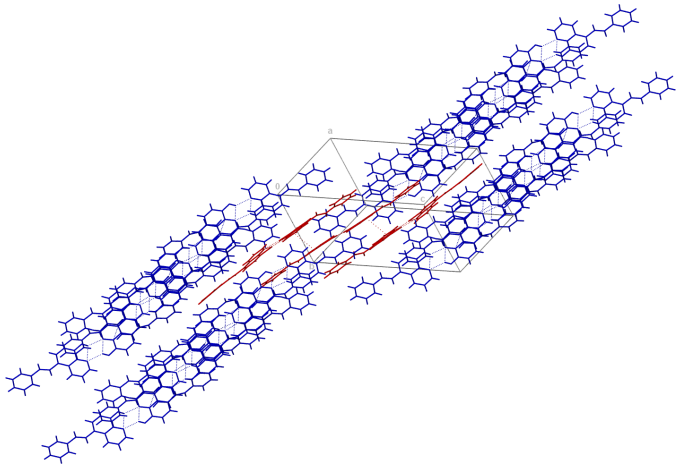


Figure 4
Central hexamer with C—H···π interactions to other hexamers.

Experimental

The title compound was synthesized *via* a Wittig reaction (Friedrich & Henning, 1959). Single crystals of (I) were produced by leaving a 3:1 mixture of (I) and $AlCl_3$ dissolved in methanol to evaporate to dryness.

Crystal data

$C_{17}H_{13}NO$
M_r = 247.28
Monoclinic, $P2_1/c$
a = 11.9280 (1) Å
b = 11.0120 (1) Å
c = 28.1700 (3) Å
β = 92.654 (1)°
V = 3696.19 (6) Å^3
Z = 12
D_x = 1.333 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 54 542 reflections
θ = 2.9–30.0°
μ = 0.08 mm^{-1}
T = 150 (2) K
Prism, translucent yellow
0.38 × 0.20 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.922, T_{max} = 0.997
65 180 measured reflections
10 796 independent reflections
6893 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 30.0°
$h = -16 \rightarrow 16$
$k = -15 \rightarrow 15$
$l = -39 \rightarrow 39$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.142
S = 1.04
10 796 reflections
526 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.3349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1A—H1A···N1B	0.88 (2)	2.15 (2)	2.8177 (16)	132.9 (17)
O1B—H1B···N1A	0.90 (2)	2.20 (2)	2.9173 (16)	135.6 (17)
O1C—H1C···N1C^{i}	0.94 (2)	2.00 (2)	2.7519 (15)	135.9 (16)

Symmetry code: (i) $1-x, 2-y, -z$.

H atoms in C—H bonds were constrained with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). Hydroxyl H atoms were located in a difference map and refined freely.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *X-Seed* (Barbour, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 280–388.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Friedrich, K. & Henning, H.-G. (1959). *Chem. Ber.* **92**, 2944–2952.
La Deda, M., Grisolia, A., Aiello, I., Crispini, A., Ghedini, M., Belviso, S., Amati, M. & Lelj, F. (2004). *Dalton Trans.* pp. 2424–2431.
Nonius (1997–2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.

supporting information

Acta Cryst. (2004). E**60**, o1981–o1983 [https://doi.org/10.1107/S1600536804025012]

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Cell parameters from 54542 reflections
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6893 reflections with $I > 2\sigma(I)$
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$\theta_{max} = 30.0°$, $\theta_{min} = 3.7°$
$h = -16 \rightarrow 16$
$k = -15 \rightarrow 15$
$l = -39 \rightarrow 39$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.142$
$S = 1.04$
10796 reflections
526 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.3349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1A	1.00536 (8)	1.15351 (10)	0.26941 (4)	0.0342 (2)
N1A	1.14573 (9)	1.28265 (10)	0.21446 (4)	0.0271 (2)
C1A	1.19146 (11)	1.22383 (11)	0.25356 (5)	0.0236 (3)
C2A	1.11634 (10)	1.15781 (12)	0.28171 (5)	0.0257 (3)
C3A	1.15606 (11)	1.09739 (12)	0.32148 (5)	0.0274 (3)
H3A	1.1054	1.0549	0.3405	0.033*
C4A	1.27068 (11)	1.09773 (12)	0.33426 (5)	0.0267 (3)
H4A	1.2961	1.0538	0.3617	0.032*
C5A	1.34898 (11)	1.15962 (11)	0.30846 (5)	0.0242 (3)
C6A	1.30817 (10)	1.22482 (11)	0.26702 (4)	0.0229 (3)
C7A	1.37663 (11)	1.29409 (12)	0.23728 (5)	0.0271 (3)
H7A	1.4552	1.2987	0.2443	0.033*
C8A	1.33061 (12)	1.35407 (12)	0.19872 (5)	0.0306 (3)
H8A	1.3766	1.4008	0.179	0.037*
C9A	1.21419 (11)	1.34600 (13)	0.18847 (5)	0.0308 (3)
H9A	1.1833	1.3882	0.1615	0.037*
C10A	1.46876 (11)	1.15961 (12)	0.32301 (5)	0.0268 (3)
H10A	1.5186	1.192	0.3009	0.032*
C11A	1.51492 (11)	1.11896 (12)	0.36401 (5)	0.0279 (3)
H11A	1.4648	1.0861	0.3859	0.034*
C12A	1.63404 (11)	1.11915 (11)	0.37918 (5)	0.0247 (3)
C13A	1.66713 (12)	1.06657 (12)	0.42280 (5)	0.0304 (3)
H13A	1.6116	1.0352	0.4426	0.036*
C14A	1.77933 (12)	1.05931 (13)	0.43781 (5)	0.0332 (3)
H14A	1.7999	1.0227	0.4675	0.04*
C15A	1.86129 (12)	1.10533 (13)	0.40960 (5)	0.0323 (3)
H15A	1.9383	1.0993	0.4195	0.039*
C16A	1.83018 (11)	1.16038 (13)	0.36668 (5)	0.0319 (3)
H16A	1.8862	1.1931	0.3474	0.038*
C17A	1.71838 (11)	1.16804 (12)	0.35167 (5)	0.0282 (3)
H17A	1.6983	1.2069	0.3224	0.034*
O1B	0.98300 (8)	1.32068 (9)	0.13534 (4)	0.0325 (2)
N1B	0.84510 (9)	1.20227 (10)	0.19523 (4)	0.0260 (2)
C1B	0.79822 (10)	1.24929 (11)	0.15391 (4)	0.0236 (3)
C2B	0.87196 (11)	1.30937 (12)	0.12321 (5)	0.0255 (3)
C3B	0.83043 (11)	1.35656 (12)	0.08096 (5)	0.0289 (3)
H3B	0.8797	1.3958	0.0603	0.035*
C4B	0.71575 (11)	1.34747 (12)	0.06792 (5)	0.0294 (3)
H4B	0.6892	1.3817	0.0386	0.035*
C5B	0.63998 (11)	1.29044 (12)	0.09626 (5)	0.0260 (3)

C6B	0.68202 (10)	1.24033 (11)	0.14043 (5)	0.0245 (3)
C7B	0.61509 (11)	1.17671 (12)	0.17251 (5)	0.0283 (3)
H7B	0.5368	1.1676	0.1656	0.034*
C8B	0.66268 (11)	1.12858 (13)	0.21328 (5)	0.0296 (3)
H8B	0.6179	1.0856	0.2347	0.036*
C9B	0.77814 (11)	1.14288 (12)	0.22339 (5)	0.0284 (3)
H9B	0.8099	1.1083	0.2518	0.034*
C10B	0.51995 (11)	1.28230 (12)	0.08217 (5)	0.0289 (3)
H10B	0.4692	1.2769	0.1071	0.035*
C11B	0.47527 (11)	1.28169 (12)	0.03795 (5)	0.0280 (3)
H11B	0.526	1.2839	0.0129	0.034*
C12B	0.35474 (11)	1.27795 (12)	0.02420 (5)	0.0266 (3)
C13B	0.31851 (12)	1.30248 (12)	−0.02270 (5)	0.0299 (3)
H13B	0.3725	1.3193	−0.0455	0.036*
C14B	0.20576 (12)	1.30281 (13)	−0.03661 (5)	0.0327 (3)
H14B	0.1832	1.3199	−0.0687	0.039*
C15B	0.12565 (12)	1.27828 (13)	−0.00391 (5)	0.0329 (3)
H15B	0.0482	1.2787	−0.0134	0.04*
C16B	0.15981 (12)	1.25300 (14)	0.04283 (5)	0.0341 (3)
H16B	0.1053	1.2359	0.0654	0.041*
C17B	0.27245 (11)	1.25247 (13)	0.05679 (5)	0.0307 (3)
H17B	0.2944	1.2346	0.0889	0.037*
O1C	0.51422 (8)	0.93682 (10)	0.06785 (4)	0.0347 (2)
N1C	0.64938 (9)	1.04801 (10)	0.00406 (4)	0.0244 (2)
C1C	0.69711 (10)	1.00783 (11)	0.04625 (4)	0.0222 (3)
C2C	0.62491 (11)	0.95194 (12)	0.07854 (5)	0.0248 (3)
C3C	0.66786 (11)	0.91111 (12)	0.12160 (5)	0.0271 (3)
H3C	0.6192	0.8752	0.1434	0.033*
C4C	0.78202 (11)	0.92167 (12)	0.13378 (5)	0.0260 (3)
H4C	0.8094	0.891	0.1636	0.031*
C5C	0.85717 (10)	0.97513 (11)	0.10404 (5)	0.0232 (3)
C6C	0.81345 (10)	1.01986 (11)	0.05913 (4)	0.0219 (3)
C7C	0.87933 (11)	1.07791 (12)	0.02501 (5)	0.0252 (3)
H7C	0.9577	1.0882	0.0313	0.03*
C8C	0.83096 (11)	1.11881 (12)	−0.01667 (5)	0.0273 (3)
H8C	0.8751	1.158	−0.0393	0.033*
C9C	0.71516 (11)	1.10263 (12)	−0.02591 (5)	0.0266 (3)
H9C	0.6825	1.1323	−0.0551	0.032*
C10C	0.97697 (11)	0.98371 (12)	0.11767 (5)	0.0261 (3)
H10C	1.0253	1.0068	0.0934	0.031*
C11C	1.02524 (11)	0.96268 (12)	0.16029 (5)	0.0270 (3)
H11C	0.9767	0.9435	0.185	0.032*
C12C	1.14578 (11)	0.96604 (11)	0.17310 (5)	0.0244 (3)
C13C	1.18417 (11)	0.92764 (12)	0.21819 (5)	0.0261 (3)
H13C	1.1315	0.9017	0.2404	0.031*
C14C	1.29790 (11)	0.92664 (12)	0.23130 (5)	0.0288 (3)
H14C	1.3224	0.9001	0.2622	0.035*
C15C	1.37544 (12)	0.96429 (12)	0.19935 (5)	0.0310 (3)

H15C	1.4533	0.9639	0.2082	0.037*
C16C	1.33884 (11)	1.00272 (13)	0.15416 (5)	0.0319 (3)
H16C	1.3919	1.0279	0.1321	0.038*
C17C	1.22566 (11)	1.00432 (13)	0.14131 (5)	0.0285 (3)
H17C	1.2016	1.0317	0.1105	0.034*
H1A	0.9927 (16)	1.1865 (18)	0.2413 (8)	0.074 (7)*
H1B	0.9981 (17)	1.289 (2)	0.1646 (8)	0.086 (8)*
H1C	0.4915 (16)	0.9616 (19)	0.0369 (8)	0.078 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0208 (5)	0.0500 (6)	0.0315 (6)	−0.0021 (4)	−0.0010 (4)	0.0098 (5)
N1A	0.0267 (6)	0.0267 (6)	0.0277 (6)	0.0003 (5)	−0.0011 (5)	0.0028 (5)
C1A	0.0240 (7)	0.0235 (6)	0.0233 (6)	0.0020 (5)	0.0005 (5)	−0.0010 (5)
C2A	0.0212 (7)	0.0294 (7)	0.0265 (7)	0.0005 (5)	0.0013 (5)	−0.0017 (5)
C3A	0.0266 (7)	0.0310 (7)	0.0249 (7)	−0.0017 (5)	0.0033 (6)	0.0019 (5)
C4A	0.0279 (7)	0.0291 (7)	0.0229 (6)	0.0017 (5)	−0.0010 (5)	0.0015 (5)
C5A	0.0247 (7)	0.0238 (6)	0.0241 (7)	0.0006 (5)	0.0010 (5)	−0.0018 (5)
C6A	0.0229 (7)	0.0217 (6)	0.0241 (6)	0.0007 (5)	0.0005 (5)	−0.0023 (5)
C7A	0.0250 (7)	0.0268 (7)	0.0293 (7)	−0.0023 (5)	0.0002 (6)	−0.0005 (5)
C8A	0.0318 (8)	0.0286 (7)	0.0314 (7)	−0.0052 (6)	0.0014 (6)	0.0060 (6)
C9A	0.0314 (8)	0.0302 (7)	0.0306 (7)	−0.0006 (6)	−0.0024 (6)	0.0067 (6)
C10A	0.0240 (7)	0.0284 (7)	0.0280 (7)	0.0001 (5)	0.0022 (6)	0.0023 (5)
C11A	0.0254 (7)	0.0324 (7)	0.0262 (7)	0.0007 (5)	0.0040 (6)	0.0005 (6)
C12A	0.0262 (7)	0.0229 (6)	0.0249 (7)	0.0018 (5)	0.0002 (5)	−0.0019 (5)
C13A	0.0330 (8)	0.0318 (7)	0.0262 (7)	−0.0012 (6)	0.0006 (6)	0.0031 (6)
C14A	0.0365 (8)	0.0337 (8)	0.0285 (7)	0.0026 (6)	−0.0070 (6)	0.0012 (6)
C15A	0.0270 (7)	0.0317 (7)	0.0374 (8)	0.0039 (6)	−0.0070 (6)	−0.0035 (6)
C16A	0.0263 (7)	0.0334 (7)	0.0360 (8)	−0.0007 (6)	0.0029 (6)	0.0001 (6)
C17A	0.0280 (7)	0.0290 (7)	0.0275 (7)	0.0026 (5)	0.0007 (6)	0.0036 (6)
O1B	0.0203 (5)	0.0455 (6)	0.0315 (6)	−0.0029 (4)	0.0004 (4)	0.0055 (5)
N1B	0.0237 (6)	0.0289 (6)	0.0253 (6)	−0.0001 (4)	0.0005 (5)	−0.0033 (5)
C1B	0.0235 (7)	0.0244 (6)	0.0229 (6)	0.0006 (5)	0.0010 (5)	−0.0040 (5)
C2B	0.0214 (7)	0.0268 (7)	0.0284 (7)	0.0000 (5)	0.0014 (5)	−0.0039 (5)
C3B	0.0271 (7)	0.0318 (7)	0.0281 (7)	−0.0020 (6)	0.0040 (6)	0.0015 (6)
C4B	0.0301 (7)	0.0308 (7)	0.0271 (7)	0.0017 (6)	−0.0010 (6)	0.0002 (6)
C5B	0.0243 (7)	0.0266 (7)	0.0270 (7)	0.0013 (5)	0.0007 (6)	−0.0036 (5)
C6B	0.0233 (7)	0.0247 (6)	0.0256 (7)	0.0005 (5)	0.0007 (5)	−0.0046 (5)
C7B	0.0223 (7)	0.0329 (7)	0.0297 (7)	−0.0037 (5)	0.0008 (6)	−0.0037 (6)
C8B	0.0272 (7)	0.0352 (7)	0.0265 (7)	−0.0057 (6)	0.0025 (6)	0.0003 (6)
C9B	0.0280 (7)	0.0330 (7)	0.0240 (7)	−0.0022 (6)	0.0002 (6)	−0.0009 (6)
C10B	0.0257 (7)	0.0327 (7)	0.0282 (7)	0.0004 (6)	0.0004 (6)	0.0012 (6)
C11B	0.0242 (7)	0.0304 (7)	0.0293 (7)	0.0029 (5)	0.0016 (6)	−0.0006 (6)
C12B	0.0275 (7)	0.0251 (7)	0.0268 (7)	0.0012 (5)	−0.0011 (6)	−0.0006 (5)
C13B	0.0313 (8)	0.0320 (7)	0.0263 (7)	−0.0002 (6)	0.0013 (6)	−0.0001 (6)
C14B	0.0362 (8)	0.0350 (8)	0.0263 (7)	−0.0013 (6)	−0.0075 (6)	0.0015 (6)
C15B	0.0251 (7)	0.0343 (8)	0.0386 (8)	−0.0040 (6)	−0.0068 (6)	0.0026 (6)

C16B	0.0270 (7)	0.0394 (8)	0.0358 (8)	−0.0061 (6)	0.0003 (6)	0.0038 (6)
C17B	0.0301 (8)	0.0353 (8)	0.0264 (7)	−0.0026 (6)	−0.0027 (6)	0.0037 (6)
O1C	0.0188 (5)	0.0568 (7)	0.0283 (5)	−0.0048 (4)	−0.0009 (4)	0.0130 (5)
N1C	0.0220 (6)	0.0277 (6)	0.0234 (6)	0.0009 (4)	−0.0003 (4)	0.0015 (4)
C1C	0.0218 (6)	0.0226 (6)	0.0221 (6)	0.0012 (5)	−0.0001 (5)	0.0003 (5)
C2C	0.0201 (7)	0.0286 (7)	0.0258 (7)	0.0001 (5)	0.0017 (5)	0.0003 (5)
C3C	0.0226 (7)	0.0323 (7)	0.0265 (7)	−0.0014 (5)	0.0028 (5)	0.0059 (6)
C4C	0.0253 (7)	0.0290 (7)	0.0235 (6)	0.0004 (5)	−0.0017 (5)	0.0035 (5)
C5C	0.0213 (6)	0.0237 (6)	0.0245 (7)	0.0009 (5)	−0.0002 (5)	−0.0004 (5)
C6C	0.0203 (6)	0.0221 (6)	0.0232 (6)	0.0001 (5)	0.0004 (5)	−0.0012 (5)
C7C	0.0194 (6)	0.0283 (7)	0.0278 (7)	−0.0021 (5)	−0.0002 (5)	−0.0006 (5)
C8C	0.0249 (7)	0.0306 (7)	0.0267 (7)	−0.0048 (5)	0.0034 (6)	0.0030 (6)
C9C	0.0262 (7)	0.0306 (7)	0.0229 (6)	−0.0002 (5)	−0.0002 (5)	0.0027 (5)
C10C	0.0222 (7)	0.0301 (7)	0.0258 (7)	−0.0011 (5)	0.0009 (5)	0.0028 (5)
C11C	0.0221 (7)	0.0326 (7)	0.0263 (7)	−0.0002 (5)	0.0018 (5)	0.0024 (6)
C12C	0.0231 (7)	0.0243 (6)	0.0254 (7)	0.0016 (5)	−0.0011 (5)	−0.0012 (5)
C13C	0.0274 (7)	0.0256 (7)	0.0251 (7)	0.0005 (5)	0.0004 (6)	0.0004 (5)
C14C	0.0324 (8)	0.0252 (7)	0.0281 (7)	0.0018 (5)	−0.0071 (6)	−0.0010 (5)
C15C	0.0224 (7)	0.0303 (7)	0.0395 (8)	−0.0007 (5)	−0.0064 (6)	−0.0018 (6)
C16C	0.0242 (7)	0.0380 (8)	0.0336 (8)	−0.0048 (6)	0.0016 (6)	0.0003 (6)
C17C	0.0257 (7)	0.0346 (7)	0.0248 (7)	−0.0018 (6)	−0.0019 (6)	0.0021 (6)

Geometric parameters (Å, º)

O1A—C2A	1.3536 (16)	C8B—H8B	0.95
O1A—H1A	0.88 (2)	C9B—H9B	0.95
N1A—C9A	1.3210 (17)	C10B—C11B	1.3320 (19)
N1A—C1A	1.3693 (16)	C10B—H10B	0.95
C1A—C2A	1.4234 (17)	C11B—C12B	1.4721 (18)
C1A—C6A	1.4258 (17)	C11B—H11B	0.95
C2A—C3A	1.3685 (19)	C12B—C13B	1.3971 (19)
C3A—C4A	1.3977 (18)	C12B—C17B	1.4032 (18)
C3A—H3A	0.95	C13B—C14B	1.3833 (19)
C4A—C5A	1.3885 (18)	C13B—H13B	0.95
C4A—H4A	0.95	C14B—C15B	1.3842 (19)
C5A—C6A	1.4361 (18)	C14B—H14B	0.95
C5A—C10A	1.4680 (18)	C15B—C16B	1.388 (2)
C6A—C7A	1.4192 (17)	C15B—H15B	0.95
C7A—C8A	1.3646 (19)	C16B—C17B	1.3823 (19)
C7A—H7A	0.95	C16B—H16B	0.95
C8A—C9A	1.4081 (19)	C17B—H17B	0.95
C8A—H8A	0.95	O1C—C2C	1.3509 (15)
C9A—H9A	0.95	O1C—H1C	0.94 (2)
C10A—C11A	1.3335 (18)	N1C—C9C	1.3235 (16)
C10A—H10A	0.95	N1C—C1C	1.3674 (16)
C11A—C12A	1.4647 (18)	C1C—C2C	1.4212 (17)
C11A—H11A	0.95	C1C—C6C	1.4242 (17)
C12A—C13A	1.3985 (18)	C2C—C3C	1.3707 (18)

C12A—C17A	1.4054 (17)	C3C—C4C	1.3937 (18)
C13A—C14A	1.3869 (19)	C3C—H3C	0.95
C13A—H13A	0.95	C4C—C5C	1.3862 (17)
C14A—C15A	1.384 (2)	C4C—H4C	0.95
C14A—H14A	0.95	C5C—C6C	1.4332 (18)
C15A—C16A	1.388 (2)	C5C—C10C	1.4654 (18)
C15A—H15A	0.95	C6C—C7C	1.4212 (17)
C16A—C17A	1.3827 (19)	C7C—C8C	1.3606 (18)
C16A—H16A	0.95	C7C—H7C	0.95
C17A—H17A	0.95	C8C—C9C	1.4051 (18)
O1B—C2B	1.3582 (16)	C8C—H8C	0.95
O1B—H1B	0.90 (2)	C9C—H9C	0.95
N1B—C9B	1.3243 (16)	C10C—C11C	1.3277 (18)
N1B—C1B	1.3693 (17)	C10C—H10C	0.95
C1B—C6B	1.4236 (17)	C11C—C12C	1.4666 (18)
C1B—C2B	1.4248 (17)	C11C—H11C	0.95
C2B—C3B	1.3700 (19)	C12C—C13C	1.3958 (18)
C3B—C4B	1.4034 (19)	C12C—C17C	1.4023 (17)
C3B—H3B	0.95	C13C—C14C	1.3894 (18)
C4B—C5B	1.3841 (18)	C13C—H13C	0.95
C4B—H4B	0.95	C14C—C15C	1.3836 (19)
C5B—C6B	1.4304 (18)	C14C—H14C	0.95
C5B—C10B	1.4707 (18)	C15C—C16C	1.392 (2)
C6B—C7B	1.4184 (18)	C15C—H15C	0.95
C7B—C8B	1.3644 (19)	C16C—C17C	1.3815 (19)
C7B—H7B	0.95	C16C—H16C	0.95
C8B—C9B	1.4023 (18)	C17C—H17C	0.95

C2A—O1A—H1A	110.0 (13)	N1B—C9B—H9B	118.4
C9A—N1A—C1A	117.53 (11)	C8B—C9B—H9B	118.4
N1A—C1A—C2A	116.88 (11)	C11B—C10B—C5B	126.52 (12)
N1A—C1A—C6A	123.92 (11)	C11B—C10B—H10B	116.7
C2A—C1A—C6A	119.20 (12)	C5B—C10B—H10B	116.7
O1A—C2A—C3A	119.34 (11)	C10B—C11B—C12B	126.14 (12)
O1A—C2A—C1A	120.57 (12)	C10B—C11B—H11B	116.9
C3A—C2A—C1A	120.08 (12)	C12B—C11B—H11B	116.9
C2A—C3A—C4A	120.47 (12)	C13B—C12B—C17B	117.53 (12)
C2A—C3A—H3A	119.8	C13B—C12B—C11B	119.93 (12)
C4A—C3A—H3A	119.8	C17B—C12B—C11B	122.53 (13)
C5A—C4A—C3A	122.69 (13)	C14B—C13B—C12B	121.51 (12)
C5A—C4A—H4A	118.7	C14B—C13B—H13B	119.2
C3A—C4A—H4A	118.7	C12B—C13B—H13B	119.2
C4A—C5A—C6A	117.38 (12)	C13B—C14B—C15B	120.19 (14)
C4A—C5A—C10A	121.56 (12)	C13B—C14B—H14B	119.9
C6A—C5A—C10A	121.06 (11)	C15B—C14B—H14B	119.9
C7A—C6A—C1A	115.37 (12)	C14B—C15B—C16B	119.27 (13)
C7A—C6A—C5A	124.46 (12)	C14B—C15B—H15B	120.4
C1A—C6A—C5A	120.16 (11)	C16B—C15B—H15B	120.4

C8A—C7A—C6A	120.59 (12)	C17B—C16B—C15B	120.62 (13)
C8A—C7A—H7A	119.7	C17B—C16B—H16B	119.7
C6A—C7A—H7A	119.7	C15B—C16B—H16B	119.7
C7A—C8A—C9A	119.29 (12)	C16B—C17B—C12B	120.87 (13)
C7A—C8A—H8A	120.4	C16B—C17B—H17B	119.6
C9A—C8A—H8A	120.4	C12B—C17B—H17B	119.6
N1A—C9A—C8A	123.28 (13)	C2C—O1C—H1C	114.0 (12)
N1A—C9A—H9A	118.4	C9C—N1C—C1C	117.80 (11)
C8A—C9A—H9A	118.4	N1C—C1C—C2C	117.14 (11)
C11A—C10A—C5A	126.82 (12)	N1C—C1C—C6C	123.55 (11)
C11A—C10A—H10A	116.6	C2C—C1C—C6C	119.31 (12)
C5A—C10A—H10A	116.6	O1C—C2C—C3C	118.57 (11)
C10A—C11A—C12A	127.47 (12)	O1C—C2C—C1C	121.71 (12)
C10A—C11A—H11A	116.3	C3C—C2C—C1C	119.72 (12)
C12A—C11A—H11A	116.3	C2C—C3C—C4C	120.75 (12)
C13A—C12A—C17A	117.58 (12)	C2C—C3C—H3C	119.6
C13A—C12A—C11A	119.11 (12)	C4C—C3C—H3C	119.6
C17A—C12A—C11A	123.30 (12)	C5C—C4C—C3C	122.58 (12)
C14A—C13A—C12A	121.38 (13)	C5C—C4C—H4C	118.7
C14A—C13A—H13A	119.3	C3C—C4C—H4C	118.7
C12A—C13A—H13A	119.3	C4C—C5C—C6C	117.42 (12)
C15A—C14A—C13A	120.07 (13)	C4C—C5C—C10C	121.27 (12)
C15A—C14A—H14A	120	C6C—C5C—C10C	121.31 (11)
C13A—C14A—H14A	120	C7C—C6C—C1C	115.62 (12)
C14A—C15A—C16A	119.51 (13)	C7C—C6C—C5C	124.17 (12)
C14A—C15A—H15A	120.2	C1C—C6C—C5C	120.22 (11)
C16A—C15A—H15A	120.2	C8C—C7C—C6C	120.45 (12)
C17A—C16A—C15A	120.55 (13)	C8C—C7C—H7C	119.8
C17A—C16A—H16A	119.7	C6C—C7C—H7C	119.8
C15A—C16A—H16A	119.7	C7C—C8C—C9C	119.47 (12)
C16A—C17A—C12A	120.85 (13)	C7C—C8C—H8C	120.3
C16A—C17A—H17A	119.6	C9C—C8C—H8C	120.3
C12A—C17A—H17A	119.6	N1C—C9C—C8C	123.09 (12)
C2B—O1B—H1B	110.2 (13)	N1C—C9C—H9C	118.5
C9B—N1B—C1B	117.52 (11)	C8C—C9C—H9C	118.5
N1B—C1B—C6B	123.69 (11)	C11C—C10C—C5C	127.05 (12)
N1B—C1B—C2B	116.90 (11)	C11C—C10C—H10C	116.5
C6B—C1B—C2B	119.41 (12)	C5C—C10C—H10C	116.5
O1B—C2B—C3B	119.53 (12)	C10C—C11C—C12C	126.67 (12)
O1B—C2B—C1B	120.80 (12)	C10C—C11C—H11C	116.7
C3B—C2B—C1B	119.67 (12)	C12C—C11C—H11C	116.7
C2B—C3B—C4B	120.61 (12)	C13C—C12C—C17C	117.92 (12)
C2B—C3B—H3B	119.7	C13C—C12C—C11C	119.52 (11)
C4B—C3B—H3B	119.7	C17C—C12C—C11C	122.54 (12)
C5B—C4B—C3B	122.40 (13)	C14C—C13C—C12C	121.28 (12)
C5B—C4B—H4B	118.8	C14C—C13C—H13C	119.4
C3B—C4B—H4B	118.8	C12C—C13C—H13C	119.4
C4B—C5B—C6B	117.70 (12)	C15C—C14C—C13C	119.91 (13)

C4B—C5B—C10B	121.70 (12)	C15C—C14C—H14C	120
C6B—C5B—C10B	120.59 (11)	C13C—C14C—H14C	120
C7B—C6B—C1B	115.72 (12)	C14C—C15C—C16C	119.68 (13)
C7B—C6B—C5B	124.04 (12)	C14C—C15C—H15C	120.2
C1B—C6B—C5B	120.20 (11)	C16C—C15C—H15C	120.2
C8B—C7B—C6B	120.24 (12)	C17C—C16C—C15C	120.30 (12)
C8B—C7B—H7B	119.9	C17C—C16C—H16C	119.8
C6B—C7B—H7B	119.9	C15C—C16C—H16C	119.8
C7B—C8B—C9B	119.59 (12)	C16C—C17C—C12C	120.90 (13)
C7B—C8B—H8B	120.2	C16C—C17C—H17C	119.6
C9B—C8B—H8B	120.2	C12C—C17C—H17C	119.6
N1B—C9B—C8B	123.21 (13)		

C9A—N1A—C1A—C2A	178.86 (12)	C1B—C6B—C7B—C8B	−0.05 (18)
C9A—N1A—C1A—C6A	−1.53 (19)	C5B—C6B—C7B—C8B	178.00 (13)
N1A—C1A—C2A—O1A	0.72 (18)	C6B—C7B—C8B—C9B	0.3 (2)
C6A—C1A—C2A—O1A	−178.91 (11)	C1B—N1B—C9B—C8B	−1.35 (19)
N1A—C1A—C2A—C3A	−179.61 (12)	C7B—C8B—C9B—N1B	0.4 (2)
C6A—C1A—C2A—C3A	0.76 (18)	C4B—C5B—C10B—C11B	27.5 (2)
O1A—C2A—C3A—C4A	178.30 (12)	C6B—C5B—C10B—C11B	−153.21 (14)
C1A—C2A—C3A—C4A	−1.4 (2)	C5B—C10B—C11B—C12B	−177.63 (12)
C2A—C3A—C4A—C5A	1.1 (2)	C10B—C11B—C12B—C13B	166.97 (14)
C3A—C4A—C5A—C6A	−0.21 (19)	C10B—C11B—C12B—C17B	−11.9 (2)
C3A—C4A—C5A—C10A	179.27 (12)	C17B—C12B—C13B—C14B	0.5 (2)
N1A—C1A—C6A—C7A	1.13 (18)	C11B—C12B—C13B—C14B	−178.34 (12)
C2A—C1A—C6A—C7A	−179.26 (11)	C12B—C13B—C14B—C15B	−0.1 (2)
N1A—C1A—C6A—C5A	−179.47 (12)	C13B—C14B—C15B—C16B	−0.2 (2)
C2A—C1A—C6A—C5A	0.13 (18)	C14B—C15B—C16B—C17B	0.1 (2)
C4A—C5A—C6A—C7A	178.94 (12)	C15B—C16B—C17B—C12B	0.3 (2)
C10A—C5A—C6A—C7A	−0.54 (19)	C13B—C12B—C17B—C16B	−0.6 (2)
C4A—C5A—C6A—C1A	−0.40 (18)	C11B—C12B—C17B—C16B	178.23 (13)
C10A—C5A—C6A—C1A	−179.88 (11)	C9C—N1C—C1C—C2C	178.55 (11)
C1A—C6A—C7A—C8A	−0.14 (18)	C9C—N1C—C1C—C6C	−1.09 (18)
C5A—C6A—C7A—C8A	−179.50 (13)	N1C—C1C—C2C—O1C	1.22 (18)
C6A—C7A—C8A—C9A	−0.4 (2)	C6C—C1C—C2C—O1C	−179.12 (11)
C1A—N1A—C9A—C8A	0.9 (2)	N1C—C1C—C2C—C3C	−179.29 (12)
C7A—C8A—C9A—N1A	0.0 (2)	C6C—C1C—C2C—C3C	0.37 (18)
C4A—C5A—C10A—C11A	−10.4 (2)	O1C—C2C—C3C—C4C	178.29 (12)
C6A—C5A—C10A—C11A	169.09 (13)	C1C—C2C—C3C—C4C	−1.2 (2)
C5A—C10A—C11A—C12A	−179.51 (12)	C2C—C3C—C4C—C5C	1.2 (2)
C10A—C11A—C12A—C13A	−176.76 (14)	C3C—C4C—C5C—C6C	−0.34 (19)
C10A—C11A—C12A—C17A	2.1 (2)	C3C—C4C—C5C—C10C	−179.35 (12)
C17A—C12A—C13A—C14A	−1.99 (19)	N1C—C1C—C6C—C7C	0.27 (18)
C11A—C12A—C13A—C14A	176.96 (12)	C2C—C1C—C6C—C7C	−179.36 (11)
C12A—C13A—C14A—C15A	0.4 (2)	N1C—C1C—C6C—C5C	−179.88 (11)
C13A—C14A—C15A—C16A	1.0 (2)	C2C—C1C—C6C—C5C	0.49 (18)
C14A—C15A—C16A—C17A	−0.9 (2)	C4C—C5C—C6C—C7C	179.34 (12)
C15A—C16A—C17A—C12A	−0.8 (2)	C10C—C5C—C6C—C7C	−1.66 (19)

C13A—C12A—C17A—C16A	2.15 (19)	C4C—C5C—C6C—C1C	−0.50 (17)
C11A—C12A—C17A—C16A	−176.75 (13)	C10C—C5C—C6C—C1C	178.50 (11)
C9B—N1B—C1B—C6B	1.63 (18)	C1C—C6C—C7C—C8C	0.46 (18)
C9B—N1B—C1B—C2B	−177.93 (11)	C5C—C6C—C7C—C8C	−179.39 (12)
N1B—C1B—C2B—O1B	−1.21 (18)	C6C—C7C—C8C—C9C	−0.36 (19)
C6B—C1B—C2B—O1B	179.20 (11)	C1C—N1C—C9C—C8C	1.21 (19)
N1B—C1B—C2B—C3B	178.91 (12)	C7C—C8C—C9C—N1C	−0.5 (2)
C6B—C1B—C2B—C3B	−0.68 (18)	C4C—C5C—C10C—C11C	−11.8 (2)
O1B—C2B—C3B—C4B	−179.14 (12)	C6C—C5C—C10C—C11C	169.28 (13)
C1B—C2B—C3B—C4B	0.73 (19)	C5C—C10C—C11C—C12C	176.97 (12)
C2B—C3B—C4B—C5B	−0.6 (2)	C10C—C11C—C12C—C13C	−172.42 (13)
C3B—C4B—C5B—C6B	0.40 (19)	C10C—C11C—C12C—C17C	6.2 (2)
C3B—C4B—C5B—C10B	179.67 (12)	C17C—C12C—C13C—C14C	−0.30 (19)
N1B—C1B—C6B—C7B	−0.95 (18)	C11C—C12C—C13C—C14C	178.42 (12)
C2B—C1B—C6B—C7B	178.61 (11)	C12C—C13C—C14C—C15C	0.04 (19)
N1B—C1B—C6B—C5B	−179.08 (12)	C13C—C14C—C15C—C16C	−0.2 (2)
C2B—C1B—C6B—C5B	0.48 (18)	C14C—C15C—C16C—C17C	0.5 (2)
C4B—C5B—C6B—C7B	−178.31 (12)	C15C—C16C—C17C—C12C	−0.8 (2)
C10B—C5B—C6B—C7B	2.41 (19)	C13C—C12C—C17C—C16C	0.7 (2)
C4B—C5B—C6B—C1B	−0.34 (18)	C11C—C12C—C17C—C16C	−177.99 (13)
C10B—C5B—C6B—C1B	−179.62 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···N1*B*	0.88 (2)	2.15 (2)	2.8177 (16)	132.9 (17)
O1*A*—H1*A*···N1*A*	0.88 (2)	2.27 (2)	2.7316 (15)	112.7 (16)
O1*B*—H1*B*···N1*A*	0.90 (2)	2.20 (2)	2.9173 (16)	135.6 (17)
O1*B*—H1*B*···N1*B*	0.90 (2)	2.27 (2)	2.7403 (14)	112.2 (16)
O1*C*—H1*C*···N1*C*^{i}	0.94 (2)	2.00 (2)	2.7519 (15)	135.9 (16)

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