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Synthesis and structure of 2,4-di-*tert*-butyl-6-[(naphthalen-2-ylimino)methyl]phenol

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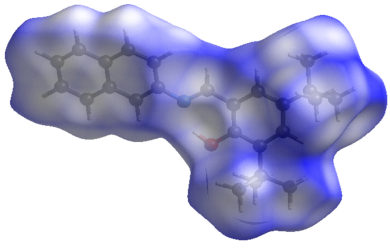
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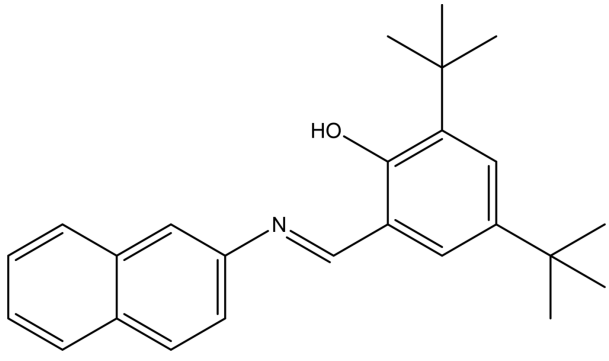
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In the title compound, $C_{25}H_{29}NO$, the dihedral angle between the naphthyl ring system and the phenol ring is 16.41 (4)°. An intramolecular O—H···N hydrogen bond is observed. The extended structure features a weak C—H···O interaction. Hirshfeld surface analysis showed that H···H contacts contribute the highest contact percentage (69.3%), followed by C···H/H···C (23.1%), C···C (2.9%), N···H/H···N (2.6%), and O···H/H···O (2.1%).

1. Chemical context

Salicylaldimine-type Schiff bases with a hydroxyl group *ortho* to the azomethine (–C═N–) linkage are known for their photochromic behaviour, and Schiff bases of this type usually feature an intramolecular O—H···N hydrogen bond (Carreño *et al.*, 2025; Kansiz *et al.*, 2018). Schiff bases derived from 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde can show proton tautomerization, which plays an important role in chemistry and biochemistry (Mason *et al.*, 2021; Carreno *et al.*, 2025). The bulky *tert*-butyl groups at the 3- and 5-positions add steric protection around the phenolic oxygen atom. They also improve solubility in organic solvents and stabilize the resulting complexes (Cozzi, 2004; Çelik *et al.*, 2009). Its crystal structure exhibits intramolecular hydrogen-bonding interactions between the phenol OH grouping and the carbonal oxygen atom that generates a six-membered ring (Chu *et al.*, 2004;), while the steric repulsion of the tert-butyl groups prevents aromatic π–π stacking between the otherwise parallel aromatic rings (Ng, 2013; Gayathri *et al.*, 2026). As part of our studies in this area, we now describe the synthesis and structure of the title compound, $C_{25}H_{29}NO$ (**I**).





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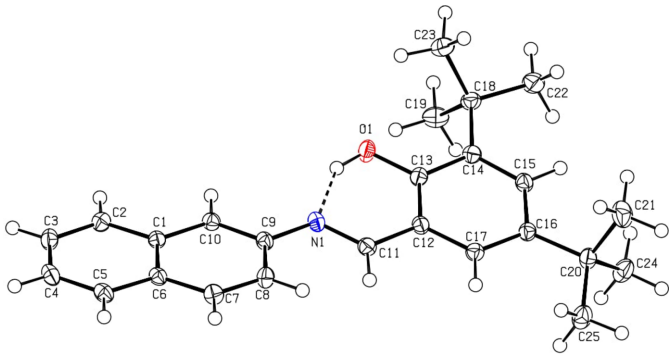


Figure 1
The molecular structure of (**I**) showing 50% displacement ellipsoids.

2. Structural commentary

Compound (I) crystallizes in space group $P2_1/c$ with one molecule in the asymmetric unit. Fig. 1 shows that the expected condensation product has arisen and the C11═N1 bond length of 1.2879 (12) Å agrees well with those observed in other azomethines. The dihedral angle between the C1–C10 naphthyl ring system (r.m.s. deviation = 0.014 Å) and the C12–C17 phenol ring is 16.41 (4)°. The near parallel orientation of these rings is supported by an intramolecular O1—H1*A*···N1 hydrogen bond (Table 1). The key torsion angles associated with the C═N bond are 176.93 (9)° (C9—N1—C11—C12), −176.25 (9)° (N1—C11—C12—C17) and 1.49 (15)° (N1—C11—C12—C13). For the C18 *t*-butyl group, one methyl C atom lies close to the plane of the aromatic ring [C22, deviation = 0.067 (1) Å], one above [C23, 1.229 (1) Å] and one below [C19, −1.288 (1) Å]. A similar situation occurs for the C20 group, with C25 close to coplanar [–0.223 (1) Å], C21 above [1.411 (1) Å] and C24 below [–1.050 (1) Å].

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N1	0.93 (1)	1.74 (1)	2.5704 (11)	148 (1)
C4—H4···O1^{i}	0.95	2.50	3.0874 (12)	120

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$.

3. Supramolecular features

The extended structure of (**I**) is shown in Fig. 2. A weak C4—H4···O1 hydrogen bond (Table 1) links the molecules into [010] chains. The molecules adopt an offset-stacked, antiparallel arrangements, with the bulky *tert*-butyl groups influencing their packing. A π–π stacking interaction occurs between inversion-related C1–C6 rings with a centroid-to-centroid distance of 3.6146 (6) Å and a slippage of 1.190 Å (Fig. 3). In contrast, there no stacking interactions were observed between the phenyl rings, presumably due to the steric repulsions of the *tert*-butyl groups.

4. Hirshfeld surface analyses

The Hirshfeld surface of (I), calculated with *Crystal Explorer 17* (Turner *et al.*, 2017; Arunagiri *et al.*, 2025), is shown in Fig. 4. The two-dimensional fingerprint plots (Fig. 5) reveal that H···H contacts contribute the highest percentage (69.3%) to the intermolecular interactions followed by C···H/H···C contacts (23.1%). The O···H/H···O, C···C and N···H/H···N contacts contributed 2.1%, 2.9% and 2.6%, respectively. The predominance of H···H contacts may be related to the presence of the *tert*-butyl groups in (**I**).

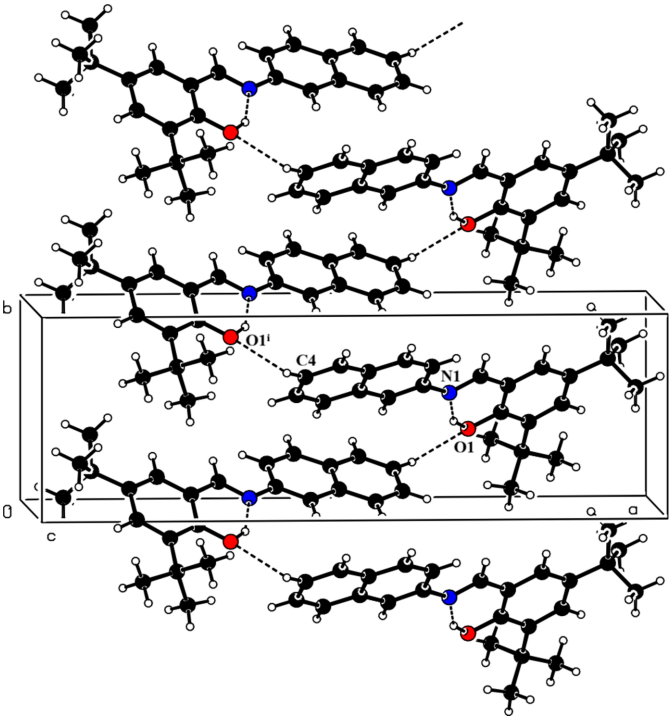


Figure 2
C—H···O hydrogen bonding interactions in (**I**).

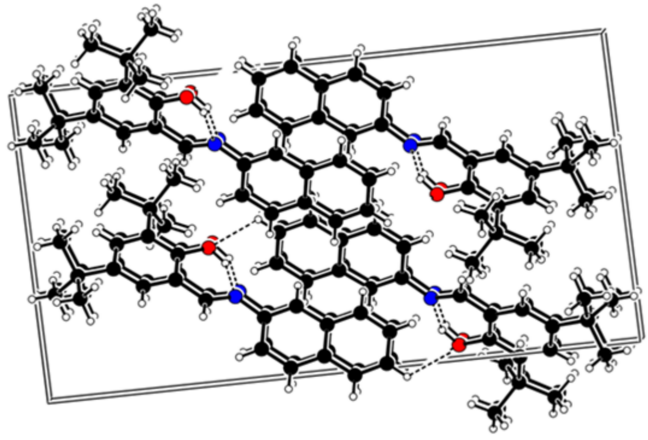


Figure 3
The packing of (**I**).

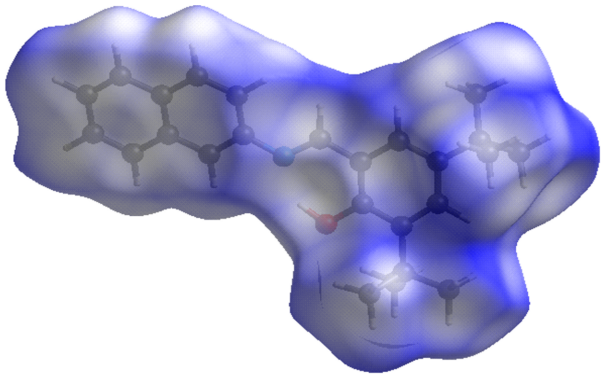


Figure 4
The Hirshfeld surface of (**I**) plotted over d_{norm}.

5. Database survey

The crystal structure of the starting material, 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (DTBHB; CCDC reference code: 239143) was reported by Tooke & Spek (2004). The crystal structure of a second monoclinic polymorph of DTBHB has also been described (Chu *et al.* 2004; Ng, 2013).

6. Synthesis and crystallization

Compound (**I**) was synthesized by the condensation of 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (0.234 g, 1.0 mmol) and 2-naphthylamine (0.143 g, 1.0 mmol) in ethanol solution. The reaction mixture was refluxed with continuous stirring for 4 h. Upon completion of the reaction, the mixture was allowed to cool to room temperature, resulting in the formation of a flaky yellow precipitate. It was collected by filtration and subsequently purified by recrystallization from ethanol solution. Slow cooling of the recrystallized solution afforded yellow block-shaped single crystals suitable for further characterization and crystallographic studies. Yield = 85% (0.306 g), with a melting point of 393 K.

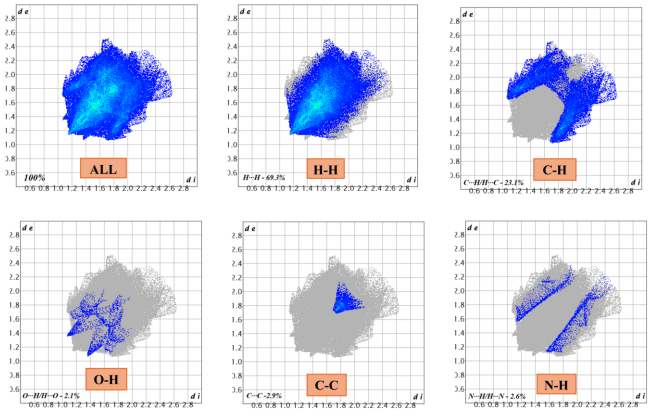


Figure 5
Two-dimensional fingerprint plots with the relative contributions of the various interactions to the Hirshfeld surface of (**I**).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{29}NO$
M_r	359.49
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	120
a, b, c (Å)	22.8874 (7), 7.4765 (2), 11.9540 (3)
β (°)	91.183 (1)
V (Å^3)	2045.10 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.45 × 0.45 × 0.09
Data collection	
Diffractometer	Bruker D8 QUEST
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.969, 0.994
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30189, 5049, 4399
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.128, 1.05
No. of reflections	5049
No. of parameters	252
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.35

Computer programs: *SAINT* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2020).

FT–IR (KBr, cm^{-1}): 3378 [ν(O—H)], 2952 [ν(C—H)], 2868 [ν(aliphatic C—H)], 1631 [ν(C═N)], 1607, 1571 [ν(C═C)], 1273, 1248 [ν(C—O)]. UV–Vis (λ_{max}, nm): 329 [$\pi \rightarrow \pi^*$], 373 [$\pi \rightarrow \pi^*$], 417 [$n \rightarrow \pi^*$].

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were placed in calculated positions (C—H = 0.95–0.98 Å) and refined using a riding model, while the O-bound H atom was refined independently. The constraint U_{iso}(H) = 1.2U_{eq}(aromatic) or 1.5U_{eq}(methyl carrier) was applied as appropriate.

Acknowledgements

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Palaniappan Meenavarsha, Iravatham Rama, Anantha Narayanan Sri Gayathri, Annamalai Subashini, Chidambaram Arunagiri and Govindaraj Krishnan

Computing details

2,4-Di-*tert*-butyl-6-[(naphthalen-2-ylimino)methyl]phenol

Crystal data

$C_{25}H_{29}NO$
M_r = 359.49
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 22.8874 (7) Å
b = 7.4765 (2) Å
c = 11.9540 (3) Å
β = 91.183 (1)°
V = 2045.10 (10) Å^3
Z = 4
$F(000)$ = 776
D_x = 1.168 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9848 reflections
θ = 2.7–28.3°
μ = 0.07 mm^{-1}
T = 120 K
Block, clear light yellow
0.45 × 0.45 × 0.09 mm

Data collection

Bruker D8 QUEST diffractometer
Radiation source: fine-focus sealed tube
Multilayer mirror monochromator
Detector resolution: 7.391 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.969, T_{max} = 0.994
30189 measured reflections
5049 independent reflections
4399 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 28.3°, θ_{min} = 2.7°
h = −30→30
k = −9→8
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.128
S = 1.05
5049 reflections
252 parameters
Primary atom site location: dual
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/[$\Sigma^2(FO^2)$ + (0.0754P)^2 + 0.4688P] WHERE P = (FO^2 + 2FC^2)/3
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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}
O1	0.69672 (3)	0.39417 (10)	0.54909 (6)	0.0222 (2)
N1	0.66106 (3)	0.58900 (11)	0.71116 (7)	0.0181 (2)
C1	0.51379 (4)	0.61573 (13)	0.83164 (8)	0.0162 (3)
C2	0.45586 (4)	0.55852 (14)	0.80585 (8)	0.0194 (3)
C3	0.41103 (4)	0.60045 (14)	0.87557 (9)	0.0215 (3)
C4	0.42176 (4)	0.69893 (15)	0.97448 (9)	0.0215 (3)
C5	0.47707 (4)	0.75707 (14)	1.00091 (8)	0.0198 (3)
C6	0.52431 (4)	0.71860 (13)	0.92993 (8)	0.0168 (3)
C7	0.58225 (4)	0.77638 (14)	0.95507 (8)	0.0196 (3)
C8	0.62730 (4)	0.73712 (14)	0.88588 (8)	0.0199 (3)
C9	0.61686 (4)	0.63488 (13)	0.78724 (8)	0.0169 (3)
C10	0.56147 (4)	0.57282 (13)	0.76266 (8)	0.0168 (3)
C11	0.71084 (4)	0.66933 (13)	0.71153 (8)	0.0186 (3)
C12	0.75712 (4)	0.61599 (13)	0.63701 (8)	0.0172 (3)
C13	0.74898 (4)	0.47636 (13)	0.55916 (8)	0.0173 (3)
C14	0.79554 (4)	0.41979 (13)	0.49161 (8)	0.0179 (3)
C15	0.84829 (4)	0.50992 (13)	0.50581 (8)	0.0186 (3)
C16	0.85784 (4)	0.65199 (13)	0.58121 (8)	0.0171 (3)
C17	0.81152 (4)	0.70232 (13)	0.64641 (8)	0.0176 (3)
C18	0.78743 (4)	0.26614 (13)	0.40741 (9)	0.0204 (3)
C19	0.74122 (5)	0.31876 (15)	0.31793 (9)	0.0267 (3)
C20	0.91848 (4)	0.73828 (14)	0.59082 (8)	0.0203 (3)
C21	0.96095 (5)	0.60389 (18)	0.64548 (11)	0.0320 (3)
C22	0.84412 (5)	0.22322 (15)	0.34694 (10)	0.0288 (3)
C23	0.76827 (5)	0.09486 (14)	0.46771 (9)	0.0257 (3)
C24	0.94031 (5)	0.78844 (16)	0.47440 (9)	0.0266 (3)
C25	0.91786 (5)	0.90864 (16)	0.66166 (10)	0.0270 (3)
H1A	0.6718 (4)	0.4379 (15)	0.6033 (11)	0.0330*
H2	0.44814	0.49083	0.73993	0.0230*
H3	0.37238	0.56280	0.85705	0.0260*
H4	0.39050	0.72503	1.02295	0.0260*
H5	0.48386	0.82389	1.06751	0.0240*
H7	0.58982	0.84360	1.02124	0.0240*
H8	0.66565	0.77823	0.90375	0.0240*
H10	0.55507	0.50004	0.69843	0.0200*

H11	0.71749	0.76595	0.76181	0.0220*
H15	0.88011	0.47304	0.46153	0.0220*
H17	0.81653	0.79714	0.69864	0.0210*
H19A	0.75508	0.42245	0.27591	0.0400*
H19B	0.70455	0.34914	0.35431	0.0400*
H19C	0.73463	0.21820	0.26662	0.0400*
H21A	0.96234	0.49520	0.59980	0.0480*
H21B	0.94756	0.57370	0.72050	0.0480*
H21C	1.00005	0.65696	0.65105	0.0480*
H22A	0.83713	0.12523	0.29389	0.0430*
H22B	0.87431	0.18756	0.40184	0.0430*
H22C	0.85718	0.32943	0.30643	0.0430*
H23A	0.76630	−0.00429	0.41414	0.0390*
H23B	0.72968	0.11345	0.49979	0.0390*
H23C	0.79662	0.06627	0.52762	0.0390*
H24A	0.94370	0.68014	0.42882	0.0400*
H24B	0.97864	0.84620	0.48180	0.0400*
H24C	0.91254	0.87100	0.43826	0.0400*
H25A	0.95715	0.96076	0.66481	0.0400*
H25B	0.90558	0.87947	0.73756	0.0400*
H25C	0.89046	0.99484	0.62799	0.0400*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0157 (3)	0.0269 (4)	0.0241 (4)	−0.0044 (3)	0.0025 (3)	−0.0055 (3)
N1	0.0157 (4)	0.0210 (4)	0.0177 (4)	0.0022 (3)	0.0022 (3)	0.0007 (3)
C1	0.0160 (4)	0.0162 (5)	0.0165 (4)	0.0012 (3)	0.0013 (3)	0.0025 (3)
C2	0.0189 (4)	0.0199 (5)	0.0193 (5)	−0.0009 (4)	−0.0001 (3)	0.0005 (4)
C3	0.0152 (4)	0.0243 (5)	0.0251 (5)	0.0004 (4)	0.0008 (4)	0.0049 (4)
C4	0.0191 (5)	0.0245 (5)	0.0212 (5)	0.0064 (4)	0.0049 (4)	0.0045 (4)
C5	0.0214 (5)	0.0206 (5)	0.0175 (5)	0.0044 (4)	0.0029 (4)	0.0007 (4)
C6	0.0176 (4)	0.0171 (5)	0.0158 (4)	0.0026 (3)	0.0017 (3)	0.0021 (3)
C7	0.0203 (5)	0.0225 (5)	0.0160 (5)	0.0004 (4)	−0.0003 (3)	−0.0024 (4)
C8	0.0161 (4)	0.0240 (5)	0.0197 (5)	−0.0010 (4)	−0.0004 (3)	−0.0005 (4)
C9	0.0166 (4)	0.0181 (5)	0.0162 (4)	0.0020 (3)	0.0024 (3)	0.0015 (3)
C10	0.0179 (4)	0.0169 (5)	0.0157 (4)	0.0006 (3)	0.0014 (3)	−0.0002 (3)
C11	0.0190 (4)	0.0175 (5)	0.0193 (5)	0.0013 (3)	0.0022 (3)	0.0000 (4)
C12	0.0160 (4)	0.0177 (5)	0.0180 (4)	0.0013 (3)	0.0020 (3)	0.0012 (3)
C13	0.0157 (4)	0.0184 (5)	0.0179 (4)	−0.0008 (3)	−0.0001 (3)	0.0019 (4)
C14	0.0194 (4)	0.0171 (5)	0.0171 (4)	0.0002 (3)	0.0014 (3)	0.0002 (3)
C15	0.0174 (4)	0.0195 (5)	0.0189 (5)	0.0014 (4)	0.0032 (3)	0.0002 (4)
C16	0.0155 (4)	0.0180 (5)	0.0177 (4)	0.0000 (3)	0.0002 (3)	0.0018 (4)
C17	0.0180 (4)	0.0171 (5)	0.0178 (5)	0.0000 (3)	0.0004 (3)	−0.0005 (4)
C18	0.0233 (5)	0.0170 (5)	0.0209 (5)	−0.0015 (4)	0.0030 (4)	−0.0023 (4)
C19	0.0362 (6)	0.0229 (5)	0.0208 (5)	0.0001 (4)	−0.0026 (4)	−0.0031 (4)
C20	0.0158 (4)	0.0238 (5)	0.0214 (5)	−0.0021 (4)	0.0014 (3)	−0.0021 (4)
C21	0.0199 (5)	0.0388 (7)	0.0371 (6)	0.0037 (4)	−0.0036 (4)	0.0020 (5)

C22	0.0310 (6)	0.0234 (5)	0.0324 (6)	−0.0024 (4)	0.0107 (5)	−0.0086 (4)
C23	0.0314 (5)	0.0181 (5)	0.0277 (5)	−0.0030 (4)	0.0020 (4)	0.0008 (4)
C24	0.0261 (5)	0.0292 (6)	0.0247 (5)	−0.0085 (4)	0.0067 (4)	−0.0025 (4)
C25	0.0220 (5)	0.0310 (6)	0.0279 (6)	−0.0066 (4)	0.0007 (4)	−0.0082 (4)

Geometric parameters (Å, º)

O1—C13	1.3479 (12)	C20—C21	1.5346 (16)
N1—C9	1.4164 (12)	C2—H2	0.9500
N1—C11	1.2879 (12)	C3—H3	0.9500
O1—H1A	0.931 (12)	C4—H4	0.9500
C1—C2	1.4209 (13)	C5—H5	0.9500
C1—C10	1.4181 (13)	C7—H7	0.9500
C1—C6	1.4207 (14)	C8—H8	0.9500
C2—C3	1.3715 (14)	C10—H10	0.9500
C3—C4	1.4101 (15)	C11—H11	0.9500
C4—C5	1.3692 (13)	C15—H15	0.9500
C5—C6	1.4176 (13)	C17—H17	0.9500
C6—C7	1.4209 (13)	C19—H19A	0.9800
C7—C8	1.3670 (13)	C19—H19B	0.9800
C8—C9	1.4213 (14)	C19—H19C	0.9800
C9—C10	1.3760 (13)	C21—H21A	0.9800
C11—C12	1.4538 (13)	C21—H21B	0.9800
C12—C17	1.4049 (13)	C21—H21C	0.9800
C12—C13	1.4083 (14)	C22—H22A	0.9800
C13—C14	1.4149 (13)	C22—H22B	0.9800
C14—C15	1.3900 (13)	C22—H22C	0.9800
C14—C18	1.5361 (14)	C23—H23A	0.9800
C15—C16	1.4072 (14)	C23—H23B	0.9800
C16—C17	1.3810 (13)	C23—H23C	0.9800
C16—C20	1.5327 (13)	C24—H24A	0.9800
C18—C22	1.5322 (15)	C24—H24B	0.9800
C18—C23	1.5378 (15)	C24—H24C	0.9800
C18—C19	1.5397 (15)	C25—H25A	0.9800
C20—C24	1.5349 (15)	C25—H25B	0.9800
C20—C25	1.5297 (16)	C25—H25C	0.9800
C9—N1—C11	121.90 (8)	C4—C5—H5	120.00
C13—O1—H1A	109.4 (6)	C6—C5—H5	120.00
C2—C1—C6	118.94 (8)	C6—C7—H7	119.00
C2—C1—C10	122.11 (9)	C8—C7—H7	119.00
C6—C1—C10	118.95 (8)	C7—C8—H8	120.00
C1—C2—C3	120.38 (9)	C9—C8—H8	120.00
C2—C3—C4	120.62 (9)	C1—C10—H10	119.00
C3—C4—C5	120.23 (9)	C9—C10—H10	119.00
C4—C5—C6	120.69 (9)	N1—C11—H11	119.00
C1—C6—C5	119.11 (8)	C12—C11—H11	119.00
C1—C6—C7	118.75 (8)	C14—C15—H15	118.00

C5—C6—C7	122.12 (9)	C16—C15—H15	118.00
C6—C7—C8	121.27 (9)	C12—C17—H17	119.00
C7—C8—C9	120.10 (9)	C16—C17—H17	119.00
N1—C9—C10	116.64 (8)	C18—C19—H19A	109.00
C8—C9—C10	119.79 (9)	C18—C19—H19B	109.00
N1—C9—C8	123.56 (8)	C18—C19—H19C	109.00
C1—C10—C9	121.08 (9)	H19A—C19—H19B	109.00
N1—C11—C12	121.71 (9)	H19A—C19—H19C	109.00
C11—C12—C13	121.34 (8)	H19B—C19—H19C	109.00
C13—C12—C17	119.89 (9)	C20—C21—H21A	109.00
C11—C12—C17	118.73 (9)	C20—C21—H21B	109.00
O1—C13—C12	120.13 (8)	C20—C21—H21C	109.00
C12—C13—C14	120.52 (8)	H21A—C21—H21B	109.00
O1—C13—C14	119.35 (8)	H21A—C21—H21C	109.00
C13—C14—C15	116.61 (9)	H21B—C21—H21C	109.00
C13—C14—C18	121.02 (8)	C18—C22—H22A	109.00
C15—C14—C18	122.38 (8)	C18—C22—H22B	109.00
C14—C15—C16	124.55 (9)	C18—C22—H22C	109.00
C15—C16—C17	117.15 (8)	H22A—C22—H22B	109.00
C17—C16—C20	123.20 (9)	H22A—C22—H22C	109.00
C15—C16—C20	119.62 (8)	H22B—C22—H22C	109.00
C12—C17—C16	121.27 (9)	C18—C23—H23A	109.00
C14—C18—C19	109.64 (8)	C18—C23—H23B	109.00
C14—C18—C22	111.95 (8)	C18—C23—H23C	109.00
C19—C18—C22	107.58 (9)	H23A—C23—H23B	109.00
C19—C18—C23	109.88 (8)	H23A—C23—H23C	109.00
C14—C18—C23	110.33 (8)	H23B—C23—H23C	109.00
C22—C18—C23	107.41 (8)	C20—C24—H24A	109.00
C16—C20—C24	110.25 (8)	C20—C24—H24B	109.00
C16—C20—C25	111.92 (8)	C20—C24—H24C	109.00
C16—C20—C21	108.72 (9)	H24A—C24—H24B	109.00
C21—C20—C25	108.81 (9)	H24A—C24—H24C	109.00
C24—C20—C25	107.78 (9)	H24B—C24—H24C	109.00
C21—C20—C24	109.32 (9)	C20—C25—H25A	109.00
C1—C2—H2	120.00	C20—C25—H25B	109.00
C3—C2—H2	120.00	C20—C25—H25C	109.00
C2—C3—H3	120.00	H25A—C25—H25B	109.00
C4—C3—H3	120.00	H25A—C25—H25C	109.00
C3—C4—H4	120.00	H25B—C25—H25C	109.00
C5—C4—H4	120.00		

C9—N1—C11—C12	176.93 (9)	C17—C12—C13—O1	−179.40 (9)
C11—N1—C9—C10	164.75 (9)	C17—C12—C13—C14	1.20 (14)
C11—N1—C9—C8	−16.20 (15)	C11—C12—C17—C16	177.17 (9)
C2—C1—C6—C5	1.68 (14)	C13—C12—C17—C16	−0.60 (15)
C10—C1—C2—C3	179.01 (10)	O1—C13—C14—C15	179.93 (9)
C10—C1—C6—C7	0.60 (14)	O1—C13—C14—C18	−0.16 (14)
C2—C1—C10—C9	177.74 (9)	C12—C13—C14—C15	−0.67 (14)

C6—C1—C2—C3	−0.73 (15)	C12—C13—C14—C18	179.25 (9)
C6—C1—C10—C9	−2.53 (14)	C13—C14—C15—C16	−0.48 (15)
C10—C1—C6—C5	−178.07 (9)	C18—C14—C15—C16	179.61 (9)
C2—C1—C6—C7	−179.65 (9)	C13—C14—C18—C19	62.90 (12)
C1—C2—C3—C4	−0.78 (16)	C13—C14—C18—C22	−177.80 (9)
C2—C3—C4—C5	1.33 (16)	C13—C14—C18—C23	−58.24 (12)
C3—C4—C5—C6	−0.34 (16)	C15—C14—C18—C19	−117.19 (10)
C4—C5—C6—C7	−179.78 (10)	C15—C14—C18—C22	2.12 (13)
C4—C5—C6—C1	−1.16 (15)	C15—C14—C18—C23	121.67 (10)
C5—C6—C7—C8	179.64 (10)	C14—C15—C16—C17	1.05 (15)
C1—C6—C7—C8	1.01 (15)	C14—C15—C16—C20	178.80 (9)
C6—C7—C8—C9	−0.75 (15)	C15—C16—C17—C12	−0.48 (14)
C7—C8—C9—C10	−1.17 (15)	C20—C16—C17—C12	−178.14 (9)
C7—C8—C9—N1	179.82 (9)	C15—C16—C20—C21	−69.27 (12)
N1—C9—C10—C1	−178.10 (9)	C15—C16—C20—C24	50.56 (12)
C8—C9—C10—C1	2.82 (15)	C15—C16—C20—C25	170.51 (9)
N1—C11—C12—C13	1.49 (15)	C17—C16—C20—C21	108.33 (11)
N1—C11—C12—C17	−176.25 (9)	C17—C16—C20—C24	−131.84 (10)
C11—C12—C13—O1	2.89 (14)	C17—C16—C20—C25	−11.89 (13)
C11—C12—C13—C14	−176.51 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N1	0.93 (1)	1.74 (1)	2.5704 (11)	148 (1)
C4—H4···O1^{i}	0.95	2.50	3.0874 (12)	120

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+3/2.