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Selected solid-state behaviour of three di-*tert*-butyl-substituted *N*-salicylideneaniline derivatives: temperature-induced phase transitions and chromic behaviour

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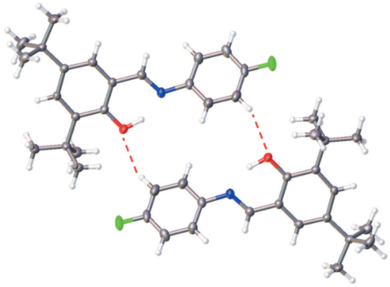


The synthesis, single-crystal structures and chromic behaviour of three related Schiff bases, namely, (*E*)-2,4-di-*tert*-butyl-6-{[(4-fluorophenyl)imino]methyl}-phenol, $C_{21}H_{26}FNO$, **1**, (*E*)-2,4-di-*tert*-butyl-6-{[(4-chlorophenyl)imino]methyl}-phenol, $C_{21}H_{26}ClNO$, **2**, and (*E*)-6-{[(4-bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol, $C_{21}H_{26}BrNO$, **3**, are reported. Two polymorphs of **1** were obtained, which were found to have different photochromic properties. Schiff bases **2** and **3** were found to be isostructural and underwent a phase transition upon cooling which was attributed to the dynamic disorder in one of the *tert*-butyl groups resolving at low temperature. All of the structures were found to exist in the enol rather than the keto form based on the C—O(H) and imine C=N bond lengths, and contained an intramolecular O—H···N hydrogen bond alongside weaker intermolecular C—H···O contacts.

1. Introduction

Compounds which display reversible property changes upon some sort of stimulus are of interest due to potential applications, including optical switches (Sliwa *et al.*, 2005), sensors (Sahu *et al.*, 2020) or optical data storage (Wang *et al.*, 2020). Within these are compounds displaying temperature-dependent thermochromic (Seeboth *et al.*, 2014; Suzuki *et al.*, 2019) or light-induced photochromic (Wu *et al.*, 2020) colour changes. One such class of compounds that has been found to exhibit both thermochromism and photochromism in the solid state are *N*-salicylideneanilines, Schiff bases of salicylaldehyde derivatives with aniline derivatives (Senier & Shepheard, 1909; Cohen & Schmidt, 1962; Cohen *et al.*, 1964). Typically, their thermochromism involves a lightening of colour from red/orange to orange/yellow upon cooling, while their photochromic colour changes usually result in a darkening of colour from yellow to orange/red upon irradiation with UV light. Initially, the two properties were thought to be mutually exclusive (Cohen & Schmidt, 1962; Cohen *et al.*, 1964); however, now it is believed that most, if not all, of *N*-salicylideneanilines display thermochromism, with some also showing photochromism (Fujiwara *et al.*, 2004).

The mechanism for the thermochromic colour change is believed to be due to an enol to *cis*-keto tautomerism, while the photochromism involves a *cis* to *trans* isomerism of the keto form (Hadjoudis & Mavridis, 2004; Robert *et al.*, 2009) (Fig. 1). Evidence of the thermoproduct has been observed for *N*-(5-chlorosalicylidene)-4-hydroxyaniline, where the population of the *cis*-keto form was found to increase upon cooling (Ogawa *et al.*, 1998, 2000), while the photoproduct has been

Table 1
Experimental details.

	1A at 100 K	**1B** at 120 K	**2** at 100 K	**3** at 100 K
Crystal data				
Chemical formula	$C_{21}H_{26}FNO$	$C_{21}H_{26}FNO$	$C_{21}H_{26}ClNO$	$C_{21}H_{26}BrNO$
M_r	327.43	327.43	343.88	388.34
Crystal system, space group	Triclinic, $P\overline{1}$	Orthorhombic, $Pna2_1$	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	100	120	100	100
a, b, c (Å)	6.5324 (3), 10.6141 (8), 14.1675 (9)	12.2569 (3), 8.9658 (2), 16.5739 (4)	17.3011 (11), 10.6780 (7), 10.1200 (6)	17.4450 (3), 10.69412 (16), 10.15010 (17)
α, β, γ (°)	80.364 (5), 81.094 (4), 74.507 (5)	90, 90, 90	90, 90.252 (6), 90	90, 90.1557 (16), 90
V (Å^3)	926.97 (10)	1821.35 (7)	1869.6 (2)	1893.58 (5)
Z	2	4	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.08	0.08	0.21	2.18
Crystal size (mm)	0.38 × 0.36 × 0.26	0.46 × 0.43 × 0.10	0.35 × 0.31 × 0.10	0.3 × 0.05 × 0.05
Data collection				
Diffractometer	Oxford Diffraction Xcalibur Sapphire3 Gemini ultra	Oxford Diffraction Xcalibur Sapphire3 Gemini ultra	Oxford Diffraction Xcalibur Sapphire3 Gemini ultra	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)	Analytical (*CrysAlis PRO*; Oxford Diffraction, 2010)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2018)	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.870, 1.000	0.973, 0.992	0.435, 1.000	0.692, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7178, 3792, 2765	25510, 3712, 3517	13865, 3830, 2740	28200, 4491, 3799
R_{int}	0.038	0.049	0.087	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.625	0.625	0.658
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.110, 1.04	0.034, 0.077, 1.05	0.071, 0.176, 1.08	0.026, 0.060, 1.04
No. of reflections	3792	3712	3830	4491
No. of parameters	227	226	227	227
No. of restraints	0	1	0	22
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.20	0.16, −0.16	0.78, −0.33	0.46, −0.22

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2010; Rigaku OD, 2018; Agilent, 2012), *SHELXS* (Sheldrick, 2008), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXL2018* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

seen crystallographically for *N*-3,5-di-*tert*-butylsalicylidene-3-nitroaniline using two-photon irradiation (Harada *et al.*, 1999). The enol form is believed to be colourless, while the keto form is coloured (Ogawa *et al.*, 1998; Fujiwara *et al.*, 2004; Harada *et al.*, 2007). However, the thermochromism cannot be fully explained by the keto–enol tautomerism alone. In order to fully explain the thermochromism, it is necessary to take into account fluorescence (Harada *et al.*, 2007). The impact of fluorescence is particularly significant for thermochromic compounds at lower temperature and can in fact be the dominant cause of colour change, while at higher temperatures, fluorescence is negligible. The presence of fluorescence at lower temperature results in different perceived colours to those observed from the diffuse reflectance spectra, *e.g.* *N*-(5-chloro-2-hydroxybenzylidene)aniline appears yellowish green at 80 K but diffuse reflectance suggests the colour to be pale yellow since fluorescence was eliminated in the measurement of diffuse reflectance spectra. The extent of the thermochromism of the *N*-salicylideneanilines has been linked to the dihedral angle (Φ) between the two aromatic rings, with those having Φ < 25° being generally strongly thermochromic, as a smaller interplanar or dihedral angle results in reduced overlap between the N-atom lone pair and the aromatic aniline moiety. This allows for easier H-atom transfer and creates a

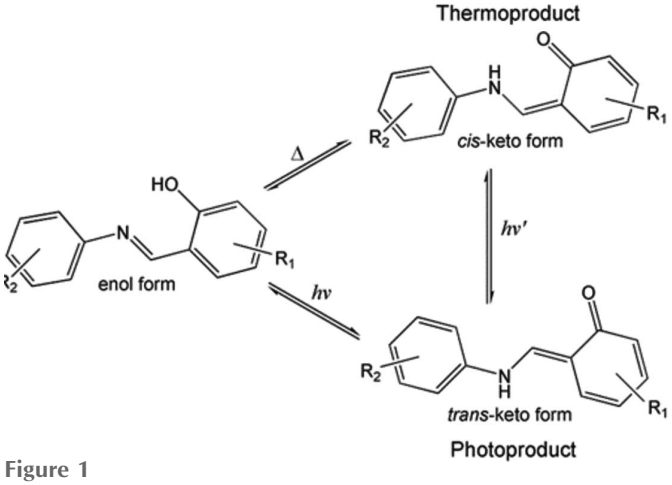
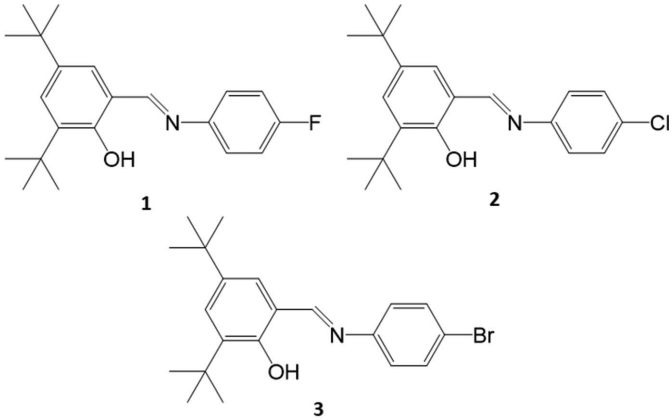


Figure 1
Illustration of the proposed mechanism for the thermo- or photochromism in *N*-salicylideneaniline derivatives.

stronger intramolecular hydrogen bond. While a larger dihedral angle increases overlap between the N-atom lone pair and the aromatic aniline moiety giving greater delocalization into the π-system and reducing the basicity of the N atom and thus the thermochromism (Hadjoudis & Mavridis, 2004; Robert *et al.*, 2009). For photochromism, the link to dihedral angle is more complicated and compounds with $\Phi < 20^\circ$ are generally nonphotochromic, those with $\Phi > 30^\circ$ are more likely to be photochromic and those in between can be either photochromic or nonphotochromic (Johmoto *et al.*, 2012). Other factors have also been found to influence the chromic behaviour of the *N*-salicylideneanilines, including substituents that weaken the O—H bond or increase the basicity of the N atoms, tending to result in more strongly thermochromic compounds (Hadjoudis & Mavridis, 2004). In addition, crystal packing also affects chromic behaviour, with more closely packed structures tending to be more strongly thermochromic and more open packed structures more likely to be photochromic (Hadjoudis & Mavridis, 2004; Robert *et al.*, 2009). The latter is likely to be due to the large conformational change required for the transition, with tightly packed structures having greater steric restrictions to conformational change. The presence of bulky groups, such as *tert*-butyl substituents, or creating cavities using hosts can help to increase space in the lattice of a structure and favour photochromism, as more space presumably reduces the steric restraint on the molecule for the significant conformational change required for *cis* to *trans* isomerism to occur (Johmoto *et al.*, 2012, Pistolis *et al.*, 1996; Koyama *et al.*, 1994).



Scheme 1

The structures of three related *N*-salicylidineanlines, namely, (*E*)-2,4-di-*tert*-butyl-6-{[(4-fluorophenyl)imino]methyl}phenol, **1**, (*E*)-2,4-di-*tert*-butyl-6-{[(4-chlorophenyl)imino]-methyl}phenol, **2**, and (*E*)-6-{[(4-bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol, **3**, are reported alongside a study into their chromic properties (Scheme 1). The structure of **2** has been reported previously at 273 K (Li *et al.*, 2007), but no investigation into the chromic properties or thermal behaviour has been reported. The structure of **3** has also been reported and is known to be photochromic; however, the thermal behaviour was not studied (Johmoto *et al.*, 2012).

2. Experimental

2.1. Synthesis

All reagents were used as supplied by Aldrich. Compounds were synthesized by direct condensation of the appropriate salicylaldehyde and aniline derivatives in ethanol. 1.25 (for **1** and **3**) or 2.5 mmoles (for **2**) of the salicylaldehyde and aniline were each dissolved in ethanol (25 ml), and the resulting solutions combined and refluxed with stirring for 4 h. Any precipitate was filtered off, rinsed with ethanol and left to dry. The (remaining) solution was then removed under reduced pressure using a rotary evaporator until (further) precipitate formed. Recrystallization was carried out by slow evaporation from ethanol.

2.2. Characterization

Elemental C, H and N content analysis was carried out by the Durham University Analytical service using an Exeter Analytical E-440 Elemental Analyzer.

2.3. Single-crystal X-ray diffraction data collection and refinement

Details of the X-ray data collection and refinement are provided in Table 1 and Table S1 in the supporting information. All H atoms, apart from the O—H hydrogen involved in the intramolecular hydrogen bonding with the imine N atom were positioned geometrically and refined using a riding model. The H atoms involved in the intramolecular hydrogen bond were located in the Fourier difference map wherever feasible. In **2** and **3**, one of the *tert*-butyl groups was disordered [apart from at 120 (2) and 100 (2) K for **2**, and at 100 (2) K for **3**], the sum of the occupancies of the disordered parts was set to equal 1. The data for **2** at 300 (2), 250 (2) and 200 (2) K drop off at high angle, presumably due to the presence of the disorder in the *tert*-butyl group; as a consequence, the data were cut at resolution limits of 0.95, 0.91 and 0.89 Å, respectively. Likewise the data for **3** were also weak at 300 (2) K and were consequently cut at a resolution limit of 0.86 Å. The interplanar dihedral angle and fold angles were calculated in *OLEX2* (Dolomanov *et al.*, 2012) by measuring the angles between planes computed through the six non-H atoms of the two rings. For the acentric structure of **1B** at 120 K, the diffraction data did not establish the absolute structure.

2.4. Raman

Irradiation was carried out using two UV LED sources ($\lambda \sim$ 365 nm) in the dark to minimize conversion back to the ground state and measurements were recorded with the 764 nm laser on a Horiba Jobin Yvon LabRAM HR Raman spectrometer.

2.5. Diffuse reflectance spectroscopy

The sample was ground to give uniform particle distribution and placed in a 40 × 10 × 2 mm quartz cuvette to ensure optical thickness. A cuvette sample holder with a white polytetrafluoroethylene (PTFE) block spacer was used to load

the sample into an Oxford Instruments Cryostat. The sample was irradiated with an Ocean Optics halogen light source and an Avantes AvaSpec-2048-2 CCD detector (placed at an acute angle to minimize detection of specular reflectance) collected the reflectance spectra, which were recorded using *AvaSoft* basic software. Cryostat temperature control was performed using an Oxford Intelligent Temperature Controller and each temperature was stabilized for 10 min or until ±0.1 K before recording the spectrum. A white PTFE block was used to record a reference spectrum before each data set collection. Irradiation was carried out using a 405 nm laser pointer or UV LEDs after an initial ground-state spectrum was collected. The diffuse reflectance spectra are illustrated as percent reflectance *versus* wavelength and Kubelka–Munk function, $F(R)$, *versus* wavelength. If S is independent of λ, then $F(R)$ *versus* λ is equivalent to the absorption spectrum for a diffuse reflector. To allow basic trends to be easily observed, moving averages were applied to data during analysis.

3. Results and discussion

3.1. Structural characterization

Compound **1** was found to produce two different polymorphs upon recrystallization, **1A** and **1B**, which had different morphologies and structures. Polymorph **1A** formed yellow rectangular block-like crystals and crystallized in the triclinic space group $P\overline{1}$, while **1B** formed bright-yellow octahedral-shaped crystals and crystallized in the orthorhombic space group $Pna2_1$. Only one polymorph was identified during these studies for **2** and **3**, both of which were yellow.

The four structures are all similar in that they have the same basic backbone with a phenyl group substituted with a hydroxy and two *tert*-butyl groups, and joined to a halogen-substituted phenyl group *via* an imine group (Fig. 2). The structures all exist in the enol form at low temperature rather than the less common keto form, with the C7═N1 bond lengths ranging from 1.279 (3) to 1.286 (2) Å and the C1—O1 bond lengths ranging from 1.353 (3) to 1.358 (2) Å, which are consistent with double C═N (typically ∼1.279 Å) and single C—O (typically ∼1.362 Å) bonds, respectively (Allen *et al.*, 1987). In all cases, the H atom was also located in the Fourier difference map in the vicinity of the O atom, supporting the presence of the enol form of the anil. All the structures contain an intramolecular O1—H1···N1 hydrogen bond with similar parameters, *e.g.* O1···N1 distances ranging from 2.544 (2) to 2.633 (3) Å (see Table 2). The structures also contain weaker intermolecular C—H···O interactions (see Table 3).

The structure of **1A** consists of molecules oriented such that the plane of the molecules is in approximately the $(\overline{1}01)$ plane, with short aromatic C—H···O contacts between pairs of adjacent molecules. The *tert*-butyl groups within these pairs are at opposite ends to each other (Fig. 3). Examining the

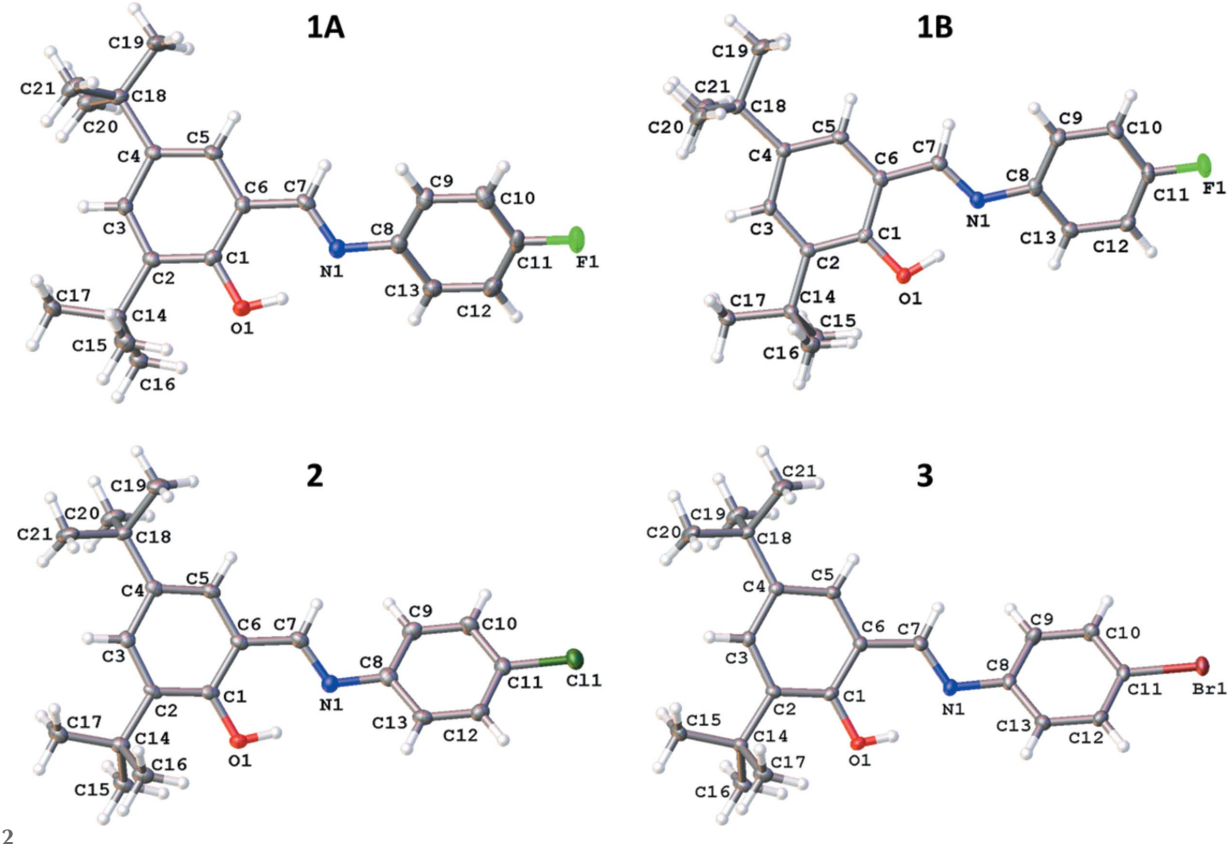


Figure 2
Illustration of the structures of **1A** [at 100 (2) K], **1B** [120 (2) K], **2** [100 (2) K] and **3** [100 (2) K], with the atomic numbering schemes depicted. Displacement ellipsoids are drawn at the 50% probability level.

Table 2
O—H···N hydrogen-bond geometry (Å, °).

	T (K)	D—H···A	D—H	H···A	D···A	D—H···A
1A	100	O1—H1···N1	0.94 (3)	1.72 (3)	2.587 (2)	151 (2)
1B	120	O1—H1···N1	0.96 (3)	1.64 (3)	2.544 (2)	155 (2)
2	300	O1—H1···N1	0.84 (4)	1.84 (4)	2.612 (4)	151 (4)
	250	O1—H1···N1	0.91 (3)	1.76 (4)	2.615 (4)	155 (3)
	200	O1—H1···N1	0.90 (3)	1.78 (3)	2.611 (3)	153 (3)
	150	O1—H1···N1	0.92 (3)	1.77 (3)	2.615 (3)	151 (3)
	120	O1—H1···N1	0.86 (4)	1.82 (4)	2.633 (3)	157 (4)
	100	O1—H1···N1	0.94 (4)	1.77 (4)	2.626 (3)	150 (3)
3	300	O1—H1···N1	0.83 (5)	1.84 (5)	2.614 (4)	154 (5)
	250	O1—H1···N1	0.84 (3)	1.83 (3)	2.612 (3)	154 (3)
	200	O1—H1···N1	0.82 (3)	1.85 (3)	2.611 (2)	153 (3)
	150	O1—H1···N1	0.86 (1)	1.83 (2)	2.612 (2)	152 (3)
	120	O1—H1···N1	0.86 (1)	1.84 (2)	2.622 (2)	151 (3)
	100	O1—H1···N1	0.85 (1)	1.84 (1)	2.6257 (18)	152 (2)

Table 3
C—H···O and C—H···F hydrogen-bond geometry (Å, °).

	T (K)	D—H···A	D—H	H···A	D···A	D—H···A
1A	100	C12—H12···O1^{i}	0.95	2.62	3.345 (2)	133
1B	120	C10—H10···O1^{ii}	0.95	2.60	3.523 (3)	165
		C19—H19*B*···O1^{iii}	0.98	2.72	3.522 (3)	140
		C17—H17*A*···F1^{iv}	0.98	2.57	3.453 (3)	150
2	300	C12—H12···O1^{v}	0.93	2.71	3.461 (4)	138
	250	C12—H12···O1^{v}	0.94	2.68	3.438 (3)	138
	200	C12—H12···O1^{v}	0.95	2.65	3.415 (2)	138
	150	C12—H12···O1^{vi}	0.95	2.56	3.359 (3)	142
	100	C12—H12···O1^{vi}	0.95	2.54	3.343 (4)	142
	150	C12—H12···O1^{v}	0.95	2.63	3.396 (3)	138
	120	C12—H12···O1^{vi}	0.95	2.56	3.359 (3)	142
3	300	C12—H12···O1^{vii}	0.93	2.76	3.522 (3)	140
	250	C12—H12···O1^{vii}	0.94	2.73	3.500 (2)	140
	200	C12—H12···O1^{vii}	0.94	2.71	3.483 (3)	140
	150	C12—H12···O1^{vii}	0.95	2.67	3.458 (2)	140
	120	C12—H12···O1^{vii}	0.95	2.62	3.425 (2)	142
	100	C12—H12···O1^{vii}	0.95	2.61	3.415 (2)	143

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+2, -y+1, z+\frac{1}{2}$; (v) $-x+2, -y+1, -z+1$; (vi) $-x+2, -y, -z+1$; (vii) $-x, -y, -z$.

structure of **1B** shows that the molecules are packed in a completely different manner to **1A**; in **1B**, alternate molecules in the *c*-axis direction are orientated in either the [101] or [10$\bar{1}$] direction (Fig. 3). Intermolecular interactions in this case are (i) short C—H···O contacts involving the H atoms on a methyl group and an aromatic H atom, and (ii) C—H···F contacts involving methyl-group H atoms (see Fig. 4 and Table 3). The structures of **2** and **3** were found to be isostructural, crystallizing in the monoclinic space group $P2_1/c$. All of the molecules are oriented such that the plane of the molecules is in approximately the (101) plane, with short aromatic C—H···O contacts between pairs of adjacent molecules. Within these pairs, the molecules are arranged such that the *tert*-butyl groups are at opposite ends to each other (Fig. S1). Although in a different crystal system and space group, the structures of **2** and **3** are similar to that of **1A** in terms of the packing and intermolecular interactions.

3.2. Thermal behaviour

The structures of **2** and **3** are isostructural and upon cooling both undergo a phase transition somewhere between 150 and 120 K, during which the *a*-axis length decreases by ∼0.37 Å for **2** and by ∼0.27 Å for **3**, while the *b* axis increases by ∼0.20 Å for **2** and by ∼0.10 Å for **3**. These changes are accompanied by a decrease in the β angle of just over 1° in both cases (see Figs. S2 and S3 in the supporting information). Across the full temperature range measured, the behaviour of the unit-cell parameters is slightly different for the two compounds but shows many similarities. For **2**, the *a* axis decreases almost linearly until 150 K and then shows a sharp decrease after the phase transition; the *b* axis decreases approximately linearly until 200 K, increases slightly to 150 K and then increases sharply by 120 K; the β angle decreases approximately linearly until 150 K, then shows a sharp decrease to 120 K before increasing slightly at 100 K; and the *c* axis and unit-cell volume decrease almost linearly throughout, with slight inflections at around 175 and 150 K. For **3** overall across the temperature range, upon cooling, the *a* and *c* cell-axes lengths, β angle and unit-cell volume decrease approximately linearly prior to the phase transition and continue to decrease

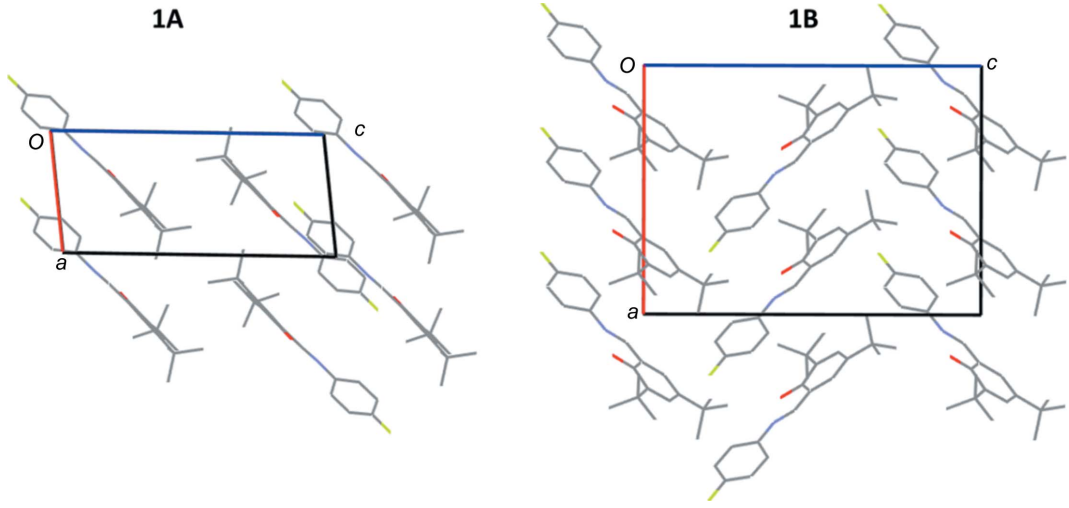


Figure 3
Illustration of the packing of **1A** at 100 (2) K and **1B** at 120 (2) K, looking down the *b* axis. H atoms have been omitted for clarity.

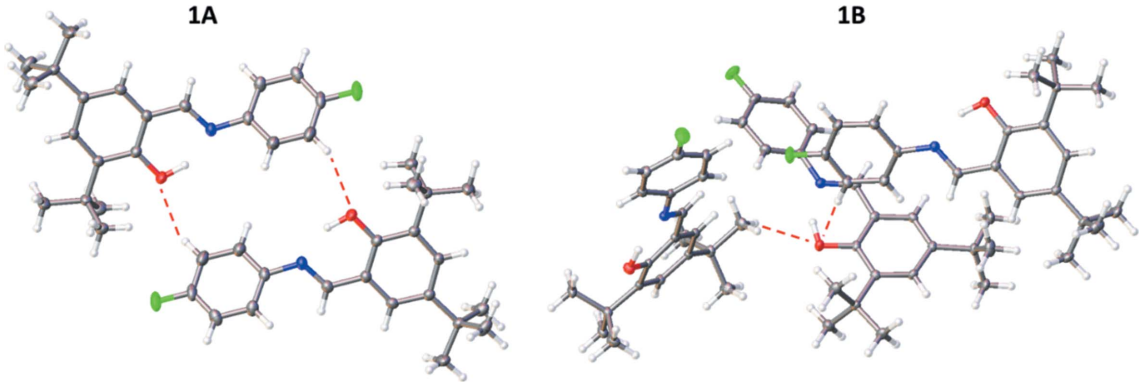


Figure 4
Intermolecular hydrogen bonding (dashed lines) in **1A** at 100 (2) K and **1B** at 120 (2) K.

after the phase transition. In the case of the *b* axis, it initially decreases until ∼200 K, increases slightly at 150 K and then increases sharply through the phase transition.

Examining the crystal structures above and below the transition, the cause of the phase transition appears to be dynamic disorder in one of the *tert*-butyl groups; at higher temperature, the group is disordered, while at low temperature, the disorder resolves. In the case of **2**, the disordered *tert*-butyl group is modelled over three positions at 150 (2) K, but is fully ordered at 120 (2) K, while for **3** at 150 (2) K, the *tert*-butyl group is also modelled over three positions, at 120 (2) K it was modelled over two positions and it was only at 100 (2) K that it was fully ordered.

The majority of the *N*-salicylideneanilines show thermochromism upon cooling, with compounds that are red/orange at room temperature becoming paler or yellow and those that are yellow at room temperature becoming paler. However, it was interesting to note that upon cooling, the crystals of **2** and **3** showed an apparent 'reverse thermochromism' around the phase-transition temperature, with the crystals becoming more red (Fig. 5 and Fig. S4 in the supporting information). Diffuse reflectance spectra were also collected for all of the compounds and are available in the supporting information (Figs. S5 and S6). No account was taken of the potential effect of fluorescence, which can affect the observed colour upon cooling (Harada *et al.*, 2007); however, the spectra are presented to support the visually observed trends. In the case of the reflectance spectra for **1**, which is likely to be a mixture of both polymorphs, the shoulder shifts to lower wavelengths upon cooling suggesting a lightening in colour. In the cases of **2** and **3**, there is also a shift in the position of the main shoulder to lower wavelengths upon cooling, but this is also accompanied by additional changes in the spectra. The spectrum for **2** shows additional changes in the ∼500–580 nm region with additional shoulders appearing. These appear to start by around 200 K and become more pronounced upon further cooling, which is consistent with results observed visually in Fig. 5. A similar situation, although less pronounced, is observed for **3**, where additional shoulders appear in the range ∼500–580 nm for the spectra at 200 K and below. The apparent 'reverse thermochromism' is believed to be related to the phase transition that has occurred rather than the

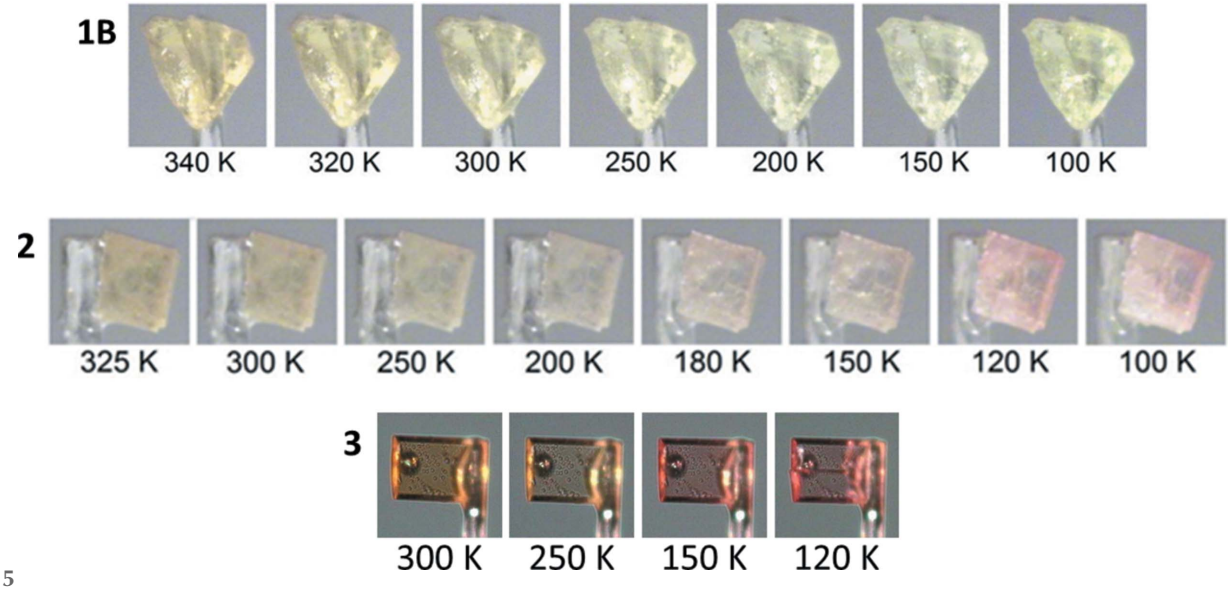


Figure 5
Illustration of the colour change of **1B**, **2** and **3** upon cooling.

Table 4
Dihedral angles (°) between planes calculated through the six atoms of the two rings.

	T (K)	Dihedral angle (°)	Fold angle (°)
1A	100	39.03 (5)	8.68 (5)
1B	120	20.61 (7)	3.24 (7)
2	300	26.75 (7)	9.01 (9)
	250	26.56 (8)	8.87 (8)
	200	26.33 (6)	9.09 (6)
	150	25.80 (9)	9.28 (9)
	120	24.96 (10)	11.84 (10)
	100	24.83 (9)	12.05 (9)
3	300	25.83 (8)	9.29 (9)
	250	25.49 (6)	9.45 (6)
	200	25.33 (8)	9.69 (7)
	150	24.88 (7)	10.16 (7)
	120	24.70 (7)	12.49 (7)
	100	24.63 (5)	13.20 (5)

normal thermochromism seen in *N*-salicylideneanilines. It was noted that the dihedral angle between the two six-membered rings decreases by around 1.2–1.9° as the temperature is reduced and in the case of **2**, there is a noticeably larger step around the phase transition between 150 (2) and 120 (2) K. In both cases, the fold angle increases as the temperature is reduced and there is a large step increase of ∼2.3–2.5° between 150 (2) and 120 (2) K (see Table 4). Although relatively small, it is possible that these structural changes may be related to the observed colour change, as structures with smaller dihedral angles have reduced overlap between the N-atom lone pair and the aromatic aniline, allowing for a stronger O—H···N hydrogen bond favoured by the strongly thermochromic compounds (Hadjoudis & Mavridis, 2004; Robert *et al.*, 2009). In the case of *N*-salicylideneaniline, a similar reverse thermochromism has been seen, whereupon heating above 306 K the colour changes from red to yellow. This was associated with the planar β-form transitioning to the nonplanar disordered α_1-form; however, the change in structure in this case was much more significant, with a change in the dihedral angle from (β) ∼2° to (α_1) ∼49° (Arod *et al.*, 2007). More examples and further studies would be required to confirm a correlation between the colour change observed here and the phase transition having occurred.

Table 5
Position of main peaks that appear in Raman upon irradiation.

Compound	New peaks (cm^{-1})
1A	1651, 1525, 1373, 1302 and 1143
1B	–
2	1528, 1423, 1311 and 1152
3	1518, 1418, 1301 and 1134

3.3. Photochromism

Upon irradiation, three of the crystals (**1A**, **2** and **3**) were found to display photochromism, becoming much darker in colour when irradiated with UV light. On the other hand, polymorph **1B** did not show a colour change even upon prolonged irradiation (Fig. 6). The occurrence of photochromism for **3** had been reported previously (Johmoto *et al.*, 2012).

Raman data were collected before irradiation and after irradiation with a UV LED (Fig. 7). The three crystals displaying photochromism (**1A**, **2** and **3**) all showed the appearance of new peaks upon irradiation; the main peak positions are given in Table 5. As expected, the spectrum of **1B** showed no change in the Raman spectra upon irradiation. It is clear that only a small amount of the photoproduct has been formed, which is not uncommon as photoyield is often low, particularly without two-photon excitation, and the change is often restricted to the surface of the crystal (Harada *et al.*, 2008). Therefore, it is unsurprising that even after irradiation with a UV laser, no changes were observed in the single-crystal X-ray structures. Diffuse reflectance spectra before and after irradiation for samples of **2** and **3** are presented in the supporting information (Fig. S7); these support the observation by eye and from the Raman with significant changes in the

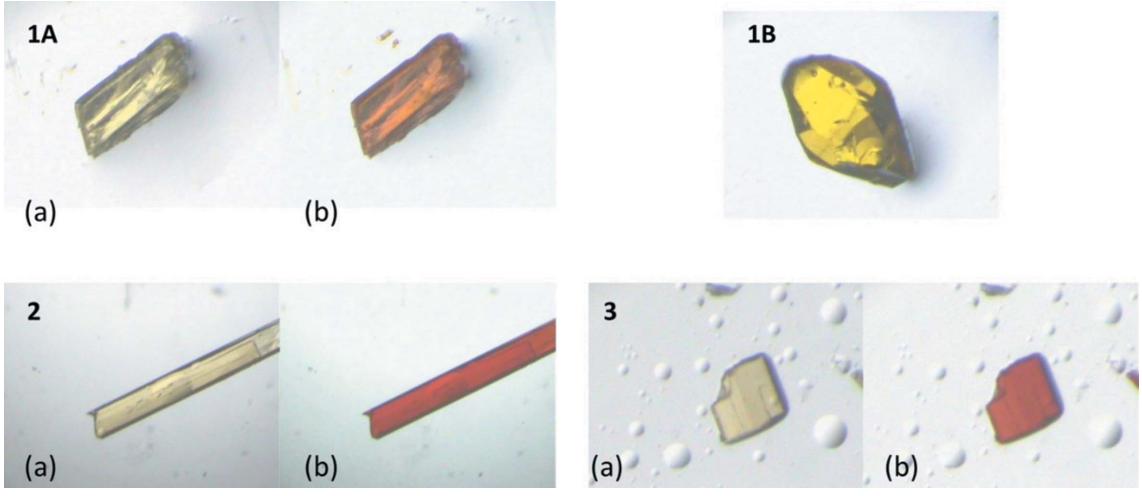


Figure 6
Illustration of the behaviour of each of the crystal structures at room temperature upon irradiation with a UV LED (λ ∼ 365 nm) for (*a*) unirradiated and (*b*) irradiated.

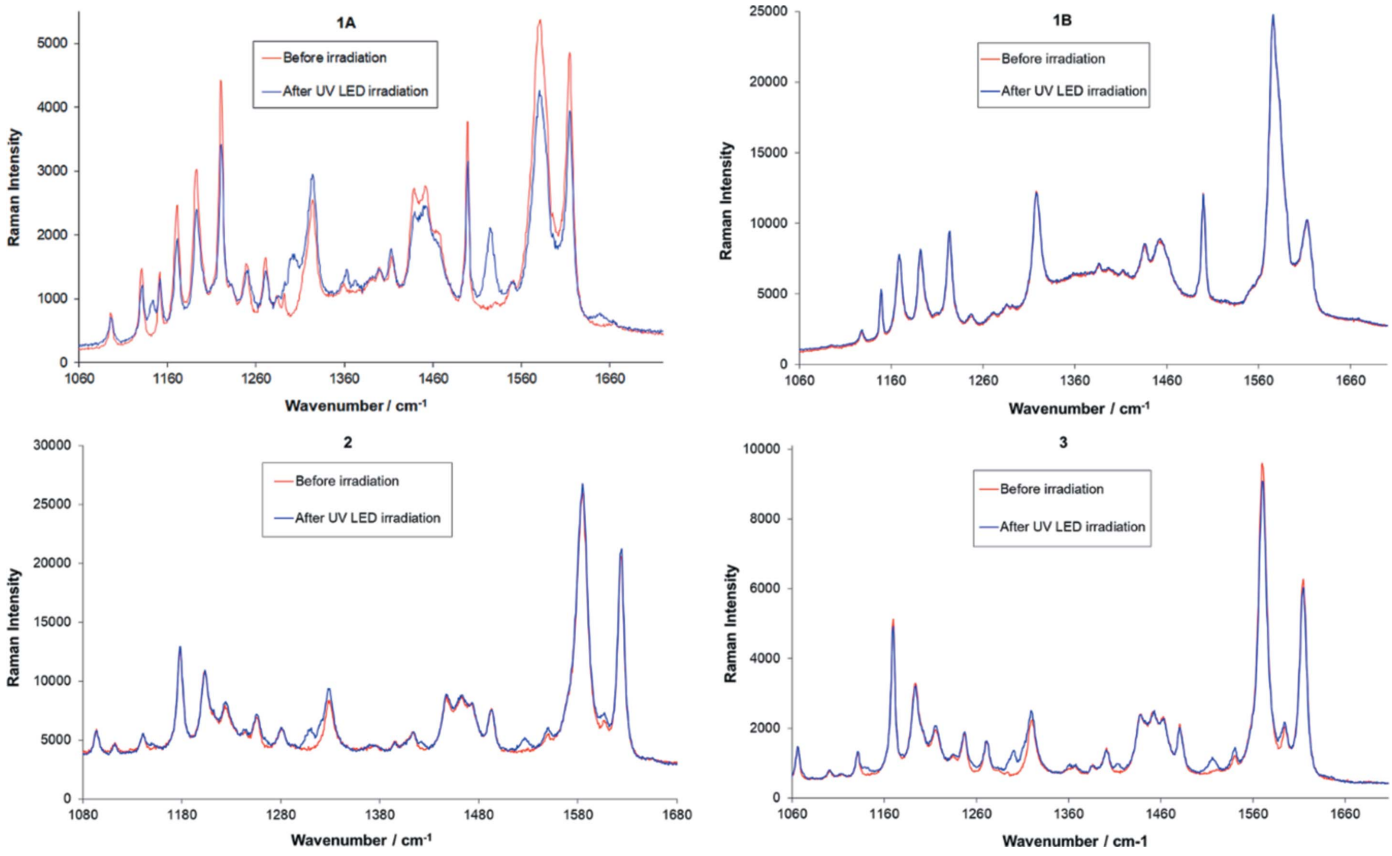


Figure 7
Raman spectra of **1A**, **1B**, **2** and **3** before irradiation (red) and after irradiation (blue) with UV LEDs.

spectra upon irradiation. In both cases, the position of the shoulder in the reflectance spectra shifts to higher wavelengths upon irradiation. No diffuse reflectance spectra upon irradiation are presented for **1** due to the sample likely being a mixture of polymoprhs.

It has also been found that compounds with more 'space' in the crystal lattice are more likely to show photochromism as it is easier for the compound to undergo the necessary *cis* to *trans* isomerism. The presence of bulky *tert*-butyl groups can help create space and potentially enable photochromism to be displayed (Johmoto *et al.*, 2012). However, only three of the structures reported herein (**1A**, **2** and **3**) display photochromism. The packing and intermolecular interactions in **1A**, **2** and **3** are relatively similar, as discussed earlier; however, **1B** has significantly different packing and intermolecular interactions. It seems reasonable to suggest that these differences may well link to the different photochromic behaviour of the compounds. A link has been proposed between the interplanar or dihedral angle between the two aromatic rings and the likelihood of this type of compound showing photochromism with the observation that photochromic compounds tend to have a larger dihedral angle, typically dihedral angles below 20° are associated with nonphotochromic compounds, those above 30° are more likely to be photochromic and those between 20 and 30° can display photochromism (Johmoto *et al.*, 2012). The structures reported here fit in with these general observations and those with the larger dihedral angles between the two aromatic rings are the ones displaying photochromism (see Table 4). It is possible that in order to form the aromatic C—H···O interaction present in **1A**, **2** and **3**, a larger dihedral angle is required between the two rings, while the C—H···O interactions in **1B** do not require this twisting, hence photochromism may be favoured for **1A**, **2** and **3** with the larger dihedral angle but is not seen for **1B** due to the smaller dihedral angle.

4. Conclusions

The structures of three related Schiff base compounds are reported; for one, (*E*)-2,4-di-*tert*-butyl-6-{[(4-fluorophenyl)-imino]methyl}phenol, **1**, two polymorphic structures are reported. The basic structures of the compounds are very similar, all existing in the enol form and showing an intermolecular O—H···N hydrogen bond and short C—H···O contacts. However, the packing of the two polymorphs of **1** were found to be significantly different. Compounds **2** and **3** were found to be isostructural with each other and displayed a temperature-induced phase transition upon cooling, this was attributed to the disorder in one of the *tert*-butyl groups resolving at low temperature, which was linked to a colour change from yellow to red around the phase transition. Three of the structures, *i.e.* **1A**, **2** and **3**, were found to show photochromism upon irradiation with UV LEDs, while **1B** did not; this was linked with differences in the packing and to the

interplanar or dihedral angle between the two aromatic rings being greater than 25° for the photochromic structures and being less than 25° for **1B**. The presence of photochromism was identified both by eye and Raman spectroscopy.

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supporting information

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Selected solid-state behaviour of three di-*tert*-butyl-substituted *N*-salicylideneaniline derivatives: temperature-induced phase transitions and chromic behaviour

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010) for 1A_100K, 1B_120K, 2_300K, 2_250K, 2_200K; *CrysAlis PRO* (Agilent, 2011) for 2_150K; *CrysAlis PRO* (Rigaku OD, 2018) for 2_120K, 2_100K; *CrysAlis PRO* (Agilent, 2013) for 3_300K, 3_250K, 3_200K, 3_150K, 3_120K; *CrysAlis PRO* (Agilent, 2012) for 3_100K. Cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010) for 1A_100K, 1B_120K, 2_300K, 2_250K, 2_200K; *CrysAlis PRO* (Agilent, 2011) for 2_150K; *CrysAlis PRO* (Rigaku OD, 2018) for 2_120K, 2_100K; *CrysAlis PRO* (Agilent, 2013) for 3_300K, 3_250K, 3_200K, 3_150K, 3_120K; *CrysAlis PRO* (Agilent, 2012) for 3_100K. Data reduction: *CrysAlis PRO* (Oxford Diffraction, 2010) for 1A_100K, 1B_120K, 2_300K, 2_250K, 2_200K; *CrysAlis PRO* (Agilent, 2011) for 2_150K; *CrysAlis PRO* (Rigaku OD, 2018) for 2_120K, 2_100K; *CrysAlis PRO* (Agilent, 2013) for 3_300K, 3_250K, 3_200K, 3_150K, 3_120K; *CrysAlis PRO* (Agilent, 2012) for 3_100K. Program(s) used to solve structure: *SHELXS* (Sheldrick, 2008) for 1A_100K, 1B_120K, 2_300K, 2_250K, 2_200K, 2_150K, 2_120K, 2_100K, 3_200K, 3_150K, 3_120K; olex2.solve 1.3 (Bourhis *et al.*, 2015) for 3_300K, 3_250K, 3_100K. For all structures, program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-fluorophenyl)imino]methyl}phenol (1A_100K)

Crystal data

$C_{21}H_{26}FNO$
$M_r = 327.43$
Triclinic, $P\overline{1}$
$a = 6.5324$ (3) Å
$b = 10.6141$ (8) Å
$c = 14.1675$ (9) Å
$\alpha = 80.364$ (5)°
$\beta = 81.094$ (4)°
$\gamma = 74.507$ (5)°
$V = 926.97$ (10) Å^3
$Z = 2$
$F(000) = 352$
$D_x = 1.173$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2473 reflections
$\theta = 2.6$–32.5°
$\mu = 0.08$ mm^{-1}
$T = 100$ K
Block, yellow
0.38 × 0.36 × 0.26 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2010)
$T_{min} = 0.870$, $T_{max} = 1.000$

7178 measured reflections
3792 independent reflections
2765 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.6°$
$h = -7 \rightarrow 8$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.110$
$S = 1.04$
3792 reflections
227 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.0587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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}
F1	−0.43318 (16)	0.71941 (11)	−0.13456 (8)	0.0341 (3)
N1	0.1460 (2)	0.73505 (14)	0.10716 (10)	0.0193 (3)
C6	0.4004 (2)	0.63436 (17)	0.22077 (12)	0.0166 (4)
C5	0.5210 (2)	0.51460 (17)	0.26395 (12)	0.0177 (4)
H5	0.496704	0.434037	0.253266	0.021*
C2	0.5864 (2)	0.75621 (17)	0.29626 (12)	0.0170 (4)
C3	0.7022 (2)	0.63411 (17)	0.33586 (12)	0.0169 (4)
H3	0.807813	0.633280	0.375301	0.020*
C4	0.6751 (2)	0.51175 (16)	0.32204 (12)	0.0157 (4)
C1	0.4334 (2)	0.75440 (17)	0.23617 (12)	0.0173 (4)
C8	−0.0021 (2)	0.72584 (17)	0.04634 (12)	0.0189 (4)
C7	0.2494 (2)	0.63086 (17)	0.15637 (12)	0.0178 (4)
H7	0.226130	0.548061	0.150415	0.021*
C18	0.8113 (3)	0.38311 (17)	0.37083 (13)	0.0195 (4)
C9	−0.1292 (3)	0.63623 (18)	0.06969 (13)	0.0218 (4)
H9	−0.117031	0.576535	0.127715	0.026*
C16	0.6915 (3)	0.96656 (17)	0.22125 (13)	0.0220 (4)
H16A	0.582832	0.984284	0.176938	0.033*
H16B	0.827729	0.916033	0.191653	0.033*
H16C	0.709342	1.050248	0.234961	0.033*
C10	−0.2737 (3)	0.63413 (19)	0.00811 (13)	0.0235 (4)
H10	−0.360534	0.572898	0.023102	0.028*
C17	0.7940 (3)	0.86411 (18)	0.38272 (14)	0.0263 (4)
H17A	0.929421	0.812771	0.353077	0.039*
H17B	0.751724	0.815744	0.444701	0.039*

H17C	0.811646	0.949405	0.393113	0.039*
C14	0.6201 (3)	0.88670 (17)	0.31578 (12)	0.0188 (4)
C13	−0.0239 (3)	0.81493 (18)	−0.03769 (13)	0.0251 (4)
H13	0.060152	0.877703	−0.052792	0.030*
C11	−0.2889 (3)	0.72204 (18)	−0.07475 (13)	0.0238 (4)
C12	−0.1674 (3)	0.81263 (19)	−0.09945 (14)	0.0289 (5)
H12	−0.181486	0.872258	−0.157455	0.035*
C20	1.0496 (3)	0.37493 (18)	0.33704 (13)	0.0242 (4)
H20A	1.087653	0.450900	0.354014	0.036*
H20B	1.075966	0.375376	0.266994	0.036*
H20C	1.136794	0.293325	0.368600	0.036*
C15	0.4108 (3)	0.96707 (19)	0.36626 (14)	0.0268 (4)
H15A	0.370138	0.916171	0.427347	0.040*
H15B	0.296854	0.985761	0.324589	0.040*
H15C	0.432778	1.050248	0.378886	0.040*
C21	0.7722 (3)	0.38104 (19)	0.48069 (13)	0.0273 (5)
H21A	0.621169	0.385042	0.502833	0.041*
H21B	0.809360	0.457200	0.497878	0.041*
H21C	0.861308	0.299554	0.511497	0.041*
C19	0.7593 (3)	0.26188 (18)	0.34583 (16)	0.0322 (5)
H19A	0.783536	0.262049	0.275802	0.048*
H19B	0.609189	0.263528	0.368646	0.048*
H19C	0.851584	0.182059	0.376970	0.048*
O1	0.31911 (19)	0.87039 (12)	0.19288 (9)	0.0222 (3)
H1	0.230 (4)	0.850 (2)	0.1544 (18)	0.067 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0347 (6)	0.0368 (7)	0.0347 (7)	−0.0015 (5)	−0.0196 (5)	−0.0129 (6)
N1	0.0183 (7)	0.0203 (8)	0.0199 (8)	−0.0047 (6)	−0.0044 (6)	−0.0024 (7)
C6	0.0153 (8)	0.0192 (9)	0.0160 (9)	−0.0062 (7)	−0.0007 (6)	−0.0021 (8)
C5	0.0200 (9)	0.0141 (9)	0.0199 (10)	−0.0069 (7)	−0.0002 (7)	−0.0024 (8)
C2	0.0184 (9)	0.0160 (9)	0.0167 (9)	−0.0061 (7)	0.0008 (7)	−0.0021 (8)
C3	0.0163 (8)	0.0197 (9)	0.0158 (9)	−0.0062 (7)	−0.0023 (6)	−0.0025 (8)
C4	0.0168 (8)	0.0152 (9)	0.0150 (9)	−0.0058 (7)	0.0005 (6)	−0.0006 (7)
C1	0.0151 (8)	0.0161 (9)	0.0188 (10)	−0.0018 (7)	−0.0017 (7)	−0.0007 (8)
C8	0.0171 (9)	0.0199 (9)	0.0189 (10)	−0.0008 (7)	−0.0027 (7)	−0.0064 (8)
C7	0.0174 (9)	0.0171 (9)	0.0204 (10)	−0.0073 (7)	0.0017 (7)	−0.0056 (8)
C18	0.0198 (9)	0.0158 (9)	0.0218 (10)	−0.0042 (7)	−0.0029 (7)	0.0001 (8)
C9	0.0185 (9)	0.0287 (11)	0.0170 (10)	−0.0036 (8)	−0.0017 (7)	−0.0033 (8)
C16	0.0230 (9)	0.0160 (9)	0.0281 (11)	−0.0067 (7)	−0.0039 (7)	−0.0022 (8)
C10	0.0184 (9)	0.0297 (11)	0.0247 (10)	−0.0072 (8)	0.0014 (7)	−0.0113 (9)
C17	0.0343 (11)	0.0176 (10)	0.0314 (11)	−0.0076 (8)	−0.0126 (8)	−0.0057 (9)
C14	0.0235 (9)	0.0138 (9)	0.0210 (10)	−0.0053 (7)	−0.0062 (7)	−0.0033 (8)
C13	0.0300 (10)	0.0189 (10)	0.0275 (11)	−0.0059 (8)	−0.0091 (8)	−0.0012 (9)
C11	0.0194 (9)	0.0271 (11)	0.0248 (11)	0.0036 (8)	−0.0099 (7)	−0.0119 (9)
C12	0.0345 (11)	0.0232 (11)	0.0287 (11)	−0.0021 (9)	−0.0141 (8)	−0.0008 (9)

C20	0.0227 (9)	0.0191 (10)	0.0289 (11)	−0.0033 (7)	−0.0020 (7)	−0.0016 (8)
C15	0.0326 (10)	0.0214 (10)	0.0276 (11)	−0.0054 (8)	−0.0037 (8)	−0.0087 (9)
C21	0.0269 (10)	0.0256 (11)	0.0220 (11)	0.0008 (8)	−0.0026 (7)	0.0053 (9)
C19	0.0347 (11)	0.0157 (10)	0.0480 (14)	−0.0057 (8)	−0.0176 (9)	0.0022 (10)
O1	0.0244 (7)	0.0138 (6)	0.0289 (8)	−0.0028 (5)	−0.0114 (5)	−0.0003 (6)

Geometric parameters (Å, º)

F1—C11	1.370 (2)	C16—C14	1.539 (2)
N1—C8	1.423 (2)	C10—H10	0.9500
N1—C7	1.286 (2)	C10—C11	1.371 (3)
C6—C5	1.402 (2)	C17—H17A	0.9800
C6—C1	1.404 (2)	C17—H17B	0.9800
C6—C7	1.455 (2)	C17—H17C	0.9800
C5—H5	0.9500	C17—C14	1.536 (2)
C5—C4	1.387 (2)	C14—C15	1.545 (2)
C2—C3	1.390 (2)	C13—H13	0.9500
C2—C1	1.415 (2)	C13—C12	1.385 (2)
C2—C14	1.534 (2)	C11—C12	1.373 (3)
C3—H3	0.9500	C12—H12	0.9500
C3—C4	1.406 (2)	C20—H20A	0.9800
C4—C18	1.536 (2)	C20—H20B	0.9800
C1—O1	1.3592 (19)	C20—H20C	0.9800
C8—C9	1.391 (3)	C15—H15A	0.9800
C8—C13	1.391 (2)	C15—H15B	0.9800
C7—H7	0.9500	C15—H15C	0.9800
C18—C20	1.540 (2)	C21—H21A	0.9800
C18—C21	1.535 (2)	C21—H21B	0.9800
C18—C19	1.523 (3)	C21—H21C	0.9800
C9—H9	0.9500	C19—H19A	0.9800
C9—C10	1.388 (2)	C19—H19B	0.9800
C16—H16A	0.9800	C19—H19C	0.9800
C16—H16B	0.9800	O1—H1	0.94 (3)
C16—H16C	0.9800		
C7—N1—C8	120.33 (16)	H17B—C17—H17C	109.5
C5—C6—C1	120.21 (15)	C14—C17—H17A	109.5
C5—C6—C7	118.57 (16)	C14—C17—H17B	109.5
C1—C6—C7	121.15 (15)	C14—C17—H17C	109.5
C6—C5—H5	119.4	C2—C14—C16	110.64 (14)
C4—C5—C6	121.10 (17)	C2—C14—C17	111.82 (14)
C4—C5—H5	119.4	C2—C14—C15	109.58 (14)
C3—C2—C1	116.26 (16)	C16—C14—C15	110.44 (14)
C3—C2—C14	122.59 (15)	C17—C14—C16	107.11 (15)
C1—C2—C14	121.15 (14)	C17—C14—C15	107.17 (15)
C2—C3—H3	117.5	C8—C13—H13	119.8
C2—C3—C4	125.01 (16)	C12—C13—C8	120.38 (18)
C4—C3—H3	117.5	C12—C13—H13	119.8

C5—C4—C3	116.80 (15)	F1—C11—C10	118.13 (17)
C5—C4—C18	123.02 (16)	F1—C11—C12	119.07 (16)
C3—C4—C18	120.17 (15)	C10—C11—C12	122.80 (17)
C6—C1—C2	120.59 (14)	C13—C12—H12	120.8
O1—C1—C6	120.16 (15)	C11—C12—C13	118.35 (17)
O1—C1—C2	119.24 (16)	C11—C12—H12	120.8
C9—C8—N1	122.77 (15)	C18—C20—H20A	109.5
C9—C8—C13	119.78 (16)	C18—C20—H20B	109.5
C13—C8—N1	117.39 (16)	C18—C20—H20C	109.5
N1—C7—C6	122.81 (17)	H20A—C20—H20B	109.5
N1—C7—H7	118.6	H20A—C20—H20C	109.5
C6—C7—H7	118.6	H20B—C20—H20C	109.5
C4—C18—C20	109.36 (14)	C14—C15—H15A	109.5
C21—C18—C4	109.72 (14)	C14—C15—H15B	109.5
C21—C18—C20	109.01 (14)	C14—C15—H15C	109.5
C19—C18—C4	111.96 (14)	H15A—C15—H15B	109.5
C19—C18—C20	108.05 (15)	H15A—C15—H15C	109.5
C19—C18—C21	108.67 (15)	H15B—C15—H15C	109.5
C8—C9—H9	120.0	C18—C21—H21A	109.5
C10—C9—C8	119.91 (17)	C18—C21—H21B	109.5
C10—C9—H9	120.0	C18—C21—H21C	109.5
H16A—C16—H16B	109.5	H21A—C21—H21B	109.5
H16A—C16—H16C	109.5	H21A—C21—H21C	109.5
H16B—C16—H16C	109.5	H21B—C21—H21C	109.5
C14—C16—H16A	109.5	C18—C19—H19A	109.5
C14—C16—H16B	109.5	C18—C19—H19B	109.5
C14—C16—H16C	109.5	C18—C19—H19C	109.5
C9—C10—H10	120.6	H19A—C19—H19B	109.5
C11—C10—C9	118.76 (18)	H19A—C19—H19C	109.5
C11—C10—H10	120.6	H19B—C19—H19C	109.5
H17A—C17—H17B	109.5	C1—O1—H1	107.1 (15)
H17A—C17—H17C	109.5		

F1—C11—C12—C13	179.32 (15)	C1—C6—C7—N1	3.2 (3)
N1—C8—C9—C10	178.67 (15)	C1—C2—C3—C4	−1.3 (2)
N1—C8—C13—C12	−179.09 (16)	C1—C2—C14—C16	−60.64 (19)
C6—C5—C4—C3	0.6 (2)	C1—C2—C14—C17	−179.95 (15)
C6—C5—C4—C18	−179.95 (15)	C1—C2—C14—C15	61.4 (2)
C5—C6—C1—C2	−0.8 (2)	C8—N1—C7—C6	−179.10 (15)
C5—C6—C1—O1	178.83 (14)	C8—C9—C10—C11	−0.5 (2)
C5—C6—C7—N1	−173.76 (15)	C8—C13—C12—C11	1.0 (3)
C5—C4—C18—C20	120.93 (18)	C7—N1—C8—C9	35.5 (2)
C5—C4—C18—C21	−119.54 (18)	C7—N1—C8—C13	−147.21 (16)
C5—C4—C18—C19	1.2 (2)	C7—C6—C5—C4	176.67 (15)
C2—C3—C4—C5	0.3 (3)	C7—C6—C1—C2	−177.70 (15)
C2—C3—C4—C18	−179.23 (15)	C7—C6—C1—O1	1.9 (2)
C3—C2—C1—C6	1.5 (2)	C9—C8—C13—C12	−1.7 (3)
C3—C2—C1—O1	−178.09 (15)	C9—C10—C11—F1	−179.59 (15)

C3—C2—C14—C16	119.41 (17)	C9—C10—C11—C12	−0.2 (3)
C3—C2—C14—C17	0.1 (2)	C10—C11—C12—C13	−0.1 (3)
C3—C2—C14—C15	−118.58 (17)	C14—C2—C3—C4	178.65 (15)
C3—C4—C18—C20	−59.6 (2)	C14—C2—C1—C6	−178.43 (15)
C3—C4—C18—C21	59.9 (2)	C14—C2—C1—O1	2.0 (2)
C3—C4—C18—C19	−179.34 (15)	C13—C8—C9—C10	1.4 (2)
C1—C6—C5—C4	−0.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.94 (3)	1.72 (3)	2.587 (2)	151 (2)

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-fluorophenyl)imino]methyl}phenol (1B_120K)

Crystal data

$C_{21}H_{26}FNO$
$M_r = 327.43$
Orthorhombic, $Pna2_1$
$a = 12.2569$ (3) Å
$b = 8.9658$ (2) Å
$c = 16.5739$ (4) Å
$V = 1821.35$ (7) Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.194$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9836 reflections
$\theta = 2.6$–$30.7°$
$\mu = 0.08$ mm^{-1}
$T = 120$ K
Block, yellow
0.46 × 0.43 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: analytical (CrysAlis PRO; Oxford Diffraction, 2010)
$T_{min} = 0.973$, $T_{max} = 0.992$
25510 measured reflections
3712 independent reflections
3517 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.6°$
$h = -15 \rightarrow 15$
$k = -11 \rightarrow 11$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.077$
$S = 1.05$
3712 reflections
226 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.3311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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	0.83391 (12)	0.36730 (17)	0.43826 (9)	0.0179 (3)
H1	0.882 (2)	0.444 (3)	0.4185 (15)	0.021*
F1	1.24654 (12)	0.88292 (16)	0.22645 (8)	0.0315 (4)
N1	0.93534 (14)	0.61161 (19)	0.41684 (10)	0.0158 (4)
C2	0.70056 (17)	0.3514 (2)	0.54254 (12)	0.0145 (4)
C5	0.75575 (17)	0.6436 (2)	0.59100 (12)	0.0155 (4)
H5	0.774023	0.742442	0.606537	0.019*
C3	0.65163 (17)	0.4218 (2)	0.60789 (13)	0.0153 (4)
H3	0.596886	0.368751	0.636573	0.018*
C4	0.67783 (16)	0.5664 (2)	0.63433 (12)	0.0146 (4)
C1	0.78248 (17)	0.4315 (2)	0.50160 (12)	0.0142 (4)
C8	1.01342 (17)	0.6906 (2)	0.37055 (13)	0.0155 (4)
C18	0.61916 (18)	0.6314 (2)	0.70838 (12)	0.0175 (5)
C6	0.80852 (17)	0.5789 (2)	0.52448 (13)	0.0152 (4)
C7	0.88583 (17)	0.6668 (2)	0.47806 (12)	0.0163 (5)
H7	0.899927	0.767122	0.493360	0.020*
C12	1.11018 (18)	0.7010 (2)	0.24320 (13)	0.0197 (5)
H12	1.123058	0.664221	0.190304	0.024*
C9	1.07431 (18)	0.8109 (3)	0.39872 (14)	0.0192 (5)
H9	1.062722	0.847815	0.451764	0.023*
C17	0.5735 (2)	0.1317 (3)	0.56633 (14)	0.0220 (5)
H17A	0.598115	0.126224	0.622515	0.033*
H17B	0.554491	0.031596	0.547268	0.033*
H17C	0.509338	0.196592	0.562816	0.033*
C10	1.15182 (19)	0.8770 (3)	0.34937 (13)	0.0207 (5)
H10	1.192878	0.960147	0.367779	0.025*
C14	0.66538 (17)	0.1957 (2)	0.51368 (13)	0.0170 (5)
C11	1.16826 (18)	0.8199 (3)	0.27322 (14)	0.0201 (5)
C13	1.03219 (18)	0.6367 (2)	0.29277 (13)	0.0182 (5)
H13	0.990796	0.554569	0.273465	0.022*
C19	0.6631 (2)	0.7856 (2)	0.73042 (14)	0.0236 (5)
H19A	0.741662	0.778955	0.740718	0.035*
H19B	0.625960	0.821884	0.778961	0.035*
H19C	0.649793	0.854751	0.685706	0.035*
C21	0.4968 (2)	0.6469 (3)	0.68953 (16)	0.0294 (6)
H21A	0.486801	0.716706	0.644634	0.044*
H21B	0.458545	0.684626	0.737292	0.044*
H21C	0.467005	0.549245	0.674676	0.044*
C15	0.6215 (2)	0.2072 (3)	0.42655 (13)	0.0228 (5)

H15A	0.599473	0.108066	0.407705	0.034*
H15B	0.678804	0.246519	0.391215	0.034*
H15C	0.558419	0.274304	0.425441	0.034*
C20	0.6349 (2)	0.5281 (3)	0.78124 (14)	0.0245 (5)
H20A	0.605052	0.429291	0.768805	0.037*
H20B	0.596803	0.569737	0.828083	0.037*
H20C	0.712876	0.519130	0.793363	0.037*
C16	0.7618 (2)	0.0853 (2)	0.51666 (15)	0.0245 (5)
H16A	0.788001	0.076477	0.572321	0.037*
H16B	0.820968	0.121976	0.482192	0.037*
H16C	0.737691	−0.012602	0.497374	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0187 (8)	0.0178 (8)	0.0172 (8)	−0.0018 (6)	0.0048 (6)	−0.0023 (6)
F1	0.0307 (8)	0.0376 (8)	0.0262 (8)	−0.0148 (7)	0.0106 (6)	0.0024 (6)
N1	0.0140 (9)	0.0167 (9)	0.0166 (9)	0.0000 (7)	−0.0001 (7)	0.0014 (7)
C2	0.0144 (10)	0.0157 (10)	0.0135 (10)	0.0007 (8)	−0.0029 (8)	−0.0006 (8)
C5	0.0175 (11)	0.0136 (10)	0.0154 (11)	0.0000 (9)	−0.0036 (8)	−0.0016 (8)
C3	0.0140 (10)	0.0186 (11)	0.0133 (10)	−0.0024 (8)	0.0009 (8)	0.0018 (8)
C4	0.0136 (10)	0.0168 (10)	0.0133 (10)	0.0012 (8)	−0.0013 (8)	−0.0013 (8)
C1	0.0141 (10)	0.0175 (10)	0.0109 (10)	0.0021 (8)	−0.0019 (8)	−0.0008 (8)
C8	0.0123 (10)	0.0172 (10)	0.0172 (11)	0.0013 (8)	−0.0008 (8)	0.0051 (9)
C18	0.0177 (11)	0.0205 (11)	0.0142 (11)	0.0013 (9)	0.0019 (9)	−0.0039 (9)
C6	0.0124 (10)	0.0174 (10)	0.0158 (11)	0.0004 (8)	−0.0021 (8)	0.0014 (8)
C7	0.0166 (11)	0.0155 (10)	0.0168 (11)	−0.0013 (8)	−0.0026 (9)	0.0005 (8)
C12	0.0238 (12)	0.0210 (11)	0.0142 (10)	−0.0001 (9)	0.0020 (9)	−0.0011 (9)
C9	0.0201 (11)	0.0232 (12)	0.0142 (10)	−0.0015 (9)	−0.0005 (8)	−0.0003 (9)
C17	0.0265 (13)	0.0206 (11)	0.0188 (11)	−0.0080 (10)	0.0012 (9)	−0.0026 (9)
C10	0.0191 (11)	0.0226 (12)	0.0202 (12)	−0.0073 (10)	−0.0025 (9)	0.0005 (9)
C14	0.0209 (11)	0.0154 (10)	0.0147 (11)	−0.0034 (9)	0.0013 (9)	−0.0010 (9)
C11	0.0168 (11)	0.0241 (12)	0.0193 (12)	−0.0033 (9)	0.0030 (9)	0.0054 (10)
C13	0.0185 (11)	0.0168 (10)	0.0195 (12)	−0.0019 (9)	−0.0013 (9)	−0.0005 (9)
C19	0.0299 (13)	0.0223 (12)	0.0186 (12)	0.0020 (10)	0.0035 (10)	−0.0057 (9)
C21	0.0195 (12)	0.0404 (15)	0.0283 (13)	0.0041 (10)	0.0027 (10)	−0.0092 (11)
C15	0.0275 (12)	0.0248 (12)	0.0162 (11)	−0.0091 (10)	−0.0018 (10)	−0.0024 (9)
C20	0.0340 (13)	0.0245 (12)	0.0149 (11)	0.0018 (10)	0.0057 (9)	−0.0010 (10)
C16	0.0301 (13)	0.0179 (11)	0.0255 (12)	0.0011 (10)	0.0033 (10)	−0.0009 (10)

Geometric parameters (Å, º)

O1—H1	0.96 (3)	C9—C10	1.386 (3)
O1—C1	1.353 (3)	C17—H17A	0.9800
F1—C11	1.357 (2)	C17—H17B	0.9800
N1—C8	1.416 (3)	C17—H17C	0.9800
N1—C7	1.282 (3)	C17—C14	1.536 (3)
C2—C3	1.390 (3)	C10—H10	0.9500

C2—C1	1.408 (3)	C10—C11	1.377 (3)
C2—C14	1.538 (3)	C14—C15	1.544 (3)
C5—H5	0.9500	C14—C16	1.542 (3)
C5—C4	1.381 (3)	C13—H13	0.9500
C5—C6	1.404 (3)	C19—H19A	0.9800
C3—H3	0.9500	C19—H19B	0.9800
C3—C4	1.405 (3)	C19—H19C	0.9800
C4—C18	1.537 (3)	C21—H21A	0.9800
C1—C6	1.411 (3)	C21—H21B	0.9800
C8—C9	1.393 (3)	C21—H21C	0.9800
C8—C13	1.396 (3)	C15—H15A	0.9800
C18—C19	1.528 (3)	C15—H15B	0.9800
C18—C21	1.539 (3)	C15—H15C	0.9800
C18—C20	1.534 (3)	C20—H20A	0.9800
C6—C7	1.453 (3)	C20—H20B	0.9800
C7—H7	0.9500	C20—H20C	0.9800
C12—H12	0.9500	C16—H16A	0.9800
C12—C11	1.375 (3)	C16—H16B	0.9800
C12—C13	1.386 (3)	C16—H16C	0.9800
C9—H9	0.9500		

C1—O1—H1	104.0 (15)	C11—C10—C9	118.8 (2)
C7—N1—C8	123.75 (19)	C11—C10—H10	120.6
C3—C2—C1	116.84 (18)	C2—C14—C15	109.13 (17)
C3—C2—C14	122.27 (19)	C2—C14—C16	110.96 (18)
C1—C2—C14	120.85 (18)	C17—C14—C2	111.58 (18)
C4—C5—H5	119.3	C17—C14—C15	107.52 (18)
C4—C5—C6	121.34 (19)	C17—C14—C16	107.71 (18)
C6—C5—H5	119.3	C16—C14—C15	109.86 (19)
C2—C3—H3	117.9	F1—C11—C12	118.8 (2)
C2—C3—C4	124.29 (19)	F1—C11—C10	118.20 (19)
C4—C3—H3	117.9	C12—C11—C10	123.0 (2)
C5—C4—C3	117.27 (19)	C8—C13—H13	119.4
C5—C4—C18	123.26 (19)	C12—C13—C8	121.2 (2)
C3—C4—C18	119.47 (18)	C12—C13—H13	119.4
O1—C1—C2	119.29 (17)	C18—C19—H19A	109.5
O1—C1—C6	120.08 (18)	C18—C19—H19B	109.5
C2—C1—C6	120.60 (18)	C18—C19—H19C	109.5
C9—C8—N1	124.60 (19)	H19A—C19—H19B	109.5
C9—C8—C13	119.29 (19)	H19A—C19—H19C	109.5
C13—C8—N1	116.04 (18)	H19B—C19—H19C	109.5
C4—C18—C21	109.16 (18)	C18—C21—H21A	109.5
C19—C18—C4	111.67 (18)	C18—C21—H21B	109.5
C19—C18—C21	108.09 (19)	C18—C21—H21C	109.5
C19—C18—C20	108.30 (18)	H21A—C21—H21B	109.5
C20—C18—C4	109.90 (17)	H21A—C21—H21C	109.5
C20—C18—C21	109.7 (2)	H21B—C21—H21C	109.5
C5—C6—C1	119.58 (19)	C14—C15—H15A	109.5

C5—C6—C7	119.48 (19)	C14—C15—H15B	109.5
C1—C6—C7	120.89 (19)	C14—C15—H15C	109.5
N1—C7—C6	121.20 (19)	H15A—C15—H15B	109.5
N1—C7—H7	119.4	H15A—C15—H15C	109.5
C6—C7—H7	119.4	H15B—C15—H15C	109.5
C11—C12—H12	121.1	C18—C20—H20A	109.5
C11—C12—C13	117.7 (2)	C18—C20—H20B	109.5
C13—C12—H12	121.1	C18—C20—H20C	109.5
C8—C9—H9	120.0	H20A—C20—H20B	109.5
C10—C9—C8	120.0 (2)	H20A—C20—H20C	109.5
C10—C9—H9	120.0	H20B—C20—H20C	109.5
H17A—C17—H17B	109.5	C14—C16—H16A	109.5
H17A—C17—H17C	109.5	C14—C16—H16B	109.5
H17B—C17—H17C	109.5	C14—C16—H16C	109.5
C14—C17—H17A	109.5	H16A—C16—H16B	109.5
C14—C17—H17B	109.5	H16A—C16—H16C	109.5
C14—C17—H17C	109.5	H16B—C16—H16C	109.5
C9—C10—H10	120.6		

O1—C1—C6—C5	−179.09 (19)	C1—C2—C3—C4	0.8 (3)
O1—C1—C6—C7	3.5 (3)	C1—C2—C14—C17	−178.77 (19)
N1—C8—C9—C10	177.5 (2)	C1—C2—C14—C15	−60.1 (3)
N1—C8—C13—C12	−177.18 (19)	C1—C2—C14—C16	61.1 (3)
C2—C3—C4—C5	1.4 (3)	C1—C6—C7—N1	−2.5 (3)
C2—C3—C4—C18	−179.0 (2)	C8—N1—C7—C6	−178.37 (19)
C2—C1—C6—C5	3.0 (3)	C8—C9—C10—C11	−1.0 (3)
C2—C1—C6—C7	−174.40 (19)	C6—C5—C4—C3	−1.5 (3)
C5—C4—C18—C19	−3.7 (3)	C6—C5—C4—C18	178.99 (19)
C5—C4—C18—C21	115.8 (2)	C7—N1—C8—C9	23.7 (3)
C5—C4—C18—C20	−123.9 (2)	C7—N1—C8—C13	−159.3 (2)
C5—C6—C7—N1	−179.83 (19)	C9—C8—C13—C12	−0.1 (3)
C3—C2—C1—O1	179.04 (18)	C9—C10—C11—F1	−178.1 (2)
C3—C2—C1—C6	−3.0 (3)	C9—C10—C11—C12	0.8 (3)
C3—C2—C14—C17	−0.8 (3)	C14—C2—C3—C4	−177.2 (2)
C3—C2—C14—C15	117.8 (2)	C14—C2—C1—O1	−2.9 (3)
C3—C2—C14—C16	−121.0 (2)	C14—C2—C1—C6	175.04 (19)
C3—C4—C18—C19	176.84 (19)	C11—C12—C13—C8	−0.1 (3)
C3—C4—C18—C21	−63.7 (3)	C13—C8—C9—C10	0.7 (3)
C3—C4—C18—C20	56.6 (3)	C13—C12—C11—F1	178.72 (19)
C4—C5—C6—C1	−0.6 (3)	C13—C12—C11—C10	−0.3 (3)
C4—C5—C6—C7	176.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.96 (3)	1.64 (3)	2.544 (2)	155 (2)

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-chlorophenyl)imino]methyl}phenol (2_300K)

Crystal data

$C_{21}H_{26}ClNO$
$M_r = 343.88$
Monoclinic, $P2_1/c$
$a = 17.9412$ (17) Å
$b = 10.5067$ (7) Å
$c = 10.3890$ (7) Å
$\beta = 92.719$ (7)°
$V = 1956.2$ (3) Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.168$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 956 reflections
$\theta = 2.8$–30.5°
$\mu = 0.20$ mm^{-1}
$T = 300$ K
Block, yellow
0.33 × 0.28 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlis PRO (Oxford Diffraction, 2010), based on expressions derived by Clark & Reid (1995)]
$T_{min} = 0.947$, $T_{max} = 0.981$
5532 measured reflections
2382 independent reflections
1501 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 22.0°$, $\theta_{min} = 2.8°$
$h = -18\rightarrow17$
$k = -10\rightarrow11$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.133$
$S = 1.02$
2382 reflections
277 parameters
169 restraints
Primary atom site location: structure-invariant direct methods
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}
$\Delta\rho_{min} = -0.15$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	1.13127 (6)	0.94077 (11)	0.78074 (11)	0.0864 (5)	
N1	0.88659 (17)	0.7046 (3)	0.4603 (3)	0.0577 (9)	
C2	0.71192 (19)	0.5474 (3)	0.2099 (3)	0.0417 (9)	
C6	0.7739 (2)	0.7231 (4)	0.3260 (3)	0.0509 (10)	
C1	0.7694 (2)	0.5931 (3)	0.2934 (3)	0.0455 (9)	
C5	0.7198 (2)	0.8061 (3)	0.2758 (3)	0.0539 (11)	

H5	0.722929	0.891663	0.298151	0.065*	
C8	0.94315 (13)	0.7639 (2)	0.5400 (2)	0.0534 (10)	
C13	1.01328 (16)	0.7074 (2)	0.5444 (2)	0.0673 (12)	
H13	1.021169	0.633327	0.497925	0.081*	
C12	1.07161 (11)	0.7615 (3)	0.6183 (3)	0.0687 (12)	
H12	1.118527	0.723674	0.621292	0.082*	
C11	1.05982 (14)	0.8721 (3)	0.6878 (2)	0.0598 (11)	
C10	0.98969 (17)	0.9286 (2)	0.6834 (2)	0.0783 (13)	
H10	0.981802	1.002679	0.729932	0.094*	
C9	0.93136 (12)	0.8745 (3)	0.6095 (3)	0.0774 (14)	
H9	0.884442	0.912334	0.606566	0.093*	
C3	0.6604 (2)	0.6373 (3)	0.1635 (3)	0.0478 (10)	
H3	0.621941	0.609106	0.107416	0.057*	
C7	0.8344 (2)	0.7724 (4)	0.4090 (3)	0.0604 (11)	
H7	0.835128	0.859377	0.425792	0.073*	
C4	0.6619 (2)	0.7667 (4)	0.1945 (3)	0.0478 (10)	
C14	0.7057 (2)	0.4067 (3)	0.1714 (3)	0.0506 (10)	
C18	0.6025 (2)	0.8590 (3)	0.1398 (3)	0.0554 (11)	
C15	0.6986 (2)	0.3242 (3)	0.2922 (3)	0.0698 (13)	
H15A	0.652863	0.344446	0.332146	0.105*	
H15B	0.740011	0.340579	0.351764	0.105*	
H15C	0.698360	0.235895	0.268355	0.105*	
C17	0.6373 (2)	0.3794 (4)	0.0812 (4)	0.0743 (13)	
H17A	0.641743	0.425296	0.002083	0.111*	
H17B	0.592947	0.405904	0.121779	0.111*	
H17C	0.634600	0.289779	0.063425	0.111*	
C16	0.7751 (2)	0.3662 (4)	0.1004 (3)	0.0730 (13)	
H16A	0.818965	0.380550	0.155003	0.110*	
H16B	0.778138	0.415251	0.022900	0.110*	
H16C	0.771535	0.277421	0.079019	0.110*	
O1	0.82124 (15)	0.5111 (2)	0.3445 (3)	0.0639 (8)	
H1	0.853 (2)	0.554 (4)	0.387 (4)	0.077*	
C19A	0.5902 (11)	0.9776 (12)	0.2223 (15)	0.071 (5)	0.348 (3)
H19A	0.582635	0.952321	0.309481	0.107*	0.348 (3)
H19B	0.547155	1.022905	0.188555	0.107*	0.348 (3)
H19C	0.633287	1.031712	0.220415	0.107*	0.348 (3)
C20A	0.6171 (10)	0.8942 (18)	0.0009 (9)	0.085 (4)	0.348 (3)
H20A	0.654070	0.960210	0.000102	0.127*	0.348 (3)
H20B	0.571649	0.923981	−0.041491	0.127*	0.348 (3)
H20C	0.634671	0.820738	−0.043377	0.127*	0.348 (3)
C21A	0.5261 (5)	0.7865 (12)	0.1402 (17)	0.072 (4)	0.348 (3)
H21A	0.525038	0.721327	0.075285	0.108*	0.348 (3)
H21B	0.486020	0.845298	0.122298	0.108*	0.348 (3)
H21C	0.520544	0.748315	0.223123	0.108*	0.348 (3)
C21	0.5389 (8)	0.7991 (13)	0.0562 (16)	0.092 (4)	0.387 (3)
H21D	0.556355	0.780235	−0.027665	0.139*	0.387 (3)
H21E	0.497910	0.857653	0.048018	0.139*	0.387 (3)
H21F	0.522836	0.722010	0.095920	0.139*	0.387 (3)

C20	0.6423 (7)	0.9586 (12)	0.0563 (14)	0.079 (4)	0.387 (3)
H20D	0.678231	1.004780	0.109455	0.118*	0.387 (3)
H20E	0.606077	1.016785	0.019098	0.118*	0.387 (3)
H20F	0.667169	0.915818	−0.011081	0.118*	0.387 (3)
C19	0.5693 (9)	0.9308 (13)	0.2522 (11)	0.065 (4)	0.387 (3)
H19D	0.543619	0.871873	0.305125	0.098*	0.387 (3)
H19E	0.534861	0.993995	0.219036	0.098*	0.387 (3)
H19F	0.608657	0.971369	0.302811	0.098*	0.387 (3)
C20B	0.6363 (10)	0.9942 (11)	0.134 (2)	0.083 (5)	0.265 (3)
H20G	0.645438	1.026285	0.219502	0.124*	0.265 (3)
H20H	0.602103	1.049534	0.086998	0.124*	0.265 (3)
H20I	0.682498	0.990794	0.090649	0.124*	0.265 (3)
C19B	0.5357 (8)	0.861 (2)	0.2244 (17)	0.078 (5)	0.265 (3)
H19G	0.510486	0.780208	0.218299	0.118*	0.265 (3)
H19H	0.502067	0.927205	0.196191	0.118*	0.265 (3)
H19I	0.552382	0.875814	0.312275	0.118*	0.265 (3)
C21B	0.5783 (12)	0.8217 (18)	0.0000 (10)	0.067 (5)	0.265 (3)
H21G	0.621832	0.809134	−0.048904	0.100*	0.265 (3)
H21H	0.548346	0.888447	−0.038577	0.100*	0.265 (3)
H21I	0.549880	0.744357	0.000638	0.100*	0.265 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0734 (9)	0.0860 (9)	0.0969 (9)	−0.0178 (7)	−0.0263 (6)	0.0001 (7)
N1	0.054 (2)	0.055 (2)	0.063 (2)	0.0031 (18)	−0.0124 (17)	0.0032 (17)
C2	0.042 (2)	0.043 (2)	0.040 (2)	−0.0002 (19)	−0.0029 (18)	0.0064 (18)
C6	0.046 (3)	0.045 (3)	0.060 (2)	−0.004 (2)	−0.010 (2)	0.001 (2)
C1	0.045 (2)	0.045 (2)	0.047 (2)	0.010 (2)	0.0011 (19)	0.013 (2)
C5	0.059 (3)	0.040 (2)	0.061 (2)	0.005 (2)	−0.011 (2)	−0.005 (2)
C8	0.045 (3)	0.059 (3)	0.055 (2)	0.000 (2)	−0.009 (2)	0.005 (2)
C13	0.062 (3)	0.055 (3)	0.083 (3)	0.009 (2)	−0.020 (2)	−0.009 (2)
C12	0.046 (3)	0.066 (3)	0.092 (3)	0.009 (2)	−0.014 (2)	−0.003 (3)
C11	0.053 (3)	0.062 (3)	0.063 (3)	−0.007 (2)	−0.014 (2)	0.006 (2)
C10	0.068 (3)	0.087 (3)	0.078 (3)	0.020 (3)	−0.019 (2)	−0.028 (3)
C9	0.057 (3)	0.092 (4)	0.081 (3)	0.021 (3)	−0.014 (2)	−0.028 (3)
C3	0.050 (3)	0.053 (3)	0.040 (2)	0.001 (2)	−0.0041 (18)	−0.0018 (19)
C7	0.063 (3)	0.045 (2)	0.071 (3)	−0.004 (2)	−0.010 (2)	0.004 (2)
C4	0.049 (3)	0.048 (3)	0.046 (2)	0.007 (2)	−0.0028 (19)	0.005 (2)
C14	0.055 (3)	0.042 (2)	0.054 (2)	0.001 (2)	0.002 (2)	−0.004 (2)
C18	0.057 (3)	0.049 (3)	0.059 (2)	0.012 (2)	−0.007 (2)	−0.001 (2)
C15	0.091 (4)	0.047 (3)	0.072 (3)	−0.010 (2)	0.004 (2)	0.007 (2)
C17	0.077 (3)	0.060 (3)	0.084 (3)	−0.006 (2)	−0.017 (2)	−0.014 (2)
C16	0.083 (3)	0.055 (3)	0.081 (3)	0.010 (2)	0.006 (3)	−0.009 (2)
O1	0.058 (2)	0.0503 (18)	0.081 (2)	0.0048 (15)	−0.0197 (15)	0.0022 (15)
C19A	0.086 (11)	0.065 (9)	0.063 (9)	0.033 (9)	−0.003 (7)	0.006 (8)
C20A	0.105 (10)	0.102 (11)	0.046 (7)	0.048 (8)	−0.004 (7)	0.011 (8)
C21A	0.068 (8)	0.080 (8)	0.067 (9)	0.033 (7)	−0.014 (8)	0.004 (8)

C21	0.102 (9)	0.098 (8)	0.073 (9)	0.032 (8)	−0.046 (8)	−0.015 (9)
C20	0.093 (9)	0.106 (10)	0.037 (7)	0.046 (7)	0.014 (7)	0.012 (7)
C19	0.069 (10)	0.071 (10)	0.058 (7)	0.017 (8)	0.008 (6)	0.015 (7)
C20B	0.101 (10)	0.079 (9)	0.065 (10)	0.031 (9)	−0.020 (9)	0.003 (9)
C19B	0.083 (10)	0.095 (11)	0.057 (9)	0.039 (9)	0.005 (9)	0.014 (8)
C21B	0.072 (10)	0.081 (10)	0.046 (8)	0.025 (9)	−0.013 (7)	0.015 (8)

Geometric parameters (Å, º)

Cl1—C11	1.726 (2)	C15—H15A	0.9600
N1—C8	1.422 (3)	C15—H15B	0.9600
N1—C7	1.274 (4)	C15—H15C	0.9600
C2—C1	1.400 (5)	C17—H17A	0.9600
C2—C3	1.392 (4)	C17—H17B	0.9600
C2—C14	1.534 (4)	C17—H17C	0.9600
C6—C1	1.409 (5)	C16—H16A	0.9600
C6—C5	1.388 (4)	C16—H16B	0.9600
C6—C7	1.449 (5)	C16—H16C	0.9600
C1—O1	1.358 (4)	O1—H1	0.84 (4)
C5—H5	0.9300	C19A—H19A	0.9600
C5—C4	1.370 (4)	C19A—H19B	0.9600
C8—C13	1.3900	C19A—H19C	0.9600
C8—C9	1.3900	C20A—H20A	0.9600
C13—H13	0.9300	C20A—H20B	0.9600
C13—C12	1.3900	C20A—H20C	0.9600
C12—H12	0.9300	C21A—H21A	0.9600
C12—C11	1.3900	C21A—H21B	0.9600
C11—C10	1.3900	C21A—H21C	0.9600
C10—H10	0.9300	C21—H21D	0.9600
C10—C9	1.3900	C21—H21E	0.9600
C9—H9	0.9300	C21—H21F	0.9600
C3—H3	0.9300	C20—H20D	0.9600
C3—C4	1.397 (5)	C20—H20E	0.9600
C7—H7	0.9300	C20—H20F	0.9600
C4—C18	1.531 (5)	C19—H19D	0.9600
C14—C15	1.536 (4)	C19—H19E	0.9600
C14—C17	1.534 (5)	C19—H19F	0.9600
C14—C16	1.538 (5)	C20B—H20G	0.9600
C18—C19A	1.534 (7)	C20B—H20H	0.9600
C18—C20A	1.524 (7)	C20B—H20I	0.9600
C18—C21A	1.568 (7)	C19B—H19G	0.9600
C18—C21	1.535 (7)	C19B—H19H	0.9600
C18—C20	1.554 (7)	C19B—H19I	0.9600
C18—C19	1.534 (7)	C21B—H21G	0.9600
C18—C20B	1.548 (7)	C21B—H21H	0.9600
C18—C19B	1.520 (7)	C21B—H21I	0.9600
C18—C21B	1.546 (7)		

C7—N1—C8	119.3 (3)	H15B—C15—H15C	109.5
C1—C2—C14	122.3 (3)	C14—C17—H17A	109.5
C3—C2—C1	116.0 (3)	C14—C17—H17B	109.5
C3—C2—C14	121.7 (3)	C14—C17—H17C	109.5
C1—C6—C7	121.5 (3)	H17A—C17—H17B	109.5
C5—C6—C1	119.1 (3)	H17A—C17—H17C	109.5
C5—C6—C7	119.3 (4)	H17B—C17—H17C	109.5
C2—C1—C6	120.9 (3)	C14—C16—H16A	109.5
O1—C1—C2	119.7 (3)	C14—C16—H16B	109.5
O1—C1—C6	119.4 (3)	C14—C16—H16C	109.5
C6—C5—H5	118.7	H16A—C16—H16B	109.5
C4—C5—C6	122.5 (4)	H16A—C16—H16C	109.5
C4—C5—H5	118.7	H16B—C16—H16C	109.5
C13—C8—N1	116.9 (2)	C1—O1—H1	108 (3)
C13—C8—C9	120.0	C18—C19A—H19A	109.5
C9—C8—N1	123.1 (2)	C18—C19A—H19B	109.5
C8—C13—H13	120.0	C18—C19A—H19C	109.5
C8—C13—C12	120.0	H19A—C19A—H19B	109.5
C12—C13—H13	120.0	H19A—C19A—H19C	109.5
C13—C12—H12	120.0	H19B—C19A—H19C	109.5
C13—C12—C11	120.0	C18—C20A—H20A	109.5
C11—C12—H12	120.0	C18—C20A—H20B	109.5
C12—C11—Cl1	120.85 (19)	C18—C20A—H20C	109.5
C10—C11—Cl1	119.15 (19)	H20A—C20A—H20B	109.5
C10—C11—C12	120.0	H20A—C20A—H20C	109.5
C11—C10—H10	120.0	H20B—C20A—H20C	109.5
C9—C10—C11	120.0	C18—C21A—H21A	109.5
C9—C10—H10	120.0	C18—C21A—H21B	109.5
C8—C9—H9	120.0	C18—C21A—H21C	109.5
C10—C9—C8	120.0	H21A—C21A—H21B	109.5
C10—C9—H9	120.0	H21A—C21A—H21C	109.5
C2—C3—H3	117.4	H21B—C21A—H21C	109.5
C2—C3—C4	125.1 (3)	C18—C21—H21D	109.5
C4—C3—H3	117.4	C18—C21—H21E	109.5
N1—C7—C6	124.3 (4)	C18—C21—H21F	109.5
N1—C7—H7	117.8	H21D—C21—H21E	109.5
C6—C7—H7	117.8	H21D—C21—H21F	109.5
C5—C4—C3	116.2 (3)	H21E—C21—H21F	109.5
C5—C4—C18	122.1 (3)	C18—C20—H20D	109.5
C3—C4—C18	121.6 (3)	C18—C20—H20E	109.5
C2—C14—C15	109.8 (3)	C18—C20—H20F	109.5
C2—C14—C16	109.9 (3)	H20D—C20—H20E	109.5
C15—C14—C16	109.7 (3)	H20D—C20—H20F	109.5
C17—C14—C2	112.7 (3)	H20E—C20—H20F	109.5
C17—C14—C15	107.4 (3)	C18—C19—H19D	109.5
C17—C14—C16	107.3 (3)	C18—C19—H19E	109.5
C4—C18—C19A	115.0 (8)	C18—C19—H19F	109.5
C4—C18—C21A	106.5 (6)	H19D—C19—H19E	109.5

C4—C18—C21	115.9 (6)	H19D—C19—H19F	109.5
C4—C18—C20	107.7 (6)	H19E—C19—H19F	109.5
C4—C18—C19	108.5 (7)	C18—C20B—H20G	109.5
C4—C18—C20B	109.2 (7)	C18—C20B—H20H	109.5
C4—C18—C21B	110.3 (8)	C18—C20B—H20I	109.5
C19A—C18—C21A	104.2 (7)	H20G—C20B—H20H	109.5
C20A—C18—C4	111.0 (6)	H20G—C20B—H20I	109.5
C20A—C18—C19A	111.5 (7)	H20H—C20B—H20I	109.5
C20A—C18—C21A	108.0 (7)	C18—C19B—H19G	109.5
C21—C18—C20	108.0 (6)	C18—C19B—H19H	109.5
C19—C18—C21	109.1 (7)	C18—C19B—H19I	109.5
C19—C18—C20	107.4 (6)	H19G—C19B—H19H	109.5
C19B—C18—C4	110.3 (7)	H19G—C19B—H19I	109.5
C19B—C18—C20B	109.6 (8)	H19H—C19B—H19I	109.5
C19B—C18—C21B	110.7 (8)	C18—C21B—H21G	109.5
C21B—C18—C20B	106.7 (7)	C18—C21B—H21H	109.5
C14—C15—H15A	109.5	C18—C21B—H21I	109.5
C14—C15—H15B	109.5	H21G—C21B—H21H	109.5
C14—C15—H15C	109.5	H21G—C21B—H21I	109.5
H15A—C15—H15B	109.5	H21H—C21B—H21I	109.5
H15A—C15—H15C	109.5		

Cl1—C11—C10—C9	−179.77 (17)	C13—C12—C11—Cl1	179.76 (18)
N1—C8—C13—C12	178.8 (2)	C13—C12—C11—C10	0.0
N1—C8—C9—C10	−178.7 (2)	C12—C11—C10—C9	0.0
C2—C3—C4—C5	0.9 (5)	C11—C10—C9—C8	0.0
C2—C3—C4—C18	−179.5 (3)	C9—C8—C13—C12	0.0
C6—C5—C4—C3	−0.5 (5)	C3—C2—C1—C6	−0.6 (5)
C6—C5—C4—C18	179.9 (3)	C3—C2—C1—O1	179.0 (3)
C1—C2—C3—C4	−0.4 (5)	C3—C2—C14—C15	−120.7 (3)
C1—C2—C14—C15	59.2 (4)	C3—C2—C14—C17	−1.1 (5)
C1—C2—C14—C17	178.9 (3)	C3—C2—C14—C16	118.6 (3)
C1—C2—C14—C16	−61.5 (4)	C3—C4—C18—C19A	154.4 (8)
C1—C6—C5—C4	−0.4 (5)	C3—C4—C18—C20A	−77.8 (10)
C1—C6—C7—N1	−1.3 (6)	C3—C4—C18—C21A	39.5 (8)
C5—C6—C1—C2	1.0 (5)	C3—C4—C18—C21	3.7 (9)
C5—C6—C1—O1	−178.6 (3)	C3—C4—C18—C20	−117.3 (7)
C5—C6—C7—N1	179.7 (4)	C3—C4—C18—C19	126.8 (7)
C5—C4—C18—C19A	−26.0 (9)	C3—C4—C18—C20B	−152.7 (10)
C5—C4—C18—C20A	101.7 (10)	C3—C4—C18—C19B	86.8 (11)
C5—C4—C18—C21A	−140.9 (7)	C3—C4—C18—C21B	−35.8 (10)
C5—C4—C18—C21	−176.7 (9)	C7—N1—C8—C13	−150.7 (3)
C5—C4—C18—C20	62.3 (8)	C7—N1—C8—C9	28.1 (4)
C5—C4—C18—C19	−53.6 (8)	C7—C6—C1—C2	−177.9 (3)
C5—C4—C18—C20B	26.8 (10)	C7—C6—C1—O1	2.5 (5)
C5—C4—C18—C19B	−93.6 (11)	C7—C6—C5—C4	178.5 (3)
C5—C4—C18—C21B	143.8 (10)	C14—C2—C1—C6	179.5 (3)
C8—N1—C7—C6	179.9 (3)	C14—C2—C1—O1	−1.0 (5)

C8—C13—C12—C11	0.0	C14—C2—C3—C4	179.6 (3)
C13—C8—C9—C10	0.0		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.84 (4)	1.84 (4)	2.612 (4)	151 (4)

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-chlorophenyl)imino]methyl}phenol (2_250K)

Crystal data

$C_{21}H_{26}ClNO$
$M_r = 343.88$
Monoclinic, $P2_1/c$
$a = 17.8739$ (13) Å
$b = 10.4846$ (7) Å
$c = 10.3312$ (6) Å
$\beta = 92.296$ (5)°
$V = 1934.5$ (2) Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.181$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1038 reflections
$\theta = 2.8$–30.5°
$\mu = 0.20$ mm^{-1}
$T = 250$ K
Block, yellow
0.33 × 0.28 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: multi-scan [CrysAlis PRO (Oxford Diffraction, 2010), based on expressions derived by Clark & Reid (1995)]
$T_{min} = 0.651$, $T_{max} = 1.000$
5874 measured reflections
2688 independent reflections
1737 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 23.0°$, $\theta_{min} = 2.8°$
$h = -19\rightarrow19$
$k = -7\rightarrow11$
$l = -8\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.145$
$S = 1.06$
2688 reflections
277 parameters
181 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.0321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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}	Occ. (<1)
Cl1	1.13193 (6)	0.94179 (11)	0.78151 (10)	0.0691 (4)	
N1	0.88654 (16)	0.7052 (3)	0.4607 (3)	0.0459 (8)	
C2	0.71228 (19)	0.5467 (3)	0.2106 (3)	0.0349 (9)	
C6	0.77403 (19)	0.7227 (4)	0.3262 (3)	0.0418 (9)	
C1	0.76985 (19)	0.5921 (3)	0.2939 (3)	0.0386 (9)	
C5	0.71951 (19)	0.8063 (3)	0.2757 (3)	0.0434 (10)	
H5	0.722514	0.893005	0.298350	0.052*	
C8	0.94377 (11)	0.7642 (2)	0.5401 (2)	0.0432 (10)	
C13	1.01412 (13)	0.70754 (19)	0.5448 (2)	0.0538 (11)	
H13	1.022330	0.632377	0.497882	0.065*	
C12	1.07234 (10)	0.7620 (2)	0.6190 (2)	0.0542 (11)	
H12	1.119915	0.723660	0.622222	0.065*	
C11	1.06020 (11)	0.8731 (2)	0.6884 (2)	0.0464 (10)	
C10	0.98984 (14)	0.9298 (2)	0.6837 (2)	0.0603 (12)	
H10	0.981636	1.005007	0.730646	0.072*	
C9	0.93163 (10)	0.8754 (2)	0.6095 (2)	0.0596 (12)	
H9	0.884051	0.913726	0.606306	0.072*	
C3	0.6605 (2)	0.6363 (4)	0.1633 (3)	0.0405 (9)	
H3	0.621839	0.607366	0.106242	0.049*	
C7	0.8341 (2)	0.7737 (4)	0.4093 (3)	0.0479 (10)	
H7	0.834531	0.861802	0.426299	0.057*	
C4	0.66174 (19)	0.7664 (3)	0.1944 (3)	0.0387 (9)	
C14	0.7063 (2)	0.4057 (3)	0.1714 (3)	0.0420 (9)	
C18	0.6015 (2)	0.8594 (3)	0.1406 (3)	0.0442 (10)	
C15	0.6983 (2)	0.3227 (4)	0.2931 (3)	0.0573 (12)	
H15A	0.652023	0.343992	0.334006	0.086*	
H15B	0.740319	0.338326	0.353403	0.086*	
H15C	0.697570	0.233342	0.268618	0.086*	
C17	0.6382 (2)	0.3786 (4)	0.0810 (3)	0.0601 (12)	
H17A	0.642360	0.426888	0.001536	0.090*	
H17B	0.592913	0.403505	0.123160	0.090*	
H17C	0.636144	0.288238	0.061051	0.090*	
C16	0.7765 (2)	0.3644 (4)	0.1009 (3)	0.0562 (11)	
H16A	0.820429	0.375223	0.158144	0.084*	
H16B	0.781606	0.416537	0.024131	0.084*	
H16C	0.771877	0.275530	0.075867	0.084*	
O1	0.82155 (14)	0.5102 (2)	0.3454 (2)	0.0505 (7)	
H1	0.854 (2)	0.560 (3)	0.393 (3)	0.061*	
C19A	0.6145 (15)	0.9993 (10)	0.177 (3)	0.071 (5)	0.186 (3)
H19A	0.625435	1.005722	0.269877	0.107*	0.186 (3)
H19B	0.569945	1.048448	0.154559	0.107*	0.186 (3)
H19C	0.656466	1.032480	0.130986	0.107*	0.186 (3)
C20A	0.5964 (16)	0.848 (3)	−0.0077 (8)	0.062 (5)	0.186 (3)
H20A	0.642755	0.877533	−0.043130	0.093*	0.186 (3)
H20B	0.555090	0.899299	−0.041914	0.093*	0.186 (3)

H20C	0.588199	0.759355	−0.031762	0.093*	0.186 (3)
C21A	0.5258 (8)	0.817 (3)	0.191 (3)	0.072 (5)	0.186 (3)
H21A	0.510607	0.737444	0.149171	0.108*	0.186 (3)
H21B	0.488492	0.881758	0.172063	0.108*	0.186 (3)
H21C	0.530645	0.803503	0.284028	0.108*	0.186 (3)
C21	0.5267 (5)	0.7884 (9)	0.1091 (14)	0.067 (3)	0.430 (3)
H21D	0.533628	0.727840	0.039633	0.101*	0.430 (3)
H21E	0.488407	0.849654	0.082473	0.101*	0.430 (3)
H21F	0.511235	0.743347	0.185598	0.101*	0.430 (3)
C20	0.6277 (7)	0.9232 (14)	0.0188 (10)	0.078 (4)	0.430 (3)
H20D	0.673949	0.968784	0.038304	0.117*	0.430 (3)
H20E	0.589704	0.982636	−0.013368	0.117*	0.430 (3)
H20F	0.636022	0.858912	−0.046640	0.117*	0.430 (3)
C19	0.5826 (7)	0.9595 (11)	0.2424 (10)	0.058 (3)	0.430 (3)
H19D	0.569757	0.917114	0.321951	0.086*	0.430 (3)
H19E	0.540506	1.010508	0.210528	0.086*	0.430 (3)
H19F	0.625644	1.014351	0.259222	0.086*	0.430 (3)
C20B	0.6455 (6)	0.9763 (10)	0.0889 (13)	0.070 (4)	0.384 (3)
H20G	0.674235	1.015577	0.159852	0.106*	0.384 (3)
H20H	0.610355	1.037986	0.051520	0.106*	0.384 (3)
H20I	0.679044	0.948126	0.023244	0.106*	0.384 (3)
C19B	0.5531 (8)	0.9061 (16)	0.2476 (10)	0.067 (4)	0.384 (3)
H19G	0.522430	0.836418	0.277077	0.100*	0.384 (3)
H19H	0.521145	0.974629	0.215108	0.100*	0.384 (3)
H19I	0.584808	0.937131	0.319260	0.100*	0.384 (3)
C21B	0.5564 (8)	0.8076 (12)	0.0236 (12)	0.076 (4)	0.384 (3)
H21G	0.590289	0.777256	−0.040629	0.114*	0.384 (3)
H21H	0.525093	0.874864	−0.013633	0.114*	0.384 (3)
H21I	0.525061	0.737719	0.050679	0.114*	0.384 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0589 (7)	0.0702 (9)	0.0765 (7)	−0.0139 (7)	−0.0192 (5)	0.0017 (6)
N1	0.0395 (18)	0.046 (2)	0.0517 (18)	−0.0014 (18)	−0.0062 (15)	0.0021 (15)
C2	0.038 (2)	0.035 (2)	0.0313 (18)	0.000 (2)	0.0008 (16)	0.0022 (16)
C6	0.044 (2)	0.038 (2)	0.042 (2)	0.002 (2)	−0.0059 (18)	0.0013 (18)
C1	0.039 (2)	0.038 (2)	0.039 (2)	0.005 (2)	0.0005 (17)	0.0088 (18)
C5	0.050 (2)	0.031 (2)	0.048 (2)	0.004 (2)	−0.0048 (19)	−0.0024 (17)
C8	0.038 (2)	0.046 (3)	0.045 (2)	0.000 (2)	−0.0004 (17)	0.0026 (19)
C13	0.050 (3)	0.047 (3)	0.064 (2)	0.011 (2)	−0.009 (2)	−0.002 (2)
C12	0.037 (2)	0.062 (3)	0.063 (2)	0.007 (2)	−0.0048 (19)	0.001 (2)
C11	0.044 (2)	0.050 (3)	0.045 (2)	−0.002 (2)	−0.0018 (17)	0.0043 (19)
C10	0.059 (3)	0.068 (3)	0.053 (2)	0.018 (3)	−0.010 (2)	−0.018 (2)
C9	0.041 (2)	0.078 (3)	0.059 (2)	0.015 (2)	−0.008 (2)	−0.020 (2)
C3	0.043 (2)	0.045 (2)	0.0328 (18)	0.001 (2)	−0.0015 (16)	−0.0032 (17)
C7	0.048 (2)	0.041 (2)	0.054 (2)	−0.004 (2)	−0.004 (2)	0.0044 (19)
C4	0.043 (2)	0.040 (2)	0.0336 (19)	0.005 (2)	−0.0005 (16)	0.0008 (17)

C14	0.047 (2)	0.039 (2)	0.0393 (19)	−0.001 (2)	0.0009 (17)	−0.0010 (17)
C18	0.047 (2)	0.045 (2)	0.040 (2)	0.015 (2)	−0.0019 (18)	−0.0025 (19)
C15	0.077 (3)	0.042 (3)	0.053 (2)	−0.008 (2)	0.007 (2)	0.0074 (19)
C17	0.071 (3)	0.043 (3)	0.066 (2)	−0.007 (2)	−0.009 (2)	−0.013 (2)
C16	0.065 (3)	0.047 (3)	0.058 (2)	0.006 (2)	0.009 (2)	−0.005 (2)
O1	0.0480 (17)	0.0390 (17)	0.0633 (17)	0.0041 (14)	−0.0135 (13)	0.0005 (13)
C19A	0.073 (10)	0.093 (11)	0.049 (9)	0.040 (9)	−0.004 (8)	0.000 (9)
C20A	0.061 (11)	0.077 (11)	0.050 (9)	0.038 (10)	0.011 (9)	0.008 (9)
C21A	0.057 (10)	0.100 (11)	0.060 (10)	0.035 (9)	0.014 (9)	0.008 (10)
C21	0.052 (6)	0.079 (7)	0.070 (7)	0.027 (6)	−0.019 (6)	−0.021 (7)
C20	0.088 (8)	0.108 (9)	0.038 (6)	0.044 (7)	0.011 (6)	0.029 (6)
C19	0.047 (8)	0.073 (8)	0.053 (6)	0.017 (6)	0.014 (5)	0.012 (6)
C20B	0.079 (8)	0.085 (8)	0.048 (7)	0.039 (7)	0.016 (6)	0.023 (6)
C19B	0.047 (9)	0.097 (10)	0.057 (6)	0.029 (8)	0.008 (6)	0.006 (7)
C21B	0.080 (9)	0.088 (8)	0.058 (7)	0.044 (7)	−0.025 (7)	−0.019 (7)

Geometric parameters (Å, º)

Cl1—C11	1.7285 (18)	C15—H15A	0.9700
N1—C8	1.426 (3)	C15—H15B	0.9700
N1—C7	1.280 (4)	C15—H15C	0.9700
C2—C1	1.398 (4)	C17—H17A	0.9700
C2—C3	1.394 (4)	C17—H17B	0.9700
C2—C14	1.536 (5)	C17—H17C	0.9700
C6—C1	1.411 (5)	C16—H16A	0.9700
C6—C5	1.396 (4)	C16—H16B	0.9700
C6—C7	1.450 (4)	C16—H16C	0.9700
C1—O1	1.354 (4)	O1—H1	0.91 (3)
C5—H5	0.9400	C19A—H19A	0.9700
C5—C4	1.370 (4)	C19A—H19B	0.9700
C8—C13	1.3900	C19A—H19C	0.9700
C8—C9	1.3900	C20A—H20A	0.9700
C13—H13	0.9400	C20A—H20B	0.9700
C13—C12	1.3900	C20A—H20C	0.9700
C12—H12	0.9400	C21A—H21A	0.9700
C12—C11	1.3900	C21A—H21B	0.9700
C11—C10	1.3900	C21A—H21C	0.9700
C10—H10	0.9400	C21—H21D	0.9700
C10—C9	1.3900	C21—H21E	0.9700
C9—H9	0.9400	C21—H21F	0.9700
C3—H3	0.9400	C20—H20D	0.9700
C3—C4	1.401 (5)	C20—H20E	0.9700
C7—H7	0.9400	C20—H20F	0.9700
C4—C18	1.540 (5)	C19—H19D	0.9700
C14—C15	1.541 (4)	C19—H19E	0.9700
C14—C17	1.531 (4)	C19—H19F	0.9700
C14—C16	1.539 (5)	C20B—H20G	0.9700
C18—C19A	1.531 (8)	C20B—H20H	0.9700

C18—C20A	1.536 (7)	C20B—H20I	0.9700
C18—C21A	1.537 (8)	C19B—H19G	0.9700
C18—C21	1.554 (6)	C19B—H19H	0.9700
C18—C20	1.515 (6)	C19B—H19I	0.9700
C18—C19	1.534 (6)	C21B—H21G	0.9700
C18—C20B	1.561 (7)	C21B—H21H	0.9700
C18—C19B	1.512 (6)	C21B—H21I	0.9700
C18—C21B	1.526 (6)		

C7—N1—C8	119.5 (3)	H15B—C15—H15C	109.5
C1—C2—C14	122.1 (3)	C14—C17—H17A	109.5
C3—C2—C1	116.7 (3)	C14—C17—H17B	109.5
C3—C2—C14	121.2 (3)	C14—C17—H17C	109.5
C1—C6—C7	121.9 (3)	H17A—C17—H17B	109.5
C5—C6—C1	119.4 (3)	H17A—C17—H17C	109.5
C5—C6—C7	118.6 (3)	H17B—C17—H17C	109.5
C2—C1—C6	120.4 (3)	C14—C16—H16A	109.5
O1—C1—C2	120.0 (3)	C14—C16—H16B	109.5
O1—C1—C6	119.6 (3)	C14—C16—H16C	109.5
C6—C5—H5	118.8	H16A—C16—H16B	109.5
C4—C5—C6	122.4 (3)	H16A—C16—H16C	109.5
C4—C5—H5	118.8	H16B—C16—H16C	109.5
C13—C8—N1	117.5 (2)	C1—O1—H1	105 (2)
C13—C8—C9	120.0	C18—C19A—H19A	109.5
C9—C8—N1	122.5 (2)	C18—C19A—H19B	109.5
C8—C13—H13	120.0	C18—C19A—H19C	109.5
C8—C13—C12	120.0	H19A—C19A—H19B	109.5
C12—C13—H13	120.0	H19A—C19A—H19C	109.5
C13—C12—H12	120.0	H19B—C19A—H19C	109.5
C11—C12—C13	120.0	C18—C20A—H20A	109.5
C11—C12—H12	120.0	C18—C20A—H20B	109.5
C12—C11—Cl1	120.56 (15)	C18—C20A—H20C	109.5
C10—C11—Cl1	119.44 (15)	H20A—C20A—H20B	109.5
C10—C11—C12	120.0	H20A—C20A—H20C	109.5
C11—C10—H10	120.0	H20B—C20A—H20C	109.5
C11—C10—C9	120.0	C18—C21A—H21A	109.5
C9—C10—H10	120.0	C18—C21A—H21B	109.5
C8—C9—H9	120.0	C18—C21A—H21C	109.5
C10—C9—C8	120.0	H21A—C21A—H21B	109.5
C10—C9—H9	120.0	H21A—C21A—H21C	109.5
C2—C3—H3	117.6	H21B—C21A—H21C	109.5
C2—C3—C4	124.8 (3)	C18—C21—H21D	109.5
C4—C3—H3	117.6	C18—C21—H21E	109.5
N1—C7—C6	123.5 (4)	C18—C21—H21F	109.5
N1—C7—H7	118.3	H21D—C21—H21E	109.5
C6—C7—H7	118.3	H21D—C21—H21F	109.5
C5—C4—C3	116.3 (3)	H21E—C21—H21F	109.5
C5—C4—C18	121.8 (3)	C18—C20—H20D	109.5

C3—C4—C18	121.9 (3)	C18—C20—H20E	109.5
C2—C14—C15	109.7 (3)	C18—C20—H20F	109.5
C2—C14—C16	110.3 (3)	H20D—C20—H20E	109.5
C17—C14—C2	112.6 (3)	H20D—C20—H20F	109.5
C17—C14—C15	107.2 (3)	H20E—C20—H20F	109.5
C17—C14—C16	107.6 (3)	C18—C19—H19D	109.5
C16—C14—C15	109.4 (3)	C18—C19—H19E	109.5
C4—C18—C21	110.8 (5)	C18—C19—H19F	109.5
C4—C18—C20B	105.5 (5)	H19D—C19—H19E	109.5
C19A—C18—C4	114.9 (9)	H19D—C19—H19F	109.5
C19A—C18—C20A	109.0 (9)	H19E—C19—H19F	109.5
C19A—C18—C21A	108.8 (9)	C18—C20B—H20G	109.5
C20A—C18—C4	108.8 (10)	C18—C20B—H20H	109.5
C20A—C18—C21A	107.3 (8)	C18—C20B—H20I	109.5
C21A—C18—C4	107.7 (9)	H20G—C20B—H20H	109.5
C20—C18—C4	110.2 (5)	H20G—C20B—H20I	109.5
C20—C18—C21	109.2 (5)	H20H—C20B—H20I	109.5
C20—C18—C19	110.6 (6)	C18—C19B—H19G	109.5
C19—C18—C4	110.9 (5)	C18—C19B—H19H	109.5
C19—C18—C21	105.1 (6)	C18—C19B—H19I	109.5
C19B—C18—C4	110.7 (6)	H19G—C19B—H19H	109.5
C19B—C18—C20B	107.8 (6)	H19G—C19B—H19I	109.5
C19B—C18—C21B	113.2 (6)	H19H—C19B—H19I	109.5
C21B—C18—C4	113.6 (5)	C18—C21B—H21G	109.5
C21B—C18—C20B	105.4 (6)	C18—C21B—H21H	109.5
C14—C15—H15A	109.5	C18—C21B—H21I	109.5
C14—C15—H15B	109.5	H21G—C21B—H21H	109.5
C14—C15—H15C	109.5	H21G—C21B—H21I	109.5
H15A—C15—H15B	109.5	H21H—C21B—H21I	109.5
H15A—C15—H15C	109.5		

Cl1—C11—C10—C9	−179.81 (17)	C13—C12—C11—Cl1	179.81 (17)
N1—C8—C13—C12	179.0 (2)	C13—C12—C11—C10	0.0
N1—C8—C9—C10	−179.0 (2)	C12—C11—C10—C9	0.0
C2—C3—C4—C5	1.2 (5)	C11—C10—C9—C8	0.0
C2—C3—C4—C18	−178.6 (3)	C9—C8—C13—C12	0.0
C6—C5—C4—C3	−0.5 (5)	C3—C2—C1—C6	−0.3 (5)
C6—C5—C4—C18	179.4 (3)	C3—C2—C1—O1	179.0 (3)
C1—C2—C3—C4	−0.8 (5)	C3—C2—C14—C15	−120.7 (3)
C1—C2—C14—C15	60.0 (4)	C3—C2—C14—C17	−1.4 (4)
C1—C2—C14—C17	179.3 (3)	C3—C2—C14—C16	118.8 (3)
C1—C2—C14—C16	−60.5 (4)	C3—C4—C18—C19A	−176.1 (13)
C1—C6—C5—C4	−0.6 (5)	C3—C4—C18—C20A	−53.6 (13)
C1—C6—C7—N1	−1.1 (6)	C3—C4—C18—C21A	62.4 (13)
C5—C6—C1—C2	1.0 (5)	C3—C4—C18—C21	26.7 (7)
C5—C6—C1—O1	−178.3 (3)	C3—C4—C18—C20	−94.2 (8)
C5—C6—C7—N1	179.7 (3)	C3—C4—C18—C19	143.0 (6)
C5—C4—C18—C19A	4.0 (13)	C3—C4—C18—C20B	−132.1 (6)

C5—C4—C18—C20A	126.5 (13)	C3—C4—C18—C19B	111.5 (8)
C5—C4—C18—C21A	−117.4 (13)	C3—C4—C18—C21B	−17.1 (9)
C5—C4—C18—C21	−153.1 (6)	C7—N1—C8—C13	−150.8 (3)
C5—C4—C18—C20	85.9 (8)	C7—N1—C8—C9	28.2 (4)
C5—C4—C18—C19	−36.8 (7)	C7—C6—C1—C2	−178.2 (3)
C5—C4—C18—C20B	48.1 (7)	C7—C6—C1—O1	2.5 (5)
C5—C4—C18—C19B	−68.3 (8)	C7—C6—C5—C4	178.7 (3)
C5—C4—C18—C21B	163.0 (8)	C14—C2—C1—C6	179.1 (3)
C8—N1—C7—C6	179.3 (3)	C14—C2—C1—O1	−1.7 (5)
C8—C13—C12—C11	0.0	C14—C2—C3—C4	179.8 (3)
C13—C8—C9—C10	0.0		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.91 (3)	1.76 (4)	2.615 (4)	155 (3)

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-chlorophenyl)imino]methyl}phenol (2_200K)

Crystal data

$C_{21}H_{26}ClNO$
$M_r = 343.88$
Monoclinic, $P2_1/c$
$a = 17.8132$ (12) Å
$b = 10.4564$ (6) Å
$c = 10.2814$ (6) Å
$\beta = 91.965$ (5)°
$V = 1913.9$ (2) Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.193$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3727 reflections
$\theta = 2.8$–$32.7°$
$\mu = 0.21$ mm^{-1}
$T = 200$ K
Block, yellow
0.33 × 0.28 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2010)
$T_{min} = 0.947$, $T_{max} = 1.000$
11973 measured reflections
2833 independent reflections
2216 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 23.5°$, $\theta_{min} = 2.8°$
$h = -20 \rightarrow 20$
$k = -11 \rightarrow 11$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.120$
$S = 1.03$
2833 reflections
277 parameters
163 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 1.0995P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	1.13257 (4)	0.94230 (7)	0.78211 (7)	0.0522 (3)	
N1	0.88679 (12)	0.7051 (2)	0.4613 (2)	0.0366 (6)	
C2	0.71237 (14)	0.5467 (2)	0.2096 (2)	0.0279 (6)	
C6	0.77395 (14)	0.7224 (2)	0.3267 (2)	0.0320 (6)	
C1	0.76975 (14)	0.5920 (2)	0.2943 (2)	0.0298 (6)	
C5	0.71934 (15)	0.8066 (2)	0.2762 (2)	0.0355 (7)	
H5	0.722372	0.894424	0.299316	0.043*	
C8	0.94401 (8)	0.76410 (16)	0.54074 (15)	0.0336 (6)	
C13	1.01456 (9)	0.70715 (13)	0.54523 (16)	0.0397 (7)	
H13	1.022917	0.630890	0.497633	0.048*	
C12	1.07287 (7)	0.76177 (16)	0.61938 (17)	0.0407 (7)	
H12	1.121089	0.722839	0.622454	0.049*	
C11	1.06064 (8)	0.87334 (16)	0.68903 (15)	0.0362 (7)	
C10	0.99009 (10)	0.93030 (14)	0.68453 (16)	0.0449 (7)	
H10	0.981735	1.006557	0.732132	0.054*	
C9	0.93178 (7)	0.87568 (16)	0.61039 (17)	0.0451 (8)	
H9	0.883562	0.914610	0.607313	0.054*	
C3	0.66019 (14)	0.6359 (2)	0.1628 (2)	0.0313 (6)	
H3	0.620954	0.606407	0.105560	0.038*	
C7	0.83424 (15)	0.7737 (3)	0.4096 (2)	0.0383 (7)	
H7	0.834762	0.863013	0.426378	0.046*	
C4	0.66142 (14)	0.7664 (2)	0.1943 (2)	0.0307 (6)	
C14	0.70657 (15)	0.4046 (2)	0.1712 (2)	0.0332 (6)	
C18	0.60133 (15)	0.8594 (2)	0.1404 (2)	0.0367 (7)	
C15	0.69801 (17)	0.3222 (3)	0.2931 (3)	0.0439 (7)	
H15A	0.650891	0.343982	0.334274	0.066*	
H15B	0.740316	0.338251	0.354345	0.066*	
H15C	0.697359	0.231602	0.268541	0.066*	
C17	0.63888 (17)	0.3774 (3)	0.0794 (3)	0.0465 (8)	
H17A	0.644000	0.425686	−0.001560	0.070*	
H17B	0.592681	0.403478	0.121175	0.070*	
H17C	0.636648	0.285761	0.059765	0.070*	
C16	0.77756 (16)	0.3643 (3)	0.0999 (3)	0.0428 (7)	
H16A	0.821972	0.377903	0.157111	0.064*	
H16B	0.781899	0.415848	0.020850	0.064*	
H16C	0.773942	0.273671	0.076322	0.064*	
O1	0.82194 (11)	0.50987 (17)	0.34582 (18)	0.0402 (5)	

H1	0.8546 (16)	0.558 (3)	0.393 (3)	0.048*	
C19A	0.5841 (6)	0.9688 (8)	0.2335 (9)	0.056 (2)	0.397 (3)
H19A	0.578196	0.934541	0.321271	0.084*	0.397 (3)
H19B	0.537477	1.011330	0.204144	0.084*	0.397 (3)
H19C	0.625456	1.030547	0.234649	0.084*	0.397 (3)
C20A	0.6207 (5)	0.9049 (9)	0.0084 (6)	0.0584 (17)	0.397 (3)
H20A	0.668299	0.951978	0.014029	0.088*	0.397 (3)
H20B	0.580867	0.961318	−0.026060	0.088*	0.397 (3)
H20C	0.625793	0.831309	−0.049733	0.088*	0.397 (3)
C21A	0.5242 (4)	0.7860 (7)	0.1286 (9)	0.0549 (18)	0.397 (3)
H21A	0.528405	0.715012	0.067022	0.082*	0.397 (3)
H21B	0.484766	0.844851	0.097309	0.082*	0.397 (3)
H21C	0.511489	0.752489	0.214062	0.082*	0.397 (3)
C21	0.5428 (6)	0.7975 (9)	0.0490 (11)	0.059 (2)	0.352 (3)
H21D	0.567894	0.757403	−0.023963	0.089*	0.352 (3)
H21E	0.507726	0.862852	0.015734	0.089*	0.352 (3)
H21F	0.515184	0.732302	0.096381	0.089*	0.352 (3)
C20	0.6425 (5)	0.9631 (9)	0.0597 (10)	0.0515 (19)	0.352 (3)
H20D	0.679851	1.007013	0.115857	0.077*	0.352 (3)
H20E	0.605841	1.025285	0.025090	0.077*	0.352 (3)
H20F	0.667725	0.921987	−0.012572	0.077*	0.352 (3)
C19	0.5651 (7)	0.9280 (11)	0.2518 (9)	0.052 (2)	0.352 (3)
H19D	0.539501	0.865724	0.305942	0.078*	0.352 (3)
H19E	0.528618	0.990367	0.216956	0.078*	0.352 (3)
H19F	0.603881	0.972415	0.304559	0.078*	0.352 (3)
C20B	0.6386 (7)	0.9930 (8)	0.1258 (13)	0.058 (2)	0.251 (3)
H20G	0.653661	1.025970	0.211976	0.086*	0.251 (3)
H20H	0.602626	1.051980	0.083568	0.086*	0.251 (3)
H20I	0.682966	0.985101	0.072560	0.086*	0.251 (3)
C19B	0.5392 (6)	0.8693 (14)	0.2343 (11)	0.056 (2)	0.251 (3)
H19G	0.512683	0.787352	0.238268	0.085*	0.251 (3)
H19H	0.503938	0.936304	0.205344	0.085*	0.251 (3)
H19I	0.560231	0.890857	0.320895	0.085*	0.251 (3)
C21B	0.5742 (8)	0.8229 (13)	0.0027 (8)	0.052 (2)	0.251 (3)
H21G	0.617596	0.811044	−0.052123	0.078*	0.251 (3)
H21H	0.542180	0.891235	−0.033717	0.078*	0.251 (3)
H21I	0.545401	0.743186	0.005536	0.078*	0.251 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0446 (5)	0.0534 (5)	0.0575 (5)	−0.0118 (4)	−0.0160 (3)	0.0012 (4)
N1	0.0321 (13)	0.0390 (13)	0.0384 (12)	−0.0005 (11)	−0.0057 (10)	−0.0001 (10)
C2	0.0293 (15)	0.0303 (14)	0.0241 (12)	−0.0015 (12)	0.0004 (11)	0.0034 (11)
C6	0.0318 (15)	0.0323 (14)	0.0317 (13)	0.0003 (12)	−0.0022 (11)	0.0006 (12)
C1	0.0280 (14)	0.0319 (14)	0.0294 (13)	0.0044 (12)	0.0004 (11)	0.0068 (11)
C5	0.0398 (17)	0.0264 (14)	0.0400 (15)	0.0036 (13)	−0.0049 (13)	−0.0008 (12)
C8	0.0290 (15)	0.0388 (15)	0.0327 (14)	−0.0008 (13)	−0.0024 (11)	0.0000 (12)

C13	0.0360 (17)	0.0376 (15)	0.0448 (16)	0.0061 (14)	−0.0072 (13)	−0.0049 (13)
C12	0.0292 (16)	0.0444 (17)	0.0483 (16)	0.0078 (14)	−0.0039 (13)	0.0035 (14)
C11	0.0334 (16)	0.0408 (16)	0.0339 (14)	−0.0063 (13)	−0.0039 (12)	0.0043 (13)
C10	0.0424 (18)	0.0496 (18)	0.0421 (16)	0.0099 (15)	−0.0080 (13)	−0.0145 (14)
C9	0.0328 (17)	0.0578 (19)	0.0444 (16)	0.0137 (15)	−0.0052 (13)	−0.0134 (15)
C3	0.0307 (15)	0.0372 (15)	0.0257 (13)	0.0004 (12)	−0.0018 (11)	−0.0005 (11)
C7	0.0397 (17)	0.0320 (14)	0.0429 (16)	−0.0021 (13)	−0.0043 (13)	0.0009 (13)
C4	0.0325 (15)	0.0322 (14)	0.0273 (13)	0.0044 (12)	−0.0021 (11)	0.0013 (11)
C14	0.0362 (16)	0.0298 (14)	0.0336 (14)	−0.0008 (12)	−0.0005 (12)	−0.0004 (12)
C18	0.0394 (17)	0.0371 (15)	0.0333 (14)	0.0111 (13)	−0.0036 (12)	−0.0019 (12)
C15	0.055 (2)	0.0340 (15)	0.0423 (16)	−0.0049 (15)	0.0023 (14)	0.0032 (13)
C17	0.0493 (19)	0.0377 (16)	0.0519 (17)	−0.0046 (15)	−0.0081 (14)	−0.0083 (14)
C16	0.0474 (18)	0.0367 (15)	0.0444 (16)	0.0057 (14)	0.0038 (14)	−0.0038 (13)
O1	0.0377 (12)	0.0338 (10)	0.0482 (11)	0.0038 (9)	−0.0120 (9)	0.0007 (9)
C19A	0.055 (4)	0.063 (4)	0.049 (3)	0.028 (4)	−0.005 (3)	0.001 (4)
C20A	0.062 (4)	0.071 (4)	0.042 (3)	0.030 (3)	−0.006 (3)	0.008 (3)
C21A	0.052 (4)	0.059 (4)	0.053 (4)	0.022 (3)	−0.012 (3)	0.001 (3)
C21	0.063 (4)	0.065 (4)	0.049 (4)	0.028 (4)	−0.022 (4)	−0.003 (4)
C20	0.058 (4)	0.067 (4)	0.030 (4)	0.031 (3)	0.006 (3)	0.012 (3)
C19	0.048 (5)	0.064 (5)	0.044 (3)	0.024 (4)	0.003 (3)	0.007 (4)
C20B	0.060 (4)	0.064 (4)	0.048 (4)	0.026 (4)	−0.009 (3)	0.007 (4)
C19B	0.054 (5)	0.067 (5)	0.048 (4)	0.026 (4)	−0.002 (4)	0.005 (4)
C21B	0.056 (4)	0.062 (4)	0.038 (4)	0.028 (4)	−0.007 (3)	0.004 (4)

Geometric parameters (Å, º)

Cl1—C11	1.7302 (13)	C15—H15A	0.9800
N1—C8	1.425 (2)	C15—H15B	0.9800
N1—C7	1.280 (3)	C15—H15C	0.9800
C2—C1	1.402 (3)	C17—H17A	0.9800
C2—C3	1.391 (3)	C17—H17B	0.9800
C2—C14	1.540 (3)	C17—H17C	0.9800
C6—C1	1.405 (3)	C16—H16A	0.9800
C6—C5	1.398 (3)	C16—H16B	0.9800
C6—C7	1.450 (4)	C16—H16C	0.9800
C1—O1	1.360 (3)	O1—H1	0.90 (3)
C5—H5	0.9500	C19A—H19A	0.9800
C5—C4	1.375 (3)	C19A—H19B	0.9800
C8—C13	1.3900	C19A—H19C	0.9800
C8—C9	1.3900	C20A—H20A	0.9800
C13—H13	0.9500	C20A—H20B	0.9800
C13—C12	1.3900	C20A—H20C	0.9800
C12—H12	0.9500	C21A—H21A	0.9800
C12—C11	1.3900	C21A—H21B	0.9800
C11—C10	1.3900	C21A—H21C	0.9800
C10—H10	0.9500	C21—H21D	0.9800
C10—C9	1.3900	C21—H21E	0.9800
C9—H9	0.9500	C21—H21F	0.9800

C3—H3	0.9500	C20—H20D	0.9800
C3—C4	1.402 (4)	C20—H20E	0.9800
C7—H7	0.9500	C20—H20F	0.9800
C4—C18	1.535 (3)	C19—H19D	0.9800
C14—C15	1.533 (4)	C19—H19E	0.9800
C14—C17	1.532 (4)	C19—H19F	0.9800
C14—C16	1.542 (4)	C20B—H20G	0.9800
C18—C19A	1.530 (6)	C20B—H20H	0.9800
C18—C20A	1.490 (6)	C20B—H20I	0.9800
C18—C21A	1.574 (6)	C19B—H19G	0.9800
C18—C21	1.524 (6)	C19B—H19H	0.9800
C18—C20	1.564 (6)	C19B—H19I	0.9800
C18—C19	1.515 (6)	C21B—H21G	0.9800
C18—C20B	1.556 (7)	C21B—H21H	0.9800
C18—C19B	1.498 (7)	C21B—H21I	0.9800
C18—C21B	1.528 (6)		

C7—N1—C8	119.6 (2)	H15B—C15—H15C	109.5
C1—C2—C14	121.8 (2)	C14—C17—H17A	109.5
C3—C2—C1	116.9 (2)	C14—C17—H17B	109.5
C3—C2—C14	121.4 (2)	C14—C17—H17C	109.5
C1—C6—C7	122.0 (2)	H17A—C17—H17B	109.5
C5—C6—C1	119.5 (2)	H17A—C17—H17C	109.5
C5—C6—C7	118.5 (2)	H17B—C17—H17C	109.5
C2—C1—C6	120.5 (2)	C14—C16—H16A	109.5
O1—C1—C2	120.2 (2)	C14—C16—H16B	109.5
O1—C1—C6	119.4 (2)	C14—C16—H16C	109.5
C6—C5—H5	118.9	H16A—C16—H16B	109.5
C4—C5—C6	122.2 (2)	H16A—C16—H16C	109.5
C4—C5—H5	118.9	H16B—C16—H16C	109.5
C13—C8—N1	117.49 (14)	C1—O1—H1	106.1 (18)
C13—C8—C9	120.0	C18—C19A—H19A	109.5
C9—C8—N1	122.50 (14)	C18—C19A—H19B	109.5
C8—C13—H13	120.0	C18—C19A—H19C	109.5
C8—C13—C12	120.0	H19A—C19A—H19B	109.5
C12—C13—H13	120.0	H19A—C19A—H19C	109.5
C13—C12—H12	120.0	H19B—C19A—H19C	109.5
C11—C12—C13	120.0	C18—C20A—H20A	109.5
C11—C12—H12	120.0	C18—C20A—H20B	109.5
C12—C11—Cl1	120.57 (10)	C18—C20A—H20C	109.5
C12—C11—C10	120.0	H20A—C20A—H20B	109.5
C10—C11—Cl1	119.43 (10)	H20A—C20A—H20C	109.5
C11—C10—H10	120.0	H20B—C20A—H20C	109.5
C9—C10—C11	120.0	C18—C21A—H21A	109.5
C9—C10—H10	120.0	C18—C21A—H21B	109.5
C8—C9—H9	120.0	C18—C21A—H21C	109.5
C10—C9—C8	120.0	H21A—C21A—H21B	109.5
C10—C9—H9	120.0	H21A—C21A—H21C	109.5

C2—C3—H3	117.7	H21B—C21A—H21C	109.5
C2—C3—C4	124.6 (2)	C18—C21—H21D	109.5
C4—C3—H3	117.7	C18—C21—H21E	109.5
N1—C7—C6	123.6 (2)	C18—C21—H21F	109.5
N1—C7—H7	118.2	H21D—C21—H21E	109.5
C6—C7—H7	118.2	H21D—C21—H21F	109.5
C5—C4—C3	116.3 (2)	H21E—C21—H21F	109.5
C5—C4—C18	121.8 (2)	C18—C20—H20D	109.5
C3—C4—C18	121.8 (2)	C18—C20—H20E	109.5
C2—C14—C16	109.7 (2)	C18—C20—H20F	109.5
C15—C14—C2	109.9 (2)	H20D—C20—H20E	109.5
C15—C14—C16	110.0 (2)	H20D—C20—H20F	109.5
C17—C14—C2	112.4 (2)	H20E—C20—H20F	109.5
C17—C14—C15	107.5 (2)	C18—C19—H19D	109.5
C17—C14—C16	107.3 (2)	C18—C19—H19E	109.5
C4—C18—C21A	108.4 (3)	C18—C19—H19F	109.5
C4—C18—C20	107.3 (4)	H19D—C19—H19E	109.5
C4—C18—C20B	108.0 (5)	H19D—C19—H19F	109.5
C19A—C18—C4	113.6 (5)	H19E—C19—H19F	109.5
C19A—C18—C21A	102.6 (5)	C18—C20B—H20G	109.5
C20A—C18—C4	110.5 (4)	C18—C20B—H20H	109.5
C20A—C18—C19A	112.9 (5)	C18—C20B—H20I	109.5
C20A—C18—C21A	108.3 (5)	H20G—C20B—H20H	109.5
C21—C18—C4	114.1 (4)	H20G—C20B—H20I	109.5
C21—C18—C20	106.9 (5)	H20H—C20B—H20I	109.5
C19—C18—C4	109.7 (5)	C18—C19B—H19G	109.5
C19—C18—C21	111.6 (6)	C18—C19B—H19H	109.5
C19—C18—C20	107.0 (5)	C18—C19B—H19I	109.5
C19B—C18—C4	109.4 (5)	H19G—C19B—H19H	109.5
C19B—C18—C20B	109.1 (6)	H19G—C19B—H19I	109.5
C19B—C18—C21B	113.4 (7)	H19H—C19B—H19I	109.5
C21B—C18—C4	111.8 (5)	C18—C21B—H21G	109.5
C21B—C18—C20B	104.9 (6)	C18—C21B—H21H	109.5
C14—C15—H15A	109.5	C18—C21B—H21I	109.5
C14—C15—H15B	109.5	H21G—C21B—H21H	109.5
C14—C15—H15C	109.5	H21G—C21B—H21I	109.5
H15A—C15—H15B	109.5	H21H—C21B—H21I	109.5
H15A—C15—H15C	109.5		

Cl1—C11—C10—C9	−179.83 (13)	C13—C12—C11—Cl1	179.83 (13)
N1—C8—C13—C12	178.92 (17)	C13—C12—C11—C10	0.0
N1—C8—C9—C10	−178.86 (18)	C12—C11—C10—C9	0.0
C2—C3—C4—C5	0.7 (4)	C11—C10—C9—C8	0.0
C2—C3—C4—C18	−179.2 (2)	C9—C8—C13—C12	0.0
C6—C5—C4—C3	−0.5 (4)	C3—C2—C1—C6	−1.3 (3)
C6—C5—C4—C18	179.4 (2)	C3—C2—C1—O1	178.8 (2)
C1—C2—C3—C4	0.2 (4)	C3—C2—C14—C15	−119.8 (3)
C1—C2—C14—C15	59.5 (3)	C3—C2—C14—C17	0.0 (3)

C1—C2—C14—C17	179.2 (2)	C3—C2—C14—C16	119.2 (3)
C1—C2—C14—C16	−61.5 (3)	C3—C4—C18—C19A	147.8 (5)
C1—C6—C5—C4	−0.6 (4)	C3—C4—C18—C20A	−84.1 (5)
C1—C6—C7—N1	−1.5 (4)	C3—C4—C18—C21A	34.5 (4)
C5—C6—C1—C2	1.5 (4)	C3—C4—C18—C21	−1.3 (6)
C5—C6—C1—O1	−178.6 (2)	C3—C4—C18—C20	−119.5 (5)
C5—C6—C7—N1	179.6 (2)	C3—C4—C18—C19	124.6 (5)
C5—C4—C18—C19A	−32.1 (5)	C3—C4—C18—C20B	−148.9 (6)
C5—C4—C18—C20A	96.0 (5)	C3—C4—C18—C19B	92.5 (7)
C5—C4—C18—C21A	−145.4 (4)	C3—C4—C18—C21B	−34.0 (7)
C5—C4—C18—C21	178.7 (6)	C7—N1—C8—C13	−150.8 (2)
C5—C4—C18—C20	60.5 (5)	C7—N1—C8—C9	28.1 (3)
C5—C4—C18—C19	−55.3 (6)	C7—C6—C1—C2	−177.3 (2)
C5—C4—C18—C20B	31.2 (6)	C7—C6—C1—O1	2.6 (4)
C5—C4—C18—C19B	−87.4 (7)	C7—C6—C5—C4	178.3 (2)
C5—C4—C18—C21B	146.1 (7)	C14—C2—C1—C6	179.4 (2)
C8—N1—C7—C6	179.6 (2)	C14—C2—C1—O1	−0.5 (3)
C8—C13—C12—C11	0.0	C14—C2—C3—C4	179.4 (2)
C13—C8—C9—C10	0.0		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.90 (3)	1.78 (3)	2.611 (3)	153 (3)

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-chlorophenyl)imino]methyl}phenol (2_150K)

Crystal data

$C_{21}H_{26}ClNO$
$M_r = 343.88$
Monoclinic, $P2_1/c$
$a = 17.7326$ (13) Å
$b = 10.4696$ (7) Å
$c = 10.2385$ (7) Å
$\beta = 91.536$ (6)°
$V = 1900.1$ (2) Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.202$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1441 reflections
$\theta = 2.8$–30.5°
$\mu = 0.21$ mm^{-1}
$T = 150$ K
Block, yellow
0.33 × 0.28 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2010)
$T_{min} = 0.795$, $T_{max} = 1.000$
8155 measured reflections
3481 independent reflections
2376 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 25.4°$, $\theta_{min} = 2.8°$
$h = -21 \rightarrow 17$
$k = -8 \rightarrow 12$
$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.138$
$S = 1.08$
3481 reflections
289 parameters
151 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.2028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	1.13334 (4)	0.94171 (8)	0.78231 (7)	0.0418 (3)	
N1	0.88685 (13)	0.7046 (2)	0.4618 (2)	0.0297 (6)	
C2	0.71247 (15)	0.5465 (3)	0.2086 (2)	0.0245 (6)	
C6	0.77422 (15)	0.7228 (3)	0.3264 (3)	0.0280 (7)	
C1	0.76983 (15)	0.5921 (3)	0.2944 (2)	0.0250 (6)	
C5	0.71949 (16)	0.8067 (3)	0.2757 (3)	0.0302 (7)	
H5	0.722319	0.894499	0.298693	0.036*	
C8	0.94438 (15)	0.7641 (3)	0.5403 (2)	0.0287 (7)	
C13	1.01462 (16)	0.7066 (3)	0.5473 (3)	0.0321 (7)	
H13	1.022808	0.629200	0.501449	0.038*	
C12	1.07347 (16)	0.7610 (3)	0.6210 (3)	0.0321 (7)	
H12	1.121797	0.721810	0.624755	0.039*	
C11	1.06059 (16)	0.8723 (3)	0.6883 (3)	0.0297 (7)	
C10	0.99071 (17)	0.9303 (3)	0.6841 (3)	0.0351 (8)	
H10	0.982626	1.007216	0.730892	0.042*	
C9	0.93248 (17)	0.8753 (3)	0.6110 (3)	0.0363 (8)	
H9	0.883967	0.913852	0.609226	0.044*	
C3	0.66052 (15)	0.6364 (3)	0.1612 (2)	0.0272 (7)	
H3	0.621635	0.607362	0.102877	0.033*	
C7	0.83423 (16)	0.7736 (3)	0.4093 (3)	0.0317 (7)	
H7	0.834888	0.862856	0.425839	0.038*	
C4	0.66156 (15)	0.7661 (3)	0.1933 (2)	0.0270 (7)	
C14	0.70711 (16)	0.4052 (3)	0.1698 (3)	0.0287 (7)	
C18	0.60129 (16)	0.8594 (3)	0.1399 (2)	0.0321 (7)	
C15	0.69702 (17)	0.3223 (3)	0.2924 (3)	0.0363 (8)	
H15A	0.649041	0.343670	0.332380	0.054*	
H15B	0.738638	0.338686	0.355051	0.054*	

H15C	0.696970	0.231892	0.267668	0.054*	
C17	0.63941 (17)	0.3789 (3)	0.0769 (3)	0.0403 (8)	
H17A	0.644986	0.427880	−0.003839	0.060*	
H17B	0.592770	0.404457	0.118977	0.060*	
H17C	0.637276	0.287527	0.056258	0.060*	
C16	0.77834 (17)	0.3638 (3)	0.0987 (3)	0.0354 (8)	
H16A	0.822729	0.376740	0.156286	0.053*	
H16B	0.783395	0.414892	0.019286	0.053*	
H16C	0.774305	0.273199	0.075345	0.053*	
O1	0.82193 (11)	0.50931 (19)	0.34592 (18)	0.0328 (5)	
H1	0.8557 (16)	0.557 (3)	0.395 (3)	0.039*	
C19A	0.5825 (6)	0.9664 (8)	0.2365 (8)	0.043 (2)	0.407 (3)
H19A	0.567673	0.928696	0.319604	0.064*	0.407 (3)
H19B	0.540770	1.017991	0.200353	0.064*	0.407 (3)
H19C	0.626896	1.020681	0.251144	0.064*	0.407 (3)
C20A	0.6231 (5)	0.9095 (9)	0.0092 (6)	0.0491 (17)	0.407 (3)
H20A	0.664481	0.970860	0.020627	0.074*	0.407 (3)
H20B	0.579588	0.952041	−0.032896	0.074*	0.407 (3)
H20C	0.639393	0.838544	−0.045638	0.074*	0.407 (3)
C21A	0.5240 (4)	0.7858 (7)	0.1221 (9)	0.0483 (18)	0.407 (3)
H21A	0.529982	0.715328	0.060292	0.072*	0.407 (3)
H21B	0.485159	0.844677	0.088449	0.072*	0.407 (3)
H21C	0.508887	0.751749	0.206657	0.072*	0.407 (3)
C21	0.5479 (6)	0.8008 (11)	0.0366 (10)	0.051 (2)	0.355 (3)
H21D	0.577046	0.769907	−0.036924	0.076*	0.355 (3)
H21E	0.511748	0.865597	0.005605	0.076*	0.355 (3)
H21F	0.520528	0.729261	0.075035	0.076*	0.355 (3)
C20	0.6437 (5)	0.9698 (9)	0.0682 (9)	0.044 (2)	0.355 (3)
H20D	0.671569	1.021830	0.132766	0.067*	0.355 (3)
H20E	0.606890	1.023480	0.020727	0.067*	0.355 (3)
H20F	0.678952	0.933012	0.006542	0.067*	0.355 (3)
C19	0.5599 (6)	0.9184 (11)	0.2518 (8)	0.041 (3)	0.355 (3)
H19D	0.533487	0.851489	0.299348	0.062*	0.355 (3)
H19E	0.523300	0.980935	0.217642	0.062*	0.355 (3)
H19F	0.596164	0.961166	0.311072	0.062*	0.355 (3)
C20B	0.6394 (8)	0.9925 (10)	0.1248 (14)	0.047 (2)	0.238 (3)
H20G	0.656770	1.023417	0.210814	0.071*	0.238 (3)
H20H	0.602862	1.052981	0.086629	0.071*	0.238 (3)
H20I	0.682573	0.984762	0.067536	0.071*	0.238 (3)
C19B	0.5385 (7)	0.8741 (16)	0.2359 (12)	0.044 (2)	0.238 (3)
H19G	0.508464	0.795580	0.237052	0.066*	0.238 (3)
H19H	0.506234	0.946000	0.209426	0.066*	0.238 (3)
H19I	0.560280	0.890126	0.323341	0.066*	0.238 (3)
C21B	0.5727 (9)	0.8205 (16)	0.0033 (9)	0.046 (2)	0.238 (3)
H21G	0.615410	0.815201	−0.055321	0.069*	0.238 (3)
H21H	0.536654	0.884326	−0.029949	0.069*	0.238 (3)
H21I	0.547892	0.737087	0.007774	0.069*	0.238 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0364 (5)	0.0420 (5)	0.0462 (5)	−0.0084 (4)	−0.0123 (3)	0.0002 (4)
N1	0.0267 (14)	0.0293 (15)	0.0330 (13)	−0.0019 (12)	−0.0032 (10)	0.0010 (11)
C2	0.0247 (15)	0.0264 (17)	0.0224 (14)	−0.0003 (13)	0.0026 (11)	0.0019 (12)
C6	0.0260 (16)	0.0272 (18)	0.0308 (15)	0.0000 (13)	−0.0021 (12)	0.0010 (13)
C1	0.0231 (15)	0.0256 (17)	0.0264 (15)	0.0018 (13)	0.0013 (11)	0.0039 (12)
C5	0.0353 (18)	0.0204 (17)	0.0347 (16)	0.0010 (13)	−0.0046 (13)	−0.0009 (13)
C8	0.0268 (16)	0.0319 (18)	0.0271 (15)	−0.0007 (14)	−0.0040 (12)	0.0013 (13)
C13	0.0320 (17)	0.0276 (18)	0.0364 (17)	0.0075 (14)	−0.0033 (13)	−0.0021 (13)
C12	0.0259 (16)	0.0330 (19)	0.0373 (17)	0.0049 (14)	−0.0037 (13)	0.0020 (14)
C11	0.0271 (17)	0.0342 (19)	0.0275 (15)	−0.0046 (14)	−0.0050 (12)	0.0029 (13)
C10	0.0332 (18)	0.0371 (19)	0.0350 (17)	0.0079 (15)	−0.0027 (13)	−0.0107 (14)
C9	0.0278 (17)	0.044 (2)	0.0372 (17)	0.0088 (15)	−0.0041 (13)	−0.0064 (15)
C3	0.0281 (16)	0.0328 (18)	0.0204 (14)	0.0010 (13)	−0.0041 (11)	−0.0032 (12)
C7	0.0325 (18)	0.0258 (17)	0.0366 (17)	−0.0002 (14)	−0.0032 (13)	0.0006 (13)
C4	0.0266 (16)	0.0297 (18)	0.0247 (15)	0.0031 (13)	−0.0013 (11)	0.0010 (12)
C14	0.0285 (17)	0.0258 (17)	0.0317 (16)	0.0004 (13)	−0.0021 (12)	−0.0018 (13)
C18	0.0361 (18)	0.0294 (18)	0.0304 (16)	0.0097 (14)	−0.0037 (13)	−0.0012 (13)
C15	0.044 (2)	0.0284 (18)	0.0362 (17)	−0.0061 (15)	0.0008 (14)	0.0018 (14)
C17	0.043 (2)	0.033 (2)	0.0442 (19)	−0.0035 (16)	−0.0077 (14)	−0.0060 (15)
C16	0.0400 (19)	0.0301 (18)	0.0360 (17)	0.0042 (15)	0.0003 (13)	−0.0038 (14)
O1	0.0302 (12)	0.0266 (12)	0.0410 (12)	0.0040 (10)	−0.0103 (9)	0.0000 (9)
C19A	0.036 (4)	0.053 (5)	0.038 (3)	0.018 (4)	0.000 (3)	0.002 (4)
C20A	0.051 (4)	0.060 (4)	0.036 (4)	0.028 (3)	−0.003 (3)	0.008 (3)
C21A	0.041 (4)	0.052 (4)	0.051 (4)	0.022 (3)	−0.012 (3)	−0.002 (3)
C21	0.051 (4)	0.056 (4)	0.043 (4)	0.028 (4)	−0.017 (3)	−0.001 (4)
C20	0.049 (4)	0.059 (5)	0.026 (5)	0.027 (4)	0.007 (4)	0.016 (4)
C19	0.031 (5)	0.055 (6)	0.039 (4)	0.018 (4)	0.003 (4)	0.003 (4)
C20B	0.048 (4)	0.055 (5)	0.039 (5)	0.022 (4)	−0.005 (4)	0.007 (4)
C19B	0.037 (5)	0.053 (5)	0.042 (4)	0.019 (4)	−0.004 (4)	0.000 (4)
C21B	0.044 (5)	0.054 (4)	0.041 (4)	0.028 (4)	−0.011 (4)	0.004 (4)

Geometric parameters (Å, º)

Cl1—C11	1.747 (3)	C15—H15A	0.9800
N1—C8	1.425 (3)	C15—H15B	0.9800
N1—C7	1.287 (3)	C15—H15C	0.9800
C2—C1	1.409 (3)	C17—H17A	0.9800
C2—C3	1.395 (4)	C17—H17B	0.9800
C2—C14	1.535 (4)	C17—H17C	0.9800
C6—C1	1.409 (4)	C16—H16A	0.9800
C6—C5	1.398 (4)	C16—H16B	0.9800
C6—C7	1.444 (4)	C16—H16C	0.9800
C1—O1	1.363 (3)	O1—H1	0.92 (3)
C5—H5	0.9500	C19A—H19A	0.9800
C5—C4	1.379 (4)	C19A—H19B	0.9800

C8—C13	1.383 (4)	C19A—H19C	0.9800
C8—C9	1.390 (4)	C20A—H20A	0.9800
C13—H13	0.9500	C20A—H20B	0.9800
C13—C12	1.393 (4)	C20A—H20C	0.9800
C12—H12	0.9500	C21A—H21A	0.9800
C12—C11	1.376 (4)	C21A—H21B	0.9800
C11—C10	1.379 (4)	C21A—H21C	0.9800
C10—H10	0.9500	C21—H21D	0.9800
C10—C9	1.384 (4)	C21—H21E	0.9800
C9—H9	0.9500	C21—H21F	0.9800
C3—H3	0.9500	C20—H20D	0.9800
C3—C4	1.396 (4)	C20—H20E	0.9800
C7—H7	0.9500	C20—H20F	0.9800
C4—C18	1.538 (4)	C19—H19D	0.9800
C14—C15	1.540 (4)	C19—H19E	0.9800
C14—C17	1.537 (4)	C19—H19F	0.9800
C14—C16	1.537 (4)	C20B—H20G	0.9800
C18—C19A	1.537 (6)	C20B—H20H	0.9800
C18—C20A	1.497 (6)	C20B—H20I	0.9800
C18—C21A	1.579 (6)	C19B—H19G	0.9800
C18—C21	1.529 (6)	C19B—H19H	0.9800
C18—C20	1.571 (6)	C19B—H19I	0.9800
C18—C19	1.509 (6)	C21B—H21G	0.9800
C18—C20B	1.558 (7)	C21B—H21H	0.9800
C18—C19B	1.512 (7)	C21B—H21I	0.9800
C18—C21B	1.529 (7)		

C7—N1—C8	119.4 (2)	H15B—C15—H15C	109.5
C1—C2—C14	121.8 (2)	C14—C17—H17A	109.5
C3—C2—C1	116.6 (3)	C14—C17—H17B	109.5
C3—C2—C14	121.6 (2)	C14—C17—H17C	109.5
C1—C6—C7	122.0 (2)	H17A—C17—H17B	109.5
C5—C6—C1	119.3 (2)	H17A—C17—H17C	109.5
C5—C6—C7	118.7 (3)	H17B—C17—H17C	109.5
C6—C1—C2	120.5 (2)	C14—C16—H16A	109.5
O1—C1—C2	119.8 (2)	C14—C16—H16B	109.5
O1—C1—C6	119.7 (2)	C14—C16—H16C	109.5
C6—C5—H5	118.9	H16A—C16—H16B	109.5
C4—C5—C6	122.1 (3)	H16A—C16—H16C	109.5
C4—C5—H5	118.9	H16B—C16—H16C	109.5
C13—C8—N1	118.0 (3)	C1—O1—H1	107.0 (18)
C13—C8—C9	119.1 (3)	C18—C19A—H19A	109.5
C9—C8—N1	122.9 (3)	C18—C19A—H19B	109.5
C8—C13—H13	119.6	C18—C19A—H19C	109.5
C8—C13—C12	120.7 (3)	H19A—C19A—H19B	109.5
C12—C13—H13	119.6	H19A—C19A—H19C	109.5
C13—C12—H12	120.5	H19B—C19A—H19C	109.5
C11—C12—C13	119.0 (3)	C18—C20A—H20A	109.5

C11—C12—H12	120.5	C18—C20A—H20B	109.5
C12—C11—Cl1	119.9 (2)	C18—C20A—H20C	109.5
C12—C11—C10	121.2 (3)	H20A—C20A—H20B	109.5
C10—C11—Cl1	118.9 (2)	H20A—C20A—H20C	109.5
C11—C10—H10	120.3	H20B—C20A—H20C	109.5
C11—C10—C9	119.4 (3)	C18—C21A—H21A	109.5
C9—C10—H10	120.3	C18—C21A—H21B	109.5
C8—C9—H9	119.7	C18—C21A—H21C	109.5
C10—C9—C8	120.6 (3)	H21A—C21A—H21B	109.5
C10—C9—H9	119.7	H21A—C21A—H21C	109.5
C2—C3—H3	117.6	H21B—C21A—H21C	109.5
C2—C3—C4	124.7 (2)	C18—C21—H21D	109.5
C4—C3—H3	117.6	C18—C21—H21E	109.5
N1—C7—C6	123.6 (3)	C18—C21—H21F	109.5
N1—C7—H7	118.2	H21D—C21—H21E	109.5
C6—C7—H7	118.2	H21D—C21—H21F	109.5
C5—C4—C3	116.7 (3)	H21E—C21—H21F	109.5
C5—C4—C18	121.4 (3)	C18—C20—H20D	109.5
C3—C4—C18	122.0 (2)	C18—C20—H20E	109.5
C2—C14—C15	109.9 (2)	C18—C20—H20F	109.5
C2—C14—C17	112.0 (2)	H20D—C20—H20E	109.5
C2—C14—C16	110.4 (2)	H20D—C20—H20F	109.5
C17—C14—C15	107.3 (2)	H20E—C20—H20F	109.5
C17—C14—C16	107.1 (2)	C18—C19—H19D	109.5
C16—C14—C15	110.0 (2)	C18—C19—H19E	109.5
C4—C18—C21A	108.9 (4)	C18—C19—H19F	109.5
C4—C18—C20	107.3 (4)	H19D—C19—H19E	109.5
C4—C18—C20B	107.7 (6)	H19D—C19—H19F	109.5
C19A—C18—C4	113.3 (4)	H19E—C19—H19F	109.5
C19A—C18—C21A	103.1 (5)	C18—C20B—H20G	109.5
C20A—C18—C4	110.3 (4)	C18—C20B—H20H	109.5
C20A—C18—C19A	112.7 (5)	C18—C20B—H20I	109.5
C20A—C18—C21A	108.2 (4)	H20G—C20B—H20H	109.5
C21—C18—C4	113.7 (5)	H20G—C20B—H20I	109.5
C21—C18—C20	105.5 (5)	H20H—C20B—H20I	109.5
C19—C18—C4	109.7 (5)	C18—C19B—H19G	109.5
C19—C18—C21	112.6 (6)	C18—C19B—H19H	109.5
C19—C18—C20	107.6 (5)	C18—C19B—H19I	109.5
C19B—C18—C4	110.5 (7)	H19G—C19B—H19H	109.5
C19B—C18—C20B	107.6 (7)	H19G—C19B—H19I	109.5
C19B—C18—C21B	113.0 (7)	H19H—C19B—H19I	109.5
C21B—C18—C4	111.4 (7)	C18—C21B—H21G	109.5
C21B—C18—C20B	106.4 (7)	C18—C21B—H21H	109.5
C14—C15—H15A	109.5	C18—C21B—H21I	109.5
C14—C15—H15B	109.5	H21G—C21B—H21H	109.5
C14—C15—H15C	109.5	H21G—C21B—H21I	109.5
H15A—C15—H15B	109.5	H21H—C21B—H21I	109.5
H15A—C15—H15C	109.5		

Cl1—C11—C10—C9	−179.3 (2)	C13—C12—C11—Cl1	179.5 (2)
N1—C8—C13—C12	179.2 (2)	C13—C12—C11—C10	0.1 (4)
N1—C8—C9—C10	−179.0 (3)	C12—C11—C10—C9	0.1 (5)
C2—C3—C4—C5	1.5 (4)	C11—C10—C9—C8	−1.3 (5)
C2—C3—C4—C18	−178.5 (2)	C9—C8—C13—C12	−1.9 (4)
C6—C5—C4—C3	−0.8 (4)	C3—C2—C1—C6	−1.5 (4)
C6—C5—C4—C18	179.2 (3)	C3—C2—C1—O1	179.1 (2)
C1—C2—C3—C4	−0.3 (4)	C3—C2—C14—C15	−119.6 (3)
C1—C2—C14—C15	60.1 (3)	C3—C2—C14—C17	−0.4 (4)
C1—C2—C14—C17	179.3 (2)	C3—C2—C14—C16	118.9 (3)
C1—C2—C14—C16	−61.4 (3)	C3—C4—C18—C19A	146.3 (5)
C1—C6—C5—C4	−1.0 (4)	C3—C4—C18—C20A	−86.3 (5)
C1—C6—C7—N1	−1.4 (5)	C3—C4—C18—C21A	32.3 (5)
C5—C6—C1—C2	2.1 (4)	C3—C4—C18—C21	−7.6 (6)
C5—C6—C1—O1	−178.5 (2)	C3—C4—C18—C20	−123.9 (5)
C5—C6—C7—N1	179.3 (3)	C3—C4—C18—C19	119.6 (5)
C5—C4—C18—C19A	−33.6 (5)	C3—C4—C18—C20B	−148.3 (6)
C5—C4—C18—C20A	93.7 (5)	C3—C4—C18—C19B	94.4 (7)
C5—C4—C18—C21A	−147.7 (4)	C3—C4—C18—C21B	−32.0 (7)
C5—C4—C18—C21	172.5 (6)	C7—N1—C8—C13	−151.7 (3)
C5—C4—C18—C20	56.2 (5)	C7—N1—C8—C9	29.4 (4)
C5—C4—C18—C19	−60.4 (6)	C7—C6—C1—C2	−177.1 (3)
C5—C4—C18—C20B	31.7 (6)	C7—C6—C1—O1	2.2 (4)
C5—C4—C18—C19B	−85.6 (7)	C7—C6—C5—C4	178.3 (3)
C5—C4—C18—C21B	148.0 (7)	C14—C2—C1—C6	178.8 (3)
C8—N1—C7—C6	178.9 (2)	C14—C2—C1—O1	−0.6 (4)
C8—C13—C12—C11	0.8 (4)	C14—C2—C3—C4	179.4 (3)
C13—C8—C9—C10	2.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.92 (3)	1.77 (3)	2.615 (3)	151 (3)

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-chlorophenyl)imino]methyl}phenol (2_120K)

Crystal data

$C_{21}H_{26}ClNO$
$M_r = 343.88$
Monoclinic, $P2_1/c$
$a = 17.3623$ (8) Å
$b = 10.6691$ (4) Å
$c = 10.1512$ (6) Å
$\beta = 90.123$ (5)°
$V = 1880.41$ (15) Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.215$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3057 reflections
$\theta = 2.8$–29.4°
$\mu = 0.21$ mm^{-1}
$T = 120$ K
Block, yellow
0.35 × 0.31 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2018)
T_{min} = 0.846, T_{max} = 1.000
14119 measured reflections
3860 independent reflections
2869 reflections with $I > 2\sigma(I)$
R_{int} = 0.080
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −21→21
k = −12→13
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.184
S = 1.08
3860 reflections
227 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0974P)^2 + 0.0284P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	1.13720 (4)	0.42872 (7)	0.21972 (7)	0.0291 (2)
O1	0.81756 (11)	0.01140 (18)	0.6549 (2)	0.0234 (5)
N1	0.88643 (13)	0.2000 (2)	0.5364 (2)	0.0221 (5)
C1	0.76870 (15)	0.0957 (2)	0.7100 (3)	0.0190 (6)
C2	0.71226 (15)	0.0563 (2)	0.8000 (2)	0.0176 (6)
C3	0.66347 (15)	0.1482 (2)	0.8507 (2)	0.0181 (6)
H3	0.625047	0.122581	0.911448	0.022*
C4	0.66710 (15)	0.2756 (2)	0.8182 (2)	0.0185 (6)
C5	0.72423 (16)	0.3103 (2)	0.7315 (3)	0.0207 (6)
H5	0.728888	0.396075	0.707699	0.025*
C6	0.77554 (15)	0.2236 (2)	0.6774 (3)	0.0206 (6)
C7	0.83633 (16)	0.2707 (3)	0.5927 (3)	0.0222 (6)
H7	0.839241	0.358479	0.578040	0.027*
C8	0.94437 (16)	0.2567 (3)	0.4578 (3)	0.0220 (6)
C9	0.93356 (16)	0.3698 (3)	0.3908 (3)	0.0259 (7)
H9	0.885128	0.410993	0.395257	0.031*
C10	0.99246 (17)	0.4225 (3)	0.3180 (3)	0.0263 (7)
H10	0.984787	0.499450	0.272853	0.032*
C11	1.06281 (16)	0.3616 (3)	0.3118 (3)	0.0228 (6)

C12	1.07459 (15)	0.2483 (3)	0.3757 (3)	0.0237 (6)
H12	1.122888	0.206920	0.369549	0.028*
C13	1.01569 (16)	0.1963 (3)	0.4480 (3)	0.0232 (6)
H13	1.023543	0.118641	0.491774	0.028*
C14	0.70465 (16)	−0.0826 (2)	0.8414 (3)	0.0202 (6)
C15	0.68718 (17)	−0.1644 (2)	0.7200 (3)	0.0250 (6)
H15A	0.638221	−0.138041	0.680534	0.037*
H15B	0.683619	−0.252443	0.746784	0.037*
H15C	0.728589	−0.154781	0.655291	0.037*
C16	0.77948 (17)	−0.1277 (3)	0.9081 (3)	0.0248 (6)
H16A	0.822818	−0.116117	0.847594	0.037*
H16B	0.774709	−0.216640	0.930608	0.037*
H16C	0.788512	−0.078912	0.988470	0.037*
C17	0.63909 (17)	−0.1029 (3)	0.9408 (3)	0.0256 (6)
H17A	0.649505	−0.054348	1.020799	0.038*
H17B	0.635716	−0.192137	0.963089	0.038*
H17C	0.590270	−0.075304	0.901822	0.038*
C18	0.60941 (15)	0.3719 (2)	0.8713 (3)	0.0190 (6)
C19	0.65006 (19)	0.4970 (3)	0.9009 (3)	0.0372 (8)
H19A	0.692735	0.482484	0.962350	0.056*
H19B	0.613254	0.555566	0.940291	0.056*
H19C	0.670102	0.532543	0.818786	0.056*
C20	0.54766 (18)	0.3952 (3)	0.7656 (3)	0.0349 (8)
H20A	0.572239	0.425402	0.684790	0.052*
H20B	0.511059	0.458194	0.797330	0.052*
H20C	0.520259	0.316787	0.747190	0.052*
C21	0.57028 (19)	0.3278 (3)	0.9979 (3)	0.0338 (8)
H21A	0.538460	0.254103	0.978936	0.051*
H21B	0.537700	0.395173	1.032490	0.051*
H21C	0.609591	0.305934	1.063367	0.051*
H1	0.848 (2)	0.056 (3)	0.607 (4)	0.055 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0211 (4)	0.0345 (5)	0.0318 (4)	−0.0069 (3)	0.0043 (3)	0.0002 (3)
O1	0.0179 (11)	0.0238 (11)	0.0283 (11)	0.0021 (8)	0.0017 (9)	−0.0006 (8)
N1	0.0149 (12)	0.0279 (13)	0.0236 (12)	−0.0010 (9)	0.0006 (10)	0.0004 (10)
C1	0.0133 (13)	0.0232 (14)	0.0205 (13)	0.0009 (11)	−0.0057 (11)	−0.0049 (11)
C2	0.0137 (13)	0.0211 (14)	0.0181 (13)	0.0005 (10)	−0.0076 (11)	−0.0006 (10)
C3	0.0135 (13)	0.0250 (15)	0.0158 (13)	−0.0021 (11)	−0.0039 (10)	−0.0001 (10)
C4	0.0155 (13)	0.0223 (14)	0.0178 (13)	0.0006 (10)	−0.0066 (11)	−0.0018 (10)
C5	0.0226 (15)	0.0180 (14)	0.0213 (14)	0.0004 (11)	−0.0030 (12)	0.0013 (11)
C6	0.0159 (13)	0.0248 (15)	0.0209 (14)	−0.0018 (11)	−0.0011 (11)	−0.0001 (11)
C7	0.0210 (14)	0.0208 (14)	0.0247 (14)	−0.0016 (11)	−0.0030 (12)	−0.0005 (11)
C8	0.0208 (14)	0.0255 (15)	0.0196 (13)	−0.0037 (12)	−0.0022 (11)	−0.0014 (11)
C9	0.0187 (15)	0.0339 (17)	0.0252 (15)	0.0071 (12)	−0.0025 (12)	0.0032 (12)
C10	0.0230 (16)	0.0296 (16)	0.0261 (15)	0.0035 (12)	−0.0027 (12)	0.0060 (12)

C11	0.0202 (15)	0.0260 (15)	0.0221 (14)	−0.0053 (11)	0.0016 (12)	−0.0042 (11)
C12	0.0152 (14)	0.0279 (15)	0.0279 (15)	0.0015 (11)	−0.0021 (12)	−0.0020 (12)
C13	0.0211 (15)	0.0232 (14)	0.0253 (15)	0.0037 (11)	−0.0030 (12)	0.0005 (11)
C14	0.0205 (14)	0.0189 (14)	0.0213 (14)	0.0003 (11)	−0.0047 (11)	0.0000 (10)
C15	0.0291 (16)	0.0202 (15)	0.0255 (15)	−0.0030 (12)	−0.0046 (13)	−0.0003 (11)
C16	0.0244 (15)	0.0229 (15)	0.0272 (15)	0.0029 (12)	−0.0057 (12)	0.0014 (11)
C17	0.0249 (16)	0.0249 (15)	0.0270 (15)	−0.0001 (12)	−0.0039 (13)	0.0048 (12)
C18	0.0160 (14)	0.0221 (14)	0.0188 (13)	0.0040 (11)	−0.0026 (11)	0.0002 (10)
C19	0.0349 (19)	0.0291 (17)	0.048 (2)	0.0036 (14)	0.0013 (16)	−0.0103 (14)
C20	0.0297 (18)	0.047 (2)	0.0276 (16)	0.0168 (14)	−0.0075 (14)	−0.0077 (14)
C21	0.0357 (19)	0.0346 (18)	0.0313 (17)	0.0117 (14)	0.0083 (15)	0.0015 (13)

Geometric parameters (Å, º)

Cl1—C11	1.750 (3)	C13—H13	0.9500
O1—C1	1.357 (3)	C14—C15	1.540 (4)
O1—H1	0.86 (4)	C14—C16	1.541 (4)
N1—C7	1.286 (3)	C14—C17	1.538 (4)
N1—C8	1.421 (3)	C15—H15A	0.9800
C1—C2	1.406 (4)	C15—H15B	0.9800
C1—C6	1.409 (4)	C15—H15C	0.9800
C2—C3	1.395 (4)	C16—H16A	0.9800
C2—C14	1.545 (4)	C16—H16B	0.9800
C3—H3	0.9500	C16—H16C	0.9800
C3—C4	1.400 (4)	C17—H17A	0.9800
C4—C5	1.378 (4)	C17—H17B	0.9800
C4—C18	1.534 (3)	C17—H17C	0.9800
C5—H5	0.9500	C18—C19	1.539 (4)
C5—C6	1.398 (4)	C18—C20	1.535 (4)
C6—C7	1.453 (4)	C18—C21	1.529 (4)
C7—H7	0.9500	C19—H19A	0.9800
C8—C9	1.397 (4)	C19—H19B	0.9800
C8—C13	1.400 (4)	C19—H19C	0.9800
C9—H9	0.9500	C20—H20A	0.9800
C9—C10	1.382 (4)	C20—H20B	0.9800
C10—H10	0.9500	C20—H20C	0.9800
C10—C11	1.385 (4)	C21—H21A	0.9800
C11—C12	1.386 (4)	C21—H21B	0.9800
C12—H12	0.9500	C21—H21C	0.9800
C12—C13	1.377 (4)		
C1—O1—H1	104 (2)	C17—C14—C15	107.5 (2)
C7—N1—C8	118.7 (2)	C17—C14—C16	107.0 (2)
O1—C1—C2	120.5 (2)	C14—C15—H15A	109.5
O1—C1—C6	119.5 (2)	C14—C15—H15B	109.5
C2—C1—C6	120.1 (2)	C14—C15—H15C	109.5
C1—C2—C14	121.6 (2)	H15A—C15—H15B	109.5
C3—C2—C1	117.0 (2)	H15A—C15—H15C	109.5

C3—C2—C14	121.4 (2)	H15B—C15—H15C	109.5
C2—C3—H3	117.7	C14—C16—H16A	109.5
C2—C3—C4	124.7 (2)	C14—C16—H16B	109.5
C4—C3—H3	117.7	C14—C16—H16C	109.5
C3—C4—C18	122.6 (2)	H16A—C16—H16B	109.5
C5—C4—C3	116.3 (2)	H16A—C16—H16C	109.5
C5—C4—C18	121.1 (2)	H16B—C16—H16C	109.5
C4—C5—H5	118.9	C14—C17—H17A	109.5
C4—C5—C6	122.2 (2)	C14—C17—H17B	109.5
C6—C5—H5	118.9	C14—C17—H17C	109.5
C1—C6—C7	122.4 (2)	H17A—C17—H17B	109.5
C5—C6—C1	119.7 (2)	H17A—C17—H17C	109.5
C5—C6—C7	117.9 (2)	H17B—C17—H17C	109.5
N1—C7—C6	123.6 (3)	C4—C18—C19	110.5 (2)
N1—C7—H7	118.2	C4—C18—C20	108.6 (2)
C6—C7—H7	118.2	C20—C18—C19	108.4 (2)
C9—C8—N1	123.2 (2)	C21—C18—C4	112.4 (2)
C9—C8—C13	118.7 (2)	C21—C18—C19	107.9 (2)
C13—C8—N1	118.1 (2)	C21—C18—C20	109.0 (2)
C8—C9—H9	119.6	C18—C19—H19A	109.5
C10—C9—C8	120.8 (3)	C18—C19—H19B	109.5
C10—C9—H9	119.6	C18—C19—H19C	109.5
C9—C10—H10	120.4	H19A—C19—H19B	109.5
C9—C10—C11	119.2 (3)	H19A—C19—H19C	109.5
C11—C10—H10	120.4	H19B—C19—H19C	109.5
C10—C11—Cl1	119.0 (2)	C18—C20—H20A	109.5
C10—C11—C12	121.1 (2)	C18—C20—H20B	109.5
C12—C11—Cl1	119.9 (2)	C18—C20—H20C	109.5
C11—C12—H12	120.3	H20A—C20—H20B	109.5
C13—C12—C11	119.4 (3)	H20A—C20—H20C	109.5
C13—C12—H12	120.3	H20B—C20—H20C	109.5
C8—C13—H13	119.7	C18—C21—H21A	109.5
C12—C13—C8	120.7 (3)	C18—C21—H21B	109.5
C12—C13—H13	119.7	C18—C21—H21C	109.5
C15—C14—C2	110.0 (2)	H21A—C21—H21B	109.5
C15—C14—C16	109.8 (2)	H21A—C21—H21C	109.5
C16—C14—C2	110.3 (2)	H21B—C21—H21C	109.5
C17—C14—C2	112.2 (2)		

Cl1—C11—C12—C13	179.9 (2)	C3—C4—C18—C21	22.2 (4)
O1—C1—C2—C3	−179.0 (2)	C4—C5—C6—C1	1.0 (4)
O1—C1—C2—C14	1.1 (4)	C4—C5—C6—C7	−176.7 (3)
O1—C1—C6—C5	178.5 (2)	C5—C4—C18—C19	−39.5 (3)
O1—C1—C6—C7	−3.9 (4)	C5—C4—C18—C20	79.2 (3)
N1—C8—C9—C10	178.5 (3)	C5—C4—C18—C21	−160.1 (3)
N1—C8—C13—C12	−178.6 (2)	C5—C6—C7—N1	−179.3 (3)
C1—C2—C3—C4	−0.1 (4)	C6—C1—C2—C3	1.8 (4)
C1—C2—C14—C15	−60.5 (3)	C6—C1—C2—C14	−178.1 (2)

C1—C2—C14—C16	60.8 (3)	C7—N1—C8—C9	−29.0 (4)
C1—C2—C14—C17	179.9 (2)	C7—N1—C8—C13	150.7 (3)
C1—C6—C7—N1	3.0 (4)	C8—N1—C7—C6	−178.6 (2)
C2—C1—C6—C5	−2.3 (4)	C8—C9—C10—C11	0.1 (4)
C2—C1—C6—C7	175.3 (3)	C9—C8—C13—C12	1.1 (4)
C2—C3—C4—C5	−1.0 (4)	C9—C10—C11—Cl1	−180.0 (2)
C2—C3—C4—C18	176.8 (2)	C9—C10—C11—C12	0.9 (4)
C3—C2—C14—C15	119.6 (3)	C10—C11—C12—C13	−0.9 (4)
C3—C2—C14—C16	−119.1 (3)	C11—C12—C13—C8	−0.1 (4)
C3—C2—C14—C17	0.0 (3)	C13—C8—C9—C10	−1.2 (4)
C3—C4—C5—C6	0.6 (4)	C14—C2—C3—C4	179.7 (2)
C3—C4—C18—C19	142.8 (3)	C18—C4—C5—C6	−177.3 (2)
C3—C4—C18—C20	−98.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.86 (4)	1.82 (4)	2.633 (3)	157 (4)

(*E*)-2,4-Di-*tert*-butyl-6-{[(4-chlorophenyl)imino]methyl}phenol (2_100K)

Crystal data

$C_{21}H_{26}ClNO$
M_r = 343.88
Monoclinic, $P2_1/c$
a = 17.3011 (11) Å
b = 10.6780 (7) Å
c = 10.1200 (6) Å
β = 90.252 (6)°
V = 1869.6 (2) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.222 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2408 reflections
θ = 3.0–28.5°
μ = 0.21 mm^{-1}
T = 100 K
Block, yellow
0.35 × 0.31 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 Gemini ultra diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1511 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2018)
T_{min} = 0.435, T_{max} = 1.000
13865 measured reflections
3830 independent reflections
2740 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −21→21
k = −13→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.176
S = 1.08
3830 reflections
227 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2 + 0.1484P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.78 e Å^{-3} $\Delta\rho_{min}$ = −0.33 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.13773 (4)	0.42791 (8)	0.21945 (7)	0.0256 (2)
O1	0.81741 (11)	0.0118 (2)	0.6546 (2)	0.0204 (5)
N1	0.88628 (13)	0.1997 (2)	0.5360 (2)	0.0188 (5)
C1	0.76828 (15)	0.0953 (3)	0.7102 (3)	0.0166 (6)
C2	0.71225 (15)	0.0567 (3)	0.8006 (3)	0.0158 (6)
C3	0.66361 (15)	0.1488 (3)	0.8519 (3)	0.0174 (6)
H3	0.625221	0.123319	0.913072	0.021*
C4	0.66743 (15)	0.2770 (3)	0.8192 (3)	0.0169 (6)
C5	0.72457 (15)	0.3112 (3)	0.7318 (3)	0.0185 (6)
H5	0.729376	0.396807	0.707748	0.022*
C6	0.77587 (15)	0.2237 (3)	0.6773 (3)	0.0182 (6)
C7	0.83659 (15)	0.2709 (3)	0.5925 (3)	0.0202 (6)
H7	0.839745	0.358649	0.578040	0.024*
C8	0.94457 (16)	0.2562 (3)	0.4575 (3)	0.0207 (7)
C9	0.93401 (16)	0.3697 (3)	0.3906 (3)	0.0219 (7)
H9	0.885555	0.411241	0.395504	0.026*
C10	0.99279 (16)	0.4219 (3)	0.3179 (3)	0.0230 (7)
H10	0.985164	0.498936	0.272778	0.028*
C11	1.06341 (16)	0.3605 (3)	0.3115 (3)	0.0195 (6)
C12	1.07512 (16)	0.2469 (3)	0.3751 (3)	0.0207 (7)
H12	1.123484	0.205169	0.369027	0.025*
C13	1.01552 (16)	0.1952 (3)	0.4473 (3)	0.0210 (7)
H13	1.022982	0.117143	0.490631	0.025*
C14	0.70433 (16)	−0.0810 (3)	0.8423 (3)	0.0200 (6)
C15	0.68658 (17)	−0.1637 (3)	0.7208 (3)	0.0231 (7)
H15A	0.637498	−0.137423	0.680836	0.035*
H15B	0.682833	−0.251498	0.748351	0.035*
H15C	0.728151	−0.154809	0.655975	0.035*
C16	0.77979 (17)	−0.1272 (3)	0.9085 (3)	0.0229 (7)
H16A	0.823093	−0.115608	0.847655	0.034*
H16B	0.774832	−0.216273	0.930465	0.034*
H16C	0.789282	−0.079174	0.989484	0.034*
C17	0.63903 (17)	−0.1017 (3)	0.9424 (3)	0.0246 (7)
H17A	0.648940	−0.051191	1.021584	0.037*
H17B	0.636894	−0.190453	0.966803	0.037*
H17C	0.589610	−0.076628	0.902822	0.037*
C18	0.60929 (15)	0.3727 (3)	0.8717 (3)	0.0177 (6)
C19	0.64974 (18)	0.4978 (3)	0.9001 (3)	0.0286 (7)

H19A	0.692356	0.484323	0.962575	0.043*
H19B	0.612582	0.556769	0.938221	0.043*
H19C	0.670105	0.532357	0.817525	0.043*
C20	0.54720 (17)	0.3955 (3)	0.7653 (3)	0.0264 (7)
H20A	0.571882	0.424736	0.683940	0.040*
H20B	0.510720	0.459064	0.796448	0.040*
H20C	0.519426	0.317246	0.747587	0.040*
C21	0.57033 (18)	0.3288 (3)	0.9980 (3)	0.0278 (8)
H21A	0.538892	0.254485	0.979150	0.042*
H21B	0.537177	0.395670	1.032112	0.042*
H21C	0.609837	0.307842	1.064106	0.042*
H1	0.850 (2)	0.056 (4)	0.597 (3)	0.041 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0244 (4)	0.0243 (5)	0.0281 (4)	−0.0057 (3)	0.0030 (3)	0.0002 (3)
O1	0.0221 (11)	0.0134 (12)	0.0257 (11)	0.0022 (8)	0.0037 (9)	−0.0002 (9)
N1	0.0183 (12)	0.0200 (15)	0.0179 (12)	0.0003 (10)	0.0002 (10)	0.0008 (10)
C1	0.0157 (13)	0.0139 (16)	0.0202 (14)	−0.0001 (11)	−0.0065 (11)	−0.0030 (12)
C2	0.0179 (14)	0.0112 (16)	0.0182 (13)	−0.0017 (11)	−0.0079 (11)	0.0008 (11)
C3	0.0180 (14)	0.0178 (17)	0.0163 (13)	−0.0034 (11)	−0.0017 (11)	−0.0013 (11)
C4	0.0177 (14)	0.0158 (17)	0.0171 (14)	−0.0008 (11)	−0.0057 (11)	0.0004 (11)
C5	0.0238 (15)	0.0127 (16)	0.0189 (14)	−0.0001 (12)	−0.0032 (12)	0.0007 (11)
C6	0.0196 (14)	0.0153 (16)	0.0196 (14)	−0.0013 (12)	−0.0037 (12)	−0.0008 (12)
C7	0.0230 (15)	0.0164 (17)	0.0212 (14)	−0.0010 (12)	−0.0031 (12)	0.0023 (12)
C8	0.0226 (15)	0.0212 (18)	0.0183 (14)	−0.0033 (12)	−0.0034 (12)	−0.0025 (12)
C9	0.0215 (15)	0.0241 (18)	0.0202 (14)	0.0048 (12)	−0.0033 (12)	0.0007 (12)
C10	0.0247 (15)	0.0205 (18)	0.0236 (15)	0.0022 (13)	−0.0025 (12)	0.0072 (13)
C11	0.0215 (15)	0.0198 (18)	0.0172 (14)	−0.0026 (12)	0.0013 (11)	−0.0011 (12)
C12	0.0187 (15)	0.0208 (18)	0.0227 (15)	0.0026 (12)	−0.0014 (12)	−0.0023 (12)
C13	0.0254 (15)	0.0149 (17)	0.0228 (15)	0.0023 (12)	−0.0024 (12)	−0.0010 (12)
C14	0.0231 (15)	0.0165 (17)	0.0204 (14)	0.0009 (12)	−0.0026 (12)	−0.0010 (12)
C15	0.0280 (16)	0.0146 (17)	0.0267 (16)	−0.0018 (13)	−0.0044 (13)	−0.0001 (12)
C16	0.0277 (16)	0.0180 (18)	0.0229 (15)	0.0032 (13)	−0.0052 (13)	0.0005 (12)
C17	0.0299 (17)	0.0188 (18)	0.0253 (16)	−0.0020 (13)	0.0005 (13)	0.0039 (13)
C18	0.0207 (14)	0.0149 (16)	0.0173 (13)	0.0022 (12)	0.0002 (11)	−0.0015 (11)
C19	0.0321 (17)	0.0182 (19)	0.0355 (18)	0.0023 (14)	−0.0012 (14)	−0.0068 (14)
C20	0.0267 (16)	0.026 (2)	0.0264 (15)	0.0121 (14)	−0.0051 (13)	−0.0048 (14)
C21	0.0372 (18)	0.0204 (19)	0.0260 (16)	0.0111 (14)	0.0042 (14)	−0.0005 (13)

Geometric parameters (Å, º)

Cl1—C11	1.746 (3)	C13—H13	0.9500
O1—C1	1.356 (3)	C14—C15	1.544 (4)
O1—H1	0.94 (4)	C14—C16	1.546 (4)
N1—C7	1.284 (4)	C14—C17	1.537 (4)
N1—C8	1.421 (4)	C15—H15A	0.9800

C1—C2	1.399 (4)	C15—H15B	0.9800
C1—C6	1.417 (4)	C15—H15C	0.9800
C2—C3	1.395 (4)	C16—H16A	0.9800
C2—C14	1.537 (4)	C16—H16B	0.9800
C3—H3	0.9500	C16—H16C	0.9800
C3—C4	1.409 (4)	C17—H17A	0.9800
C4—C5	1.378 (4)	C17—H17B	0.9800
C4—C18	1.531 (4)	C17—H17C	0.9800
C5—H5	0.9500	C18—C19	1.535 (4)
C5—C6	1.404 (4)	C18—C20	1.537 (4)
C6—C7	1.450 (4)	C18—C21	1.522 (4)
C7—H7	0.9500	C19—H19A	0.9800
C8—C9	1.399 (4)	C19—H19B	0.9800
C8—C13	1.394 (4)	C19—H19C	0.9800
C9—H9	0.9500	C20—H20A	0.9800
C9—C10	1.376 (4)	C20—H20B	0.9800
C10—H10	0.9500	C20—H20C	0.9800
C10—C11	1.389 (4)	C21—H21A	0.9800
C11—C12	1.388 (4)	C21—H21B	0.9800
C12—H12	0.9500	C21—H21C	0.9800
C12—C13	1.382 (4)		

C1—O1—H1	108 (2)	C17—C14—C15	107.4 (2)
C7—N1—C8	118.4 (3)	C17—C14—C16	106.9 (2)
O1—C1—C2	121.0 (3)	C14—C15—H15A	109.5
O1—C1—C6	118.7 (2)	C14—C15—H15B	109.5
C2—C1—C6	120.3 (3)	C14—C15—H15C	109.5
C1—C2—C14	121.6 (2)	H15A—C15—H15B	109.5
C3—C2—C1	117.2 (3)	H15A—C15—H15C	109.5
C3—C2—C14	121.2 (2)	H15B—C15—H15C	109.5
C2—C3—H3	117.7	C14—C16—H16A	109.5
C2—C3—C4	124.6 (3)	C14—C16—H16B	109.5
C4—C3—H3	117.7	C14—C16—H16C	109.5
C3—C4—C18	122.4 (2)	H16A—C16—H16B	109.5
C5—C4—C3	116.2 (3)	H16A—C16—H16C	109.5
C5—C4—C18	121.3 (3)	H16B—C16—H16C	109.5
C4—C5—H5	118.9	C14—C17—H17A	109.5
C4—C5—C6	122.2 (3)	C14—C17—H17B	109.5
C6—C5—H5	118.9	C14—C17—H17C	109.5
C1—C6—C7	122.9 (3)	H17A—C17—H17B	109.5
C5—C6—C1	119.5 (3)	H17A—C17—H17C	109.5
C5—C6—C7	117.5 (3)	H17B—C17—H17C	109.5
N1—C7—C6	123.1 (3)	C4—C18—C19	110.3 (2)
N1—C7—H7	118.5	C4—C18—C20	108.7 (2)
C6—C7—H7	118.5	C19—C18—C20	108.0 (3)
C9—C8—N1	123.1 (3)	C21—C18—C4	112.3 (2)
C13—C8—N1	118.0 (3)	C21—C18—C19	108.3 (2)
C13—C8—C9	118.8 (3)	C21—C18—C20	109.1 (2)

C8—C9—H9	119.5	C18—C19—H19A	109.5
C10—C9—C8	120.9 (3)	C18—C19—H19B	109.5
C10—C9—H9	119.5	C18—C19—H19C	109.5
C9—C10—H10	120.5	H19A—C19—H19B	109.5
C9—C10—C11	119.1 (3)	H19A—C19—H19C	109.5
C11—C10—H10	120.5	H19B—C19—H19C	109.5
C10—C11—Cl1	118.7 (2)	C18—C20—H20A	109.5
C12—C11—Cl1	120.1 (2)	C18—C20—H20B	109.5
C12—C11—C10	121.2 (3)	C18—C20—H20C	109.5
C11—C12—H12	120.4	H20A—C20—H20B	109.5
C13—C12—C11	119.1 (3)	H20A—C20—H20C	109.5
C13—C12—H12	120.4	H20B—C20—H20C	109.5
C8—C13—H13	119.6	C18—C21—H21A	109.5
C12—C13—C8	120.8 (3)	C18—C21—H21B	109.5
C12—C13—H13	119.6	C18—C21—H21C	109.5
C2—C14—C15	110.3 (2)	H21A—C21—H21B	109.5
C2—C14—C16	110.4 (2)	H21A—C21—H21C	109.5
C2—C14—C17	112.6 (2)	H21B—C21—H21C	109.5
C15—C14—C16	109.1 (2)		

Cl1—C11—C12—C13	−180.0 (2)	C3—C4—C18—C21	22.7 (4)
O1—C1—C2—C3	−179.3 (2)	C4—C5—C6—C1	1.4 (4)
O1—C1—C2—C14	0.7 (4)	C4—C5—C6—C7	−176.5 (2)
O1—C1—C6—C5	178.7 (2)	C5—C4—C18—C19	−39.5 (3)
O1—C1—C6—C7	−3.5 (4)	C5—C4—C18—C20	78.8 (3)
N1—C8—C9—C10	178.7 (3)	C5—C4—C18—C21	−160.4 (3)
N1—C8—C13—C12	−178.4 (2)	C5—C6—C7—N1	−179.2 (2)
C1—C2—C3—C4	−0.3 (4)	C6—C1—C2—C3	2.2 (4)
C1—C2—C14—C15	−60.0 (3)	C6—C1—C2—C14	−177.8 (2)
C1—C2—C14—C16	60.6 (3)	C7—N1—C8—C9	−29.0 (4)
C1—C2—C14—C17	180.0 (2)	C7—N1—C8—C13	150.8 (3)
C1—C6—C7—N1	3.0 (4)	C8—N1—C7—C6	−178.5 (2)
C2—C1—C6—C5	−2.7 (4)	C8—C9—C10—C11	0.0 (4)
C2—C1—C6—C7	175.0 (2)	C9—C8—C13—C12	1.4 (4)
C2—C3—C4—C5	−1.0 (4)	C9—C10—C11—Cl1	−179.8 (2)
C2—C3—C4—C18	176.0 (2)	C9—C10—C11—C12	1.1 (5)
C3—C2—C14—C15	120.0 (3)	C10—C11—C12—C13	−0.8 (4)
C3—C2—C14—C16	−119.3 (3)	C11—C12—C13—C8	−0.5 (4)
C3—C2—C14—C17	0.0 (3)	C13—C8—C9—C10	−1.2 (4)
C3—C4—C5—C6	0.5 (4)	C14—C2—C3—C4	179.7 (2)
C3—C4—C18—C19	143.6 (3)	C18—C4—C5—C6	−176.6 (2)
C3—C4—C18—C20	−98.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.94 (4)	1.77 (4)	2.626 (3)	150 (3)

(*E*)-6-{[(4-Bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol (3_300K)

Crystal data

$C_{21}H_{26}BrNO$
$M_r = 388.34$
Monoclinic, $P2_1/c$
$a = 18.0356$ (7) Å
$b = 10.5891$ (3) Å
$c = 10.3641$ (3) Å
$\beta = 92.894$ (3)°
$V = 1976.82$ (11) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.305$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5921 reflections
$\theta = 3.8$–$26.3°$
$\mu = 2.09$ mm^{-1}
$T = 300$ K
Needle, yellow
0.3 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.3620 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2013)
$T_{min} = 0.744$, $T_{max} = 1.000$
13771 measured reflections
3195 independent reflections
2444 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 24.4°$, $\theta_{min} = 2.9°$
$h = -20 \rightarrow 20$
$k = -12 \rightarrow 12$
$l = -9 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.118$
$S = 1.05$
3195 reflections
278 parameters
181 restraints
Primary atom site location: iterative
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 1.8801P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	−0.13439 (2)	0.44494 (4)	−0.28958 (4)	0.0747 (2)	
O1	0.18011 (15)	0.0118 (2)	0.1572 (3)	0.0579 (7)	
N1	0.11610 (16)	0.2045 (3)	0.0400 (3)	0.0537 (8)	
C1	0.23225 (19)	0.0925 (3)	0.2067 (3)	0.0430 (8)	
C2	0.28963 (19)	0.0485 (3)	0.2917 (3)	0.0420 (8)	
C3	0.34106 (19)	0.1369 (3)	0.3377 (3)	0.0431 (8)	
H3	0.379201	0.108749	0.394293	0.052*	

C4	0.34003 (19)	0.2656 (3)	0.3056 (3)	0.0435 (8)	
C5	0.2828 (2)	0.3041 (3)	0.2226 (3)	0.0500 (9)	
H5	0.280144	0.388602	0.198256	0.060*	
C6	0.22857 (19)	0.2213 (3)	0.1737 (3)	0.0457 (8)	
C7	0.1689 (2)	0.2713 (3)	0.0889 (4)	0.0552 (9)	
H7	0.169479	0.357012	0.069392	0.066*	
C8	0.05915 (11)	0.2622 (2)	−0.0400 (2)	0.0508 (9)	
C9	0.07093 (11)	0.3723 (2)	−0.1091 (3)	0.0766 (13)	
H9	0.117599	0.409847	−0.105520	0.092*	
C10	0.01295 (14)	0.4263 (2)	−0.1834 (3)	0.0785 (14)	
H10	0.020835	0.499922	−0.229591	0.094*	
C11	−0.05680 (11)	0.3701 (2)	−0.1887 (2)	0.0548 (9)	
C12	−0.06858 (10)	0.2600 (2)	−0.1196 (3)	0.0639 (11)	
H12	−0.115249	0.222455	−0.123143	0.077*	
C13	−0.01060 (13)	0.20604 (19)	−0.0453 (2)	0.0632 (11)	
H13	−0.018486	0.132377	0.000930	0.076*	
C14	0.2953 (2)	−0.0918 (3)	0.3314 (3)	0.0497 (9)	
C15	0.3636 (2)	−0.1180 (4)	0.4203 (4)	0.0711 (12)	
H15A	0.360902	−0.068967	0.497857	0.107*	
H15B	0.407573	−0.095315	0.377156	0.107*	
H15C	0.365385	−0.206136	0.441881	0.107*	
C16	0.3015 (3)	−0.1740 (3)	0.2096 (4)	0.0660 (11)	
H16A	0.345758	−0.151821	0.167179	0.099*	
H16B	0.258964	−0.159794	0.151916	0.099*	
H16C	0.303551	−0.261414	0.233901	0.099*	
C17	0.2266 (2)	−0.1294 (4)	0.4035 (4)	0.0664 (11)	
H17A	0.182802	−0.114908	0.349023	0.100*	
H17B	0.224329	−0.079598	0.480615	0.100*	
H17C	0.229647	−0.217221	0.426102	0.100*	
C18	0.39918 (19)	0.3570 (3)	0.3597 (3)	0.0522 (9)	
C19	0.4482 (9)	0.4004 (17)	0.2535 (11)	0.081 (4)	0.355 (3)
H19A	0.418064	0.439075	0.185464	0.121*	0.355 (3)
H19B	0.473713	0.328962	0.219822	0.121*	0.355 (3)
H19C	0.483769	0.460442	0.287998	0.121*	0.355 (3)
C20	0.4448 (9)	0.3044 (13)	0.4756 (13)	0.082 (4)	0.355 (3)
H20A	0.476534	0.238076	0.447404	0.123*	0.355 (3)
H20B	0.412078	0.271351	0.537524	0.123*	0.355 (3)
H20C	0.474601	0.370539	0.514700	0.123*	0.355 (3)
C21	0.3571 (7)	0.4742 (11)	0.4100 (17)	0.079 (4)	0.355 (3)
H21A	0.319872	0.446979	0.466823	0.118*	0.355 (3)
H21B	0.333962	0.518954	0.338168	0.118*	0.355 (3)
H21C	0.391644	0.529029	0.456036	0.118*	0.355 (3)
C19A	0.4187 (7)	0.4572 (10)	0.2595 (10)	0.062 (3)	0.438 (3)
H19D	0.376880	0.512125	0.243062	0.094*	0.438 (3)
H19E	0.430823	0.416343	0.180623	0.094*	0.438 (3)
H19F	0.460444	0.505822	0.292182	0.094*	0.438 (3)
C21A	0.3737 (7)	0.4203 (14)	0.4805 (11)	0.090 (4)	0.438 (3)
H21D	0.363048	0.357173	0.543364	0.134*	0.438 (3)

H21E	0.329755	0.468808	0.459680	0.134*	0.438 (3)
H21F	0.412178	0.475130	0.515061	0.134*	0.438 (3)
C20A	0.4737 (5)	0.2868 (9)	0.3916 (16)	0.082 (3)	0.438 (3)
H20D	0.488342	0.242091	0.316439	0.123*	0.438 (3)
H20E	0.467291	0.228013	0.460651	0.123*	0.438 (3)
H20F	0.511371	0.347029	0.417369	0.123*	0.438 (3)
C21B	0.3838 (14)	0.4944 (10)	0.322 (3)	0.080 (5)	0.206 (3)
H21G	0.348944	0.530000	0.379038	0.120*	0.206 (3)
H21H	0.363454	0.498002	0.234797	0.120*	0.206 (3)
H21I	0.429244	0.541650	0.328991	0.120*	0.206 (3)
C19B	0.4740 (8)	0.315 (2)	0.310 (3)	0.083 (5)	0.206 (3)
H19G	0.471709	0.316358	0.217625	0.125*	0.206 (3)
H19H	0.484719	0.230211	0.339687	0.125*	0.206 (3)
H19I	0.512429	0.370550	0.342880	0.125*	0.206 (3)
C20B	0.4044 (15)	0.347 (2)	0.5076 (8)	0.069 (5)	0.206 (3)
H20G	0.408459	0.260255	0.532620	0.103*	0.206 (3)
H20H	0.360682	0.383289	0.541945	0.103*	0.206 (3)
H20I	0.447399	0.392569	0.540896	0.103*	0.206 (3)
H1	0.151 (3)	0.055 (4)	0.111 (5)	0.082 (16)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0643 (3)	0.0739 (3)	0.0832 (3)	0.0135 (2)	−0.0217 (2)	0.0037 (2)
O1	0.0565 (17)	0.0467 (14)	0.0685 (18)	−0.0075 (13)	−0.0172 (14)	−0.0028 (13)
N1	0.0446 (18)	0.0564 (17)	0.0586 (19)	0.0014 (14)	−0.0115 (15)	−0.0028 (14)
C1	0.040 (2)	0.0430 (18)	0.0458 (19)	−0.0038 (15)	−0.0031 (15)	−0.0078 (15)
C2	0.049 (2)	0.0384 (17)	0.0389 (17)	−0.0003 (15)	0.0021 (15)	−0.0060 (14)
C3	0.042 (2)	0.0489 (19)	0.0374 (17)	−0.0006 (15)	−0.0033 (14)	−0.0016 (15)
C4	0.047 (2)	0.0424 (18)	0.0409 (18)	−0.0037 (15)	−0.0032 (15)	−0.0016 (14)
C5	0.052 (2)	0.0377 (18)	0.059 (2)	−0.0018 (15)	−0.0071 (18)	−0.0008 (15)
C6	0.041 (2)	0.0441 (18)	0.051 (2)	0.0022 (15)	−0.0058 (16)	−0.0030 (15)
C7	0.053 (2)	0.0462 (19)	0.064 (2)	0.0031 (17)	−0.0114 (19)	−0.0031 (17)
C8	0.044 (2)	0.055 (2)	0.052 (2)	0.0030 (17)	−0.0072 (16)	−0.0024 (17)
C9	0.054 (3)	0.097 (3)	0.077 (3)	−0.025 (2)	−0.014 (2)	0.031 (3)
C10	0.064 (3)	0.085 (3)	0.084 (3)	−0.020 (2)	−0.022 (2)	0.034 (2)
C11	0.049 (2)	0.060 (2)	0.054 (2)	0.0020 (18)	−0.0057 (17)	−0.0001 (18)
C12	0.042 (2)	0.068 (2)	0.080 (3)	−0.0089 (18)	−0.013 (2)	0.005 (2)
C13	0.054 (3)	0.054 (2)	0.080 (3)	−0.0094 (18)	−0.014 (2)	0.0076 (19)
C14	0.057 (2)	0.0407 (18)	0.052 (2)	0.0003 (16)	−0.0017 (17)	0.0005 (15)
C15	0.082 (3)	0.051 (2)	0.079 (3)	0.006 (2)	−0.019 (2)	0.012 (2)
C16	0.087 (3)	0.047 (2)	0.064 (3)	0.008 (2)	0.002 (2)	−0.0078 (18)
C17	0.079 (3)	0.052 (2)	0.069 (3)	−0.008 (2)	0.009 (2)	0.0049 (19)
C18	0.055 (2)	0.051 (2)	0.049 (2)	−0.0173 (17)	−0.0085 (17)	0.0019 (16)
C19	0.073 (9)	0.095 (9)	0.073 (7)	−0.041 (7)	0.000 (7)	−0.007 (7)
C20	0.091 (9)	0.093 (8)	0.059 (7)	−0.048 (7)	−0.031 (7)	0.011 (7)
C21	0.089 (8)	0.073 (7)	0.074 (8)	−0.035 (6)	0.004 (7)	−0.034 (7)
C19A	0.063 (7)	0.068 (7)	0.057 (5)	−0.023 (5)	0.012 (5)	−0.007 (5)

C21A	0.099 (8)	0.112 (9)	0.058 (6)	−0.056 (7)	0.010 (6)	−0.026 (6)
C20A	0.069 (6)	0.082 (6)	0.092 (8)	−0.034 (5)	−0.033 (6)	0.017 (7)
C21B	0.093 (10)	0.078 (9)	0.067 (10)	−0.047 (9)	−0.012 (9)	0.002 (9)
C19B	0.075 (9)	0.104 (10)	0.072 (10)	−0.046 (9)	0.011 (9)	−0.013 (9)
C20B	0.071 (11)	0.075 (10)	0.059 (9)	−0.040 (9)	−0.005 (8)	−0.021 (8)

Geometric parameters (Å, º)

Br1—C11	1.8794 (16)	C17—H17C	0.9600
O1—C1	1.353 (4)	C18—C19	1.517 (7)
O1—H1	0.83 (5)	C18—C20	1.527 (7)
N1—C7	1.272 (5)	C18—C21	1.558 (7)
N1—C8	1.425 (3)	C18—C19A	1.538 (6)
C1—C2	1.404 (5)	C18—C21A	1.512 (7)
C1—C6	1.406 (4)	C18—C20A	1.557 (7)
C2—C3	1.386 (4)	C18—C21B	1.528 (8)
C2—C14	1.543 (4)	C18—C19B	1.535 (8)
C3—H3	0.9300	C18—C20B	1.535 (8)
C3—C4	1.403 (4)	C19—H19A	0.9600
C4—C5	1.372 (5)	C19—H19B	0.9600
C4—C18	1.526 (4)	C19—H19C	0.9600
C5—H5	0.9300	C20—H20A	0.9600
C5—C6	1.390 (5)	C20—H20B	0.9600
C6—C7	1.454 (5)	C20—H20C	0.9600
C7—H7	0.9300	C21—H21A	0.9600
C8—C9	1.3900	C21—H21B	0.9600
C8—C13	1.3900	C21—H21C	0.9600
C9—H9	0.9300	C19A—H19D	0.9600
C9—C10	1.3900	C19A—H19E	0.9600
C10—H10	0.9300	C19A—H19F	0.9600
C10—C11	1.3900	C21A—H21D	0.9600
C11—C12	1.3900	C21A—H21E	0.9600
C12—H12	0.9300	C21A—H21F	0.9600
C12—C13	1.3900	C20A—H20D	0.9600
C13—H13	0.9300	C20A—H20E	0.9600
C14—C15	1.527 (5)	C20A—H20F	0.9600
C14—C16	1.541 (5)	C21B—H21G	0.9600
C14—C17	1.532 (5)	C21B—H21H	0.9600
C15—H15A	0.9600	C21B—H21I	0.9600
C15—H15B	0.9600	C19B—H19G	0.9600
C15—H15C	0.9600	C19B—H19H	0.9600
C16—H16A	0.9600	C19B—H19I	0.9600
C16—H16B	0.9600	C20B—H20G	0.9600
C16—H16C	0.9600	C20B—H20H	0.9600
C17—H17A	0.9600	C20B—H20I	0.9600
C17—H17B	0.9600		

C1—O1—H1	106 (3)	C4—C18—C21B	113.3 (8)

C7—N1—C8	119.8 (3)	C4—C18—C19B	107.6 (9)
O1—C1—C2	120.3 (3)	C4—C18—C20B	109.4 (8)
O1—C1—C6	119.8 (3)	C19—C18—C4	110.3 (6)
C2—C1—C6	119.9 (3)	C19—C18—C20	111.7 (7)
C1—C2—C14	121.6 (3)	C19—C18—C21	108.3 (7)
C3—C2—C1	116.8 (3)	C20—C18—C21	106.2 (7)
C3—C2—C14	121.6 (3)	C19A—C18—C20A	104.4 (6)
C2—C3—H3	117.5	C21A—C18—C4	110.5 (5)
C2—C3—C4	125.0 (3)	C21A—C18—C19A	110.0 (6)
C4—C3—H3	117.5	C21A—C18—C20A	109.3 (6)
C3—C4—C18	121.9 (3)	C21B—C18—C19B	110.2 (9)
C5—C4—C3	116.0 (3)	C21B—C18—C20B	108.6 (8)
C5—C4—C18	122.1 (3)	C19B—C18—C20B	107.6 (8)
C4—C5—H5	118.9	C18—C19—H19A	109.5
C4—C5—C6	122.3 (3)	C18—C19—H19B	109.5
C6—C5—H5	118.9	C18—C19—H19C	109.5
C1—C6—C7	121.6 (3)	H19A—C19—H19B	109.5
C5—C6—C1	120.0 (3)	H19A—C19—H19C	109.5
C5—C6—C7	118.4 (3)	H19B—C19—H19C	109.5
N1—C7—C6	123.7 (3)	C18—C20—H20A	109.5
N1—C7—H7	118.1	C18—C20—H20B	109.5
C6—C7—H7	118.1	C18—C20—H20C	109.5
C9—C8—N1	122.33 (19)	H20A—C20—H20B	109.5
C9—C8—C13	120.0	H20A—C20—H20C	109.5
C13—C8—N1	117.65 (19)	H20B—C20—H20C	109.5
C8—C9—H9	120.0	C18—C21—H21A	109.5
C8—C9—C10	120.0	C18—C21—H21B	109.5
C10—C9—H9	120.0	C18—C21—H21C	109.5
C9—C10—H10	120.0	H21A—C21—H21B	109.5
C9—C10—C11	120.0	H21A—C21—H21C	109.5
C11—C10—H10	120.0	H21B—C21—H21C	109.5
C10—C11—Br1	119.25 (13)	C18—C19A—H19D	109.5
C12—C11—Br1	120.75 (13)	C18—C19A—H19E	109.5
C12—C11—C10	120.0	C18—C19A—H19F	109.5
C11—C12—H12	120.0	H19D—C19A—H19E	109.5
C11—C12—C13	120.0	H19D—C19A—H19F	109.5
C13—C12—H12	120.0	H19E—C19A—H19F	109.5
C8—C13—H13	120.0	C18—C21A—H21D	109.5
C12—C13—C8	120.0	C18—C21A—H21E	109.5
C12—C13—H13	120.0	C18—C21A—H21F	109.5
C15—C14—C2	112.1 (3)	H21D—C21A—H21E	109.5
C15—C14—C16	107.6 (3)	H21D—C21A—H21F	109.5
C15—C14—C17	107.8 (3)	H21E—C21A—H21F	109.5
C16—C14—C2	109.4 (3)	C18—C20A—H20D	109.5
C17—C14—C2	109.6 (3)	C18—C20A—H20E	109.5
C17—C14—C16	110.3 (3)	C18—C20A—H20F	109.5
C14—C15—H15A	109.5	H20D—C20A—H20E	109.5
C14—C15—H15B	109.5	H20D—C20A—H20F	109.5

C14—C15—H15C	109.5	H20E—C20A—H20F	109.5
H15A—C15—H15B	109.5	C18—C21B—H21G	109.5
H15A—C15—H15C	109.5	C18—C21B—H21H	109.5
H15B—C15—H15C	109.5	C18—C21B—H21I	109.5
C14—C16—H16A	109.5	H21G—C21B—H21H	109.5
C14—C16—H16B	109.5	H21G—C21B—H21I	109.5
C14—C16—H16C	109.5	H21H—C21B—H21I	109.5
H16A—C16—H16B	109.5	C18—C19B—H19G	109.5
H16A—C16—H16C	109.5	C18—C19B—H19H	109.5
H16B—C16—H16C	109.5	C18—C19B—H19I	109.5
C14—C17—H17A	109.5	H19G—C19B—H19H	109.5
C14—C17—H17B	109.5	H19G—C19B—H19I	109.5
C14—C17—H17C	109.5	H19H—C19B—H19I	109.5
H17A—C17—H17B	109.5	C18—C20B—H20G	109.5
H17A—C17—H17C	109.5	C18—C20B—H20H	109.5
H17B—C17—H17C	109.5	C18—C20B—H20I	109.5
C4—C18—C20	113.4 (5)	H20G—C20B—H20H	109.5
C4—C18—C21	106.6 (5)	H20G—C20B—H20I	109.5
C4—C18—C19A	111.6 (5)	H20H—C20B—H20I	109.5
C4—C18—C20A	110.8 (5)		

Br1—C11—C12—C13	−179.89 (19)	C3—C4—C18—C20B	−53.5 (12)
O1—C1—C2—C3	179.7 (3)	C4—C5—C6—C1	−1.5 (5)
O1—C1—C2—C14	0.0 (5)	C4—C5—C6—C7	178.5 (3)
O1—C1—C6—C5	−178.9 (3)	C5—C4—C18—C19	−69.2 (9)
O1—C1—C6—C7	1.2 (5)	C5—C4—C18—C20	164.6 (9)
N1—C8—C9—C10	−178.5 (3)	C5—C4—C18—C21	48.1 (8)
N1—C8—C13—C12	178.6 (2)	C5—C4—C18—C19A	−36.4 (7)
C1—C2—C3—C4	−0.2 (5)	C5—C4—C18—C21A	86.4 (8)
C1—C2—C14—C15	177.9 (3)	C5—C4—C18—C20A	−152.3 (7)
C1—C2—C14—C16	58.6 (4)	C5—C4—C18—C21B	5.3 (13)
C1—C2—C14—C17	−62.4 (4)	C5—C4—C18—C19B	−116.9 (13)
C1—C6—C7—N1	0.8 (6)	C5—C4—C18—C20B	126.6 (12)
C2—C1—C6—C5	1.7 (5)	C5—C6—C7—N1	−179.2 (4)
C2—C1—C6—C7	−178.3 (3)	C6—C1—C2—C3	−0.9 (5)
C2—C3—C4—C5	0.4 (5)	C6—C1—C2—C14	179.4 (3)
C2—C3—C4—C18	−179.5 (3)	C7—N1—C8—C9	26.1 (4)
C3—C2—C14—C15	−1.8 (5)	C7—N1—C8—C13	−152.5 (3)
C3—C2—C14—C16	−121.1 (4)	C8—N1—C7—C6	178.7 (3)
C3—C2—C14—C17	117.9 (4)	C8—C9—C10—C11	0.0
C3—C4—C5—C6	0.4 (5)	C9—C8—C13—C12	0.0
C3—C4—C18—C19	110.7 (9)	C9—C10—C11—Br1	179.89 (19)
C3—C4—C18—C20	−15.5 (10)	C9—C10—C11—C12	0.0
C3—C4—C18—C21	−132.0 (8)	C10—C11—C12—C13	0.0
C3—C4—C18—C19A	143.6 (6)	C11—C12—C13—C8	0.0
C3—C4—C18—C21A	−93.6 (8)	C13—C8—C9—C10	0.0
C3—C4—C18—C20A	27.7 (7)	C14—C2—C3—C4	179.5 (3)
C3—C4—C18—C21B	−174.8 (13)	C18—C4—C5—C6	−179.6 (3)

C3—C4—C18—C19B	63.1 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.83 (5)	1.84 (5)	2.614 (4)	154 (5)

(*E*)-6-{[(4-Bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol (3_250K)

Crystal data

$C_{21}H_{26}BrNO$
$M_r = 388.34$
Monoclinic, $P2_1/c$
$a = 17.9642$ (4) Å
$b = 10.5593$ (2) Å
$c = 10.3153$ (2) Å
$\beta = 92.535$ (2)°
$V = 1954.79$ (8) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.320$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8503 reflections
$\theta = 3.0$–26.0°
$\mu = 2.11$ mm^{-1}
$T = 250$ K
Needle, yellow
0.3 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.3620 pixels mm^{-1}
ω and π scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2013)
$T_{min} = 0.690$, $T_{max} = 1.000$
29546 measured reflections
4650 independent reflections
3079 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 27.9°$, $\theta_{min} = 3.0°$
$h = -23\rightarrow23$
$k = -9\rightarrow13$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.101$
$S = 1.02$
4650 reflections
278 parameters
181 restraints
Primary atom site location: iterative
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 1.096P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	−0.13496 (2)	0.44592 (3)	−0.28979 (3)	0.05979 (13)	

O1	0.17999 (10)	0.01102 (17)	0.15632 (19)	0.0470 (4)	
N1	0.11606 (11)	0.2045 (2)	0.0395 (2)	0.0437 (5)	
C1	0.23214 (13)	0.0919 (2)	0.2068 (2)	0.0364 (5)	
C2	0.28965 (13)	0.0477 (2)	0.2919 (2)	0.0340 (5)	
C3	0.34126 (13)	0.1364 (2)	0.3379 (2)	0.0364 (5)	
H3	0.379678	0.107782	0.395500	0.044*	
C4	0.34063 (13)	0.2651 (2)	0.3054 (2)	0.0372 (5)	
C5	0.28305 (13)	0.3045 (2)	0.2223 (2)	0.0409 (6)	
H5	0.280342	0.390299	0.198077	0.049*	
C6	0.22876 (13)	0.2212 (2)	0.1730 (2)	0.0383 (5)	
C7	0.16905 (14)	0.2716 (2)	0.0888 (2)	0.0455 (6)	
H7	0.169482	0.358642	0.069565	0.055*	
C8	0.05918 (7)	0.26234 (15)	−0.04062 (16)	0.0416 (6)	
C9	0.07099 (7)	0.37306 (17)	−0.10964 (19)	0.0597 (8)	
H9	0.118293	0.411270	−0.106226	0.072*	
C10	0.01284 (9)	0.42728 (15)	−0.18370 (18)	0.0599 (8)	
H10	0.020822	0.502160	−0.230379	0.072*	
C11	−0.05712 (8)	0.37079 (15)	−0.18875 (16)	0.0423 (6)	
C12	−0.06893 (7)	0.26007 (15)	−0.11973 (18)	0.0506 (7)	
H12	−0.116234	0.221861	−0.123144	0.061*	
C13	−0.01078 (9)	0.20584 (13)	−0.04566 (17)	0.0516 (7)	
H13	−0.018763	0.130968	0.001011	0.062*	
C14	0.29481 (14)	−0.0928 (2)	0.3315 (2)	0.0405 (6)	
C15	0.36308 (16)	−0.1194 (3)	0.4214 (3)	0.0569 (7)	
H15A	0.359810	−0.070153	0.500328	0.085*	
H15B	0.407899	−0.096085	0.378032	0.085*	
H15C	0.364794	−0.208829	0.442804	0.085*	
C16	0.30185 (17)	−0.1755 (2)	0.2097 (3)	0.0534 (7)	
H16A	0.347267	−0.153661	0.167372	0.080*	
H16B	0.259302	−0.160860	0.150384	0.080*	
H16C	0.303407	−0.264080	0.234574	0.080*	
C17	0.22552 (16)	−0.1310 (3)	0.4038 (3)	0.0541 (7)	
H17A	0.181299	−0.116478	0.348362	0.081*	
H17B	0.222751	−0.080801	0.482114	0.081*	
H17C	0.228648	−0.220086	0.426479	0.081*	
C18	0.40010 (14)	0.3568 (2)	0.3593 (2)	0.0436 (6)	
C19	0.4486 (6)	0.3982 (12)	0.2532 (8)	0.069 (3)	0.386 (3)
H19A	0.418279	0.438277	0.184790	0.104*	0.386 (3)
H19B	0.473708	0.325136	0.218501	0.104*	0.386 (3)
H19C	0.485412	0.458075	0.287571	0.104*	0.386 (3)
C20	0.4426 (7)	0.3056 (10)	0.4780 (10)	0.077 (3)	0.386 (3)
H20A	0.472932	0.234315	0.453319	0.116*	0.386 (3)
H20B	0.407716	0.278311	0.541453	0.116*	0.386 (3)
H20C	0.474500	0.371539	0.515415	0.116*	0.386 (3)
C21	0.3573 (5)	0.4760 (8)	0.4080 (13)	0.075 (3)	0.386 (3)
H21A	0.318768	0.449214	0.464980	0.113*	0.386 (3)
H21B	0.334813	0.520824	0.334202	0.113*	0.386 (3)
H21C	0.391988	0.531590	0.455070	0.113*	0.386 (3)

C19A	0.4199 (5)	0.4574 (7)	0.2594 (7)	0.0543 (19)	0.463 (3)
H19D	0.377781	0.513752	0.243943	0.081*	0.463 (3)
H19E	0.431789	0.416335	0.178771	0.081*	0.463 (3)
H19F	0.462593	0.505742	0.292192	0.081*	0.463 (3)
C21A	0.3752 (5)	0.4193 (11)	0.4800 (8)	0.084 (3)	0.463 (3)
H21D	0.365234	0.355196	0.544354	0.126*	0.463 (3)
H21E	0.330251	0.467593	0.460185	0.126*	0.463 (3)
H21F	0.414105	0.475547	0.513868	0.126*	0.463 (3)
C20A	0.4755 (4)	0.2863 (7)	0.3895 (12)	0.076 (2)	0.463 (3)
H20D	0.489117	0.238728	0.313655	0.113*	0.463 (3)
H20E	0.469901	0.228692	0.461698	0.113*	0.463 (3)
H20F	0.514126	0.347620	0.411821	0.113*	0.463 (3)
C21B	0.3856 (14)	0.4933 (10)	0.318 (3)	0.071 (5)	0.151 (3)
H21G	0.339329	0.522207	0.353266	0.107*	0.151 (3)
H21H	0.381979	0.498396	0.224338	0.107*	0.151 (3)
H21I	0.426286	0.546409	0.351130	0.107*	0.151 (3)
C19B	0.4755 (7)	0.312 (2)	0.313 (3)	0.075 (5)	0.151 (3)
H19G	0.474217	0.311891	0.218683	0.112*	0.151 (3)
H19H	0.485871	0.227726	0.345064	0.112*	0.151 (3)
H19I	0.514275	0.369740	0.345124	0.112*	0.151 (3)
C20B	0.4040 (16)	0.349 (3)	0.5075 (7)	0.070 (5)	0.151 (3)
H20G	0.411832	0.262314	0.534373	0.104*	0.151 (3)
H20H	0.357589	0.380216	0.540583	0.104*	0.151 (3)
H20I	0.444910	0.401318	0.541508	0.104*	0.151 (3)
H1	0.1498 (19)	0.055 (3)	0.112 (3)	0.071 (11)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.05142 (18)	0.05850 (19)	0.0676 (2)	0.01114 (13)	−0.01808 (14)	0.00286 (15)
O1	0.0448 (10)	0.0370 (9)	0.0577 (12)	−0.0065 (8)	−0.0160 (9)	−0.0026 (9)
N1	0.0388 (11)	0.0437 (12)	0.0475 (12)	0.0004 (9)	−0.0092 (9)	−0.0021 (10)
C1	0.0342 (12)	0.0359 (12)	0.0387 (13)	−0.0041 (10)	−0.0015 (10)	−0.0065 (10)
C2	0.0375 (12)	0.0332 (12)	0.0314 (11)	−0.0008 (10)	0.0015 (9)	−0.0042 (10)
C3	0.0366 (12)	0.0397 (13)	0.0323 (12)	0.0000 (10)	−0.0042 (10)	−0.0006 (10)
C4	0.0406 (13)	0.0365 (12)	0.0340 (12)	−0.0054 (10)	−0.0044 (10)	−0.0035 (10)
C5	0.0446 (14)	0.0309 (12)	0.0463 (14)	−0.0028 (10)	−0.0086 (11)	−0.0017 (10)
C6	0.0374 (12)	0.0346 (12)	0.0422 (14)	0.0015 (10)	−0.0069 (10)	−0.0033 (10)
C7	0.0477 (15)	0.0362 (13)	0.0515 (16)	0.0015 (11)	−0.0106 (12)	−0.0043 (11)
C8	0.0366 (13)	0.0432 (14)	0.0443 (14)	0.0013 (11)	−0.0076 (11)	−0.0021 (11)
C9	0.0399 (15)	0.075 (2)	0.0626 (18)	−0.0172 (14)	−0.0110 (13)	0.0220 (16)
C10	0.0523 (17)	0.0634 (18)	0.0623 (18)	−0.0147 (14)	−0.0159 (14)	0.0260 (15)
C11	0.0397 (13)	0.0445 (14)	0.0422 (14)	0.0018 (11)	−0.0047 (11)	−0.0030 (11)
C12	0.0357 (13)	0.0524 (16)	0.0627 (18)	−0.0057 (12)	−0.0084 (12)	0.0023 (13)
C13	0.0468 (15)	0.0446 (15)	0.0620 (18)	−0.0061 (12)	−0.0131 (13)	0.0075 (13)
C14	0.0463 (14)	0.0335 (12)	0.0412 (14)	0.0006 (11)	−0.0030 (11)	0.0004 (10)
C15	0.0627 (18)	0.0414 (15)	0.0649 (19)	0.0038 (13)	−0.0163 (15)	0.0113 (13)
C16	0.0692 (19)	0.0375 (14)	0.0534 (17)	0.0063 (13)	0.0024 (14)	−0.0044 (12)

C17	0.0650 (18)	0.0431 (15)	0.0544 (17)	−0.0053 (13)	0.0061 (14)	0.0041 (13)
C18	0.0476 (14)	0.0432 (14)	0.0392 (14)	−0.0143 (11)	−0.0086 (11)	0.0020 (11)
C19	0.059 (6)	0.090 (7)	0.059 (5)	−0.033 (5)	0.006 (4)	−0.007 (5)
C20	0.080 (6)	0.085 (6)	0.062 (5)	−0.051 (5)	−0.040 (5)	0.019 (5)
C21	0.077 (6)	0.067 (6)	0.080 (6)	−0.022 (5)	−0.005 (5)	−0.040 (5)
C19A	0.052 (5)	0.059 (5)	0.052 (4)	−0.020 (3)	−0.001 (3)	−0.002 (4)
C21A	0.084 (6)	0.116 (8)	0.053 (5)	−0.056 (5)	0.015 (4)	−0.037 (5)
C20A	0.051 (4)	0.066 (4)	0.106 (7)	−0.025 (3)	−0.033 (4)	0.021 (5)
C21B	0.075 (9)	0.073 (9)	0.063 (9)	−0.043 (8)	−0.018 (8)	0.003 (8)
C19B	0.064 (9)	0.090 (9)	0.070 (10)	−0.039 (8)	0.007 (9)	−0.012 (9)
C20B	0.069 (10)	0.069 (10)	0.070 (9)	−0.037 (9)	−0.008 (9)	−0.019 (8)

Geometric parameters (Å, º)

Br1—C11	1.8821 (11)	C17—H17C	0.9700
O1—C1	1.354 (3)	C18—C19	1.494 (6)
O1—H1	0.84 (3)	C18—C20	1.514 (6)
N1—C7	1.275 (3)	C18—C21	1.569 (6)
N1—C8	1.423 (2)	C18—C19A	1.533 (5)
C1—C2	1.405 (3)	C18—C21A	1.495 (5)
C1—C6	1.410 (3)	C18—C20A	1.564 (5)
C2—C3	1.386 (3)	C18—C21B	1.522 (7)
C2—C14	1.541 (3)	C18—C19B	1.531 (7)
C3—H3	0.9400	C18—C20B	1.529 (7)
C3—C4	1.401 (3)	C19—H19A	0.9700
C4—C5	1.378 (3)	C19—H19B	0.9700
C4—C18	1.528 (3)	C19—H19C	0.9700
C5—H5	0.9400	C20—H20A	0.9700
C5—C6	1.393 (3)	C20—H20B	0.9700
C6—C7	1.451 (3)	C20—H20C	0.9700
C7—H7	0.9400	C21—H21A	0.9700
C8—C9	1.3900	C21—H21B	0.9700
C8—C13	1.3900	C21—H21C	0.9700
C9—H9	0.9400	C19A—H19D	0.9700
C9—C10	1.3900	C19A—H19E	0.9700
C10—H10	0.9400	C19A—H19F	0.9700
C10—C11	1.3900	C21A—H21D	0.9700
C11—C12	1.3900	C21A—H21E	0.9700
C12—H12	0.9400	C21A—H21F	0.9700
C12—C13	1.3900	C20A—H20D	0.9700
C13—H13	0.9400	C20A—H20E	0.9700
C14—C15	1.530 (3)	C20A—H20F	0.9700
C14—C16	1.540 (4)	C21B—H21G	0.9700
C14—C17	1.533 (4)	C21B—H21H	0.9700
C15—H15A	0.9700	C21B—H21I	0.9700
C15—H15B	0.9700	C19B—H19G	0.9700
C15—H15C	0.9700	C19B—H19H	0.9700
C16—H16A	0.9700	C19B—H19I	0.9700

C16—H16B	0.9700	C20B—H20G	0.9700
C16—H16C	0.9700	C20B—H20H	0.9700
C17—H17A	0.9700	C20B—H20I	0.9700
C17—H17B	0.9700		

C1—O1—H1	106 (2)	C4—C18—C20B	109.4 (9)
C7—N1—C8	119.8 (2)	C19—C18—C4	109.9 (4)
O1—C1—C2	120.5 (2)	C19—C18—C20	114.0 (5)
O1—C1—C6	119.6 (2)	C19—C18—C21	108.0 (6)
C2—C1—C6	119.9 (2)	C20—C18—C4	112.8 (4)
C1—C2—C14	121.3 (2)	C20—C18—C21	105.3 (5)
C3—C2—C1	116.9 (2)	C19A—C18—C20A	103.9 (4)
C3—C2—C14	121.8 (2)	C21A—C18—C4	110.7 (3)
C2—C3—H3	117.5	C21A—C18—C19A	109.9 (5)
C2—C3—C4	125.1 (2)	C21A—C18—C20A	109.4 (5)
C4—C3—H3	117.5	C21B—C18—C4	113.0 (8)
C3—C4—C18	122.0 (2)	C21B—C18—C19B	110.2 (9)
C5—C4—C3	116.1 (2)	C21B—C18—C20B	109.0 (8)
C5—C4—C18	121.9 (2)	C20B—C18—C19B	107.2 (8)
C4—C5—H5	119.0	C18—C19—H19A	109.5
C4—C5—C6	122.0 (2)	C18—C19—H19B	109.5
C6—C5—H5	119.0	C18—C19—H19C	109.5
C1—C6—C7	121.7 (2)	H19A—C19—H19B	109.5
C5—C6—C1	120.0 (2)	H19A—C19—H19C	109.5
C5—C6—C7	118.3 (2)	H19B—C19—H19C	109.5
N1—C7—C6	123.6 (2)	C18—C20—H20A	109.5
N1—C7—H7	118.2	C18—C20—H20B	109.5
C6—C7—H7	118.2	C18—C20—H20C	109.5
C9—C8—N1	122.45 (13)	H20A—C20—H20B	109.5
C9—C8—C13	120.0	H20A—C20—H20C	109.5
C13—C8—N1	117.53 (13)	H20B—C20—H20C	109.5
C8—C9—H9	120.0	C18—C21—H21A	109.5
C8—C9—C10	120.0	C18—C21—H21B	109.5
C10—C9—H9	120.0	C18—C21—H21C	109.5
C9—C10—H10	120.0	H21A—C21—H21B	109.5
C11—C10—C9	120.0	H21A—C21—H21C	109.5
C11—C10—H10	120.0	H21B—C21—H21C	109.5
C10—C11—Br1	119.22 (9)	C18—C19A—H19D	109.5
C10—C11—C12	120.0	C18—C19A—H19E	109.5
C12—C11—Br1	120.78 (9)	C18—C19A—H19F	109.5
C11—C12—H12	120.0	H19D—C19A—H19E	109.5
C13—C12—C11	120.0	H19D—C19A—H19F	109.5
C13—C12—H12	120.0	H19E—C19A—H19F	109.5
C8—C13—H13	120.0	C18—C21A—H21D	109.5
C12—C13—C8	120.0	C18—C21A—H21E	109.5
C12—C13—H13	120.0	C18—C21A—H21F	109.5
C15—C14—C2	112.0 (2)	H21D—C21A—H21E	109.5
C15—C14—C16	107.3 (2)	H21D—C21A—H21F	109.5

C15—C14—C17	107.7 (2)	H21E—C21A—H21F	109.5
C16—C14—C2	109.6 (2)	C18—C20A—H20D	109.5
C17—C14—C2	110.0 (2)	C18—C20A—H20E	109.5
C17—C14—C16	110.2 (2)	C18—C20A—H20F	109.5
C14—C15—H15A	109.5	H20D—C20A—H20E	109.5
C14—C15—H15B	109.5	H20D—C20A—H20F	109.5
C14—C15—H15C	109.5	H20E—C20A—H20F	109.5
H15A—C15—H15B	109.5	C18—C21B—H21G	109.5
H15A—C15—H15C	109.5	C18—C21B—H21H	109.5
H15B—C15—H15C	109.5	C18—C21B—H21I	109.5
C14—C16—H16A	109.5	H21G—C21B—H21H	109.5
C14—C16—H16B	109.5	H21G—C21B—H21I	109.5
C14—C16—H16C	109.5	H21H—C21B—H21I	109.5
H16A—C16—H16B	109.5	C18—C19B—H19G	109.5
H16A—C16—H16C	109.5	C18—C19B—H19H	109.5
H16B—C16—H16C	109.5	C18—C19B—H19I	109.5
C14—C17—H17A	109.5	H19G—C19B—H19H	109.5
C14—C17—H17B	109.5	H19G—C19B—H19I	109.5
C14—C17—H17C	109.5	H19H—C19B—H19I	109.5
H17A—C17—H17B	109.5	C18—C20B—H20G	109.5
H17A—C17—H17C	109.5	C18—C20B—H20H	109.5
H17B—C17—H17C	109.5	C18—C20B—H20I	109.5
C4—C18—C21	106.3 (4)	H20G—C20B—H20H	109.5
C4—C18—C19A	111.9 (3)	H20G—C20B—H20I	109.5
C4—C18—C20A	110.8 (3)	H20H—C20B—H20I	109.5
C4—C18—C19B	107.8 (9)		

Br1—C11—C12—C13	179.96 (13)	C3—C4—C18—C20B	−54.6 (13)
O1—C1—C2—C3	179.2 (2)	C4—C5—C6—C1	−0.7 (4)
O1—C1—C2—C14	−0.7 (3)	C4—C5—C6—C7	178.4 (2)
O1—C1—C6—C5	−178.6 (2)	C5—C4—C18—C19	−69.7 (6)
O1—C1—C6—C7	2.3 (4)	C5—C4—C18—C20	161.9 (7)
N1—C8—C9—C10	−178.29 (18)	C5—C4—C18—C21	47.0 (6)
N1—C8—C13—C12	178.37 (17)	C5—C4—C18—C19A	−36.3 (5)
C1—C2—C3—C4	−0.5 (4)	C5—C4—C18—C21A	86.7 (7)
C1—C2—C14—C15	178.3 (2)	C5—C4—C18—C20A	−151.7 (5)
C1—C2—C14—C16	59.3 (3)	C5—C4—C18—C21B	3.6 (13)
C1—C2—C14—C17	−62.0 (3)	C5—C4—C18—C19B	−118.5 (13)
C1—C6—C7—N1	−0.1 (4)	C5—C4—C18—C20B	125.2 (13)
C2—C1—C6—C5	1.0 (4)	C5—C6—C7—N1	−179.2 (3)
C2—C1—C6—C7	−178.0 (2)	C6—C1—C2—C3	−0.4 (3)
C2—C3—C4—C5	0.9 (4)	C6—C1—C2—C14	179.7 (2)
C2—C3—C4—C18	−179.4 (2)	C7—N1—C8—C9	25.9 (3)
C3—C2—C14—C15	−1.6 (3)	C7—N1—C8—C13	−152.4 (2)
C3—C2—C14—C16	−120.6 (2)	C8—N1—C7—C6	179.1 (2)
C3—C2—C14—C17	118.1 (2)	C8—C9—C10—C11	0.0
C3—C4—C5—C6	−0.2 (4)	C9—C8—C13—C12	0.0
C3—C4—C18—C19	110.6 (6)	C9—C10—C11—Br1	−179.96 (13)

C3—C4—C18—C20	−17.8 (7)	C9—C10—C11—C12	0.0
C3—C4—C18—C21	−132.7 (6)	C10—C11—C12—C13	0.0
C3—C4—C18—C19A	144.0 (5)	C11—C12—C13—C8	0.0
C3—C4—C18—C21A	−93.0 (6)	C13—C8—C9—C10	0.0
C3—C4—C18—C20A	28.6 (6)	C14—C2—C3—C4	179.4 (2)
C3—C4—C18—C21B	−176.2 (13)	C18—C4—C5—C6	−180.0 (2)
C3—C4—C18—C19B	61.8 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.84 (3)	1.83 (3)	2.612 (3)	154 (3)

(*E*)-6-{[(4-Bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol (3_200K)

Crystal data

$C_{21}H_{26}BrNO$
$M_r = 388.34$
Monoclinic, $P2_1/c$
$a = 17.8944$ (4) Å
$b = 10.54749$ (18) Å
$c = 10.2693$ (2) Å
$\beta = 92.1529$ (18)°
$V = 1936.88$ (6) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.332$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9913 reflections
$\theta = 3.0$–$31.3°$
$\mu = 2.13$ mm^{-1}
$T = 200$ K
Needle, yellow
0.3 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.3620 pixels mm^{-1}
ω and π scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2013)
$T_{min} = 0.660$, $T_{max} = 1.000$
29301 measured reflections
4612 independent reflections
3377 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.9°$, $\theta_{min} = 3.0°$
$h = -23\rightarrow23$
$k = -9\rightarrow13$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.083$
$S = 1.02$
4612 reflections
290 parameters
175 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 1.206P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	−0.13556 (2)	0.44640 (2)	−0.28995 (2)	0.04650 (10)	
O1	0.17988 (9)	0.01054 (15)	0.15601 (16)	0.0379 (4)	
N1	0.11607 (10)	0.20409 (17)	0.03889 (18)	0.0354 (4)	
C1	0.23210 (11)	0.09160 (19)	0.2063 (2)	0.0287 (4)	
C2	0.28944 (11)	0.04716 (18)	0.29217 (19)	0.0274 (4)	
C3	0.34128 (11)	0.13600 (19)	0.33857 (19)	0.0291 (4)	
H3	0.379590	0.107416	0.396463	0.035*	
C4	0.34078 (11)	0.26462 (19)	0.3057 (2)	0.0304 (4)	
C5	0.28338 (12)	0.3045 (2)	0.2222 (2)	0.0333 (5)	
H5	0.280858	0.390340	0.197999	0.040*	
C6	0.22893 (11)	0.22103 (19)	0.1727 (2)	0.0312 (5)	
C7	0.16915 (12)	0.2718 (2)	0.0883 (2)	0.0365 (5)	
H7	0.169541	0.358974	0.069146	0.044*	
C8	0.05886 (11)	0.2631 (2)	−0.0404 (2)	0.0330 (5)	
C9	0.07038 (13)	0.3723 (2)	−0.1112 (2)	0.0464 (6)	
H9	0.118108	0.409612	−0.109893	0.056*	
C10	0.01246 (14)	0.4272 (2)	−0.1839 (2)	0.0467 (6)	
H10	0.020302	0.502549	−0.230238	0.056*	
C11	−0.05682 (12)	0.3704 (2)	−0.1877 (2)	0.0331 (5)	
C12	−0.06943 (12)	0.2601 (2)	−0.1206 (2)	0.0392 (5)	
H12	−0.116841	0.221578	−0.124418	0.047*	
C13	−0.01093 (12)	0.2067 (2)	−0.0474 (2)	0.0399 (5)	
H13	−0.018818	0.130938	−0.001687	0.048*	
C14	0.29444 (12)	−0.09343 (19)	0.3321 (2)	0.0318 (5)	
C15	0.36238 (14)	−0.1201 (2)	0.4229 (2)	0.0450 (6)	
H15A	0.358805	−0.070217	0.501743	0.068*	
H15B	0.407693	−0.097467	0.379397	0.068*	
H15C	0.363709	−0.209488	0.444988	0.068*	
C16	0.30236 (14)	−0.1762 (2)	0.2099 (2)	0.0426 (6)	
H16A	0.348326	−0.154486	0.167973	0.064*	
H16B	0.260123	−0.161363	0.149840	0.064*	
H16C	0.303615	−0.264893	0.234842	0.064*	
C17	0.22445 (14)	−0.1320 (2)	0.4042 (2)	0.0422 (5)	
H17A	0.180375	−0.117900	0.348224	0.063*	
H17B	0.221044	−0.081472	0.482708	0.063*	
H17C	0.227658	−0.221052	0.427402	0.063*	
C18	0.40043 (12)	0.3569 (2)	0.3594 (2)	0.0359 (5)	

C19	0.4494 (4)	0.3964 (9)	0.2530 (6)	0.060 (2)	0.432 (3)
H19A	0.419224	0.434554	0.183093	0.090*	0.432 (3)
H19B	0.475182	0.322769	0.220151	0.090*	0.432 (3)
H19C	0.485806	0.457503	0.286418	0.090*	0.432 (3)
C20	0.4421 (5)	0.3068 (7)	0.4791 (7)	0.067 (2)	0.432 (3)
H20A	0.470873	0.232756	0.455985	0.100*	0.432 (3)
H20B	0.406658	0.283778	0.544208	0.100*	0.432 (3)
H20C	0.475598	0.371805	0.513983	0.100*	0.432 (3)
C21	0.3577 (4)	0.4777 (6)	0.4080 (10)	0.068 (2)	0.432 (3)
H21A	0.320273	0.452044	0.468704	0.101*	0.432 (3)
H21B	0.333471	0.520176	0.334044	0.101*	0.432 (3)
H21C	0.392980	0.535039	0.451171	0.101*	0.432 (3)
C19A	0.4210 (4)	0.4572 (6)	0.2589 (6)	0.0447 (16)	0.458 (3)
H19D	0.378788	0.513469	0.242584	0.067*	0.458 (3)
H19E	0.433633	0.415800	0.178287	0.067*	0.458 (3)
H19F	0.463573	0.505865	0.292126	0.067*	0.458 (3)
C21A	0.3759 (5)	0.4188 (10)	0.4805 (7)	0.073 (3)	0.458 (3)
H21D	0.365667	0.354421	0.544960	0.110*	0.458 (3)
H21E	0.330954	0.467719	0.461465	0.110*	0.458 (3)
H21F	0.415164	0.474521	0.514327	0.110*	0.458 (3)
C20A	0.4763 (3)	0.2850 (6)	0.3889 (10)	0.065 (2)	0.458 (3)
H20D	0.490175	0.238337	0.312073	0.097*	0.458 (3)
H20E	0.470260	0.226415	0.460567	0.097*	0.458 (3)
H20F	0.515145	0.345868	0.412215	0.097*	0.458 (3)
C21B	0.3904 (16)	0.4917 (12)	0.309 (3)	0.062 (5)	0.110 (3)
H21G	0.343913	0.526115	0.339740	0.093*	0.110 (3)
H21H	0.389010	0.491338	0.214826	0.093*	0.110 (3)
H21I	0.431866	0.543554	0.341513	0.093*	0.110 (3)
C19B	0.4768 (9)	0.306 (3)	0.322 (3)	0.061 (5)	0.110 (3)
H19G	0.474575	0.280474	0.231122	0.091*	0.110 (3)
H19H	0.489919	0.233159	0.376059	0.091*	0.110 (3)
H19I	0.514310	0.371453	0.335079	0.091*	0.110 (3)
C20B	0.3986 (19)	0.356 (3)	0.5076 (8)	0.064 (6)	0.110 (3)
H20G	0.405818	0.270324	0.539420	0.096*	0.110 (3)
H20H	0.350545	0.387670	0.534274	0.096*	0.110 (3)
H20I	0.438105	0.410158	0.543479	0.096*	0.110 (3)
H1	0.1506 (16)	0.053 (3)	0.111 (3)	0.057 (9)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04069 (14)	0.04521 (15)	0.05239 (16)	0.00871 (11)	−0.01424 (10)	0.00238 (11)
O1	0.0360 (9)	0.0294 (8)	0.0470 (10)	−0.0040 (7)	−0.0140 (7)	−0.0028 (7)
N1	0.0320 (9)	0.0352 (10)	0.0384 (10)	0.0016 (8)	−0.0078 (8)	−0.0019 (8)
C1	0.0268 (10)	0.0290 (10)	0.0300 (11)	−0.0029 (8)	−0.0013 (8)	−0.0059 (8)
C2	0.0304 (10)	0.0269 (10)	0.0251 (10)	−0.0010 (8)	0.0014 (8)	−0.0031 (8)
C3	0.0293 (10)	0.0316 (11)	0.0260 (10)	0.0003 (8)	−0.0033 (8)	−0.0002 (8)
C4	0.0321 (11)	0.0298 (11)	0.0289 (11)	−0.0053 (9)	−0.0037 (8)	−0.0025 (9)

C5	0.0368 (12)	0.0252 (10)	0.0371 (12)	−0.0026 (9)	−0.0071 (9)	−0.0010 (9)
C6	0.0309 (11)	0.0291 (10)	0.0332 (11)	0.0023 (9)	−0.0054 (9)	−0.0033 (9)
C7	0.0391 (12)	0.0294 (11)	0.0404 (13)	0.0025 (9)	−0.0086 (10)	−0.0038 (9)
C8	0.0309 (11)	0.0351 (11)	0.0324 (11)	0.0022 (9)	−0.0068 (9)	−0.0019 (9)
C9	0.0314 (12)	0.0574 (16)	0.0494 (15)	−0.0131 (11)	−0.0088 (10)	0.0163 (12)
C10	0.0435 (13)	0.0501 (14)	0.0457 (14)	−0.0115 (11)	−0.0103 (11)	0.0199 (11)
C11	0.0313 (11)	0.0355 (12)	0.0322 (11)	0.0031 (9)	−0.0043 (9)	−0.0018 (9)
C12	0.0278 (11)	0.0398 (12)	0.0494 (14)	−0.0036 (9)	−0.0061 (10)	0.0015 (11)
C13	0.0389 (13)	0.0331 (12)	0.0470 (14)	−0.0043 (10)	−0.0098 (10)	0.0046 (10)
C14	0.0364 (11)	0.0262 (10)	0.0325 (11)	−0.0003 (9)	−0.0016 (9)	0.0003 (9)
C15	0.0496 (14)	0.0324 (12)	0.0520 (15)	0.0026 (11)	−0.0128 (11)	0.0088 (11)
C16	0.0553 (15)	0.0298 (11)	0.0428 (13)	0.0051 (11)	0.0016 (11)	−0.0052 (10)
C17	0.0512 (14)	0.0336 (12)	0.0421 (13)	−0.0040 (10)	0.0047 (11)	0.0037 (10)
C18	0.0400 (12)	0.0354 (11)	0.0317 (11)	−0.0123 (10)	−0.0075 (9)	0.0023 (9)
C19	0.050 (5)	0.083 (6)	0.049 (4)	−0.031 (4)	0.006 (3)	−0.009 (4)
C20	0.080 (5)	0.069 (5)	0.049 (4)	−0.044 (4)	−0.036 (4)	0.015 (4)
C21	0.065 (4)	0.055 (4)	0.082 (5)	−0.020 (4)	−0.005 (4)	−0.036 (4)
C19A	0.042 (4)	0.050 (4)	0.042 (3)	−0.019 (3)	0.000 (3)	−0.004 (3)
C21A	0.074 (5)	0.101 (7)	0.046 (4)	−0.052 (5)	0.016 (4)	−0.035 (4)
C20A	0.040 (3)	0.053 (4)	0.098 (6)	−0.021 (3)	−0.034 (4)	0.021 (4)
C21B	0.064 (10)	0.066 (9)	0.055 (9)	−0.038 (8)	−0.010 (8)	−0.002 (9)
C19B	0.054 (9)	0.071 (9)	0.058 (10)	−0.032 (8)	0.008 (9)	−0.008 (9)
C20B	0.070 (11)	0.065 (12)	0.056 (10)	−0.037 (10)	0.001 (10)	−0.037 (9)

Geometric parameters (Å, º)

Br1—C11	1.902 (2)	C17—H17C	0.9700
O1—C1	1.355 (2)	C18—C19	1.485 (5)
O1—H1	0.82 (3)	C18—C20	1.509 (5)
N1—C7	1.278 (3)	C18—C21	1.576 (5)
N1—C8	1.427 (3)	C18—C19A	1.533 (5)
C1—C2	1.408 (3)	C18—C21A	1.486 (5)
C1—C6	1.409 (3)	C18—C20A	1.574 (5)
C2—C3	1.390 (3)	C18—C21B	1.520 (7)
C2—C14	1.540 (3)	C18—C19B	1.531 (7)
C3—H3	0.9400	C18—C20B	1.524 (7)
C3—C4	1.398 (3)	C19—H19A	0.9700
C4—C5	1.378 (3)	C19—H19B	0.9700
C4—C18	1.532 (3)	C19—H19C	0.9700
C5—H5	0.9400	C20—H20A	0.9700
C5—C6	1.395 (3)	C20—H20B	0.9700
C6—C7	1.454 (3)	C20—H20C	0.9700
C7—H7	0.9400	C21—H21A	0.9700
C8—C9	1.382 (3)	C21—H21B	0.9700
C8—C13	1.383 (3)	C21—H21C	0.9700
C9—H9	0.9400	C19A—H19D	0.9700
C9—C10	1.381 (3)	C19A—H19E	0.9700
C10—H10	0.9400	C19A—H19F	0.9700

C10—C11	1.376 (3)	C21A—H21D	0.9700
C11—C12	1.376 (3)	C21A—H21E	0.9700
C12—H12	0.9400	C21A—H21F	0.9700
C12—C13	1.385 (3)	C20A—H20D	0.9700
C13—H13	0.9400	C20A—H20E	0.9700
C14—C15	1.530 (3)	C20A—H20F	0.9700
C14—C16	1.540 (3)	C21B—H21G	0.9700
C14—C17	1.534 (3)	C21B—H21H	0.9700
C15—H15A	0.9700	C21B—H21I	0.9700
C15—H15B	0.9700	C19B—H19G	0.9700
C15—H15C	0.9700	C19B—H19H	0.9700
C16—H16A	0.9700	C19B—H19I	0.9700
C16—H16B	0.9700	C20B—H20G	0.9700
C16—H16C	0.9700	C20B—H20H	0.9700
C17—H17A	0.9700	C20B—H20I	0.9700
C17—H17B	0.9700		

C1—O1—H1	106 (2)	C19—C18—C20	114.2 (5)
C7—N1—C8	119.31 (19)	C19—C18—C21	108.3 (5)
O1—C1—C2	120.32 (18)	C20—C18—C4	112.8 (3)
O1—C1—C6	119.82 (18)	C20—C18—C21	104.8 (4)
C2—C1—C6	119.86 (18)	C19A—C18—C20A	103.6 (4)
C1—C2—C14	121.40 (17)	C21A—C18—C4	110.9 (3)
C3—C2—C1	116.84 (18)	C21A—C18—C19A	110.3 (4)
C3—C2—C14	121.75 (18)	C21A—C18—C20A	109.3 (5)
C2—C3—H3	117.5	C21B—C18—C4	113.6 (9)
C2—C3—C4	124.96 (19)	C21B—C18—C19B	109.8 (9)
C4—C3—H3	117.5	C21B—C18—C20B	109.6 (9)
C3—C4—C18	122.10 (18)	C19B—C18—C4	107.6 (11)
C5—C4—C3	116.36 (18)	C20B—C18—C4	108.4 (12)
C5—C4—C18	121.54 (18)	C20B—C18—C19B	107.6 (9)
C4—C5—H5	119.1	C18—C19—H19A	109.5
C4—C5—C6	121.90 (19)	C18—C19—H19B	109.5
C6—C5—H5	119.1	C18—C19—H19C	109.5
C1—C6—C7	121.69 (18)	H19A—C19—H19B	109.5
C5—C6—C1	120.07 (19)	H19A—C19—H19C	109.5
C5—C6—C7	118.24 (19)	H19B—C19—H19C	109.5
N1—C7—C6	123.4 (2)	C18—C20—H20A	109.5
N1—C7—H7	118.3	C18—C20—H20B	109.5
C6—C7—H7	118.3	C18—C20—H20C	109.5
C9—C8—N1	123.07 (19)	H20A—C20—H20B	109.5
C9—C8—C13	118.9 (2)	H20A—C20—H20C	109.5
C13—C8—N1	118.0 (2)	H20B—C20—H20C	109.5
C8—C9—H9	119.7	C18—C21—H21A	109.5
C10—C9—C8	120.6 (2)	C18—C21—H21B	109.5
C10—C9—H9	119.7	C18—C21—H21C	109.5
C9—C10—H10	120.3	H21A—C21—H21B	109.5
C11—C10—C9	119.4 (2)	H21A—C21—H21C	109.5

C11—C10—H10	120.3	H21B—C21—H21C	109.5
C10—C11—Br1	118.72 (17)	C18—C19A—H19D	109.5
C12—C11—Br1	120.06 (16)	C18—C19A—H19E	109.5
C12—C11—C10	121.2 (2)	C18—C19A—H19F	109.5
C11—C12—H12	120.6	H19D—C19A—H19E	109.5
C11—C12—C13	118.7 (2)	H19D—C19A—H19F	109.5
C13—C12—H12	120.6	H19E—C19A—H19F	109.5
C8—C13—C12	121.1 (2)	C18—C21A—H21D	109.5
C8—C13—H13	119.5	C18—C21A—H21E	109.5
C12—C13—H13	119.5	C18—C21A—H21F	109.5
C15—C14—C2	112.09 (17)	H21D—C21A—H21E	109.5
C15—C14—C16	107.28 (19)	H21D—C21A—H21F	109.5
C15—C14—C17	107.55 (19)	H21E—C21A—H21F	109.5
C16—C14—C2	109.58 (17)	C18—C20A—H20D	109.5
C17—C14—C2	110.09 (17)	C18—C20A—H20E	109.5
C17—C14—C16	110.19 (18)	C18—C20A—H20F	109.5
C14—C15—H15A	109.5	H20D—C20A—H20E	109.5
C14—C15—H15B	109.5	H20D—C20A—H20F	109.5
C14—C15—H15C	109.5	H20E—C20A—H20F	109.5
H15A—C15—H15B	109.5	C18—C21B—H21G	109.5
H15A—C15—H15C	109.5	C18—C21B—H21H	109.5
H15B—C15—H15C	109.5	C18—C21B—H21I	109.5
C14—C16—H16A	109.5	H21G—C21B—H21H	109.5
C14—C16—H16B	109.5	H21G—C21B—H21I	109.5
C14—C16—H16C	109.5	H21H—C21B—H21I	109.5
H16A—C16—H16B	109.5	C18—C19B—H19G	109.5
H16A—C16—H16C	109.5	C18—C19B—H19H	109.5
H16B—C16—H16C	109.5	C18—C19B—H19I	109.5
C14—C17—H17A	109.5	H19G—C19B—H19H	109.5
C14—C17—H17B	109.5	H19G—C19B—H19I	109.5
C14—C17—H17C	109.5	H19H—C19B—H19I	109.5
H17A—C17—H17B	109.5	C18—C20B—H20G	109.5
H17A—C17—H17C	109.5	C18—C20B—H20H	109.5
H17B—C17—H17C	109.5	C18—C20B—H20I	109.5
C4—C18—C21	106.7 (3)	H20G—C20B—H20H	109.5
C4—C18—C19A	112.2 (3)	H20G—C20B—H20I	109.5
C4—C18—C20A	110.3 (3)	H20H—C20B—H20I	109.5
C19—C18—C4	109.6 (3)		

Br1—C11—C12—C13	179.74 (17)	C3—C4—C18—C20B	−59.0 (14)
O1—C1—C2—C3	179.38 (18)	C4—C5—C6—C1	−0.8 (3)
O1—C1—C2—C14	−0.4 (3)	C4—C5—C6—C7	178.2 (2)
O1—C1—C6—C5	−178.8 (2)	C5—C4—C18—C19	−70.2 (5)
O1—C1—C6—C7	2.2 (3)	C5—C4—C18—C20	161.3 (5)
N1—C8—C9—C10	−178.3 (2)	C5—C4—C18—C21	46.8 (5)
N1—C8—C13—C12	178.8 (2)	C5—C4—C18—C19A	−36.5 (4)
C1—C2—C3—C4	−0.5 (3)	C5—C4—C18—C21A	87.4 (6)
C1—C2—C14—C15	178.41 (19)	C5—C4—C18—C20A	−151.4 (4)

C1—C2—C14—C16	59.4 (3)	C5—C4—C18—C21B	−1.3 (14)
C1—C2—C14—C17	−61.9 (2)	C5—C4—C18—C19B	−123.2 (13)
C1—C6—C7—N1	−0.2 (4)	C5—C4—C18—C20B	120.8 (14)
C2—C1—C6—C5	1.4 (3)	C5—C6—C7—N1	−179.2 (2)
C2—C1—C6—C7	−177.67 (19)	C6—C1—C2—C3	−0.7 (3)
C2—C3—C4—C5	1.0 (3)	C6—C1—C2—C14	179.51 (19)
C2—C3—C4—C18	−179.23 (19)	C7—N1—C8—C9	27.6 (3)
C3—C2—C14—C15	−1.3 (3)	C7—N1—C8—C13	−153.2 (2)
C3—C2—C14—C16	−120.3 (2)	C8—N1—C7—C6	178.5 (2)
C3—C2—C14—C17	118.3 (2)	C8—C9—C10—C11	−1.5 (4)
C3—C4—C5—C6	−0.3 (3)	C9—C8—C13—C12	−1.9 (4)
C3—C4—C18—C19	110.0 (5)	C9—C10—C11—Br1	−179.26 (19)
C3—C4—C18—C20	−18.4 (5)	C9—C10—C11—C12	−0.1 (4)
C3—C4—C18—C21	−133.0 (4)	C10—C11—C12—C13	0.6 (4)
C3—C4—C18—C19A	143.7 (4)	C11—C12—C13—C8	0.5 (4)
C3—C4—C18—C21A	−92.4 (5)	C13—C8—C9—C10	2.4 (4)
C3—C4—C18—C20A	28.8 (5)	C14—C2—C3—C4	179.3 (2)
C3—C4—C18—C21B	178.9 (13)	C18—C4—C5—C6	179.9 (2)
C3—C4—C18—C19B	57.0 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82 (3)	1.85 (3)	2.611 (2)	153 (3)

(*E*)-6-{[(4-Bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol (3_150K)

Crystal data

$C_{21}H_{26}BrNO$
M_r = 388.34
Monoclinic, $P2_1/c$
a = 17.8028 (3) Å
b = 10.55679 (16) Å
c = 10.21910 (18) Å
β = 91.6950 (16)°
V = 1919.74 (6) Å^3
Z = 4
$F(000)$ = 808
D_x = 1.344 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 11397 reflections
θ = 3.0–31.4°
μ = 2.15 mm^{-1}
T = 150 K
Needle, yellow
0.3 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.3620 pixels mm^{-1}
ω and π scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2013)
T_{min} = 0.660, T_{max} = 1.000
28980 measured reflections
4570 independent reflections
3604 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.9°, θ_{min} = 3.0°
h = −23→23
k = −9→13
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.073$
$S = 1.03$
4570 reflections
258 parameters
67 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 1.2083P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	−0.13644 (2)	0.44578 (2)	−0.29000 (2)	0.03480 (8)	
O1	0.18011 (8)	0.01007 (13)	0.15556 (14)	0.0295 (3)	
N1	0.11607 (9)	0.20340 (15)	0.03813 (16)	0.0277 (4)	
C1	0.23231 (10)	0.09145 (17)	0.20655 (18)	0.0230 (4)	
C2	0.28925 (10)	0.04754 (16)	0.29343 (17)	0.0217 (4)	
C3	0.34096 (10)	0.13632 (17)	0.34049 (17)	0.0232 (4)	
H3	0.379382	0.107662	0.399830	0.028*	
C4	0.34061 (10)	0.26494 (17)	0.30686 (18)	0.0247 (4)	
C5	0.28326 (11)	0.30457 (17)	0.22279 (19)	0.0271 (4)	
H5	0.280656	0.391310	0.198318	0.032*	
C6	0.22892 (10)	0.22080 (17)	0.17262 (18)	0.0247 (4)	
C7	0.16923 (11)	0.27128 (18)	0.08793 (19)	0.0291 (4)	
H7	0.169624	0.359268	0.068451	0.035*	
C8	0.05884 (10)	0.26217 (18)	−0.04112 (18)	0.0261 (4)	
C9	0.07027 (11)	0.3727 (2)	−0.1113 (2)	0.0353 (5)	
H9	0.118509	0.411234	−0.109202	0.042*	
C10	0.01216 (12)	0.4273 (2)	−0.1843 (2)	0.0350 (5)	
H10	0.020081	0.503480	−0.231393	0.042*	
C11	−0.05743 (10)	0.36977 (18)	−0.18789 (18)	0.0259 (4)	
C12	−0.07008 (11)	0.25848 (19)	−0.1214 (2)	0.0298 (4)	
H12	−0.118098	0.219178	−0.125727	0.036*	
C13	−0.01139 (11)	0.20496 (19)	−0.0481 (2)	0.0305 (4)	
H13	−0.019370	0.128141	−0.002171	0.037*	
C14	0.29426 (11)	−0.09316 (17)	0.33386 (18)	0.0249 (4)	
C15	0.36176 (12)	−0.11911 (19)	0.4261 (2)	0.0350 (5)	
H15A	0.356928	−0.069418	0.506412	0.052*	
H15B	0.408107	−0.095073	0.383036	0.052*	

H15C	0.363476	−0.209480	0.447938	0.052*	
C16	0.30344 (12)	−0.17599 (18)	0.2111 (2)	0.0333 (5)	
H16A	0.350575	−0.154139	0.169403	0.050*	
H16B	0.261165	−0.160990	0.149506	0.050*	
H16C	0.304431	−0.265514	0.236523	0.050*	
C17	0.22318 (12)	−0.13215 (19)	0.4055 (2)	0.0324 (4)	
H17A	0.178929	−0.118533	0.347883	0.049*	
H17B	0.218775	−0.080873	0.484829	0.049*	
H17C	0.226510	−0.221911	0.429418	0.049*	
C18	0.40013 (11)	0.35767 (18)	0.36040 (18)	0.0291 (4)	
C19	0.4498 (3)	0.3960 (7)	0.2547 (5)	0.0518 (15)	0.535 (6)
H19A	0.419730	0.434848	0.183550	0.078*	0.535 (6)
H19B	0.475817	0.321328	0.221553	0.078*	0.535 (6)
H19C	0.486796	0.457267	0.288735	0.078*	0.535 (6)
C20	0.4414 (3)	0.3089 (5)	0.4809 (5)	0.060 (2)	0.535 (6)
H20A	0.475916	0.374283	0.514732	0.091*	0.535 (6)
H20B	0.470091	0.233045	0.458459	0.091*	0.535 (6)
H20C	0.405219	0.287585	0.547793	0.091*	0.535 (6)
C21	0.3570 (3)	0.4798 (5)	0.4092 (7)	0.0605 (17)	0.535 (6)
H21A	0.318837	0.454594	0.471226	0.091*	0.535 (6)
H21B	0.332704	0.522462	0.334007	0.091*	0.535 (6)
H21C	0.392898	0.537745	0.452383	0.091*	0.535 (6)
C19A	0.4198 (4)	0.4608 (6)	0.2615 (5)	0.0440 (15)	0.465 (6)
H19D	0.377474	0.519708	0.250993	0.066*	0.465 (6)
H19E	0.429930	0.421559	0.176886	0.066*	0.465 (6)
H19F	0.464424	0.506986	0.293242	0.066*	0.465 (6)
C21A	0.3786 (4)	0.4101 (8)	0.4865 (6)	0.066 (2)	0.465 (6)
H21D	0.419622	0.462612	0.522576	0.099*	0.465 (6)
H21E	0.368431	0.340814	0.547262	0.099*	0.465 (6)
H21F	0.333324	0.462071	0.474067	0.099*	0.465 (6)
C20A	0.4783 (3)	0.2852 (5)	0.3802 (8)	0.057 (2)	0.465 (6)
H20D	0.517875	0.346325	0.403387	0.086*	0.465 (6)
H20E	0.490672	0.242011	0.298699	0.086*	0.465 (6)
H20F	0.474232	0.222698	0.450517	0.086*	0.465 (6)
H1	0.1492 (12)	0.054 (2)	0.109 (2)	0.058 (8)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03124 (12)	0.03363 (12)	0.03882 (13)	0.00648 (9)	−0.01060 (8)	0.00195 (9)
O1	0.0294 (7)	0.0224 (7)	0.0360 (8)	−0.0032 (6)	−0.0114 (6)	−0.0015 (6)
N1	0.0259 (8)	0.0276 (8)	0.0293 (9)	0.0015 (7)	−0.0061 (7)	−0.0015 (7)
C1	0.0223 (9)	0.0227 (9)	0.0240 (9)	−0.0020 (7)	−0.0004 (7)	−0.0043 (7)
C2	0.0243 (9)	0.0209 (8)	0.0200 (8)	0.0004 (7)	0.0014 (7)	−0.0023 (7)
C3	0.0244 (9)	0.0241 (9)	0.0209 (9)	−0.0003 (7)	−0.0024 (7)	0.0011 (7)
C4	0.0268 (9)	0.0245 (9)	0.0226 (9)	−0.0037 (8)	−0.0030 (7)	−0.0013 (7)
C5	0.0320 (10)	0.0195 (9)	0.0293 (10)	−0.0012 (8)	−0.0053 (8)	−0.0004 (7)
C6	0.0243 (9)	0.0238 (9)	0.0256 (9)	0.0029 (7)	−0.0050 (7)	−0.0027 (7)

C7	0.0325 (10)	0.0226 (9)	0.0319 (10)	0.0030 (8)	−0.0070 (8)	−0.0039 (8)
C8	0.0254 (9)	0.0274 (10)	0.0253 (9)	0.0021 (8)	−0.0048 (8)	−0.0015 (8)
C9	0.0250 (10)	0.0437 (12)	0.0370 (11)	−0.0105 (9)	−0.0057 (9)	0.0103 (10)
C10	0.0334 (11)	0.0368 (11)	0.0343 (11)	−0.0071 (9)	−0.0072 (9)	0.0133 (9)
C11	0.0263 (9)	0.0265 (9)	0.0246 (9)	0.0034 (8)	−0.0034 (7)	−0.0027 (8)
C12	0.0225 (9)	0.0304 (10)	0.0361 (11)	−0.0032 (8)	−0.0036 (8)	−0.0007 (8)
C13	0.0313 (10)	0.0253 (10)	0.0344 (11)	−0.0018 (8)	−0.0067 (8)	0.0024 (8)
C14	0.0285 (10)	0.0203 (8)	0.0257 (9)	0.0005 (8)	−0.0019 (8)	0.0004 (7)
C15	0.0379 (11)	0.0258 (10)	0.0407 (12)	0.0024 (9)	−0.0101 (9)	0.0074 (9)
C16	0.0440 (12)	0.0227 (9)	0.0331 (11)	0.0039 (9)	0.0016 (9)	−0.0034 (8)
C17	0.0381 (11)	0.0265 (10)	0.0326 (11)	−0.0037 (9)	0.0032 (9)	0.0024 (8)
C18	0.0333 (10)	0.0283 (10)	0.0254 (10)	−0.0108 (8)	−0.0066 (8)	0.0021 (8)
C19	0.045 (3)	0.071 (4)	0.039 (3)	−0.031 (3)	0.006 (2)	−0.005 (3)
C20	0.072 (4)	0.057 (3)	0.050 (3)	−0.042 (3)	−0.039 (3)	0.020 (3)
C21	0.051 (3)	0.045 (3)	0.085 (4)	−0.014 (2)	−0.004 (3)	−0.038 (3)
C19A	0.044 (3)	0.042 (3)	0.046 (3)	−0.019 (3)	−0.010 (3)	−0.001 (3)
C21A	0.059 (4)	0.093 (5)	0.045 (3)	−0.046 (4)	0.012 (3)	−0.034 (4)
C20A	0.031 (3)	0.039 (3)	0.100 (5)	−0.015 (2)	−0.025 (3)	0.010 (3)

Geometric parameters (Å, º)

Br1—C11	1.9039 (18)	C15—H15C	0.9800
O1—C1	1.358 (2)	C16—H16A	0.9800
O1—H1	0.855 (10)	C16—H16B	0.9800
N1—C7	1.280 (2)	C16—H16C	0.9800
N1—C8	1.425 (2)	C17—H17A	0.9800
C1—C2	1.406 (2)	C17—H17B	0.9800
C1—C6	1.410 (3)	C17—H17C	0.9800
C2—C3	1.390 (2)	C18—C19	1.472 (4)
C2—C14	1.544 (2)	C18—C20	1.506 (4)
C3—H3	0.9500	C18—C21	1.588 (4)
C3—C4	1.401 (3)	C18—C19A	1.533 (5)
C4—C5	1.380 (3)	C18—C21A	1.464 (5)
C4—C18	1.532 (2)	C18—C20A	1.595 (4)
C5—H5	0.9500	C19—H19A	0.9800
C5—C6	1.397 (3)	C19—H19B	0.9800
C6—C7	1.452 (2)	C19—H19C	0.9800
C7—H7	0.9500	C20—H20A	0.9800
C8—C9	1.388 (3)	C20—H20B	0.9800
C8—C13	1.388 (3)	C20—H20C	0.9800
C9—H9	0.9500	C21—H21A	0.9800
C9—C10	1.383 (3)	C21—H21B	0.9800
C10—H10	0.9500	C21—H21C	0.9800
C10—C11	1.379 (3)	C19A—H19D	0.9800
C11—C12	1.379 (3)	C19A—H19E	0.9800
C12—H12	0.9500	C19A—H19F	0.9800
C12—C13	1.388 (3)	C21A—H21D	0.9800
C13—H13	0.9500	C21A—H21E	0.9800

C14—C15	1.530 (3)	C21A—H21F	0.9800
C14—C16	1.541 (3)	C20A—H20D	0.9800
C14—C17	1.537 (3)	C20A—H20E	0.9800
C15—H15A	0.9800	C20A—H20F	0.9800
C15—H15B	0.9800		

C1—O1—H1	107.2 (18)	H16A—C16—H16C	109.5
C7—N1—C8	119.33 (17)	H16B—C16—H16C	109.5
O1—C1—C2	120.40 (16)	C14—C17—H17A	109.5
O1—C1—C6	119.64 (16)	C14—C17—H17B	109.5
C2—C1—C6	119.96 (16)	C14—C17—H17C	109.5
C1—C2—C14	121.40 (15)	H17A—C17—H17B	109.5
C3—C2—C1	117.00 (16)	H17A—C17—H17C	109.5
C3—C2—C14	121.59 (16)	H17B—C17—H17C	109.5
C2—C3—H3	117.6	C4—C18—C21	107.2 (2)
C2—C3—C4	124.81 (17)	C4—C18—C19A	112.8 (2)
C4—C3—H3	117.6	C4—C18—C20A	109.3 (2)
C3—C4—C18	122.27 (16)	C19—C18—C4	109.7 (2)
C5—C4—C3	116.40 (16)	C19—C18—C20	113.8 (3)
C5—C4—C18	121.33 (16)	C19—C18—C21	108.3 (4)
C4—C5—H5	119.1	C20—C18—C4	112.9 (2)
C4—C5—C6	121.89 (17)	C20—C18—C21	104.5 (3)
C6—C5—H5	119.1	C19A—C18—C20A	102.1 (3)
C1—C6—C7	121.83 (16)	C21A—C18—C4	111.1 (3)
C5—C6—C1	119.92 (16)	C21A—C18—C19A	112.5 (4)
C5—C6—C7	118.24 (17)	C21A—C18—C20A	108.7 (4)
N1—C7—C6	123.42 (18)	C18—C19—H19A	109.5
N1—C7—H7	118.3	C18—C19—H19B	109.5
C6—C7—H7	118.3	C18—C19—H19C	109.5
C9—C8—N1	123.13 (17)	H19A—C19—H19B	109.5
C9—C8—C13	118.99 (17)	H19A—C19—H19C	109.5
C13—C8—N1	117.89 (17)	H19B—C19—H19C	109.5
C8—C9—H9	119.7	C18—C20—H20A	109.5
C10—C9—C8	120.68 (18)	C18—C20—H20B	109.5
C10—C9—H9	119.7	C18—C20—H20C	109.5
C9—C10—H10	120.4	H20A—C20—H20B	109.5
C11—C10—C9	119.19 (19)	H20A—C20—H20C	109.5
C11—C10—H10	120.4	H20B—C20—H20C	109.5
C10—C11—Br1	118.52 (15)	C18—C21—H21A	109.5
C12—C11—Br1	120.01 (14)	C18—C21—H21B	109.5
C12—C11—C10	121.45 (18)	C18—C21—H21C	109.5
C11—C12—H12	120.6	H21A—C21—H21B	109.5
C11—C12—C13	118.77 (18)	H21A—C21—H21C	109.5
C13—C12—H12	120.6	H21B—C21—H21C	109.5
C8—C13—H13	119.6	C18—C19A—H19D	109.5
C12—C13—C8	120.89 (18)	C18—C19A—H19E	109.5
C12—C13—H13	119.6	C18—C19A—H19F	109.5
C15—C14—C2	112.05 (15)	H19D—C19A—H19E	109.5

C15—C14—C16	107.42 (16)	H19D—C19A—H19F	109.5
C15—C14—C17	107.54 (16)	H19E—C19A—H19F	109.5
C16—C14—C2	109.56 (15)	C18—C21A—H21D	109.5
C17—C14—C2	110.08 (15)	C18—C21A—H21E	109.5
C17—C14—C16	110.13 (16)	C18—C21A—H21F	109.5
C14—C15—H15A	109.5	H21D—C21A—H21E	109.5
C14—C15—H15B	109.5	H21D—C21A—H21F	109.5
C14—C15—H15C	109.5	H21E—C21A—H21F	109.5
H15A—C15—H15B	109.5	C18—C20A—H20D	109.5
H15A—C15—H15C	109.5	C18—C20A—H20E	109.5
H15B—C15—H15C	109.5	C18—C20A—H20F	109.5
C14—C16—H16A	109.5	H20D—C20A—H20E	109.5
C14—C16—H16B	109.5	H20D—C20A—H20F	109.5
C14—C16—H16C	109.5	H20E—C20A—H20F	109.5
H16A—C16—H16B	109.5		

Br1—C11—C12—C13	179.77 (15)	C3—C4—C18—C20A	32.9 (4)
O1—C1—C2—C3	179.43 (16)	C4—C5—C6—C1	−0.7 (3)
O1—C1—C2—C14	−0.2 (3)	C4—C5—C6—C7	178.15 (18)
O1—C1—C6—C5	−178.80 (17)	C5—C4—C18—C19	−70.7 (4)
O1—C1—C6—C7	2.4 (3)	C5—C4—C18—C20	161.2 (3)
N1—C8—C9—C10	−178.48 (19)	C5—C4—C18—C21	46.7 (4)
N1—C8—C13—C12	178.72 (18)	C5—C4—C18—C19A	−34.6 (4)
C1—C2—C3—C4	−0.5 (3)	C5—C4—C18—C21A	92.7 (4)
C1—C2—C14—C15	178.53 (17)	C5—C4—C18—C20A	−147.4 (3)
C1—C2—C14—C16	59.4 (2)	C5—C6—C7—N1	−179.02 (19)
C1—C2—C14—C17	−61.8 (2)	C6—C1—C2—C3	−1.0 (3)
C1—C6—C7—N1	−0.2 (3)	C6—C1—C2—C14	179.39 (17)
C2—C1—C6—C5	1.6 (3)	C7—N1—C8—C9	27.0 (3)
C2—C1—C6—C7	−177.22 (17)	C7—N1—C8—C13	−153.34 (19)
C2—C3—C4—C5	1.4 (3)	C8—N1—C7—C6	178.35 (17)
C2—C3—C4—C18	−178.92 (17)	C8—C9—C10—C11	−0.7 (3)
C3—C2—C14—C15	−1.1 (2)	C9—C8—C13—C12	−1.6 (3)
C3—C2—C14—C16	−120.19 (19)	C9—C10—C11—Br1	−179.53 (16)
C3—C2—C14—C17	118.56 (19)	C9—C10—C11—C12	−0.7 (3)
C3—C4—C5—C6	−0.7 (3)	C10—C11—C12—C13	0.9 (3)
C3—C4—C18—C19	109.7 (4)	C11—C12—C13—C8	0.2 (3)
C3—C4—C18—C20	−18.5 (4)	C13—C8—C9—C10	1.8 (3)
C3—C4—C18—C21	−133.0 (3)	C14—C2—C3—C4	179.08 (17)
C3—C4—C18—C19A	145.7 (4)	C18—C4—C5—C6	179.59 (18)
C3—C4—C18—C21A	−86.9 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.86 (1)	1.83 (2)	2.612 (2)	152 (3)

(*E*)-6-{[(4-Bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol (3_120K)

Crystal data

$C_{21}H_{26}BrNO$
$M_r = 388.34$
Monoclinic, $P2_1/c$
$a = 17.5364$ (3) Å
$b = 10.65933$ (19) Å
$c = 10.1718$ (2) Å
$\beta = 90.6047$ (16)°
$V = 1901.26$ (6) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 19498 reflections
$\theta = 3.0$–$33.7°$
$\mu = 2.17$ mm^{-1}
$T = 120$ K
Needle, yellow
0.3 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.3620 pixels mm^{-1}
ω and π scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2013)
$T_{min} = 0.683$, $T_{max} = 1.000$
44888 measured reflections
4509 independent reflections
3697 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.9°$, $\theta_{min} = 3.0°$
$h = -23 \rightarrow 23$
$k = -10 \rightarrow 14$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.074$
$S = 1.05$
4509 reflections
258 parameters
103 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 1.846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ 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.

Refinement. Occupancies of the disordered tBu carbon atoms refined with their sum set to equal 1. Restraints were applied to maintain sensible thermal and geometric parameters.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	−0.13844 (2)	0.43829 (2)	−0.28813 (2)	0.02634 (7)	
O1	0.18335 (8)	0.01013 (13)	0.15526 (14)	0.0234 (3)	
N1	0.11721 (9)	0.19964 (16)	0.03565 (16)	0.0216 (4)	
C1	0.23349 (11)	0.09331 (18)	0.20854 (19)	0.0189 (4)	
C2	0.28966 (11)	0.05260 (18)	0.29902 (18)	0.0176 (4)	
C3	0.33929 (11)	0.14357 (18)	0.34904 (18)	0.0184 (4)	

H3	0.377226	0.117353	0.410491	0.022*	
C4	0.33707 (11)	0.27097 (18)	0.31492 (18)	0.0191 (4)	
C5	0.28065 (11)	0.30691 (18)	0.22702 (19)	0.0202 (4)	
H5	0.277174	0.392520	0.201705	0.024*	
C6	0.22861 (11)	0.22112 (19)	0.17431 (19)	0.0198 (4)	
C7	0.16847 (11)	0.26895 (19)	0.0887 (2)	0.0223 (4)	
H7	0.167154	0.356474	0.071266	0.027*	
C8	0.05922 (11)	0.25697 (19)	−0.04310 (19)	0.0205 (4)	
C9	0.07049 (12)	0.3685 (2)	−0.1113 (2)	0.0269 (5)	
H9	0.119013	0.408120	−0.108253	0.032*	
C10	0.01170 (12)	0.4224 (2)	−0.1835 (2)	0.0268 (5)	
H10	0.019426	0.499010	−0.229147	0.032*	
C11	−0.05848 (11)	0.36318 (19)	−0.18819 (19)	0.0201 (4)	
C12	−0.07077 (11)	0.25090 (19)	−0.1236 (2)	0.0226 (4)	
H12	−0.119082	0.210756	−0.128412	0.027*	
C13	−0.01115 (11)	0.19778 (19)	−0.0515 (2)	0.0237 (4)	
H13	−0.018687	0.120171	−0.007623	0.028*	
C14	0.29587 (11)	−0.08585 (18)	0.34107 (19)	0.0199 (4)	
C15	0.36147 (12)	−0.1077 (2)	0.4390 (2)	0.0268 (5)	
H15A	0.352459	−0.059068	0.519060	0.040*	
H15B	0.409560	−0.080971	0.399533	0.040*	
H15C	0.364385	−0.197117	0.460950	0.040*	
C16	0.31050 (13)	−0.16864 (19)	0.2197 (2)	0.0273 (5)	
H16A	0.359236	−0.145097	0.180394	0.041*	
H16B	0.269274	−0.156519	0.155142	0.041*	
H16C	0.312291	−0.256948	0.246356	0.041*	
C17	0.22224 (12)	−0.1278 (2)	0.4088 (2)	0.0256 (4)	
H17A	0.178983	−0.117698	0.347927	0.038*	
H17B	0.214040	−0.076414	0.487233	0.038*	
H17C	0.226738	−0.216188	0.434369	0.038*	
C18	0.39480 (11)	0.36655 (18)	0.36816 (18)	0.0220 (4)	
C19	0.45276 (15)	0.3956 (3)	0.2635 (2)	0.0325 (7)	0.866 (4)
H19A	0.426705	0.429933	0.185801	0.049*	0.866 (4)
H19B	0.479678	0.318507	0.239477	0.049*	0.866 (4)
H19C	0.489486	0.457189	0.297504	0.049*	0.866 (4)
C20	0.43448 (16)	0.3215 (3)	0.4933 (3)	0.0357 (7)	0.866 (4)
H20A	0.467578	0.388141	0.527699	0.054*	0.866 (4)
H20B	0.465249	0.247148	0.473742	0.054*	0.866 (4)
H20C	0.396146	0.300037	0.559027	0.054*	0.866 (4)
C21	0.35248 (15)	0.4905 (2)	0.4045 (3)	0.0345 (7)	0.866 (4)
H21A	0.313289	0.472481	0.469819	0.052*	0.866 (4)
H21B	0.328427	0.525905	0.325396	0.052*	0.866 (4)
H21C	0.389148	0.550822	0.441016	0.052*	0.866 (4)
C19A	0.4165 (10)	0.4668 (13)	0.2667 (13)	0.037 (4)	0.134 (4)
H19D	0.375157	0.528297	0.258655	0.056*	0.134 (4)
H19E	0.424704	0.426767	0.181219	0.056*	0.134 (4)
H19F	0.463361	0.509153	0.295317	0.056*	0.134 (4)
C21A	0.3726 (10)	0.4232 (17)	0.4984 (11)	0.050 (5)	0.134 (4)

H21D	0.408437	0.490241	0.521756	0.075*	0.134 (4)
H21E	0.373903	0.358192	0.566514	0.075*	0.134 (4)
H21F	0.320915	0.457808	0.491313	0.075*	0.134 (4)
C20A	0.4711 (6)	0.2925 (13)	0.3923 (18)	0.046 (5)	0.134 (4)
H20D	0.510831	0.350588	0.422946	0.070*	0.134 (4)
H20E	0.487149	0.253026	0.310116	0.070*	0.134 (4)
H20F	0.463040	0.227653	0.459071	0.070*	0.134 (4)
H1	0.1518 (13)	0.051 (2)	0.107 (2)	0.052 (9)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02311 (11)	0.02777 (12)	0.02797 (12)	0.00560 (9)	−0.00830 (8)	0.00102 (9)
O1	0.0233 (7)	0.0183 (7)	0.0285 (8)	−0.0029 (6)	−0.0093 (6)	−0.0009 (6)
N1	0.0192 (8)	0.0235 (9)	0.0220 (8)	0.0005 (7)	−0.0051 (7)	−0.0004 (7)
C1	0.0174 (9)	0.0204 (10)	0.0189 (9)	−0.0020 (7)	−0.0010 (7)	−0.0048 (8)
C2	0.0184 (9)	0.0181 (9)	0.0163 (9)	0.0008 (8)	0.0013 (7)	−0.0006 (7)
C3	0.0175 (9)	0.0212 (10)	0.0165 (9)	−0.0008 (8)	−0.0027 (7)	0.0022 (7)
C4	0.0192 (9)	0.0207 (10)	0.0173 (9)	−0.0020 (8)	−0.0018 (7)	−0.0016 (8)
C5	0.0229 (10)	0.0163 (9)	0.0212 (10)	−0.0022 (8)	−0.0027 (8)	0.0007 (8)
C6	0.0191 (9)	0.0204 (10)	0.0199 (10)	0.0016 (8)	−0.0035 (7)	−0.0014 (8)
C7	0.0233 (10)	0.0182 (10)	0.0251 (10)	0.0019 (8)	−0.0058 (8)	−0.0026 (8)
C8	0.0198 (9)	0.0228 (10)	0.0186 (9)	0.0016 (8)	−0.0039 (7)	−0.0014 (8)
C9	0.0201 (10)	0.0330 (12)	0.0274 (11)	−0.0074 (9)	−0.0047 (8)	0.0048 (9)
C10	0.0273 (11)	0.0285 (12)	0.0245 (10)	−0.0050 (9)	−0.0048 (8)	0.0084 (9)
C11	0.0201 (9)	0.0225 (10)	0.0178 (9)	0.0035 (8)	−0.0046 (7)	−0.0031 (8)
C12	0.0171 (9)	0.0240 (10)	0.0267 (10)	−0.0016 (8)	−0.0033 (8)	−0.0017 (8)
C13	0.0252 (10)	0.0200 (10)	0.0258 (11)	−0.0006 (8)	−0.0051 (8)	0.0016 (8)
C14	0.0226 (9)	0.0167 (10)	0.0203 (9)	0.0003 (8)	−0.0006 (8)	0.0003 (7)
C15	0.0285 (11)	0.0219 (10)	0.0300 (11)	0.0019 (9)	−0.0054 (9)	0.0074 (9)
C16	0.0373 (12)	0.0181 (10)	0.0264 (11)	0.0045 (9)	0.0019 (9)	−0.0011 (8)
C17	0.0285 (11)	0.0225 (11)	0.0259 (11)	−0.0028 (9)	0.0017 (8)	0.0020 (9)
C18	0.0250 (10)	0.0221 (10)	0.0189 (10)	−0.0074 (8)	−0.0053 (8)	0.0015 (8)
C19	0.0294 (14)	0.0411 (16)	0.0271 (13)	−0.0159 (13)	0.0017 (11)	−0.0037 (12)
C20	0.0416 (16)	0.0350 (15)	0.0300 (15)	−0.0172 (13)	−0.0176 (12)	0.0068 (12)
C21	0.0318 (14)	0.0272 (14)	0.0443 (17)	−0.0040 (11)	−0.0037 (12)	−0.0151 (12)
C19A	0.037 (8)	0.035 (8)	0.040 (8)	−0.006 (7)	−0.006 (7)	−0.003 (7)
C21A	0.043 (8)	0.058 (9)	0.048 (9)	−0.021 (8)	−0.012 (7)	−0.012 (8)
C20A	0.040 (8)	0.036 (8)	0.062 (9)	−0.023 (7)	−0.025 (7)	0.001 (7)

Geometric parameters (Å, º)

Br1—C11	1.9001 (19)	C15—H15C	0.9800
O1—C1	1.358 (2)	C16—H16A	0.9800
O1—H1	0.858 (10)	C16—H16B	0.9800
N1—C7	1.279 (3)	C16—H16C	0.9800
N1—C8	1.425 (2)	C17—H17A	0.9800
C1—C2	1.409 (3)	C17—H17B	0.9800

C1—C6	1.409 (3)	C17—H17C	0.9800
C2—C3	1.396 (3)	C18—C19	1.511 (3)
C2—C14	1.540 (3)	C18—C20	1.522 (3)
C3—H3	0.9500	C18—C21	1.561 (3)
C3—C4	1.402 (3)	C18—C19A	1.536 (7)
C4—C5	1.381 (3)	C18—C21A	1.510 (7)
C4—C18	1.531 (3)	C18—C20A	1.571 (7)
C5—H5	0.9500	C19—H19A	0.9800
C5—C6	1.395 (3)	C19—H19B	0.9800
C6—C7	1.453 (3)	C19—H19C	0.9800
C7—H7	0.9500	C20—H20A	0.9800
C8—C9	1.392 (3)	C20—H20B	0.9800
C8—C13	1.388 (3)	C20—H20C	0.9800
C9—H9	0.9500	C21—H21A	0.9800
C9—C10	1.384 (3)	C21—H21B	0.9800
C10—H10	0.9500	C21—H21C	0.9800
C10—C11	1.383 (3)	C19A—H19D	0.9800
C11—C12	1.383 (3)	C19A—H19E	0.9800
C12—H12	0.9500	C19A—H19F	0.9800
C12—C13	1.391 (3)	C21A—H21D	0.9800
C13—H13	0.9500	C21A—H21E	0.9800
C14—C15	1.531 (3)	C21A—H21F	0.9800
C14—C16	1.541 (3)	C20A—H20D	0.9800
C14—C17	1.536 (3)	C20A—H20E	0.9800
C15—H15A	0.9800	C20A—H20F	0.9800
C15—H15B	0.9800		

C1—O1—H1	108 (2)	H16A—C16—H16C	109.5
C7—N1—C8	118.93 (18)	H16B—C16—H16C	109.5
O1—C1—C2	120.33 (17)	C14—C17—H17A	109.5
O1—C1—C6	119.70 (17)	C14—C17—H17B	109.5
C6—C1—C2	119.97 (17)	C14—C17—H17C	109.5
C1—C2—C14	121.56 (17)	H17A—C17—H17B	109.5
C3—C2—C1	116.94 (17)	H17A—C17—H17C	109.5
C3—C2—C14	121.50 (17)	H17B—C17—H17C	109.5
C2—C3—H3	117.7	C4—C18—C21	109.41 (17)
C2—C3—C4	124.55 (18)	C4—C18—C19A	113.1 (7)
C4—C3—H3	117.7	C4—C18—C20A	106.3 (6)
C3—C4—C18	122.70 (17)	C19—C18—C4	109.53 (17)
C5—C4—C3	116.54 (17)	C19—C18—C20	110.4 (2)
C5—C4—C18	120.73 (17)	C19—C18—C21	108.6 (2)
C4—C5—H5	119.1	C20—C18—C4	112.36 (17)
C4—C5—C6	121.90 (18)	C20—C18—C21	106.5 (2)
C6—C5—H5	119.1	C19A—C18—C20A	103.8 (7)
C1—C6—C7	121.97 (17)	C21A—C18—C4	113.6 (7)
C5—C6—C1	120.07 (17)	C21A—C18—C19A	112.3 (8)
C5—C6—C7	117.91 (18)	C21A—C18—C20A	106.9 (7)
N1—C7—C6	123.57 (19)	C18—C19—H19A	109.5

N1—C7—H7	118.2	C18—C19—H19B	109.5
C6—C7—H7	118.2	C18—C19—H19C	109.5
C9—C8—N1	122.83 (18)	H19A—C19—H19B	109.5
C13—C8—N1	117.93 (18)	H19A—C19—H19C	109.5
C13—C8—C9	119.24 (18)	H19B—C19—H19C	109.5
C8—C9—H9	119.7	C18—C20—H20A	109.5
C10—C9—C8	120.66 (19)	C18—C20—H20B	109.5
C10—C9—H9	119.7	C18—C20—H20C	109.5
C9—C10—H10	120.4	H20A—C20—H20B	109.5
C11—C10—C9	119.11 (19)	H20A—C20—H20C	109.5
C11—C10—H10	120.4	H20B—C20—H20C	109.5
C10—C11—Br1	118.52 (15)	C18—C21—H21A	109.5
C12—C11—Br1	120.06 (15)	C18—C21—H21B	109.5
C12—C11—C10	121.42 (18)	C18—C21—H21C	109.5
C11—C12—H12	120.6	H21A—C21—H21B	109.5
C11—C12—C13	118.85 (18)	H21A—C21—H21C	109.5
C13—C12—H12	120.6	H21B—C21—H21C	109.5
C8—C13—C12	120.69 (19)	C18—C19A—H19D	109.5
C8—C13—H13	119.7	C18—C19A—H19E	109.5
C12—C13—H13	119.7	C18—C19A—H19F	109.5
C2—C14—C16	109.76 (16)	H19D—C19A—H19E	109.5
C15—C14—C2	112.14 (16)	H19D—C19A—H19F	109.5
C15—C14—C16	107.67 (17)	H19E—C19A—H19F	109.5
C15—C14—C17	107.06 (16)	C18—C21A—H21D	109.5
C17—C14—C2	110.26 (16)	C18—C21A—H21E	109.5
C17—C14—C16	109.88 (17)	C18—C21A—H21F	109.5
C14—C15—H15A	109.5	H21D—C21A—H21E	109.5
C14—C15—H15B	109.5	H21D—C21A—H21F	109.5
C14—C15—H15C	109.5	H21E—C21A—H21F	109.5
H15A—C15—H15B	109.5	C18—C20A—H20D	109.5
H15A—C15—H15C	109.5	C18—C20A—H20E	109.5
H15B—C15—H15C	109.5	C18—C20A—H20F	109.5
C14—C16—H16A	109.5	H20D—C20A—H20E	109.5
C14—C16—H16B	109.5	H20D—C20A—H20F	109.5
C14—C16—H16C	109.5	H20E—C20A—H20F	109.5
H16A—C16—H16B	109.5		

Br1—C11—C12—C13	179.78 (15)	C3—C4—C18—C20A	30.2 (7)
O1—C1—C2—C3	179.74 (17)	C4—C5—C6—C1	−1.1 (3)
O1—C1—C2—C14	−0.4 (3)	C4—C5—C6—C7	176.38 (18)
O1—C1—C6—C5	−179.00 (18)	C5—C4—C18—C19	−75.6 (3)
O1—C1—C6—C7	3.6 (3)	C5—C4—C18—C20	161.3 (2)
N1—C8—C9—C10	−178.1 (2)	C5—C4—C18—C21	43.2 (3)
N1—C8—C13—C12	178.08 (18)	C5—C4—C18—C19A	−35.0 (8)
C1—C2—C3—C4	−0.3 (3)	C5—C4—C18—C21A	94.6 (8)
C1—C2—C14—C15	179.49 (17)	C5—C4—C18—C20A	−148.2 (7)
C1—C2—C14—C16	59.9 (2)	C5—C6—C7—N1	−179.40 (19)
C1—C2—C14—C17	−61.3 (2)	C6—C1—C2—C3	−1.1 (3)

C1—C6—C7—N1	−1.9 (3)	C6—C1—C2—C14	178.78 (17)
C2—C1—C6—C5	1.8 (3)	C7—N1—C8—C9	28.2 (3)
C2—C1—C6—C7	−175.62 (18)	C7—N1—C8—C13	−152.0 (2)
C2—C3—C4—C5	1.0 (3)	C8—N1—C7—C6	177.84 (18)
C2—C3—C4—C18	−177.46 (18)	C8—C9—C10—C11	−0.7 (3)
C3—C2—C14—C15	−0.7 (3)	C9—C8—C13—C12	−2.1 (3)
C3—C2—C14—C16	−120.3 (2)	C9—C10—C11—Br1	−179.84 (16)
C3—C2—C14—C17	118.5 (2)	C9—C10—C11—C12	−0.7 (3)
C3—C4—C5—C6	−0.2 (3)	C10—C11—C12—C13	0.7 (3)
C3—C4—C18—C19	102.7 (2)	C11—C12—C13—C8	0.8 (3)
C3—C4—C18—C20	−20.3 (3)	C13—C8—C9—C10	2.0 (3)
C3—C4—C18—C21	−138.4 (2)	C14—C2—C3—C4	179.82 (18)
C3—C4—C18—C19A	143.4 (8)	C18—C4—C5—C6	178.26 (18)
C3—C4—C18—C21A	−87.1 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.86 (1)	1.84 (2)	2.622 (2)	151 (3)

(*E*)-6-{[(4-Bromophenyl)imino]methyl}-2,4-di-*tert*-butylphenol (3_100K)

Crystal data

$C_{21}H_{26}BrNO$
$M_r = 388.34$
Monoclinic, $P2_1/c$
$a = 17.4450$ (3) Å
$b = 10.69412$ (16) Å
$c = 10.15010$ (17) Å
$\beta = 90.1557$ (16)°
$V = 1893.58$ (5) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.362$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 13594 reflections
$\theta = 3.0$–34.3°
$\mu = 2.18$ mm^{-1}
$T = 100$ K
Needle, yellow
0.3 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.3620 pixels mm^{-1}
ω and π scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2012)
$T_{min} = 0.692$, $T_{max} = 1.000$
28200 measured reflections
4491 independent reflections
3799 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.9$°, $\theta_{min} = 3.0$°
$h = -22 \rightarrow 22$
$k = -9 \rightarrow 14$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.060$
$S = 1.04$
4491 reflections
227 parameters
22 restraints
Primary atom site location: iterative
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 1.2915P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	−0.13933 (2)	0.43538 (2)	−0.28775 (2)	0.02035 (6)
O1	0.18475 (7)	0.01027 (11)	0.15496 (11)	0.0181 (2)
N1	0.11754 (8)	0.19817 (13)	0.03472 (13)	0.0166 (3)
C1	0.23415 (9)	0.09407 (15)	0.20904 (15)	0.0146 (3)
C2	0.29006 (9)	0.05468 (14)	0.30067 (15)	0.0138 (3)
C3	0.33886 (9)	0.14656 (15)	0.35168 (15)	0.0144 (3)
H3	0.376570	0.121268	0.413895	0.017*
C4	0.33593 (9)	0.27321 (15)	0.31735 (15)	0.0142 (3)
C5	0.27967 (9)	0.30790 (15)	0.22833 (16)	0.0154 (3)
H5	0.275740	0.393149	0.202869	0.019*
C6	0.22853 (9)	0.22134 (15)	0.17486 (15)	0.0150 (3)
C7	0.16834 (9)	0.26823 (15)	0.08879 (16)	0.0174 (3)
H7	0.166524	0.355509	0.071650	0.021*
C8	0.05948 (9)	0.25507 (15)	−0.04414 (15)	0.0158 (3)
C9	0.07046 (10)	0.36729 (16)	−0.11150 (17)	0.0208 (4)
H9	0.118968	0.407533	−0.107976	0.025*
C10	0.01145 (10)	0.42060 (16)	−0.18335 (16)	0.0205 (4)
H10	0.019048	0.497335	−0.228634	0.025*
C11	−0.05873 (9)	0.36073 (15)	−0.18841 (15)	0.0160 (3)
C12	−0.07095 (9)	0.24801 (15)	−0.12469 (16)	0.0181 (3)
H12	−0.119309	0.207431	−0.129914	0.022*
C13	−0.01112 (9)	0.19534 (15)	−0.05293 (16)	0.0179 (3)
H13	−0.018570	0.117663	−0.009402	0.021*
C14	0.29671 (9)	−0.08308 (14)	0.34338 (15)	0.0153 (3)
C15	0.36162 (10)	−0.10331 (16)	0.44310 (17)	0.0206 (4)
H15A	0.351478	−0.054064	0.522594	0.031*
H15B	0.410326	−0.076645	0.404282	0.031*
H15C	0.364567	−0.192154	0.466219	0.031*
C16	0.31359 (10)	−0.16574 (15)	0.22250 (17)	0.0204 (4)
H16A	0.362649	−0.140865	0.183675	0.031*
H16B	0.272616	−0.155370	0.157158	0.031*
H16C	0.316225	−0.253535	0.249797	0.031*
C17	0.22203 (10)	−0.12617 (16)	0.40988 (17)	0.0205 (4)
H17A	0.179111	−0.116069	0.348292	0.031*
H17B	0.212820	−0.075515	0.488723	0.031*
H17C	0.226611	−0.214355	0.434947	0.031*
C18	0.39307 (9)	0.36988 (14)	0.37038 (15)	0.0152 (3)

C19	0.45373 (10)	0.39566 (18)	0.26508 (17)	0.0239 (4)
H19A	0.428702	0.426618	0.184911	0.036*
H19B	0.481412	0.318215	0.245215	0.036*
H19C	0.489891	0.458656	0.297712	0.036*
C20	0.43335 (11)	0.32435 (17)	0.49562 (17)	0.0252 (4)
H20A	0.467029	0.390454	0.529255	0.038*
H20B	0.463885	0.249890	0.475419	0.038*
H20C	0.394933	0.303543	0.562384	0.038*
C21	0.35161 (10)	0.49285 (16)	0.40367 (19)	0.0253 (4)
H21A	0.311491	0.476559	0.468845	0.038*
H21B	0.328419	0.527413	0.323523	0.038*
H21C	0.388530	0.552878	0.439846	0.038*
H1	0.1539 (11)	0.051 (2)	0.106 (2)	0.048 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01862 (9)	0.02097 (9)	0.02144 (9)	0.00471 (7)	−0.00577 (6)	0.00085 (7)
O1	0.0184 (6)	0.0135 (6)	0.0223 (6)	−0.0024 (5)	−0.0070 (5)	−0.0010 (5)
N1	0.0146 (6)	0.0178 (7)	0.0174 (7)	0.0007 (6)	−0.0028 (5)	−0.0008 (6)
C1	0.0137 (7)	0.0150 (8)	0.0151 (7)	−0.0018 (6)	0.0002 (6)	−0.0030 (6)
C2	0.0158 (7)	0.0120 (7)	0.0136 (7)	0.0000 (6)	0.0012 (6)	−0.0012 (6)
C3	0.0140 (7)	0.0159 (8)	0.0132 (7)	0.0008 (6)	−0.0006 (6)	0.0006 (6)
C4	0.0150 (7)	0.0141 (7)	0.0136 (7)	−0.0007 (6)	0.0007 (6)	−0.0011 (6)
C5	0.0177 (8)	0.0111 (7)	0.0174 (8)	−0.0005 (6)	−0.0016 (6)	0.0003 (6)
C6	0.0150 (7)	0.0151 (8)	0.0150 (8)	0.0013 (6)	−0.0011 (6)	−0.0002 (6)
C7	0.0195 (8)	0.0140 (8)	0.0186 (8)	0.0023 (6)	−0.0025 (6)	−0.0014 (6)
C8	0.0162 (8)	0.0172 (8)	0.0141 (7)	0.0024 (6)	−0.0022 (6)	−0.0022 (6)
C9	0.0168 (8)	0.0251 (9)	0.0206 (8)	−0.0057 (7)	−0.0030 (7)	0.0035 (7)
C10	0.0221 (8)	0.0207 (9)	0.0186 (8)	−0.0030 (7)	−0.0020 (7)	0.0055 (7)
C11	0.0163 (8)	0.0180 (8)	0.0137 (7)	0.0033 (6)	−0.0030 (6)	−0.0024 (6)
C12	0.0149 (8)	0.0181 (8)	0.0212 (8)	−0.0020 (7)	−0.0020 (6)	−0.0022 (7)
C13	0.0200 (8)	0.0141 (8)	0.0196 (8)	0.0003 (7)	−0.0021 (6)	0.0008 (6)
C14	0.0182 (8)	0.0117 (7)	0.0159 (8)	−0.0006 (6)	−0.0002 (6)	0.0008 (6)
C15	0.0248 (9)	0.0151 (8)	0.0219 (9)	0.0014 (7)	−0.0036 (7)	0.0046 (7)
C16	0.0275 (9)	0.0127 (8)	0.0210 (9)	0.0018 (7)	−0.0001 (7)	−0.0007 (7)
C17	0.0246 (9)	0.0160 (8)	0.0210 (8)	−0.0032 (7)	0.0019 (7)	0.0014 (7)
C18	0.0182 (8)	0.0139 (8)	0.0136 (7)	−0.0030 (6)	−0.0025 (6)	0.0001 (6)
C19	0.0230 (9)	0.0278 (9)	0.0209 (9)	−0.0098 (8)	0.0005 (7)	−0.0032 (7)
C20	0.0305 (10)	0.0228 (9)	0.0224 (9)	−0.0092 (8)	−0.0116 (7)	0.0029 (7)
C21	0.0255 (9)	0.0191 (9)	0.0314 (10)	−0.0014 (7)	−0.0030 (8)	−0.0084 (8)

Geometric parameters (Å, º)

Br1—C11	1.9034 (15)	C13—H13	0.9500
O1—C1	1.3581 (19)	C14—C15	1.532 (2)
O1—H1	0.854 (10)	C14—C16	1.541 (2)
N1—C7	1.283 (2)	C14—C17	1.540 (2)

N1—C8	1.426 (2)	C15—H15A	0.9800
C1—C2	1.410 (2)	C15—H15B	0.9800
C1—C6	1.408 (2)	C15—H15C	0.9800
C2—C3	1.399 (2)	C16—H16A	0.9800
C2—C14	1.540 (2)	C16—H16B	0.9800
C3—H3	0.9500	C16—H16C	0.9800
C3—C4	1.399 (2)	C17—H17A	0.9800
C4—C5	1.383 (2)	C17—H17B	0.9800
C4—C18	1.533 (2)	C17—H17C	0.9800
C5—H5	0.9500	C18—C19	1.531 (2)
C5—C6	1.394 (2)	C18—C20	1.530 (2)
C6—C7	1.453 (2)	C18—C21	1.539 (2)
C7—H7	0.9500	C19—H19A	0.9800
C8—C9	1.395 (2)	C19—H19B	0.9800
C8—C13	1.390 (2)	C19—H19C	0.9800
C9—H9	0.9500	C20—H20A	0.9800
C9—C10	1.383 (2)	C20—H20B	0.9800
C10—H10	0.9500	C20—H20C	0.9800
C10—C11	1.383 (2)	C21—H21A	0.9800
C11—C12	1.385 (2)	C21—H21B	0.9800
C12—H12	0.9500	C21—H21C	0.9800
C12—C13	1.390 (2)		

C1—O1—H1	107.4 (16)	C17—C14—C2	110.28 (13)
C7—N1—C8	118.68 (14)	C17—C14—C16	109.94 (13)
O1—C1—C2	120.42 (14)	C14—C15—H15A	109.5
O1—C1—C6	119.65 (14)	C14—C15—H15B	109.5
C6—C1—C2	119.92 (14)	C14—C15—H15C	109.5
C1—C2—C14	121.53 (13)	H15A—C15—H15B	109.5
C3—C2—C1	116.97 (14)	H15A—C15—H15C	109.5
C3—C2—C14	121.51 (14)	H15B—C15—H15C	109.5
C2—C3—H3	117.8	C14—C16—H16A	109.5
C2—C3—C4	124.48 (15)	C14—C16—H16B	109.5
C4—C3—H3	117.8	C14—C16—H16C	109.5
C3—C4—C18	122.83 (14)	H16A—C16—H16B	109.5
C5—C4—C3	116.59 (14)	H16A—C16—H16C	109.5
C5—C4—C18	120.55 (14)	H16B—C16—H16C	109.5
C4—C5—H5	119.1	C14—C17—H17A	109.5
C4—C5—C6	121.90 (15)	C14—C17—H17B	109.5
C6—C5—H5	119.1	C14—C17—H17C	109.5
C1—C6—C7	122.09 (14)	H17A—C17—H17B	109.5
C5—C6—C1	120.12 (14)	H17A—C17—H17C	109.5
C5—C6—C7	117.73 (14)	H17B—C17—H17C	109.5
N1—C7—C6	123.57 (15)	C4—C18—C21	110.36 (13)
N1—C7—H7	118.2	C19—C18—C4	109.05 (13)
C6—C7—H7	118.2	C19—C18—C21	109.00 (14)
C9—C8—N1	122.97 (14)	C20—C18—C4	111.95 (13)
C13—C8—N1	117.90 (14)	C20—C18—C19	108.70 (14)

C13—C8—C9	119.13 (15)	C20—C18—C21	107.73 (14)
C8—C9—H9	119.7	C18—C19—H19A	109.5
C10—C9—C8	120.68 (15)	C18—C19—H19B	109.5
C10—C9—H9	119.7	C18—C19—H19C	109.5
C9—C10—H10	120.4	H19A—C19—H19B	109.5
C11—C10—C9	119.11 (16)	H19A—C19—H19C	109.5
C11—C10—H10	120.4	H19B—C19—H19C	109.5
C10—C11—Br1	118.57 (12)	C18—C20—H20A	109.5
C10—C11—C12	121.55 (15)	C18—C20—H20B	109.5
C12—C11—Br1	119.87 (12)	C18—C20—H20C	109.5
C11—C12—H12	120.6	H20A—C20—H20B	109.5
C11—C12—C13	118.75 (15)	H20A—C20—H20C	109.5
C13—C12—H12	120.6	H20B—C20—H20C	109.5
C8—C13—C12	120.75 (15)	C18—C21—H21A	109.5
C8—C13—H13	119.6	C18—C21—H21B	109.5
C12—C13—H13	119.6	C18—C21—H21C	109.5
C2—C14—C16	109.81 (13)	H21A—C21—H21B	109.5
C15—C14—C2	112.09 (13)	H21A—C21—H21C	109.5
C15—C14—C16	107.61 (13)	H21B—C21—H21C	109.5
C15—C14—C17	107.03 (13)		

Br1—C11—C12—C13	179.90 (12)	C3—C4—C18—C21	−139.68 (16)
O1—C1—C2—C3	179.87 (14)	C4—C5—C6—C1	−1.3 (2)
O1—C1—C2—C14	−0.6 (2)	C4—C5—C6—C7	176.08 (15)
O1—C1—C6—C5	−179.06 (14)	C5—C4—C18—C19	−77.25 (19)
O1—C1—C6—C7	3.7 (2)	C5—C4—C18—C20	162.43 (15)
N1—C8—C9—C10	−177.94 (16)	C5—C4—C18—C21	42.4 (2)
N1—C8—C13—C12	177.87 (15)	C5—C6—C7—N1	−179.34 (16)
C1—C2—C3—C4	−0.4 (2)	C6—C1—C2—C3	−1.2 (2)
C1—C2—C14—C15	179.83 (14)	C6—C1—C2—C14	178.39 (14)
C1—C2—C14—C16	60.27 (19)	C7—N1—C8—C9	28.0 (2)
C1—C2—C14—C17	−61.03 (19)	C7—N1—C8—C13	−151.64 (16)
C1—C6—C7—N1	−2.1 (3)	C8—N1—C7—C6	177.74 (14)
C2—C1—C6—C5	2.0 (2)	C8—C9—C10—C11	−0.4 (3)
C2—C1—C6—C7	−175.24 (15)	C9—C8—C13—C12	−1.8 (2)
C2—C3—C4—C5	1.1 (2)	C9—C10—C11—Br1	180.00 (13)
C2—C3—C4—C18	−176.87 (15)	C9—C10—C11—C12	−0.9 (3)
C3—C2—C14—C15	−0.6 (2)	C10—C11—C12—C13	0.8 (2)
C3—C2—C14—C16	−120.18 (16)	C11—C12—C13—C8	0.6 (2)
C3—C2—C14—C17	118.52 (16)	C13—C8—C9—C10	1.7 (3)
C3—C4—C5—C6	−0.2 (2)	C14—C2—C3—C4	−179.94 (15)
C3—C4—C18—C19	100.62 (18)	C18—C4—C5—C6	177.76 (14)
C3—C4—C18—C20	−19.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.85 (1)	1.84 (1)	2.6257 (18)	152 (2)

Hydrogen-bond geometry (Å, °)

Compound	Temperature (K)	*D*—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
1A	100	O1—H1···N1	0.94 (3)	1.72 (3)	2.587 (2)	151 (2)
1B	120	O1—H1···N1	0.96 (3)	1.64 (3)	2.544 (2)	155 (2)
2	300	O1—H1···N1	0.84 (4)	1.84 (4)	2.612 (4)	151 (4)
	250	O1—H1···N1	0.91 (3)	1.76 (4)	2.615 (4)	155 (3)
	200	O1—H1···N1	0.90 (3)	1.78 (3)	2.611 (3)	153 (3)
	150	O1—H1···N1	0.92 (3)	1.77 (3)	2.615 (3)	151 (3)
	120	O1—H1···N1	0.86 (4)	1.82 (4)	2.633 (3)	157 (4)
	100	O1—H1···N1	0.94 (4)	1.77 (4)	2.626 (3)	150 (3)
3	300	O1—H1···N1	0.83 (5)	1.84 (5)	2.614 (4)	154 (5)
	250	O1—H1···N1	0.84 (3)	1.83 (3)	2.612 (3)	154 (3)
	200	O1—H1···N1	0.82 (3)	1.85 (3)	2.611 (2)	153 (3)
	150	O1—H1···N1	0.86 (1)	1.83 (2)	2.612 (2)	152 (3)
	120	O1—H1···N1	0.86 (1)	1.84 (2)	2.622 (2)	151 (3)
	100	O1—H1···N1	0.85 (1)	1.84 (1)	2.6257 (18)	152 (2)