Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS
ISSN 2056-9890

Crystal structure and Hirshfeld surface analysis of 4-bromo-2-[3-methyl-5-(2,4,6-trimethylbenzyl)-oxazolidin-2-yl]phenol

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Received 26 May 2022
Accepted 2 June 2022

Edited by B. Therrien, University of Neuchâtel, Switzerland

Keywords: crystal structure; 1,3-oxazolidine; hydrogen bond; van der Waals interactions; Hirshfeld surface analysis.

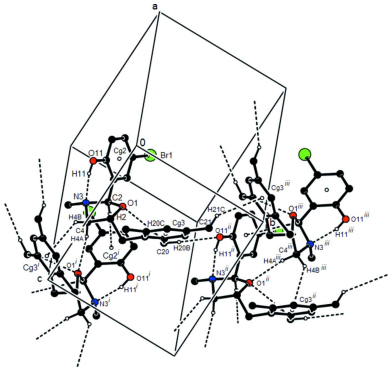
CCDC reference: 2176709

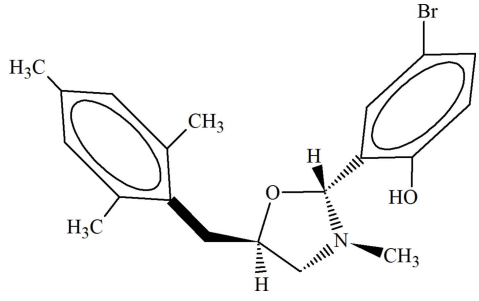
Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $C_{20}H_{24}BrNO_2$, is chiral at the carbon atoms on either side of the oxygen atom of the oxazolidine ring and crystallizes as a racemate. The 1,3-oxazolidine ring adopts an envelope conformation with the N atom in an *endo* position. The mean plane of the oxazolidine ring makes dihedral angles of 77.74 (10) and 45.50 (11)°, respectively, with the 4-bromophenol and 1,3,5-trimethylbenzene rings. In the crystal, adjacent molecules are connected *via* C—H···O hydrogen bonds and C—H···π interactions into layers parallel to the (200) plane. The packing is strengthened by van der Waals interactions between parallel molecular layers. A Hirshfeld surface analysis shows that H···H (58.2%), C···H/H···C (18.9%), and Br···H/H···Br (11.5%) interactions are the most abundant in the crystal packing.

1. Chemical context

Functionalization of amine and carbonyl compounds represents a cornerstone of organic synthesis, material science and medicinal chemistry (Zubkov *et al.*, 2018; Shikhaliyev *et al.*, 2019; Viswanathan *et al.*, 2019; Gurbanov *et al.*, 2020). In particular, the reaction of 1,2-amino alcohols with oxo compounds is an effective tool in the construction of a broad class of organic compounds such as amides, esters, enaminones, ureas, carbamates, aziridines, oxazolidines, oxazolines, oxazolidinones, oxazines, pyrroles, pyridones, morpholines, acridinones *etc* (Juhász *et al.*, 2011; Tamura *et al.*, 2014; Sepideh *et al.*, 2018; Khalilov, 2021).





In the context of our recent studies, herein we report the structural analysis of a 1,3-oxazolidine, synthesized on the base of racemic 1,2-amino alcohol. Theoretically, in the solid

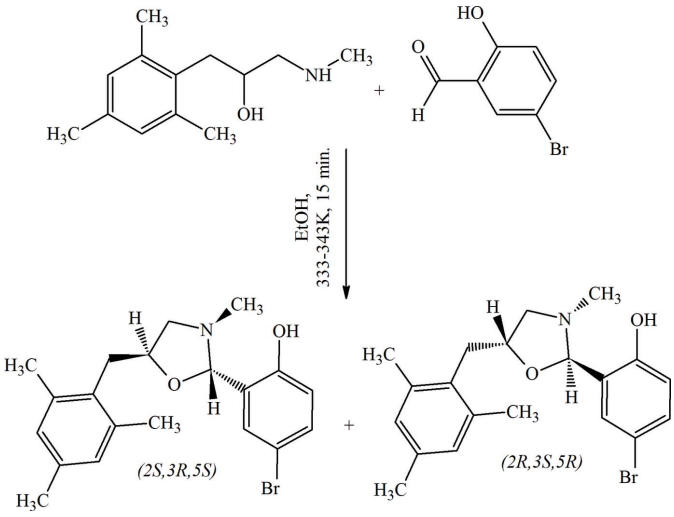


Figure 1
Synthesis of the racemic mixture of 2*R*,3*S*,5*R*- and 2*S*,3*R*,5*S*-oxazolidines.

state, this 1,3-oxazolidine can exist as eight optical isomers due to two CH and one N-chiral center. However, NMR analysis of the obtained product indicated the formation of a pair of diastereoisomers in a 1:1 ratio (Khalilov, 2021) and single-crystal X-ray analysis of the racemic mixture confirmed the 2*R*,3*S*,5*R*- and 2*S*,3*R*,5*S*-configuration of these isomers (Fig. 1).

Thus, in the framework of our ongoing structural studies (Naghiyev *et al.*, 2020, 2021, 2022; Khalilov *et al.*, 2022), we report the crystal structure and Hirshfeld surface analysis of the racemic title compound, 4-bromo-2-[3-methyl-5-(2,4,6-trimethylbenzyl)oxazolidin-2-yl]phenol.

2. Structural commentary

In the title compound, (Fig. 2), the 1,3-oxazolidine ring (O1/N3/C2/C4/C5) adopts an envelope conformation with the N atom in an *endo* position [the puckering parameters (Cremer & Pople, 1975) are $Q(2)$ = 0.413 (2) Å, $\varphi(2)$ = 256.7 (3)°]. The mean plane of th oxazolidine ring makes dihedral angles of 77.74 (10) and 45.50 (11)°, respectively, with the 4-bromophenol (C6–C11) and the 1,3,5-trimethylbenzene (C14–C19) rings. The molecular conformation is stabilized by intramolecular O11—H11···N3 and C20—H20*C*···O1 hydrogen bonds (Table 1). There are two stereogenic centers in the racaemic title compound and the chirality about the C2 and C5 atoms is *R* in the chosen asymmetric unit. The geometric properties of the title compound are normal and consistent with those of related compounds listed in the *Database survey* section.

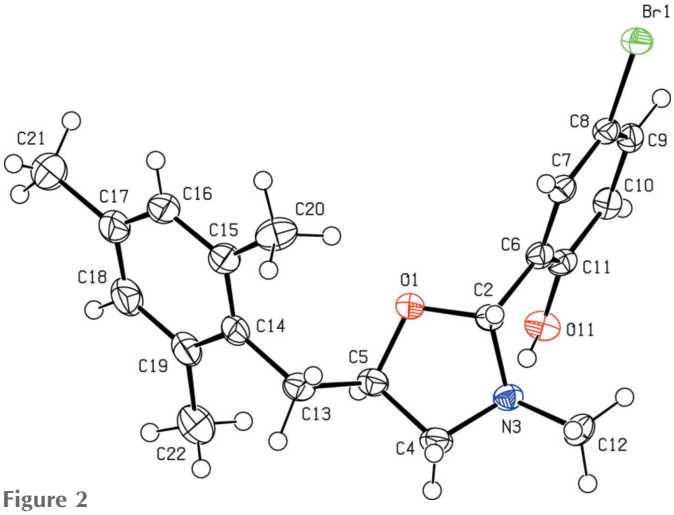


Figure 2
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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

*Cg*2 and *Cg*3 are the centroids of the 4-bromophenol (C6–C11) and 1,3,5-trimethylbenzene (C14–C19) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11···N3	0.81 (4)	1.89 (4)	2.644 (2)	155 (3)
C4—H4*A*···O1^{i}	0.99	2.58	3.564 (2)	171
C20—H20*B*···O11^{ii}	0.98	2.57	3.548 (3)	173
C20—H20*C*···O1	0.98	2.55	3.332 (3)	136
C2—H2···*Cg*2^{i}	1.00	2.91	3.908 (2)	176
C4—H4*B*···*Cg*3^{i}	0.99	2.88	3.622 (2)	132
C21—H21*C*···*Cg*3^{iii}	0.98	2.93	3.723 (4)	138

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

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, adjacent molecules are connected *via* C—H···O hydrogen bonds and C—H···π interactions into layers parallel to the (200) plane (Table 1; Figs. 3 and 4). The packing

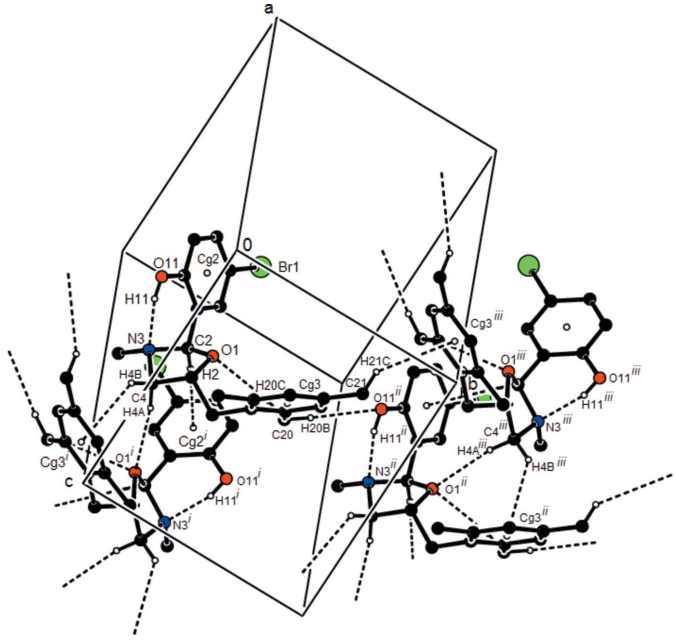


Figure 3
A general view of the C—H···O hydrogen bonding and C—H···π interactions of the title compound. Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, y+1, z$; (iii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, -y+\frac{1}{2}, z-\frac{3}{2}$.

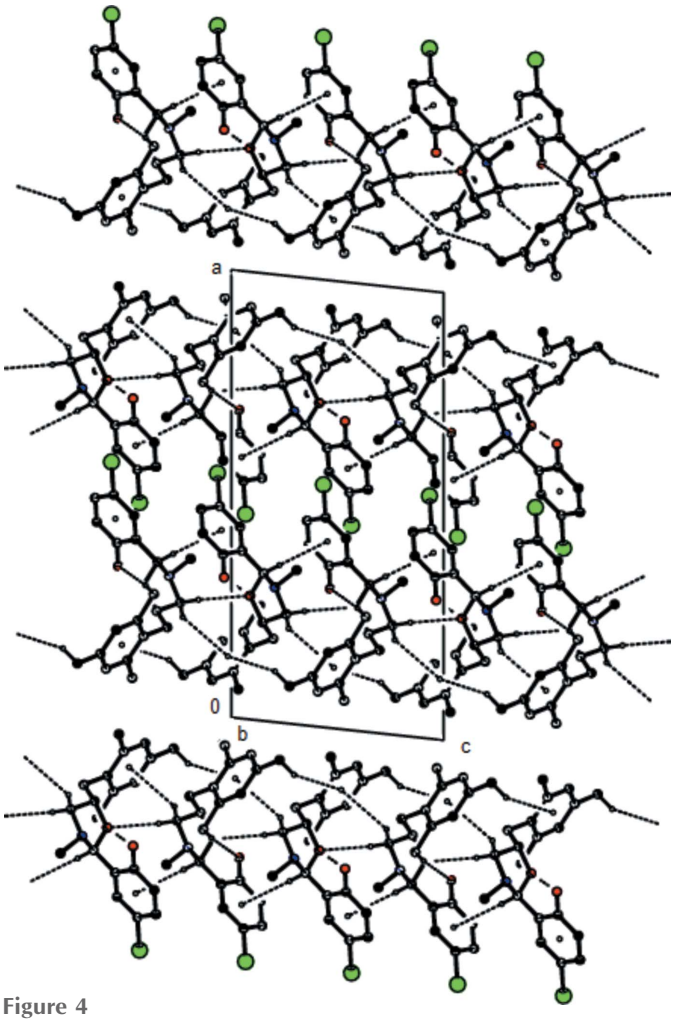


Figure 4
Packing view of the title compound along the *b* axis with the interactions depicted as in Fig. 3.

is strengthened by van der Waals interactions between parallel molecular layers.

A Hirshfeld surface analysis was performed and the associated two-dimensional fingerprint plots were obtained with *CrystalExplorer17.5* (Turner *et al.*, 2017). The overall two-dimensional fingerprint plot for the title compound is given in Fig. 5*a*, and those delineated into H···H (58.2%), C···H/H···C (18.9%), and Br···H/H···Br (11.5%) contacts are shown in Fig. 5*b–d*, while numerical details of the different contacts are given in Table 2. The O···H/H···O (8.3%), C···C (1.4%), Br···C/C···Br (1.0%), Br···O/O···Br (0.5%) and Br···Br (0.3%) contacts have little directional influence on the molecular packing. A result, in the crystal packing, C—H···π (ring) and van der Waals interactions are dominant.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016) for similar structures with a 1,3-oxazolidine ring showed that the five most closely related to the title compound are (*S*)-5-chloro-*N*-({2-oxo-3-[4-(3-oxomorpholin-4-yl)phenyl]-oxazolidin-5-yl}methyl)-thiophene-2-carboxamide [(I): Shen *et al.*, 2018], 2,2-dichloro-1-(2-phenyl-1,3-oxazolidin-3-yl)-ethanone [(II): Ye *et al.*, 2010], (4-benzyl-2-oxo-1,3-oxazolidin-5-yl)- methyl methanesulfonate [(III): Cunico *et al.*, 2010], 2-bromo-4-(3,4-dimethyl-5-phenyl-1,3-oxazolidin-2-yl)-6-methoxyphenol [(IV): Hariono *et al.*, 2012] and (*R*)-2-phenoxy-1-(4-phenyl-2-sulfanylidene-1,3-oxazolidin-3-yl)ethanone [(V): Caracelli *et al.*, 2011].

Table 2
Summary of short interatomic contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
Br1···H10	2.96	$1-x, \frac{1}{2}+y, \frac{1}{2}-z$
Br1···C12	3.598	$1-x, \frac{1}{2}+y, \frac{3}{2}-z$
C9···C8	3.409	$1-x, -y, 1-z$
H9···H7	2.45	$x, \frac{1}{2}-y, -\frac{1}{2}+z$
H11···H20*B*	2.35	$x, -1+y, z$
C15···H21*C*	2.80	$x, \frac{3}{2}-y, \frac{1}{2}+z$
H22*B*···C18	3.07	$-x, 1-y, 1-z$
H21*B*···H22*B*	2.51	$-x, \frac{1}{2}+y, \frac{1}{2}-z$

In the crystal of (I), classical N—H···O hydrogen bonds and weak C— H···O hydrogen bonds link the molecules into a three-dimensional supramolecular architecture. In (II), molecules are linked by weak intermolecular C—H···O hydrogen bonds, forming one-dimensional chains. In the crystal of (III), N—H···O hydrogen bonds, involving one of the sulfur-bound oxo groups as acceptor, lead to the formation of supramolecular chains along the *b*-axis direction. These

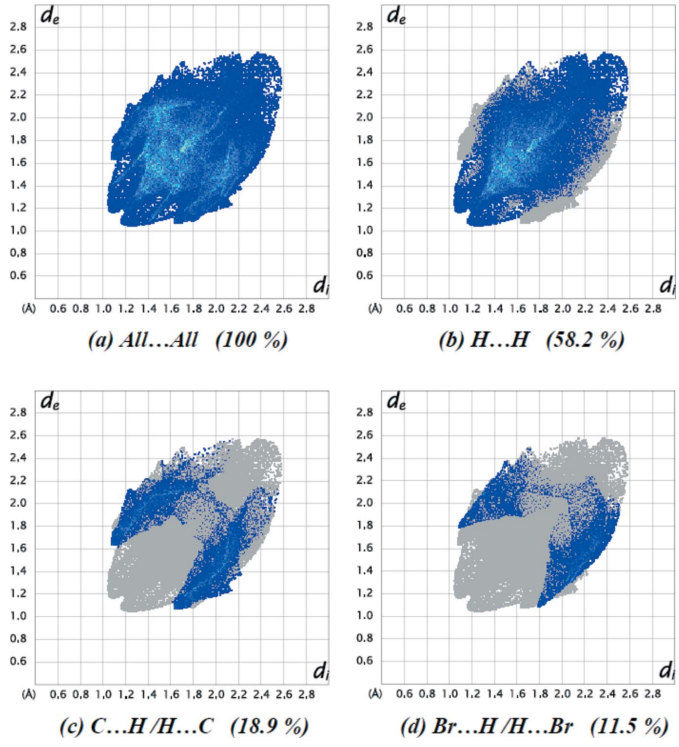


Figure 5
The two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C and (*d*) Br···H/H···Br interactions. [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively.]

chains are reinforced by C—H···O contacts, with the carbonyl O atom accepting three such interactions. In (IV), adjacent molecules are connected *via* O—H···O and C—H···O hydrogen bonds and C—H···π interactions into a zigzag chain along the *b*-axis direction. In (V), molecules are linked into supramolecular arrays two molecules thick in the *bc* plane through C—H···O, C—H···S and C—H···π interactions.

5. Synthesis and crystallization

The title compound was synthesized using our recently reported procedure (Khalilov, 2021), and colorless needle-like crystals were obtained upon recrystallization from an ethanol/water solution.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C-bound H atoms were placed at calculated positions and refined using a riding model, with C—H = 0.95 to 1.00 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). The hydroxyl H atom was found in a difference-Fourier map and was refined freely.

Acknowledgements

Authors' contributions are as follows. Conceptualization, ANK and IGM; methodology, ANK and IGM; investigation, ANK, MA and EAF; writing (original draft), MA and ANK; writing (review and editing of the manuscript), MA and ANK; visualization, MA, SÖY, ANK and IGM; funding acquisition, VNK, AB and ANK; resources, AB, VNK and EAF; supervision, ANK and MA.

Funding information

This work was supported by Baku State University and the Ministry of Science and Higher Education of the Russian Federation [award No. 075–03–2020-223 (FSSF-2020–0017)].

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{24}BrNO_2$
M_r	390.30
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	21.1019 (3), 9.01359 (11), 10.03985 (11)
β (°)	96.1425 (11)
V (Å^3)	1898.66 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	3.03
Crystal size (mm)	0.32 × 0.04 × 0.03
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.424, 0.882
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21431, 4096, 3783
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.096, 1.07
No. of reflections	4096
No. of parameters	225
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.60

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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supporting information

Acta Cryst. (2022). E**78**, 695-698 [https://doi.org/10.1107/S2056989022005928]

Crystal structure and Hirshfeld surface analysis of 4-bromo-2-[3-methyl-5-(2,4,6-trimethylbenzyl)oxazolidin-2-yl]phenol

Ali N. Khalilov, Victor N. Khrustalev, Elena A. Fortalnova, Mehmet Akkurt, Sema Öztürk Yıldırım, Ajaya Bhattarai and İbrahim G. Mamedov

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

4-Bromo-2-[3-methyl-5-(2,4,6-trimethylbenzyl)oxazolidin-2-yl]phenol

Crystal data

$C_{20}H_{24}BrNO_2$
$M_r = 390.30$
Monoclinic, $P2_1/c$
$a = 21.1019$ (3) Å
$b = 9.01359$ (11) Å
$c = 10.03985$ (11) Å
$\beta = 96.1425$ (11)°
$V = 1898.66$ (4) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.365$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 13703 reflections
$\theta = 2.1$–78.6°
$\mu = 3.03$ mm^{-1}
$T = 100$ K
Needle, colourless
0.32 × 0.04 × 0.03 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
$T_{min} = 0.424$, $T_{max} = 0.882$
21431 measured reflections
4096 independent reflections
3783 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 79.6°$, $\theta_{min} = 2.1°$
$h = -25\rightarrow26$
$k = -11\rightarrow11$
$l = -12\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.096$
$S = 1.07$
4096 reflections
225 parameters
0 restraints
Primary atom site location: difference Fourier map
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.055P)^2 + 1.11P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

Special details

Experimental. CrysAlisPro 1.171.41.117a (Rigaku OD, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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	0.54220 (2)	0.31515 (2)	0.43375 (2)	0.02813 (9)
O1	0.27633 (7)	0.25150 (17)	0.58702 (14)	0.0298 (3)
C2	0.32957 (9)	0.1726 (2)	0.65118 (19)	0.0232 (4)
H2	0.3517	0.2334	0.7256	0.028*
N3	0.30119 (8)	0.03941 (18)	0.70533 (15)	0.0240 (3)
C4	0.24396 (10)	0.0998 (2)	0.7578 (2)	0.0286 (4)
H4A	0.2548	0.1518	0.8441	0.034*
H4B	0.2124	0.0210	0.7696	0.034*
C5	0.21970 (10)	0.2075 (2)	0.6467 (2)	0.0275 (4)
H5	0.1901	0.1541	0.5785	0.033*
C6	0.37483 (9)	0.1367 (2)	0.54907 (18)	0.0226 (4)
C7	0.42805 (9)	0.2251 (2)	0.53991 (18)	0.0235 (4)
H7	0.4364	0.3066	0.5991	0.028*
C8	0.46904 (9)	0.1942 (2)	0.44404 (19)	0.0229 (4)
C9	0.45780 (9)	0.0753 (2)	0.35676 (18)	0.0238 (4)
H9	0.4865	0.0541	0.2925	0.029*
C10	0.40439 (10)	−0.0118 (2)	0.36452 (18)	0.0255 (4)
H10	0.3961	−0.0925	0.3043	0.031*
C11	0.36252 (9)	0.0175 (2)	0.45995 (18)	0.0237 (4)
O11	0.31123 (7)	−0.07205 (17)	0.46493 (15)	0.0287 (3)
H11	0.2980 (17)	−0.053 (4)	0.536 (4)	0.050 (9)*
C12	0.34457 (10)	−0.0365 (2)	0.8069 (2)	0.0295 (4)
H12A	0.3823	−0.0707	0.7665	0.044*
H12B	0.3228	−0.1218	0.8418	0.044*
H12C	0.3577	0.0323	0.8803	0.044*
C13	0.18595 (10)	0.3429 (2)	0.6965 (2)	0.0293 (4)
H13A	0.1502	0.3093	0.7453	0.035*
H13B	0.2162	0.3982	0.7606	0.035*
C14	0.16029 (10)	0.4466 (2)	0.5851 (2)	0.0288 (4)
C15	0.19383 (11)	0.5761 (2)	0.5574 (2)	0.0301 (4)
C16	0.16792 (12)	0.6723 (3)	0.4563 (2)	0.0361 (5)
H16	0.1904	0.7603	0.4389	0.043*
C17	0.11055 (12)	0.6426 (3)	0.3812 (3)	0.0430 (6)
C18	0.07858 (11)	0.5135 (4)	0.4079 (3)	0.0452 (6)

H18	0.0393	0.4915	0.3564	0.054*
C19	0.10236 (10)	0.4145 (3)	0.5084 (2)	0.0365 (5)
C20	0.25709 (13)	0.6141 (3)	0.6335 (2)	0.0393 (5)
H20A	0.2512	0.6344	0.7273	0.059*
H20B	0.2748	0.7021	0.5938	0.059*
H20C	0.2865	0.5304	0.6291	0.059*
C21	0.08362 (15)	0.7492 (5)	0.2732 (3)	0.0650 (10)
H21A	0.0776	0.8468	0.3131	0.097*
H21B	0.0425	0.7119	0.2318	0.097*
H21C	0.1133	0.7581	0.2050	0.097*
C22	0.06445 (12)	0.2765 (4)	0.5315 (3)	0.0523 (7)
H22A	0.0859	0.1897	0.4985	0.079*
H22B	0.0217	0.2853	0.4835	0.079*
H22C	0.0611	0.2651	0.6276	0.079*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02612 (13)	0.02966 (14)	0.02922 (14)	−0.00322 (7)	0.00584 (9)	0.00477 (7)
O1	0.0269 (7)	0.0344 (8)	0.0296 (7)	0.0054 (6)	0.0103 (6)	0.0108 (6)
C2	0.0242 (9)	0.0241 (9)	0.0216 (8)	−0.0010 (7)	0.0035 (7)	0.0011 (7)
N3	0.0258 (8)	0.0261 (8)	0.0201 (7)	−0.0015 (6)	0.0024 (6)	0.0029 (6)
C4	0.0291 (9)	0.0332 (10)	0.0245 (9)	−0.0019 (8)	0.0076 (7)	0.0037 (8)
C5	0.0270 (10)	0.0315 (10)	0.0249 (9)	−0.0003 (8)	0.0068 (7)	0.0021 (8)
C6	0.0254 (9)	0.0250 (9)	0.0173 (8)	0.0018 (7)	0.0018 (6)	0.0021 (7)
C7	0.0269 (9)	0.0231 (8)	0.0201 (8)	0.0005 (7)	0.0007 (7)	0.0015 (7)
C8	0.0223 (9)	0.0250 (9)	0.0212 (9)	−0.0002 (7)	0.0014 (7)	0.0040 (7)
C9	0.0257 (9)	0.0273 (9)	0.0183 (8)	0.0048 (7)	0.0018 (6)	0.0014 (7)
C10	0.0296 (9)	0.0266 (9)	0.0197 (8)	0.0039 (8)	0.0005 (7)	−0.0025 (7)
C11	0.0260 (9)	0.0238 (9)	0.0209 (8)	−0.0015 (7)	0.0002 (7)	0.0039 (7)
O11	0.0297 (7)	0.0317 (8)	0.0249 (7)	−0.0075 (6)	0.0040 (6)	−0.0043 (6)
C12	0.0347 (10)	0.0290 (10)	0.0239 (9)	0.0027 (8)	−0.0009 (8)	0.0043 (8)
C13	0.0312 (10)	0.0322 (10)	0.0260 (10)	0.0005 (8)	0.0093 (8)	0.0018 (8)
C14	0.0282 (9)	0.0335 (10)	0.0264 (9)	0.0076 (8)	0.0109 (7)	0.0004 (8)
C15	0.0369 (11)	0.0319 (10)	0.0231 (9)	0.0056 (8)	0.0102 (8)	−0.0007 (8)
C16	0.0421 (13)	0.0376 (12)	0.0314 (11)	0.0092 (9)	0.0167 (10)	0.0062 (9)
C17	0.0364 (12)	0.0587 (15)	0.0361 (12)	0.0159 (11)	0.0142 (10)	0.0169 (11)
C18	0.0252 (10)	0.0668 (17)	0.0435 (13)	0.0095 (11)	0.0032 (9)	0.0111 (12)
C19	0.0240 (9)	0.0471 (13)	0.0392 (11)	0.0059 (9)	0.0072 (8)	0.0041 (10)
C20	0.0515 (14)	0.0358 (12)	0.0306 (11)	−0.0086 (10)	0.0039 (10)	−0.0001 (9)
C21	0.0446 (15)	0.094 (3)	0.0574 (17)	0.0211 (17)	0.0119 (13)	0.0422 (19)
C22	0.0265 (11)	0.0609 (17)	0.0689 (18)	−0.0046 (12)	0.0016 (11)	0.0095 (15)

Geometric parameters (Å, º)

Br1—C8	1.9019 (19)	C12—H12B	0.9800
O1—C2	1.424 (2)	C12—H12C	0.9800
O1—C5	1.448 (2)	C13—C14	1.513 (3)

C2—N3	1.472 (2)	C13—H13A	0.9900
C2—C6	1.509 (3)	C13—H13B	0.9900
C2—H2	1.0000	C14—C19	1.404 (3)
N3—C12	1.465 (2)	C14—C15	1.407 (3)
N3—C4	1.472 (3)	C15—C16	1.401 (3)
C4—C5	1.525 (3)	C15—C20	1.505 (3)
C4—H4A	0.9900	C16—C17	1.382 (4)
C4—H4B	0.9900	C16—H16	0.9500
C5—C13	1.524 (3)	C17—C18	1.385 (4)
C5—H5	1.0000	C17—C21	1.513 (4)
C6—C7	1.388 (3)	C18—C19	1.399 (4)
C6—C11	1.404 (3)	C18—H18	0.9500
C7—C8	1.389 (3)	C19—C22	1.510 (4)
C7—H7	0.9500	C20—H20A	0.9800
C8—C9	1.388 (3)	C20—H20B	0.9800
C9—C10	1.383 (3)	C20—H20C	0.9800
C9—H9	0.9500	C21—H21A	0.9800
C10—C11	1.396 (3)	C21—H21B	0.9800
C10—H10	0.9500	C21—H21C	0.9800
C11—O11	1.356 (2)	C22—H22A	0.9800
O11—H11	0.81 (4)	C22—H22B	0.9800
C12—H12A	0.9800	C22—H22C	0.9800

C2—O1—C5	108.79 (14)	H12A—C12—H12C	109.5
O1—C2—N3	104.01 (15)	H12B—C12—H12C	109.5
O1—C2—C6	109.02 (15)	C14—C13—C5	113.25 (17)
N3—C2—C6	112.83 (16)	C14—C13—H13A	108.9
O1—C2—H2	110.3	C5—C13—H13A	108.9
N3—C2—H2	110.3	C14—C13—H13B	108.9
C6—C2—H2	110.3	C5—C13—H13B	108.9
C12—N3—C2	112.92 (16)	H13A—C13—H13B	107.7
C12—N3—C4	113.51 (15)	C19—C14—C15	119.3 (2)
C2—N3—C4	102.26 (15)	C19—C14—C13	120.0 (2)
N3—C4—C5	101.41 (15)	C15—C14—C13	120.7 (2)
N3—C4—H4A	111.5	C16—C15—C14	119.4 (2)
C5—C4—H4A	111.5	C16—C15—C20	118.9 (2)
N3—C4—H4B	111.5	C14—C15—C20	121.7 (2)
C5—C4—H4B	111.5	C17—C16—C15	121.8 (2)
H4A—C4—H4B	109.3	C17—C16—H16	119.1
O1—C5—C13	110.61 (17)	C15—C16—H16	119.1
O1—C5—C4	104.45 (16)	C16—C17—C18	118.2 (2)
C13—C5—C4	113.71 (17)	C16—C17—C21	120.5 (3)
O1—C5—H5	109.3	C18—C17—C21	121.3 (3)
C13—C5—H5	109.3	C17—C18—C19	122.1 (2)
C4—C5—H5	109.3	C17—C18—H18	119.0
C7—C6—C11	119.50 (17)	C19—C18—H18	119.0
C7—C6—C2	119.82 (17)	C18—C19—C14	119.2 (2)
C11—C6—C2	120.64 (17)	C18—C19—C22	118.8 (2)

C6—C7—C8	119.94 (18)	C14—C19—C22	122.0 (2)
C6—C7—H7	120.0	C15—C20—H20A	109.5
C8—C7—H7	120.0	C15—C20—H20B	109.5
C9—C8—C7	121.00 (18)	H20A—C20—H20B	109.5
C9—C8—Br1	119.54 (14)	C15—C20—H20C	109.5
C7—C8—Br1	119.46 (15)	H20A—C20—H20C	109.5
C10—C9—C8	119.20 (17)	H20B—C20—H20C	109.5
C10—C9—H9	120.4	C17—C21—H21A	109.5
C8—C9—H9	120.4	C17—C21—H21B	109.5
C9—C10—C11	120.70 (18)	H21A—C21—H21B	109.5
C9—C10—H10	119.7	C17—C21—H21C	109.5
C11—C10—H10	119.7	H21A—C21—H21C	109.5
O11—C11—C10	118.61 (18)	H21B—C21—H21C	109.5
O11—C11—C6	121.74 (17)	C19—C22—H22A	109.5
C10—C11—C6	119.65 (18)	C19—C22—H22B	109.5
C11—O11—H11	105 (2)	H22A—C22—H22B	109.5
N3—C12—H12A	109.5	C19—C22—H22C	109.5
N3—C12—H12B	109.5	H22A—C22—H22C	109.5
H12A—C12—H12B	109.5	H22B—C22—H22C	109.5
N3—C12—H12C	109.5		

C5—O1—C2—N3	23.8 (2)	C7—C6—C11—O11	179.93 (17)
C5—O1—C2—C6	144.39 (16)	C2—C6—C11—O11	−2.2 (3)
O1—C2—N3—C12	−163.70 (15)	C7—C6—C11—C10	0.9 (3)
C6—C2—N3—C12	78.3 (2)	C2—C6—C11—C10	178.71 (17)
O1—C2—N3—C4	−41.36 (18)	O1—C5—C13—C14	64.6 (2)
C6—C2—N3—C4	−159.35 (16)	C4—C5—C13—C14	−178.21 (18)
C12—N3—C4—C5	163.78 (17)	C5—C13—C14—C19	80.4 (2)
C2—N3—C4—C5	41.84 (18)	C5—C13—C14—C15	−99.8 (2)
C2—O1—C5—C13	125.28 (18)	C19—C14—C15—C16	1.7 (3)
C2—O1—C5—C4	2.6 (2)	C13—C14—C15—C16	−178.05 (18)
N3—C4—C5—O1	−27.6 (2)	C19—C14—C15—C20	−178.2 (2)
N3—C4—C5—C13	−148.32 (17)	C13—C14—C15—C20	2.1 (3)
O1—C2—C6—C7	98.9 (2)	C14—C15—C16—C17	−1.0 (3)
N3—C2—C6—C7	−146.13 (17)	C20—C15—C16—C17	178.9 (2)
O1—C2—C6—C11	−79.0 (2)	C15—C16—C17—C18	−0.1 (4)
N3—C2—C6—C11	36.0 (2)	C15—C16—C17—C21	179.6 (2)
C11—C6—C7—C8	−0.7 (3)	C16—C17—C18—C19	0.5 (4)
C2—C6—C7—C8	−178.59 (17)	C21—C17—C18—C19	−179.2 (3)
C6—C7—C8—C9	−0.2 (3)	C17—C18—C19—C14	0.2 (4)
C6—C7—C8—Br1	−179.44 (14)	C17—C18—C19—C22	179.8 (3)
C7—C8—C9—C10	1.0 (3)	C15—C14—C19—C18	−1.3 (3)
Br1—C8—C9—C10	−179.76 (14)	C13—C14—C19—C18	178.4 (2)
C8—C9—C10—C11	−0.9 (3)	C15—C14—C19—C22	179.1 (2)
C9—C10—C11—O11	−179.15 (17)	C13—C14—C19—C22	−1.1 (3)
C9—C10—C11—C6	−0.1 (3)		

Hydrogen-bond geometry (Å, º)

*Cg*2 and *Cg*3 are the centroids of the 4-bromophenol (C6–C11) and 1,3,5-trimethylbenzene (C14–C19) rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11···N3	0.81 (4)	1.89 (4)	2.644 (2)	155 (3)
C4—H4*A*···O1^{i}	0.99	2.58	3.564 (2)	171
C20—H20*B*···O11^{ii}	0.98	2.57	3.548 (3)	173
C20—H20*C*···O1	0.98	2.55	3.332 (3)	136
C2—H2···*Cg*2^{i}	1.00	2.91	3.908 (2)	176
C4—H4*B*···*Cg*3^{i}	0.99	2.88	3.622 (2)	132
C21—H21*C*···*Cg*3^{iii}	0.98	2.93	3.723 (4)	138

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*, *y*+1, *z*; (iii) *x*, −*y*+3/2, *z*−1/2.