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Crystal structure of 1-(3-bromopropyl)-2-((4-chlorophenoxy)methyl)-4-methyl-1*H*-benzo[*d*]imidazole, $C_{18}H_{18}BrClN_2O$

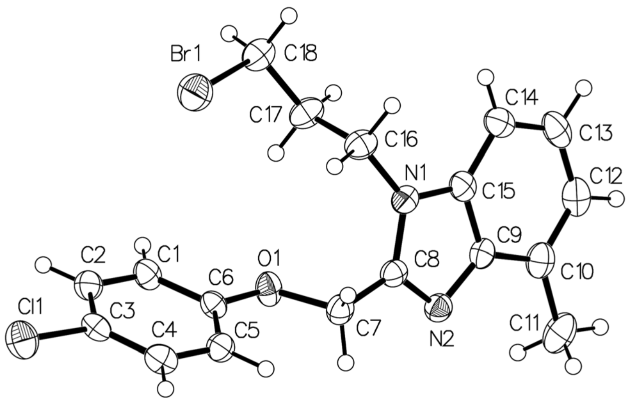

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.11 × 0.05 × 0.04 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	2.57 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	26.4°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9844, 3459, 0.040
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2773
$N(param)_{refined}$:	209
Programs:	CrysAlis^PRO [1], Olex2 [2], SHELX [3, 4]

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Abstract

$C_{18}H_{18}BrClN_2O$, triclinic, $P\bar{1}$ (no. 2), a = 9.0583(4) Å, b = 9.2694(4) Å, c = 11.1183(4) Å, α = 83.1120(10)°, β = 72.2590(10)°, γ = 73.9400(10)°, V = 853.80(6) $Å^3$, Z = 2, $R_{gt}(F)$ = 0.0381, $wR_{ref}(F^2)$ = 0.0969, T = 170 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

A mixture of 2-((4-chlorophenoxy)methyl)-4-methyl-1*H*-benzo[*d*] imidazole (136 mg, 0.5 mmol), 1,3-dibromopropane (200 mg, 1.0 mmol), DMF (8 mL), K_2CO_3 (138 mg, 1.0 mmol) was added in a tube. The reaction system was heated to 75 °C for 5 h and monitored by thin-layer chromatography. After the reaction was completed, brine (20 mL) was added. The mixture was extracted with DCM (20 mL) three times. The organic phases were combined, dried over anhydrous sodium sulfate, and evaporated under reduced pressure. The product was separated by silica gel column chromatography with ethyl acetate and petroleum ether (v/v = 15/85) to obtain the title compound (white solid, yield 75%).

Experimental details

All hydrogen atoms were placed in idealized positions. Their U_{iso} values were set to $1.2U_{eq}$ of the parent atoms.

Comment

Benzimidazole is one of the most commonly used scaffolds because it plays an important role in drug chemotherapy and occupies a significant position in the list of chemotherapeutic drugs [5]. Many crystal structures of the derivatives with benzimidazole were reported [6–13]. The activity and structural diversity exhibited by compounds containing the benzimidazole moiety have led to the development of a series of novel and valuable bioactive benzimidazole analogs.

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

Atom	x	y	z	U_{iso}*/U_{eq}
Br1	0.61078 (4)	0.55172 (5)	0.10896 (3)	0.05187 (14)
C1	0.1994 (3)	0.6215 (3)	0.2755 (3)	0.0303 (6)
H1	0.257848	0.528796	0.303693	0.036*
C2	0.1271 (3)	0.6241 (3)	0.1823 (3)	0.0325 (6)
H2	0.135570	0.533453	0.145948	0.039*
C3	0.0421 (3)	0.7598 (3)	0.1424 (3)	0.0288 (6)
C4	0.0254 (3)	0.8915 (3)	0.1956 (3)	0.0321 (6)
H4	−0.036097	0.983610	0.169096	0.038*
C5	0.0993 (3)	0.8888 (3)	0.2890 (3)	0.0298 (6)
H5	0.089663	0.979493	0.325869	0.036*
C6	0.1869 (3)	0.7540 (3)	0.3278 (3)	0.0256 (6)
C7	0.2776 (3)	0.8750 (3)	0.4593 (3)	0.0309 (6)
H7A	0.172101	0.927908	0.513871	0.037*
H7B	0.309691	0.942020	0.385231	0.037*
C8	0.3985 (3)	0.8382 (3)	0.5309 (3)	0.0267 (6)
C9	0.5131 (3)	0.8247 (3)	0.6751 (2)	0.0272 (6)
C10	0.5479 (4)	0.8320 (3)	0.7890 (3)	0.0342 (7)
C11	0.4152 (4)	0.8807 (4)	0.9075 (3)	0.0483 (9)
H11A	0.354327	0.983649	0.894534	0.072*
H11B	0.461060	0.876771	0.977482	0.072*
H11C	0.343752	0.813313	0.927833	0.072*
C12	0.7087 (4)	0.7907 (3)	0.7834 (3)	0.0371 (7)
H12	0.737855	0.794519	0.857890	0.045*
C13	0.8303 (4)	0.7435 (3)	0.6722 (3)	0.0384 (8)
H13	0.938889	0.717236	0.673529	0.046*
C14	0.7967 (3)	0.7340 (3)	0.5610 (3)	0.0331 (7)
H14	0.878849	0.701154	0.485787	0.040*
C15	0.6352 (3)	0.7756 (3)	0.5654 (3)	0.0280 (6)
C16	0.6358 (4)	0.7271 (3)	0.3463 (3)	0.0328 (7)
H16A	0.739904	0.753309	0.311051	0.039*
H16B	0.567238	0.774645	0.290704	0.039*
C17	0.6627 (4)	0.5570 (3)	0.3501 (3)	0.0362 (7)
H17A	0.728859	0.511290	0.407900	0.043*
H17B	0.557804	0.532544	0.385728	0.043*
C18	0.7436 (4)	0.4867 (4)	0.2233 (3)	0.0383 (7)
H18A	0.767282	0.375947	0.235285	0.046*
H18B	0.846586	0.514233	0.185190	0.046*
Cl1	−0.04600 (10)	0.76262 (9)	0.02227 (7)	0.0427 (2)
N1	0.5592 (3)	0.7838 (3)	0.4732 (2)	0.0268 (5)
N2	0.3646 (3)	0.8642 (3)	0.6506 (2)	0.0288 (5)
O1	0.2661 (2)	0.7387 (2)	0.41824 (19)	0.0325 (5)

As can be seen from the figure, there is one bromopropyl group that replaced the H atom on the benzimidazole. The bond length of N1–C16 is 1.459(4) Å, and the bond length of Br1–C18 is 1.943(4) Å. The dihedral angle of the two planes formed by bromophenyl and benzimidazole is 54.87°. The bond lengths and angles within these moieties are in the expected ranges [10–13].

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