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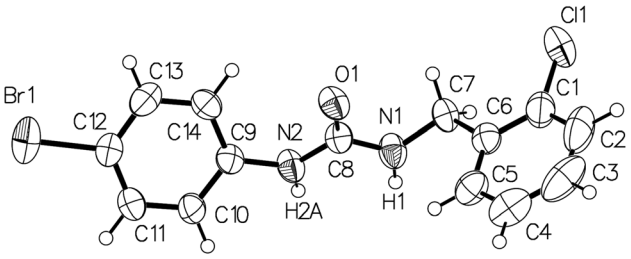
The crystal structure of 1-(4-bromophenyl)-3-(2-chlorobenzyl)urea, $C_{14}H_{12}BrClN_2O$



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Abstract

$C_{14}H_{12}BrClN_2O$, monoclinic, $P2_1/c$ (no. 14), a = 13.4072(6) Å, b = 8.6103(5) Å, c = 12.3824(6) Å, β = 100.475(4), V = 1405.60(12) Å^3, Z = 4, $R_{gt}(F)$ = 0.0499, $wR_{ref}(F^2)$ = 0.1215, T = 173 K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size	0.27 × 0.25 × 0.22 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	3.11 mm^{-1}
Diffractometer, scan mode:	Multiwire proportional, φ and ω-scans
θ_{max}, completeness:	29.3°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6337, 3236, 0.026
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1727
$N(param)_{refined}$:	173
Programs:	CrysAlis^{PRO} [1], OLEX2 [2], SHELX [3, 4]

Source of materials

The chemical reagents 1-bromo-4-isocyanatobenzene, dichloromethane, and 2-chlorobenzylamine were purchased from Aladdin Biochemical Technology Co., Ltd with no further purification. The 1-bromo-4-isocyanatobenzene (198 mg, 1 mmol), dichloromethane (10 mL), and 2-chlorobenzylamine (142 mg, 1 mmol) were mixed and stirred for 24 h under normal temperature and pressure. Then, the organic solvent was removed by vacuum distillation. The crude product (80 mg) was dissolved in 10 mL ethanol with ultrasonic dispersion. The single crystal product of the title compound was obtained after two days by slow volatilization of the organic solvent.

Experimental details

The structure of the title compound was solved with the ShelXT [4] package and refined with the ShelXL [3] program. All hydrogen atoms were placed in idealized positions and refined as riding atoms. The U_{iso} values were constrained to be 1.2 U_{eq} of the parent atoms.

Comment

The urea group is an important structural fragment of many bioactive compounds, including many drug molecules such as Sorafenib, Donafenib, and Regorafenib [5, 6], which plays a significant role in target interaction drugs and the regulation of drug formation of compounds. Many references showed crystal structures of the derivatives with the urea group [7–15]. In this work, we report the single crystal structure of 1-(4-bromophenyl)-3-(2-chlorobenzyl)-urea, which provides an essential basis for studying urea derivatives.

As shown in the figure, the title compound adopts trans conformations with respect to the position of the 3-chloropropanoyl and 4-bromophenyl groups, respectively, against the C=O bond across their C–N bonds. The

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.09861(4)	0.47977(6)	0.33688(4)	0.0922(3)
N1	0.5800(2)	0.1958(3)	0.8092(2)	0.0509(8)
H1	0.553621	0.115781	0.838190	0.061*
N2	0.4292(2)	0.2172(3)	0.6905(2)	0.0469(7)
H2A	0.416253	0.125020	0.715289	0.056*
O1	0.54552(17)	0.4131(2)	0.7065(2)	0.0484(6)
C1	0.8128(3)	0.3575(4)	0.9918(3)	0.0606(11)
C2	0.8405(4)	0.4436(5)	1.0867(4)	0.0849(16)
H2	0.910143	0.459597	1.116717	0.102*
C3	0.7666(6)	0.5061(5)	1.1373(4)	0.0912(19)
H3	0.784681	0.568010	1.201334	0.109*
C4	0.6672(5)	0.4782(5)	1.0946(4)	0.0774(14)
H4	0.616078	0.520044	1.130091	0.093*
C5	0.6394(3)	0.3903(4)	1.0005(3)	0.0566(10)
H5	0.569633	0.372965	0.971983	0.068*
C6	0.7124(3)	0.3273(4)	0.9477(3)	0.0453(9)
C7	0.6863(2)	0.2304(4)	0.8440(3)	0.0476(9)
H7A	0.710528	0.286021	0.783700	0.057*
H7B	0.724049	0.131220	0.855849	0.057*
C8	0.5202(3)	0.2830(4)	0.7336(3)	0.0415(8)
C9	0.3539(3)	0.2847(3)	0.6093(3)	0.0402(8)
C10	0.2532(3)	0.2578(4)	0.6135(3)	0.0488(9)
H10	0.236455	0.198390	0.672342	0.059*
C11	0.1765(3)	0.3148(4)	0.5344(3)	0.0583(10)
H11	0.107539	0.294104	0.538007	0.070*
C12	0.2009(3)	0.4016(4)	0.4506(3)	0.0535(10)
C13	0.3001(3)	0.4315(4)	0.4429(3)	0.0558(10)
H13	0.316002	0.492304	0.384316	0.067*
C14	0.3771(3)	0.3706(4)	0.5231(3)	0.0479(9)
H14	0.446081	0.388513	0.518132	0.058*
Cl1	0.90662(8)	0.28220(16)	0.92618(10)	0.0922(4)

Br and Cl atoms replace H atoms in the two phenyl, and the lengths of C–Br and C–Cl bonds are 1.901(4) Å and 1.742(5) Å, respectively. The two halogenophenyl rings make a dihedral angle of 10.2(4)°. In the crystal, molecules are linked by N–H···O hydrogen bonds. The angle of hydrogen bonds N2–H2A···O1 is 154.70(18)°, and the length is 2.0856(19) Å. The angle of hydrogen bonds N1–H1···O1 is 141.87(17)°, and the length is 2.2025(19) Å. It indicates that the hydrogen bond plays an important role in maintaining the crystal structure. All bond lengths and angles are within a reasonable range [7, 11, 14].

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