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Crystal structure of (2-((4-bromo-2,6-dichlorophenyl)amino)phenyl) (morpholino) methanone, $C_{17}H_{15}BrCl_2N_2O_2$

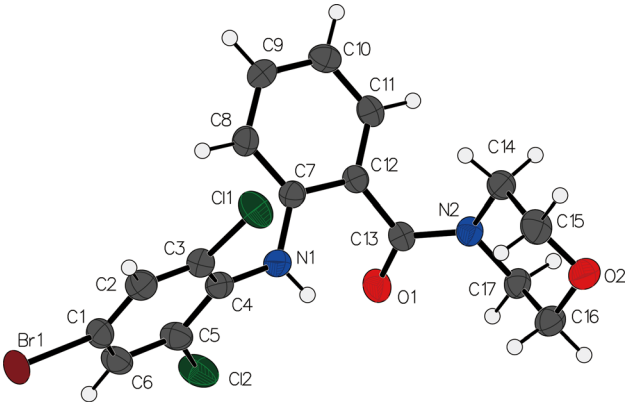

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.28 × 0.15 × 0.11 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	2.64 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.5°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14,352, 4029, 0.041
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3126
$N(param)_{refined}$:	217
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

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Abstract

$C_{17}H_{15}BrCl_2N_2O_2$, monoclinic, $P2_1/c$ (no. 14), a = 20.333(7) Å, b = 11.226(5) Å, c = 7.843(3) Å, β = 99.651(8)°, V = 1764.8(12) Å^3, Z = 4, $R_{gt}(F)$ = 0.0464, $wR_{ref}(F^2)$ = 0.1601, T = 173 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.

1 Source of materials

A mixture of 2-((4-bromo-2,6-dichlorophenyl)amino)benzoic acid (3.59 g, 10 mmol), morpholine (1.11 g, 13 mmol), 2-(7-azabenzotriazol-1-yl)-*N*,*N*,*N*′,*N*′-tetramethyluronium hexafluorophosphate (HATU) (4.18 g, 11 mmol) and *N*,*N*-diisopropylethylamine (2.58 g, 20 mmol) was dissolved in *N*,*N*-dimethylformamide (20 mL). The mixture was stirred for 3 h at room temperature, until the TLC indicated the reaction was completed. The mixture was diluted with brine, and then extracted with ethyl acetate (3 × 30 mL). The organic phase was washed with brine (30 mL), dried with anhydrous sodium sulfate, and then concentrated under pressure. The title compound was separated by silica-gel column chromatography with ethyl acetate-petroleum ether (30 %) gradient solvent system. The target product was obtained as a white solid. Yield: 83.8 %.

2 Experimental details

All hydrogen atoms were placed in idealized positions. Their U_{iso} values were set to 1.2 U_{eq} of the parent atoms. The structure was solved using ShelXT [2] and refined using ShelXL [3] in Olex2 software [4].

3 Comment

Morpholine derivatives find wide applications in the field of medicinal chemistry as a key scaffold for the development of various drugs. In addition, these derivatives are used as important building blocks for the synthesis of heterocyclic compounds with various biological activities, as highlighted in recent academic publications [5, 6]. In this study, a novel morpholine derivative was synthesized and characterized by obtaining its single-crystal structure, providing valuable insights for solid-state properties and potential applications,

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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	0.45144 (2)	0.31430 (4)	0.02326 (5)	0.03884 (17)
C1	0.54180 (19)	0.3659 (3)	0.1294 (5)	0.0352 (8)
C2	0.5516 (2)	0.4143 (4)	0.2945 (5)	0.0377 (9)
H2	0.515278	0.424312	0.355130	0.045*
C3	0.61562 (19)	0.4478 (3)	0.3692 (5)	0.0338 (8)
C4	0.67063 (18)	0.4387 (3)	0.2820 (5)	0.0317 (8)
C5	0.6572 (2)	0.3847 (4)	0.1180 (5)	0.0360 (9)
C6	0.5935 (2)	0.3488 (4)	0.0405 (6)	0.0375 (9)
H6	0.586225	0.313458	−0.071131	0.045*
C7	0.75279 (18)	0.5883 (3)	0.4131 (5)	0.0288 (7)
C8	0.70756 (19)	0.6835 (3)	0.3933 (5)	0.0335 (8)
H8	0.662592	0.670886	0.340053	0.040*
C9	0.7285 (2)	0.7964 (3)	0.4515 (5)	0.0342 (8)
H9	0.697765	0.860853	0.436010	0.041*
C10	0.7936 (2)	0.8160 (3)	0.5319 (5)	0.0348 (9)
H10	0.807111	0.892662	0.575535	0.042*
C11	0.83863 (19)	0.7230 (4)	0.5481 (5)	0.0330 (8)
H11	0.883723	0.737303	0.598896	0.040*
C12	0.81922 (18)	0.6083 (3)	0.4911 (4)	0.0283 (7)
C13	0.86979 (17)	0.5120 (3)	0.4918 (4)	0.0278 (7)
C14	0.9050 (2)	0.5306 (4)	0.8121 (5)	0.0363 (9)
H14A	0.864202	0.579752	0.804527	0.044*
H14B	0.943638	0.579903	0.863576	0.044*
C15	0.8996 (2)	0.4232 (4)	0.9250 (5)	0.0414 (10)
H15A	0.897151	0.450034	1.044008	0.050*
H15B	0.857996	0.379506	0.880435	0.050*
C16	0.9580 (2)	0.3029 (4)	0.7584 (5)	0.0383 (9)
H16A	0.916315	0.259863	0.712273	0.046*
H16B	0.995644	0.246341	0.763210	0.046*
C17	0.96734 (18)	0.4047 (3)	0.6401 (5)	0.0321 (8)
H17A	1.010868	0.443604	0.680368	0.039*
H17B	0.967290	0.374283	0.521574	0.039*
Cl1	0.62799 (6)	0.49342 (11)	0.58362 (13)	0.0475 (3)
Cl2	0.72302 (6)	0.36148 (11)	0.00644 (16)	0.0512 (3)
N1	0.73454 (16)	0.4730 (3)	0.3525 (5)	0.0366 (8)
H1	0.766180	0.418794	0.360247	0.044*
N2	0.91342 (15)	0.4916 (3)	0.6382 (4)	0.0308 (7)
O1	0.87243 (14)	0.4563 (3)	0.3558 (4)	0.0418 (7)
O2	0.95482 (17)	0.3455 (3)	0.9293 (4)	0.0437 (7)

as reported in recent publications in the field of crystallography [7–9].

The crystal structure of (2-((4-bromo-2,6-dichlorophenyl) amino) phenyl)(morpholino)methanone has been determined through single-crystal X-ray diffraction analysis.

The compound consists of the 2-((4-bromo-2,6-dichlorophenyl)amino)phenyl and the (morpholino)methanone moieties. The molecule adopts a non-planar geometry with dihedral angle of 59.3° between the two substituted benzene rings. The 4-bromo-2,6-dichlorophenyl moiety is positioned at one end of the molecule and, forms intermolecular interactions with neighboring molecules via π–π interactions, similar to structures reported in literatures [10–13].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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