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## Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.038  
 $wR$  factor = 0.100  
Data-to-parameter ratio = 15.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*o*-(2-Bromoethoxy)benzaldehydeMolecules of the title compound,  $\text{C}_9\text{H}_9\text{BrO}_2$ , form a chain, *via*  
 $\pi$ - $\pi$  stacking interactions, which runs along the *a* axis.

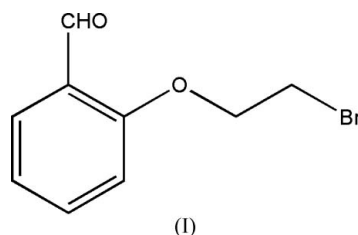
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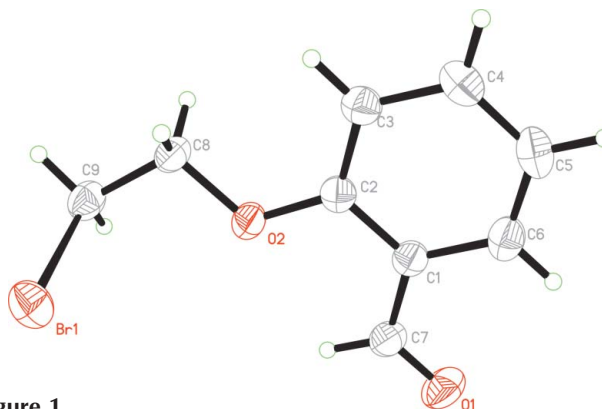
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## Comment

As a result of their good complexing properties, biological activity and analytical applications, salicylaldehyde and its Schiff bases, as well as their metal complexes, have been the subject of many studies (Hata *et al.*, 2004; Scherhag & Spicer 2000; Mukherjee *et al.*, 2001; Li *et al.*, 2000). The most numerous among them are the syntheses of new ligands based on salicylaldehyde, which may be modified in the following three ways: (i) introduction of functional groups to the benzene ring in salicylaldehyde; (ii) *o*-alkylation of the hydroxy group in salicylaldehyde; (iii) condensation of the aldehyde group to obtain many kinds of Schiff bases and their derivatives. Meanwhile, weak interactions, such as  $\text{C}-\text{H} \cdots \pi$ ,  $\pi$ - $\pi$ , and weak hydrogen bonds ( $\text{C}-\text{H} \cdots \text{X}$ ,  $\text{X} = \text{O}, \text{N}, \text{Cl}, \text{Br}$ ) are known to play crucial roles in molecular self-assembly and crystal symmetry in biology, chemistry and materials science (Leininger *et al.*, 2000; Müller-Dethlefs & Hobza, 2000; Conn & Rebek, 1997; Hunter *et al.*, 1991).



In the title molecule, (I), an intramolecular  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bond is observed (Table 1). The aldehyde group and



**Figure 1**  
View of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

the ether O atom lie almost in the plane of the benzene ring (Fig. 1). The benzene ring is offset-stacked with respect to the neighbouring benzene ring along the *a* axis (Fig. 2). The centroid (*C<sub>g</sub>*) separations between adjacent benzene rings are 4.305 (2) Å for *C<sub>g</sub>*...*C<sub>g</sub><sup>i</sup>* and 4.535 (2) Å for *C<sub>g</sub>*...*C<sub>g</sub><sup>ii</sup>* [symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*, (ii) -*x*, 1 - *y*, 1 - *z*], and the interplanar spacings are 3.511 (2) and 3.408 (2) Å. The alternating  $\pi$ - $\pi$  interactions are quite reasonable in view of Hunter's rule (Hunter & Sanders, 1990), and hence contribute greatly to the stabilization of the one-dimensional chain-like structure. There is a C-H...O hydrogen bond between adjacent chains (Table 1), resulting in a three-dimensional packing arrangement (Fig. 3).

## Experimental

A mixture of salicylaldehyde (32 mmol), 1,2-dibromoethane (320 mmol) and anhydrous K<sub>2</sub>CO<sub>3</sub> (64 mmol) was refluxed in anhydrous CH<sub>3</sub>CN (200 ml) for 30 h, and then cooled to room temperature and filtered. After washing with CH<sub>3</sub>CN, the filtrate was evaporated to dryness and purified by silica-gel column chromatography to give *o*-(2-bromoethoxy)benzaldehyde in 66% yield (Ashram, 2002). A small amount of (I) was dissolved in ethanol to give a clear solution and kept at room temperature for a week to give colourless pillar-like crystals suitable for X-ray diffraction analysis.

### Crystal data

C <sub>9</sub> H <sub>9</sub> BrO <sub>2</sub>	<i>D<sub>x</sub></i> = 1.663 Mg m <sup>-3</sup>
<i>M<sub>r</sub></i> = 229.07	Mo <i>K</i> α radiation
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Cell parameters from 3002 reflections
<i>a</i> = 7.7453 (9) Å	$\theta$ = 2.7–28.2°
<i>b</i> = 16.2325 (19) Å	$\mu$ = 4.45 mm <sup>-1</sup>
<i>c</i> = 7.3667 (9) Å	<i>T</i> = 296 (2) K
$\beta$ = 98.908 (2)°	Pillar, colourless
<i>V</i> = 915.01 (19) Å <sup>3</sup>	0.20 × 0.15 × 0.10 mm
<i>Z</i> = 4	

### Data collection

Bruker SMART APEX-II CCD diffractometer	1697 independent reflections
$\varphi$ and $\omega$ scans	1494 reflections with <i>I</i> > 2σ( <i>I</i> )
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	<i>R</i> <sub>int</sub> = 0.028
<i>T</i> <sub>min</sub> = 0.470, <i>T</i> <sub>max</sub> = 0.665	$\theta$ <sub>max</sub> = 25.5°
4818 measured reflections	<i>h</i> = -9 → 9
	<i>k</i> = -19 → 16
	<i>l</i> = -8 → 8

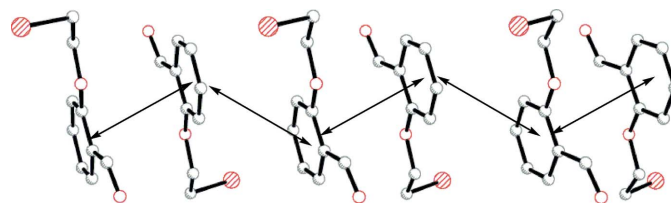
### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 0.8593P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.100$	( $\Delta/\sigma$ ) <sub>max</sub> = 0.001
<i>S</i> = 1.05	$\Delta\rho$ <sub>max</sub> = 0.69 e Å <sup>-3</sup>
1697 reflections	$\Delta\rho$ <sub>min</sub> = -0.48 e Å <sup>-3</sup>
110 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.015 (2)

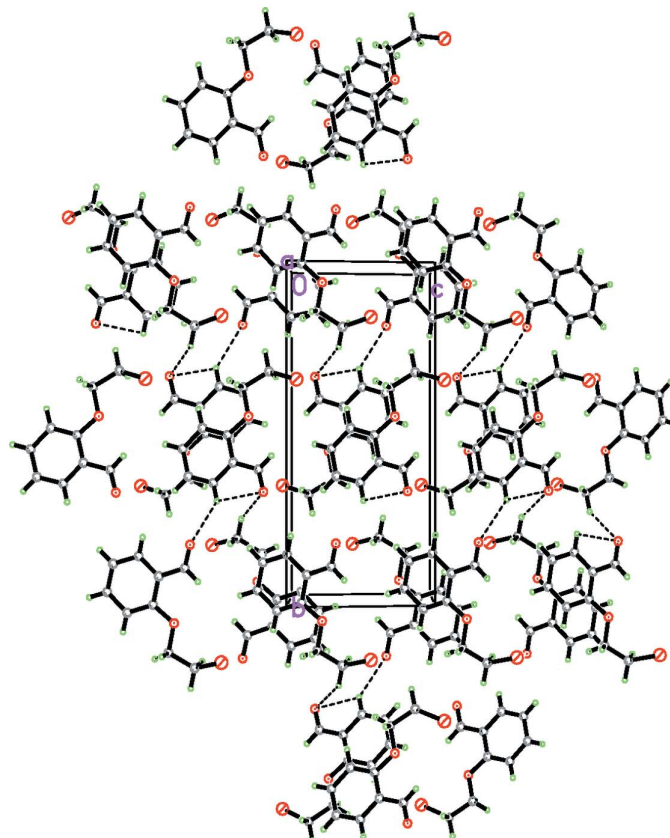
**Table 1**  
Hydrogen-bond geometry (Å, °).

<i>D</i> -H... <i>A</i>	<i>D</i> -H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> -H... <i>A</i>
C7-H7...O2	0.93	2.43	2.762 (4)	101
C9-H9A...O1 <sup>i</sup>	0.97	2.59	3.453 (5)	149

Symmetry code: (i) -*x* + 1, -*y* + 1, -*z*.



**Figure 2**  
The one-dimensional chain-like structure of (I) formed by  $\pi$ - $\pi$  interactions along the *a* axis (double-headed arrows represent the  $\pi$ - $\pi$  interactions in an offset arrangement). H atoms have been omitted.



**Figure 3**  
A packing diagram of (I), viewed down the *a* axis. Dashed lines denote C-H...O hydrogen bonds.

H atoms were included in the refinement at calculated positions in the riding-model approximation, with C-H = 0.97 or 0.93 Å and 1.2*U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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## References

- Ashram, M. (2002). *J. Chem. Soc. Perkin Trans. 2*, pp. 1662–1668.
- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Conn, M. M. & Rebek, J. Jr (1997). *Chem. Rev.* **97**, 1647–1668.
- Hata, M., Akutsu, H., Yamada, J. & Nakatsuji, S. (2004). *Molecules*, **9**, 746–756.
- Hunter, C. A. & Sanders, J. K. M. (1990). *J. Am. Chem. Soc.* **112**, 5525–5534.
- Hunter, C. A., Singh, J. & Thornton, J. M. (1991). *J. Mol. Biol.* **218**, 837–846.
- Leininger, S., Olenyuk, B. & Stang, P. J. (2000). *Chem. Rev.* **100**, 853–908.
- Li, Z. N., Liu, G. & Zheng, Z. (2000). *Tetrahedron*, **56**, 7787–7791.
- Mukherjee, P. S., Dalai, S., Mostafa, G., Lu, T.-H., Rentschler, E. & Chaudhuri, N. R. (2001). *New J. Chem.* **25**, 1203–1207.
- Müller-Dethlefs, K. & Hobza, P. (2000). *Chem. Rev.* **100**, 143–167.
- Scherhag, G. & Spicer, M. D. (2000). *J. Chem. Soc. Dalton Trans.* pp. 1237–1238.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.