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## Structure Reports

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## 1,4-Bis(4-chlorobenzoyl)piperazine

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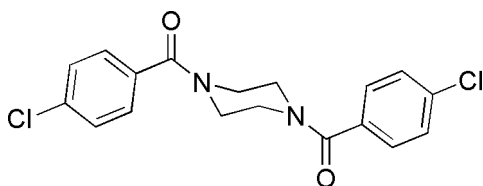
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Key indicators: single-crystal X-ray study;  $T = 294$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.043;  $wR$  factor = 0.132; data-to-parameter ratio = 16.0.

The title compound,  $\text{C}_{18}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}_2$ , crystallizes with two half-molecules in the asymmetric unit; each molecule lies on an inversion centre. The piperazine ring adopts a chair conformation and the two chlorobenzene rings in each molecule are parallel to each other due to symmetry. The crystal packing is stabilized by  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\pi$  interactions.

## Related literature

For related literature, see: Pollard &amp; Gray (1953).



## Experimental

## Crystal data

 $\text{C}_{18}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}_2$  $M_r = 363.23$ Monoclinic,  $P2_1/n$  $a = 11.892$  (2) Å $b = 11.413$  (2) Å $c = 12.653$  (2) Å $\beta = 96.959$  (3)° $V = 1704.6$  (5) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.39$  mm<sup>-1</sup> $T = 294$  (2) K $0.16 \times 0.14 \times 0.12$  mm

## Data collection

Bruker SMART 1K CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{\min} = 0.940$ ,  $T_{\max} = 0.954$ 9538 measured reflections  
3473 independent reflections  
1795 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.044$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.043$  $wR(F^2) = 0.132$  $S = 1.00$ 

3473 reflections

217 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.37$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C2}-\text{H2}\cdots\text{O1}^i$	0.93	2.42	3.350 (3)	173
$\text{C11}-\text{H11}\cdots\text{O2}^{ii}$	0.93	2.34	3.265 (3)	170
$\text{C18}-\text{H18B}\cdots\text{Cg1}$	0.97	2.91	3.812 (3)	155

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

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2456).

## References

- Bruker (1997). SMART, SAINT and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.  
Pollard, C. B. & Gray, B. S. (1953). *J. Am. Chem. Soc.* **75**, 491–491.  
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

**supplementary materials**

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## 1,4-Bis(4-chlorobenzoyl)piperazine

H.-M. Jin, P.-F. Li, C.-Y. Li and B. Liu

### Comment

Some amides of piperazines have been reported to exhibit marked activity in inhibiting growth of tubercle bacillus in serum (Pollard & Gray, 1953).

The title compound, C<sub>18</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>, crystallizes with two half molecules in the asymmetric unit (Figs. 1 and 2).

The piperazine rings adopt a chair-conformation and the two chlorobenzene rings are parallel to each due to symmetry.

In the crystal of (I), weak C—H···O interactions (Table 1) and a C—H··· $\pi$ -interaction (C18···Cg1 = 3.812 (3) Å, C18—H18B···Cg1 = 155°) stabilize the structure (Cg1 is the centroid of the C1—C6 ring).

### Experimental

A solution of 4-chlorobenzoyl chloride in CH<sub>2</sub>Cl<sub>2</sub> was added dropwise to a suspension of 1,4-piperazine in CH<sub>2</sub>Cl<sub>2</sub> at room temperature with stirring. The reaction mixture continued stirring overnight. The white solid was obtained by recrystallization from methanol. Colourless blocks of (I) were grown by natural evaporation of a methanolic solution.

### Refinement

All H atoms were positioned geometrically and refined as riding atoms. The C—H distance for CH group is 0.93 Å and that CH<sub>2</sub> group 0.97 Å both with the constraint of  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

### Figures

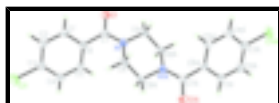


Fig. 1. The molecular structure of molecule one of the title compound with the atom-numbering scheme and 30% probability displacement ellipsoids [symmetry code:  $-x, -y + 1, -z + 1$ ].

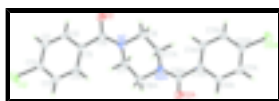


Fig. 2. The molecular structure of molecule two of the title compound with the atom-numbering scheme and 30% probability displacement ellipsoids [symmetry code:  $-x + 1, -y + 1, -z + 1$ ].

## 1,4-Bis(4-chlorobenzoyl)piperazine

### Crystal data

C<sub>18</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>

$M_r = 363.23$

Monoclinic,  $P2_1/n$

$F_{000} = 752$

$D_x = 1.415 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

# supplementary materials

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Hall symbol: -P 2yn

$a = 11.892 (2) \text{ \AA}$

$b = 11.413 (2) \text{ \AA}$

$c = 12.653 (2) \text{ \AA}$

$\beta = 96.959 (3)^\circ$

$V = 1704.6 (5) \text{ \AA}^3$

$Z = 4$

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1786 reflections

$\theta = 2.5\text{--}26.2^\circ$

$\mu = 0.39 \text{ mm}^{-1}$

$T = 294 (2) \text{ K}$

Block, colourless

$0.16 \times 0.14 \times 0.12 \text{ mm}$

## Data collection

Bruker SMART 1K CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294(2) \text{ K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.940$ ,  $T_{\max} = 0.954$

9538 measured reflections

3473 independent reflections

1795 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.4^\circ$

$\theta_{\min} = 2.2^\circ$

$h = -14 \rightarrow 14$

$k = -7 \rightarrow 14$

$l = -15 \rightarrow 15$

## Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.132$

$S = 1.00$

3473 reflections

217 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 0.0445P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.37 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.21 \text{ e \AA}^{-3}$

Extinction correction: none

## Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.07297 (8)	1.14374 (6)	0.33438 (7)	0.0734 (3)
C12	0.67186 (8)	1.15311 (6)	0.41373 (7)	0.0755 (3)
O1	0.10101 (17)	0.56724 (16)	0.25514 (15)	0.0608 (6)
O2	0.73471 (16)	0.58451 (15)	0.37660 (16)	0.0604 (6)
N1	0.05304 (18)	0.55966 (16)	0.42159 (16)	0.0431 (6)
N2	0.56644 (18)	0.56438 (18)	0.43733 (19)	0.0517 (6)
C1	0.1649 (2)	0.8111 (2)	0.30465 (19)	0.0445 (6)
H1	0.2263	0.7707	0.2835	0.053*
C2	0.1644 (2)	0.9320 (2)	0.3036 (2)	0.0485 (7)
H2	0.2255	0.9731	0.2825	0.058*
C3	0.0730 (2)	0.9914 (2)	0.3340 (2)	0.0466 (7)
C4	-0.0192 (2)	0.9316 (2)	0.3633 (2)	0.0524 (7)
H4	-0.0816	0.9725	0.3819	0.063*
C5	-0.0182 (2)	0.8109 (2)	0.3649 (2)	0.0462 (7)
H5	-0.0803	0.7705	0.3848	0.055*
C6	0.0741 (2)	0.7489 (2)	0.33721 (18)	0.0393 (6)
C7	0.0774 (2)	0.6181 (2)	0.3351 (2)	0.0407 (6)
C8	0.0563 (2)	0.6076 (2)	0.52951 (19)	0.0446 (7)
H8A	0.0580	0.6925	0.5264	0.054*
H8B	0.1248	0.5815	0.5725	0.054*
C9	0.0460 (2)	0.4316 (2)	0.4195 (2)	0.0459 (7)
H9A	0.1142	0.3984	0.4578	0.055*
H9B	0.0398	0.4041	0.3464	0.055*
C10	0.6690 (2)	0.8217 (2)	0.31981 (19)	0.0444 (7)
H10	0.6819	0.7807	0.2589	0.053*
C11	0.6757 (2)	0.9420 (2)	0.3207 (2)	0.0463 (7)
H11	0.6916	0.9825	0.2604	0.056*
C12	0.6586 (2)	1.0017 (2)	0.4119 (2)	0.0443 (6)
C13	0.6332 (2)	0.9435 (2)	0.5015 (2)	0.0468 (7)
H13	0.6215	0.9849	0.5625	0.056*
C14	0.6253 (2)	0.8229 (2)	0.4990 (2)	0.0450 (7)
H14	0.6077	0.7830	0.5589	0.054*
C15	0.64333 (19)	0.7606 (2)	0.40892 (19)	0.0386 (6)
C16	0.6512 (2)	0.6301 (2)	0.4060 (2)	0.0423 (7)
C17	0.4532 (2)	0.6053 (2)	0.4531 (2)	0.0516 (7)
H17A	0.3984	0.5761	0.3962	0.062*
H17B	0.4512	0.6902	0.4510	0.062*
C18	0.5771 (2)	0.4364 (2)	0.4426 (2)	0.0574 (8)
H18A	0.6542	0.4136	0.4347	0.069*
H18B	0.5270	0.4009	0.3852	0.069*

Atomic displacement parameters ( $\text{\AA}^2$ )

$U^{11}$        $U^{22}$        $U^{33}$        $U^{12}$        $U^{13}$        $U^{23}$

## supplementary materials

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C11	0.1044 (7)	0.0389 (4)	0.0786 (6)	-0.0003 (4)	0.0184 (5)	0.0003 (4)
C12	0.1046 (7)	0.0373 (4)	0.0892 (6)	-0.0095 (4)	0.0309 (5)	-0.0060 (4)
O1	0.0898 (15)	0.0487 (12)	0.0508 (13)	0.0040 (10)	0.0366 (11)	-0.0049 (9)
O2	0.0639 (13)	0.0467 (12)	0.0776 (14)	0.0110 (10)	0.0362 (11)	0.0041 (10)
N1	0.0661 (15)	0.0292 (11)	0.0363 (13)	0.0006 (10)	0.0153 (11)	-0.0010 (9)
N2	0.0502 (14)	0.0316 (12)	0.0789 (17)	0.0098 (10)	0.0300 (13)	0.0082 (11)
C1	0.0428 (16)	0.0472 (16)	0.0458 (16)	0.0024 (13)	0.0150 (13)	0.0029 (12)
C2	0.0487 (17)	0.0471 (17)	0.0503 (17)	-0.0051 (14)	0.0082 (14)	0.0069 (13)
C3	0.0599 (18)	0.0360 (15)	0.0440 (17)	-0.0011 (13)	0.0068 (14)	0.0022 (12)
C4	0.0542 (19)	0.0491 (17)	0.0563 (19)	0.0103 (14)	0.0161 (15)	0.0021 (14)
C5	0.0457 (16)	0.0434 (16)	0.0525 (17)	0.0016 (13)	0.0183 (13)	0.0040 (13)
C6	0.0426 (16)	0.0412 (15)	0.0351 (14)	0.0023 (12)	0.0087 (12)	0.0035 (11)
C7	0.0455 (16)	0.0395 (15)	0.0393 (16)	0.0025 (12)	0.0138 (13)	0.0011 (12)
C8	0.0654 (18)	0.0331 (14)	0.0362 (15)	0.0029 (13)	0.0095 (13)	-0.0031 (11)
C9	0.0659 (19)	0.0315 (14)	0.0422 (16)	0.0060 (13)	0.0150 (14)	-0.0033 (11)
C10	0.0545 (17)	0.0417 (15)	0.0396 (16)	-0.0018 (13)	0.0159 (13)	-0.0027 (12)
C11	0.0534 (17)	0.0451 (16)	0.0418 (17)	-0.0037 (13)	0.0119 (13)	0.0066 (13)
C12	0.0466 (16)	0.0359 (15)	0.0512 (17)	-0.0031 (12)	0.0098 (13)	-0.0028 (13)
C13	0.0536 (17)	0.0469 (17)	0.0417 (17)	0.0013 (13)	0.0128 (13)	-0.0107 (13)
C14	0.0517 (17)	0.0486 (16)	0.0370 (15)	0.0011 (13)	0.0140 (13)	0.0057 (12)
C15	0.0391 (15)	0.0375 (14)	0.0403 (15)	0.0010 (12)	0.0090 (12)	0.0013 (12)
C16	0.0474 (17)	0.0384 (16)	0.0441 (16)	0.0066 (13)	0.0176 (13)	0.0047 (12)
C17	0.0524 (18)	0.0352 (15)	0.070 (2)	0.0110 (13)	0.0181 (15)	0.0019 (14)
C18	0.0639 (19)	0.0373 (16)	0.076 (2)	0.0132 (14)	0.0274 (16)	0.0037 (14)

### *Geometric parameters (Å, °)*

C11—C3	1.739 (3)	C8—H8A	0.9700
C12—C12	1.735 (3)	C8—H8B	0.9700
O1—C7	1.228 (3)	C9—C8 <sup>i</sup>	1.513 (3)
O2—C16	1.219 (3)	C9—H9A	0.9700
N1—C7	1.343 (3)	C9—H9B	0.9700
N1—C9	1.464 (3)	C10—C11	1.376 (3)
N1—C8	1.467 (3)	C10—C15	1.391 (3)
N2—C16	1.354 (3)	C10—H10	0.9300
N2—C17	1.461 (3)	C11—C12	1.377 (3)
N2—C18	1.467 (3)	C11—H11	0.9300
C1—C2	1.380 (3)	C12—C13	1.378 (3)
C1—C6	1.395 (3)	C13—C14	1.380 (3)
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.375 (4)	C14—C15	1.382 (3)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.380 (4)	C15—C16	1.492 (3)
C4—C5	1.378 (3)	C17—C18 <sup>ii</sup>	1.488 (4)
C4—H4	0.9300	C17—H17A	0.9700
C5—C6	1.387 (3)	C17—H17B	0.9700
C5—H5	0.9300	C18—C17 <sup>ii</sup>	1.488 (4)
C6—C7	1.494 (3)	C18—H18A	0.9700

C8—C9 <sup>i</sup>	1.513 (3)	C18—H18B	0.9700
C7—N1—C9	119.9 (2)	N1—C9—H9B	109.8
C7—N1—C8	126.1 (2)	C8 <sup>i</sup> —C9—H9B	109.8
C9—N1—C8	112.61 (19)	H9A—C9—H9B	108.2
C16—N2—C17	126.4 (2)	C11—C10—C15	120.8 (2)
C16—N2—C18	120.1 (2)	C11—C10—H10	119.6
C17—N2—C18	112.8 (2)	C15—C10—H10	119.6
C2—C1—C6	120.6 (2)	C10—C11—C12	119.1 (2)
C2—C1—H1	119.7	C10—C11—H11	120.5
C6—C1—H1	119.7	C12—C11—H11	120.5
C3—C2—C1	119.5 (2)	C11—C12—C13	121.4 (2)
C3—C2—H2	120.3	C11—C12—Cl2	118.8 (2)
C1—C2—H2	120.2	C13—C12—Cl2	119.8 (2)
C2—C3—C4	120.9 (2)	C12—C13—C14	118.9 (2)
C2—C3—C11	119.6 (2)	C12—C13—H13	120.6
C4—C3—C11	119.5 (2)	C14—C13—H13	120.6
C5—C4—C3	119.5 (3)	C13—C14—C15	121.0 (2)
C5—C4—H4	120.3	C13—C14—H14	119.5
C3—C4—H4	120.3	C15—C14—H14	119.5
C4—C5—C6	120.8 (2)	C14—C15—C10	118.8 (2)
C4—C5—H5	119.6	C14—C15—C16	123.4 (2)
C6—C5—H5	119.6	C10—C15—C16	117.4 (2)
C5—C6—C1	118.7 (2)	O2—C16—N2	121.1 (2)
C5—C6—C7	122.5 (2)	O2—C16—C15	119.3 (2)
C1—C6—C7	118.7 (2)	N2—C16—C15	119.6 (2)
O1—C7—N1	122.0 (2)	N2—C17—C18 <sup>ii</sup>	110.2 (2)
O1—C7—C6	119.8 (2)	N2—C17—H17A	109.6
N1—C7—C6	118.2 (2)	C18 <sup>ii</sup> —C17—H17A	109.6
N1—C8—C9 <sup>i</sup>	110.8 (2)	N2—C17—H17B	109.6
N1—C8—H8A	109.5	C18 <sup>ii</sup> —C17—H17B	109.6
C9 <sup>i</sup> —C8—H8A	109.5	H17A—C17—H17B	108.1
N1—C8—H8B	109.5	N2—C18—C17 <sup>ii</sup>	109.3 (2)
C9 <sup>i</sup> —C8—H8B	109.5	N2—C18—H18A	109.8
H8A—C8—H8B	108.1	C17 <sup>ii</sup> —C18—H18A	109.8
N1—C9—C8 <sup>i</sup>	109.5 (2)	N2—C18—H18B	109.8
N1—C9—H9A	109.8	C17 <sup>ii</sup> —C18—H18B	109.8
C8 <sup>i</sup> —C9—H9A	109.8	H18A—C18—H18B	108.3
C6—C1—C2—C3	-0.6 (4)	C15—C10—C11—C12	1.1 (4)
C1—C2—C3—C4	-1.4 (4)	C10—C11—C12—C13	-1.0 (4)
C1—C2—C3—C11	179.15 (19)	C10—C11—C12—Cl2	177.85 (19)
C2—C3—C4—C5	1.7 (4)	C11—C12—C13—C14	0.2 (4)
C11—C3—C4—C5	-178.8 (2)	Cl2—C12—C13—C14	-178.64 (19)
C3—C4—C5—C6	-0.1 (4)	C12—C13—C14—C15	0.5 (4)
C4—C5—C6—C1	-1.9 (4)	C13—C14—C15—C10	-0.4 (4)
C4—C5—C6—C7	-178.3 (2)	C13—C14—C15—C16	171.6 (2)
C2—C1—C6—C5	2.2 (4)	C11—C10—C15—C14	-0.5 (4)

## supplementary materials

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C2—C1—C6—C7	178.8 (2)	C11—C10—C15—C16	-172.9 (2)
C9—N1—C7—O1	-4.5 (4)	C17—N2—C16—O2	-166.5 (3)
C8—N1—C7—O1	160.9 (3)	C18—N2—C16—O2	3.8 (4)
C9—N1—C7—C6	174.9 (2)	C17—N2—C16—C15	14.5 (4)
C8—N1—C7—C6	-19.6 (4)	C18—N2—C16—C15	-175.3 (2)
C5—C6—C7—O1	127.9 (3)	C14—C15—C16—O2	-124.8 (3)
C1—C6—C7—O1	-48.6 (3)	C10—C15—C16—O2	47.3 (3)
C5—C6—C7—N1	-51.5 (3)	C14—C15—C16—N2	54.3 (4)
C1—C6—C7—N1	132.0 (2)	C10—C15—C16—N2	-133.6 (3)
C7—N1—C8—C9 <sup>i</sup>	136.7 (2)	C16—N2—C17—C18 <sup>ii</sup>	-131.6 (3)
C9—N1—C8—C9 <sup>i</sup>	-57.0 (3)	C18—N2—C17—C18 <sup>ii</sup>	57.6 (3)
C7—N1—C9—C8 <sup>i</sup>	-136.4 (2)	C16—N2—C18—C17 <sup>ii</sup>	131.4 (3)
C8—N1—C9—C8 <sup>i</sup>	56.2 (3)	C17—N2—C18—C17 <sup>ii</sup>	-57.1 (3)

Symmetry codes: (i)  $-x, -y+1, -z+1$ ; (ii)  $-x+1, -y+1, -z+1$ .

### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ O1 <sup>iii</sup>	0.93	2.42	3.350 (3)	173
C11—H11 $\cdots$ O2 <sup>iv</sup>	0.93	2.34	3.265 (3)	170
C18—H18B $\cdots$ Cg1	0.97	Missing	3.812 (3)	155

Symmetry codes: (iii)  $-x+1/2, y+1/2, -z+1/2$ ; (iv)  $-x+3/2, y+1/2, -z+1/2$ .



Fig. 1

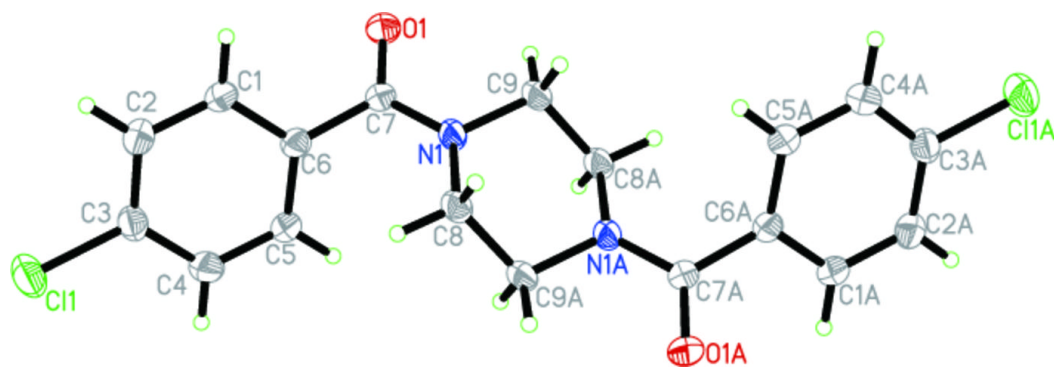


Fig. 2

