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## Structure Reports

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## (Z)-3-Chloro-3-phenyl-N-[(S)-1-phenylethyl]prop-2-enamide

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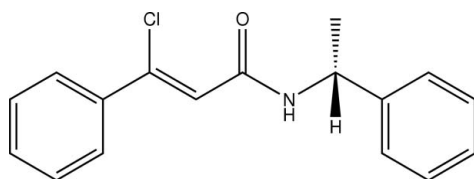
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å;  $R$  factor = 0.071;  $wR$  factor = 0.161; data-to-parameter ratio = 16.0.

The asymmetric unit of the title compound,  $\text{C}_{17}\text{H}_{16}\text{ClNO}$ , contains two crystallographically independent molecules. These molecules are connected in an alternating fashion through  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, generating one-dimensional chains of graph sets  $R_2^1(6)$  and  $C(4)$  along the  $a$  axis.

### Related literature

For related literature, see: Kishikawa *et al.*, (1997); Cherry *et al.* (2003); Pontiki & Hadjipavlou (2007); Urdaneta *et al.* (2004). For graph-set notation, see: Bernstein *et al.* (1995).



### Experimental

#### Crystal data

$\text{C}_{17}\text{H}_{16}\text{ClNO}$   
 $M_r = 285.76$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 9.803$  (3) Å  
 $b = 14.976$  (5) Å  
 $c = 20.823$  (6) Å

$V = 3057.2$  (15) Å<sup>3</sup>  
 $Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.24$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.48 \times 0.38 \times 0.28$  mm

#### Data collection

Rigaku AFC-7S Mercury diffractometer  
 Absorption correction: multi-scan (Jacobson, 1998)  
 $T_{\min} = 0.897$ ,  $T_{\max} = 0.985$   
 (expected range = 0.850–0.934)

32660 measured reflections  
 5802 independent reflections  
 3687 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.063$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.070$   
 $wR(F^2) = 0.161$   
 $S = 1.07$   
 5802 reflections  
 362 parameters  
 H-atom parameters constrained

$\Delta\rho_{\max} = 0.18$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.28$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 1693 Friedel pairs  
 Flack parameter:  $-0.03$  (9)

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O2}^i$	0.97	1.89	2.852 (4)	174
$\text{N2}-\text{H2N}\cdots\text{O1}$	0.95	2.04	2.933 (5)	157
$\text{C10}-\text{H10}\cdots\text{C11}$	0.93	2.64	3.021 (6)	105
$\text{C13}-\text{H13}\cdots\text{N1}$	0.93	2.55	2.874 (5)	101
$\text{C19}-\text{H19}\cdots\text{O1}$	0.93	2.50	3.315 (5)	146
$\text{C27}-\text{H27}\cdots\text{Cl2}$	0.93	2.65	3.028 (6)	105
$\text{C30}-\text{H30}\cdots\text{N2}$	0.93	2.65	2.951 (5)	99

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

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSK, 2004); program(s) used to solve structure: *SHELXTL-NT* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT* and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL-NT* and *PLATON* (Spek, 2003).

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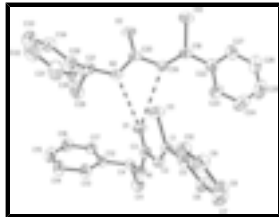
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2746).

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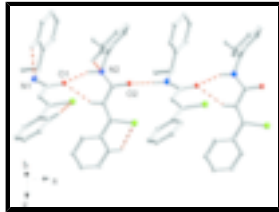
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