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N-Benzyl-3-(4-chlorophenyl)-3-phenylacrylamide

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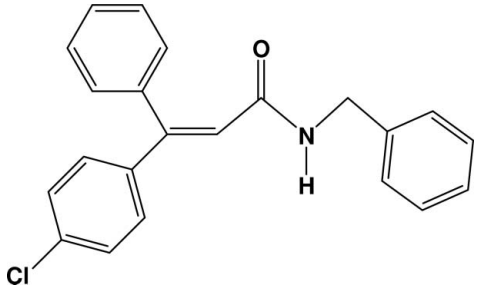
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.055; wR factor = 0.103; data-to-parameter ratio = 12.5.

In the title compound, $C_{22}H_{18}ClNO$, the aromatic substituents are not coplanar with the acrylamide unit. C—H···Cl and N—H···O hydrogen bonds link the molecules to form a three-dimensional supramolecular structure.

Related literature

For related literature, see: Hiroaki *et al.* (2005); Hu, Zhou, Lian *et al.* (2003); Hu, Zhou, Long *et al.* (2003); Mathews *et al.* (2000); Ross *et al.* (2001).



Experimental

Crystal data

$C_{22}H_{18}ClNO$
M_r = 347.82
Monoclinic, *Cc*
a = 10.352 (2) Å
b = 19.028 (4) Å
c = 9.621 (2) Å
β = 107.02 (3)°
V = 1812.1 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 291 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.95, T_{max} = 0.98
5453 measured reflections
2834 independent reflections
2248 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.103
S = 1.01
2834 reflections
226 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 1047 Friedel pairs
Flack parameter: 0.08 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O1^{i}	0.86	2.01	2.852 (4)	168

Symmetry code: (i) $x, -y+1, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Bruno *et al.*, 2002); 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: IM2014).

References

Bruker (2000). *SMART* (Version 5.625), *SAINT* (Version 6.01), *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hiroaki, O., Kumiko, M., Tsuyoshi, M. & Yoichi, K. (2005). *Chem. Eur. J.* **11**, 3728–3741.
Hu, Y.-M., Zhou, -J., Lian, H.-Z., Zhu, C.-J. & Pan, Y. (2003). *Synthesis*, pp. 1177–1180.
Hu, Y.-M., Zhou, J., Long, X.-T., Han, J.-L., Zhu, C.-J. & Pan, Y. (2003). *Tetrahedron Lett.* **44**, 5009–5010.
Mathews, C. J., Smith, P. G. & Welton, T. (2000). *Chem. Commun.* pp. 1249–1250.
Ross, J., Chen, W., Xu, L. & Xiao, J. (2001). *Organometallics*, **20**, 138–142.

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supplementary materials

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N-Benzyl-3-(4-chlorophenyl)-3-phenylacrylamide

Y.-M. Hu, D. Cheng, F.-H. Wu, D. Ren and O.-Y. Ying

Comment

The acrylamide structural features are absolutely essential for biological activity and function, it can therefore provide an impetus for synthetic chemists to design and develop efficient methods (Hiroaki, *et al.*, 2005; Mathews, *et al.*, 2000; Ross, *et al.*, 2001). We have recently developed a palladium-catalysted tandem cyclization of 1,6-dienes with aryl halides (Hu, Zhou, Long, *et al.*, 2003; Hu, Zhou, Lian *et al.*, 2003). The acrylamide derivative skeleton is formed by β-hydride elimination. Herein we describe a new compound formed by a corresponding palladium-catalyzed reaction.

In the title compound, $C_{22}H_{18}ClNO$, the atoms C7/N1/C8/C9/C10/O1 form a conjugated plane (I), whereas the planes of the other three phenyl rings, C1/C2/C3/C4/C5/C6 (II), C11/C12/C13/C14/C15/C16 (III) and C17/C18/C19/C20/C21/C22 (IV), are around the plane (I) and the dihedral angel for (I) and (II), (I) and (III), (I) and (IV) are 66.83 (1), 55.04 (2) and 55.75 (2)°, respectively.

In the crystal packing C–H···Cl and N–H···O hydrogen bonds (C1–H1A···Cl1^{i}; i: $-1/2+x, 1/2+y, -1+z$; N1–H1B···O1^{ii}, ii: $x, -y+1, z+1/2$) play an important role by linking the molecules to form the three-dimensional network structure (Fig. 2).

Experimental

An oven-dried Schlenk flask was evacuated, filled with nitrogen, and then charged with *N*-benzyl-3-phenylacrylamide (1.18 g, 5 mmol), 1-bromo-4-chlorobenzene (1.24 g, 6.5 mmol), tributylamine (1.8 ml), PPh_3 (53 mg, 0.2 mmol), $Pd(OAc)_2$ (23 mg, 1 mol %), and DMF (5 ml) to give a yellow solution. The reaction mixture was heated at 393 K with stirring. The reaction mixture was cooled to room temperature after 24 h and the resultant red-orange mixture was diluted with Et_2O(10 ml). The mixture was washed with H_2O(15 ml) and the aqueous layer was extracted with Et_2O (3 *X* 10 ml). The combined organic layers were dried ($MgSO_4$), filtered, and concentrated in vacuo. The crude material was purified by flash column chromatography on silica gel (light petroleum/EtOAc, 5:1) to obtain the prsoduct (1.36 g, 78%). Colorless crystals of the title compound suitable for X-ray diffraction were obtained from an ethyl acetate solution after 1 week.

Refinement

H atoms were placed in calculated positions, with C—H = 0.96–0.97 Å, N—H = 0.86 Å and included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C or N).

Figures

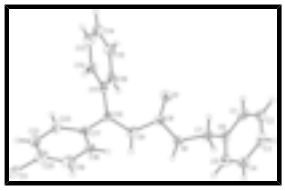

Fig. 1. : The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Fig. 2. : A view of the hydrogen bonds (i: −1/2 + *x*, 1/2 + *y*, −1 + *z*; ii: *x*, −*y* + 1, *z* + 1/2)

N-benzyl-3-(4-chlorophenyl)-3-phenylacrylamide

Crystal data

$C_{22}H_{18}ClNO$	F_{000} = 728
M_r = 347.82	D_x = 1.275 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 764 reflections
a = 10.352 (2) Å	θ = 2.1–25.5º
b = 19.028 (4) Å	μ = 0.22 mm^{-1}
c = 9.621 (2) Å	*T* = 291 (2) K
β = 107.02 (3)º	Block, orange
V = 1812.1 (7) Å^3	0.30 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	2834 independent reflections
Radiation source: sealed tube	2248 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 291(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −12→12
T_{min} = 0.95, T_{max} = 0.98	*k* = 0→23
5453 measured reflections	*l* = −11→11

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.88P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.103$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
2834 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
226 parameters	Extinction correction: none
2 restraints	Absolute structure: Flack (1983), 1047 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.08 (9)
Secondary atom site location: difference Fourier map	

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.

Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)

9.0508 (0.0077) *x* + 8.7550 (0.0172) *y* − 1.0401 (0.0187) *z* = 9.9745 (0.0076)

* −0.0235 (0.0023) C7 * 0.0438 (0.0026) N1 * 0.0139 (0.0033) C8 * −0.0498 (0.0028) C9 * 0.0204 (0.0024) C10 * −0.0048 (0.0013) O1

Rms deviation of fitted atoms = 0.0305

1.9715 (0.0153) *x* + 11.4206 (0.0246) *y* + 6.6104 (0.0118) *z* = 7.5091 (0.0102)

Angle to previous plane (with approximate e.s.d.) = 55.75 (0.15)

* −0.0006 (0.0025) C17 * 0.0041 (0.0028) C18 * 0.0155 (0.0029) C19 * −0.0388 (0.0030) C20 * 0.0420 (0.0029) C21 * −0.0221 (0.0027) C22

Rms deviation of fitted atoms = 0.0259

9.0508 (0.0077) *x* + 8.7550 (0.0172) *y* − 1.0401 (0.0187) *z* = 9.9745 (0.0076)

Angle to previous plane (with approximate e.s.d.) = 55.75 (0.15)

* −0.0235 (0.0023) C7 * 0.0438 (0.0026) N1 * 0.0139 (0.0033) C8 * −0.0498 (0.0028) C9 * 0.0204 (0.0024) C10 * −0.0048 (0.0013) O1

Rms deviation of fitted atoms = 0.0305

7.9952 (0.0115) *x* − 7.4330 (0.0303) *y* + 2.4331 (0.0147) *z* = 4.4092 (0.0177)

Angle to previous plane (with approximate e.s.d.) = 55.04 (0.12)

* −0.0327 (0.0025) C11 * 0.0264 (0.0028) C12 * −0.0110 (0.0030) C13 * 0.0030 (0.0030) C14 * −0.0102 (0.0028) C15 * 0.0245 (0.0025) C16

Rms deviation of fitted atoms = 0.0208

9.0508 (0.0077) *x* + 8.7550 (0.0172) *y* − 1.0401 (0.0187) *z* = 9.9745 (0.0076)

Angle to previous plane (with approximate e.s.d.) = 55.04 (0.12)

* −0.0235 (0.0023) C7 * 0.0438 (0.0026) N1 * 0.0139 (0.0033) C8 * −0.0498 (0.0028) C9 * 0.0204 (0.0024) C10 * −0.0048 (0.0013) O1

Rms deviation of fitted atoms = 0.0305

− 1.0169 (0.0171) *x* + 18.5528 (0.0120) *y* + 2.1090 (0.0156) *z* = 10.7462 (0.0084)

Angle to previous plane (with approximate e.s.d.) = 66.83 (0.11)

* −0.0023 (0.0030) C1 * −0.0128 (0.0028) C2 * 0.0167 (0.0029) C3 * −0.0054 (0.0032) C4 * −0.0094 (0.0031) C5 * 0.0133 (0.0028) C6

Rms deviation of fitted atoms = 0.0111

9.0508 (0.0077) *x* + 8.7550 (0.0172) *y* − 1.0401 (0.0187) *z* = 9.9745 (0.0076)

Angle to previous plane (with approximate e.s.d.) = 66.83 (0.11)

* −0.0235 (0.0023) C7 * 0.0438 (0.0026) N1 * 0.0139 (0.0033) C8 * −0.0498 (0.0028) C9 * 0.0204 (0.0024) C10 * −0.0048 (0.0013) O1

Rms deviation of fitted atoms = 0.0305

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3256 (5)	0.5940 (2)	0.0255 (5)	0.0568 (12)
H1A	0.3668	0.6042	−0.0460	0.068*
C2	0.1873 (4)	0.5902 (2)	−0.0124 (4)	0.0484 (10)
H2A	0.1361	0.5969	−0.1085	0.058*
C3	0.1236 (4)	0.5761 (2)	0.0948 (5)	0.0528 (11)
H3A	0.0298	0.5756	0.0703	0.063*
C4	0.2007 (5)	0.5627 (2)	0.2394 (5)	0.0572 (12)
H4A	0.1593	0.5518	0.3103	0.069*
C5	0.3410 (5)	0.5664 (2)	0.2727 (5)	0.0568 (11)
H5A	0.3933	0.5575	0.3675	0.068*
C6	0.4059 (4)	0.5832 (2)	0.1667 (5)	0.0488 (10)
C7	0.5526 (4)	0.58951 (18)	0.2037 (4)	0.0398 (9)
H7A	0.5769	0.5978	0.1151	0.048*
H7B	0.5807	0.6303	0.2656	0.048*
C8	0.6674 (4)	0.47547 (18)	0.2064 (4)	0.0364 (8)

C9	0.7269 (4)	0.41857 (19)	0.3067 (4)	0.0373 (8)
H9A	0.7231	0.4228	0.4017	0.045*
C10	0.7888 (4)	0.35857 (17)	0.2730 (4)	0.0383 (8)
C11	0.8325 (3)	0.35184 (18)	0.1378 (4)	0.0349 (8)
C12	0.8087 (4)	0.2920 (2)	0.0575 (4)	0.0435 (9)
H12A	0.7712	0.2536	0.0913	0.052*
C13	0.8386 (4)	0.2866 (2)	−0.0724 (5)	0.0500 (10)
H13A	0.8140	0.2464	−0.1289	0.060*
C14	0.9032 (4)	0.3392 (2)	−0.1183 (5)	0.0557 (11)
H14A	0.9271	0.3344	−0.2038	0.067*
C15	0.9344 (4)	0.4016 (2)	−0.0357 (5)	0.0511 (11)
H15A	0.9753	0.4390	−0.0688	0.061*
C16	0.9041 (4)	0.4069 (2)	0.0945 (4)	0.0421 (9)
H16A	0.9304	0.4463	0.1532	0.050*
C17	0.8120 (3)	0.30118 (18)	0.3733 (4)	0.0334 (8)
C18	0.7130 (4)	0.28042 (19)	0.4394 (4)	0.0395 (9)
H18A	0.6328	0.3057	0.4189	0.047*
C19	0.7300 (4)	0.2261 (2)	0.5300 (5)	0.0490 (10)
H19A	0.6642	0.2153	0.5750	0.059*
C20	0.8443 (4)	0.1861 (2)	0.5568 (5)	0.0510 (11)
C21	0.9479 (4)	0.2056 (2)	0.5044 (4)	0.0457 (9)
H21A	1.0303	0.1823	0.5350	0.055*
C22	0.9301 (4)	0.25964 (19)	0.4066 (4)	0.0405 (9)
H22A	0.9965	0.2691	0.3617	0.049*
Cl1	0.86209 (10)	0.11174 (5)	0.66618 (11)	0.0527 (3)
N1	0.6263 (3)	0.52965 (15)	0.2760 (3)	0.0379 (7)
H1B	0.6458	0.5278	0.3692	0.045*
O1	0.6475 (3)	0.47862 (16)	0.0779 (3)	0.0537 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.060 (3)	0.059 (3)	0.062 (3)	0.023 (2)	0.033 (2)	0.007 (2)
C2	0.054 (2)	0.041 (2)	0.037 (2)	0.0041 (19)	−0.0071 (18)	−0.0141 (17)
C3	0.039 (2)	0.033 (2)	0.084 (3)	0.0071 (17)	0.013 (2)	0.002 (2)
C4	0.062 (3)	0.058 (3)	0.064 (3)	0.014 (2)	0.038 (3)	0.005 (2)
C5	0.062 (3)	0.049 (2)	0.058 (3)	0.015 (2)	0.015 (2)	−0.002 (2)
C6	0.056 (3)	0.0328 (19)	0.057 (2)	0.0176 (17)	0.016 (2)	−0.0114 (18)
C7	0.054 (2)	0.0301 (19)	0.047 (2)	0.0100 (16)	0.031 (2)	0.0087 (16)
C8	0.044 (2)	0.0316 (18)	0.040 (2)	−0.0041 (15)	0.0222 (17)	−0.0092 (15)
C9	0.042 (2)	0.0351 (19)	0.044 (2)	0.0004 (15)	0.0269 (18)	−0.0052 (15)
C10	0.050 (2)	0.0256 (17)	0.041 (2)	0.0134 (16)	0.0155 (18)	−0.0053 (15)
C11	0.0226 (16)	0.040 (2)	0.042 (2)	0.0092 (14)	0.0086 (14)	0.0067 (16)
C12	0.043 (2)	0.047 (2)	0.044 (2)	0.0024 (18)	0.0182 (18)	−0.0057 (18)
C13	0.058 (3)	0.042 (2)	0.055 (2)	0.0018 (19)	0.025 (2)	−0.003 (2)
C14	0.060 (3)	0.049 (3)	0.065 (3)	0.019 (2)	0.030 (2)	0.014 (2)
C15	0.060 (3)	0.047 (2)	0.059 (3)	0.009 (2)	0.036 (2)	0.016 (2)
C16	0.036 (2)	0.039 (2)	0.049 (2)	0.0084 (16)	0.0099 (18)	0.0174 (16)

C17	0.0355 (19)	0.0403 (19)	0.0222 (15)	−0.0009 (15)	0.0050 (14)	−0.0101 (14)
C18	0.043 (2)	0.042 (2)	0.040 (2)	0.0030 (17)	0.0224 (18)	−0.0056 (16)
C19	0.044 (2)	0.058 (2)	0.057 (3)	−0.0171 (19)	0.033 (2)	0.001 (2)
C20	0.051 (2)	0.048 (2)	0.063 (3)	−0.0120 (19)	0.029 (2)	−0.007 (2)
C21	0.045 (2)	0.044 (2)	0.050 (2)	0.0092 (18)	0.0172 (19)	−0.0010 (19)
C22	0.039 (2)	0.0301 (19)	0.047 (2)	0.0067 (15)	0.0051 (17)	0.0018 (16)
Cl1	0.0585 (6)	0.0502 (5)	0.0533 (6)	0.0194 (5)	0.0228 (5)	−0.0061 (5)
N1	0.0575 (19)	0.0266 (14)	0.0267 (14)	−0.0007 (14)	0.0080 (13)	−0.0026 (11)
O1	0.0596 (17)	0.0705 (19)	0.0311 (14)	0.0153 (16)	0.0135 (13)	0.0131 (14)

Geometric parameters (Å, °)

C1—C2	1.372 (6)	C11—C16	1.415 (5)
C1—C6	1.385 (6)	C12—C13	1.376 (5)
C1—H1A	0.9300	C12—H12A	0.9300
C2—C3	1.403 (6)	C13—C14	1.348 (6)
C2—H2A	0.9300	C13—H13A	0.9300
C3—C4	1.409 (7)	C14—C15	1.412 (6)
C3—H3A	0.9300	C14—H14A	0.9300
C4—C5	1.394 (6)	C15—C16	1.382 (5)
C4—H4A	0.9300	C15—H15A	0.9300
C5—C6	1.412 (6)	C16—H16A	0.9300
C5—H5A	0.9300	C17—C22	1.412 (5)
C6—C7	1.460 (6)	C17—C18	1.412 (5)
C7—N1	1.432 (4)	C18—C19	1.331 (5)
C7—H7A	0.9700	C18—H18A	0.9300
C7—H7B	0.9700	C19—C20	1.366 (6)
C8—O1	1.194 (4)	C19—H19A	0.9300
C8—N1	1.364 (4)	C20—C21	1.363 (5)
C8—C9	1.461 (5)	C20—Cl1	1.740 (4)
C9—C10	1.393 (5)	C21—C22	1.369 (5)
C9—H9A	0.9300	C21—H21A	0.9300
C10—C17	1.431 (5)	C22—H22A	0.9300
C10—C11	1.502 (5)	N1—H1B	0.8600
C11—C12	1.357 (5)		
C2—C1—C6	122.2 (4)	C11—C12—C13	121.9 (4)
C2—C1—H1A	118.9	C11—C12—H12A	119.1
C6—C1—H1A	118.9	C13—C12—H12A	119.1
C1—C2—C3	119.5 (4)	C14—C13—C12	120.4 (4)
C1—C2—H2A	120.2	C14—C13—H13A	119.8
C3—C2—H2A	120.2	C12—C13—H13A	119.8
C2—C3—C4	120.5 (4)	C13—C14—C15	119.6 (4)
C2—C3—H3A	119.7	C13—C14—H14A	120.2
C4—C3—H3A	119.7	C15—C14—H14A	120.2
C5—C4—C3	118.0 (4)	C16—C15—C14	119.8 (4)
C5—C4—H4A	121.0	C16—C15—H15A	120.1
C3—C4—H4A	121.0	C14—C15—H15A	120.1
C4—C5—C6	121.9 (5)	C15—C16—C11	119.4 (4)
C4—C5—H5A	119.0	C15—C16—H16A	120.3

C6—C5—H5A	119.0	C11—C16—H16A	120.3
C1—C6—C5	117.8 (4)	C22—C17—C18	115.9 (3)
C1—C6—C7	120.6 (4)	C22—C17—C10	122.9 (3)
C5—C6—C7	121.6 (4)	C18—C17—C10	121.1 (3)
N1—C7—C6	114.9 (3)	C19—C18—C17	122.6 (3)
N1—C7—H7A	108.5	C19—C18—H18A	118.7
C6—C7—H7A	108.5	C17—C18—H18A	118.7
N1—C7—H7B	108.5	C18—C19—C20	119.8 (3)
C6—C7—H7B	108.5	C18—C19—H19A	120.1
H7A—C7—H7B	107.5	C20—C19—H19A	120.1
O1—C8—N1	119.1 (4)	C21—C20—C19	120.7 (4)
O1—C8—C9	129.2 (3)	C21—C20—Cl1	119.3 (3)
N1—C8—C9	111.6 (3)	C19—C20—Cl1	120.0 (3)
C10—C9—C8	126.0 (3)	C20—C21—C22	119.8 (4)
C10—C9—H9A	117.0	C20—C21—H21A	120.1
C8—C9—H9A	117.0	C22—C21—H21A	120.1
C9—C10—C17	117.8 (3)	C21—C22—C17	120.6 (4)
C9—C10—C11	123.1 (3)	C21—C22—H22A	119.7
C17—C10—C11	119.0 (3)	C17—C22—H22A	119.7
C12—C11—C16	118.5 (4)	C8—N1—C7	124.1 (3)
C12—C11—C10	120.9 (3)	C8—N1—H1B	117.9
C16—C11—C10	120.5 (3)	C7—N1—H1B	117.9

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1B···O1^{i}	0.86	2.01	2.852 (4)	168

Symmetry codes: (i) *x*, −*y*+1, *z*+1/2.

Fig. 1

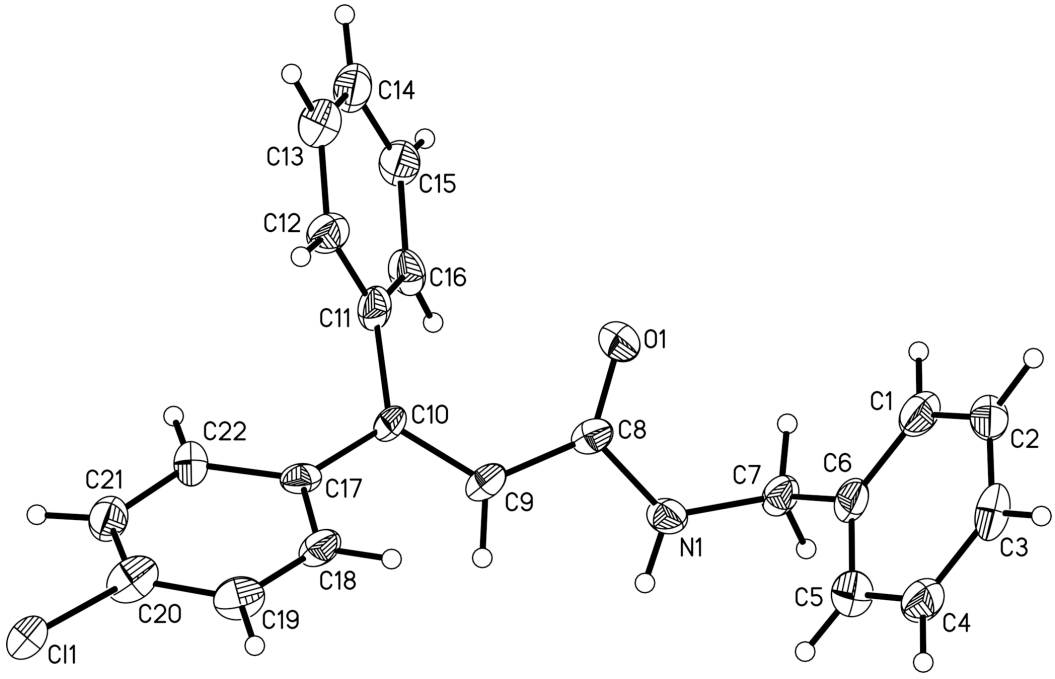
C14
C13
C15
C12
C16
C11
O1
C10
C8
C1
C2
C22
C6
C7
C21
C17
C9
N1
C3
C18
C5
C20
C19
C4
Cl1

Fig. 2