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2-Benzoyl-1-benzylmethyl-3-phenylguanidine

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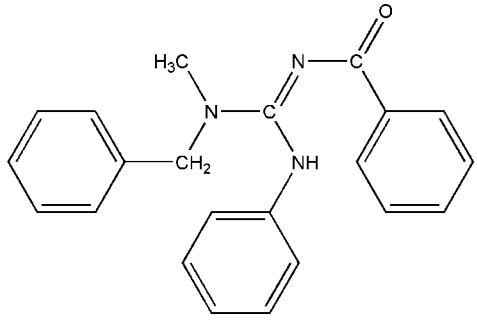
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.105; data-to-parameter ratio = 17.4.

The title compound, $C_{22}H_{21}N_3O$, is a typical polysubstituted guanidine with normal geometric parameters. The torsion angles indicate that the guanidine unit and the carbonyl group are not coplanar. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds which link the molecules into a continuous zigzag chain. The benzyl group is almost perpendicular to the guanidine unit, making a dihedral angle of 88.38 (5)°.

Related literature

For related literature, see: Aldhaheri (1998); Cunha *et al.* (2005); Kohn *et al.* (2004); Moroni *et al.* (2001); Taniguchi *et al.* (1993); Yoshiizumi *et al.* (1998).



Experimental

Crystal data

$C_{22}H_{21}N_3O$
M_r = 343.42
Monoclinic, $P2_1/c$
a = 12.887 (6) Å
b = 9.298 (4) Å
c = 18.286 (6) Å
β = 123.534 (5)°
V = 1826.4 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 113 (2) K
0.50 × 0.40 × 0.20 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: none
14468 measured reflections
4168 independent reflections
3842 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.105
S = 1.19
4168 reflections
240 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.891 (19)	1.89 (2)	2.7757 (17)	172.0 (17)

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku Corporation, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Molecular Structure Corporation & Rigaku Corporation, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2339).

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supplementary materials

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2-Benzoyl-1-benzylmethyl-3-phenylguanidine

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Comment

N,N′,N″-Trisubstituted Guanidines are useful compounds used in medicine as an analgesic, antihypertensive, antibacterial, cancerostatic and cytotoxic agents (Taniguchi *et al.*, 1993; Yoshiizumi *et al.*, 1998; Moroni *et al.*, 2001). They have potential applications in the field of analytical and synthetic organic chemistry (Aldhaheri *et al.*, 1998; Kohn *et al.*, 2004). The title compound (I), (Fig. 1) is a typical *N,N′,N″*-Trisubstituted guanidine with normal geometric parameters (Cunha *et al.*, 2005). The C(1)—O(1) bond shows expected full double bond character while the short values for C(1)—N(1), C(2)—N(1), C(2)—N(2), and C(2)—N(3) bond lengths indicate partial double bond character. The dihedral angles between the guanidine plane [C(2)/N(1)/N(2)/N(3)] and the phenyl ring C(11)–C(16), benzoyl and benzyl planes are 47.89 (8)°, 33.11 (9)° & 88.38 (5)°, respectively. The guanidine moiety and carbonyl group are not coplanar, as reflected by the torsion angles O(1)—C(1)—N(1)—C(2), N(2)—C(2)—N(1)—C(1), N(3)—C(2)—N(1)—C(1) and C(2)—N(1)—C(1)—C(3), expectedly this is due to the absence of intramolecular N—H···O hydrogen bonding, forming a six-membered ring commonly observed in this class of compounds (Cunha *et al.*, 2005). The crystal packing shows intermolecular N—H···O hydrogen bonds which link the molecules into a continuous zigzag chain (Fig. 2).

Experimental

N-Benzoyl-*N*′-phenylthiourea (0.512 g, 2 mmol) was dissolved in 10 ml of DMF and was taken in a two neck round bottom flask. Triethylamine (0.56 ml, 4 mmol) and benzylmethyl amine (0.3 ml, 2 mmol) was added to it and the mixture was stirred well. Then mercuric chloride (0.544 g, 2 mmol) was added and vigorously stirred for 12 h and progress of reaction was monitored by TLC. When the thiourea was consumed, 20 ml of chloroform was added and the suspension was filtered through sintered glass funnel to remove HgS formed during reaction. The solvent was evaporated under reduced pressure and the residue was dissolved in 20 ml of CH_2Cl_2 and byproducts were extracted with water (4 × 30 ml). The organic phase was dried over anhydrous $MgSO_4$ and then filtered. After filtration the solvent was evaporated and the guanidine was recrystallized in ethanol.

Refinement

Hydrogen atoms bonded to C were included in calculated positions and refined as riding on their parent C atom with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). The H atoms bonded to N were freely refined.

Figures

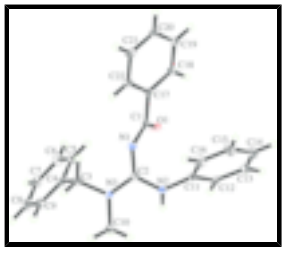

Fig. 1. Molecular structure of (I) showing atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

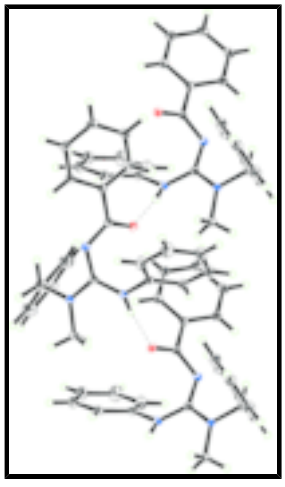

Fig. 2. Hydrogen bonding chain of (I). Hydrogen bonds shown as dashed lines.

2-Benzoyl-1-benzylmethyl-3-phenylguanidine

Crystal data

$C_{22}H_{21}N_3O$	F_{000} = 728
M_r = 343.42	D_x = 1.249 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: -P 2ybc	Cell parameters from 4921 reflections
a = 12.887 (6) Å	θ = 3.2–27.5º
b = 9.298 (4) Å	μ = 0.08 mm^{-1}
c = 18.286 (6) Å	T = 113 (2) K
β = 123.534 (5)º	Block, colourless
V = 1826.4 (13) Å^3	0.50 × 0.40 × 0.20 mm
Z = 4	

Data collection

Rigaku/MSC Mercury CCD diffractometer	4168 independent reflections
Radiation source: fine-focus sealed tube	3842 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 14.62 pixels mm^{-1}	θ_{max} = 27.5º

T = 113(2) K	θ_{min} = 3.2°
ω scans	h = −14→16
Absorption correction: none	k = −11→12
14468 measured reflections	l = −23→14

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 0.8451P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.19	$(\Delta/\sigma)_{max} < 0.001$
4168 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
240 parameters	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.47386 (10)	0.79221 (11)	0.20921 (6)	0.0238 (2)
N1	0.43613 (11)	0.68638 (13)	0.08296 (7)	0.0198 (3)
N2	0.40990 (11)	0.49147 (13)	0.15547 (8)	0.0195 (3)
H2	0.4509 (17)	0.424 (2)	0.1965 (12)	0.033 (5)*
N3	0.55340 (11)	0.47769 (12)	0.11860 (7)	0.0190 (3)
C1	0.43019 (13)	0.79478 (15)	0.12897 (9)	0.0182 (3)
C2	0.46771 (13)	0.55557 (15)	0.12081 (8)	0.0179 (3)
C3	0.63975 (13)	0.54547 (16)	0.10072 (9)	0.0213 (3)
H3A	0.6064	0.6404	0.0730	0.026*
H3B	0.6466	0.4851	0.0590	0.026*
C4	0.76762 (14)	0.56506 (16)	0.18374 (9)	0.0208 (3)
C5	0.78900 (15)	0.67564 (17)	0.24179 (10)	0.0262 (3)
H5	0.7234	0.7397	0.2287	0.031*

C6	0.90559 (16)	0.6928 (2)	0.31870 (11)	0.0331 (4)
H6	0.9202	0.7700	0.3573	0.040*
C7	1.00079 (16)	0.5973 (2)	0.33920 (11)	0.0356 (4)
H7	1.0801	0.6079	0.3924	0.043*
C8	0.98010 (15)	0.4872 (2)	0.28232 (12)	0.0344 (4)
H8	1.0452	0.4216	0.2964	0.041*
C9	0.86422 (15)	0.47171 (18)	0.20443 (11)	0.0277 (3)
H9	0.8510	0.3965	0.1650	0.033*
C10	0.57864 (14)	0.32698 (15)	0.14542 (10)	0.0239 (3)
H10A	0.5008	0.2788	0.1285	0.036*
H10B	0.6373	0.3213	0.2092	0.036*
H10C	0.6147	0.2797	0.1165	0.036*
C11	0.30173 (13)	0.54399 (15)	0.14878 (10)	0.0208 (3)
C12	0.29603 (14)	0.53620 (15)	0.22243 (10)	0.0231 (3)
H12	0.3649	0.4996	0.2760	0.028*
C13	0.19031 (15)	0.58166 (17)	0.21805 (11)	0.0288 (3)
H13	0.1866	0.5744	0.2684	0.035*
C14	0.09040 (16)	0.6373 (2)	0.14121 (12)	0.0361 (4)
H14	0.0186	0.6702	0.1385	0.043*
C15	0.09647 (16)	0.6445 (2)	0.06818 (12)	0.0422 (5)
H15	0.0280	0.6829	0.0151	0.051*
C16	0.20020 (15)	0.5969 (2)	0.07080 (11)	0.0330 (4)
H16	0.2019	0.6004	0.0196	0.040*
C17	0.36914 (13)	0.92985 (15)	0.07780 (9)	0.0184 (3)
C18	0.31789 (15)	1.02614 (16)	0.10768 (10)	0.0251 (3)
H18	0.3220	1.0061	0.1602	0.030*
C19	0.26077 (15)	1.15124 (17)	0.06129 (11)	0.0280 (3)
H19	0.2249	1.2157	0.0816	0.034*
C20	0.25594 (14)	1.18226 (16)	−0.01436 (10)	0.0264 (3)
H20	0.2168	1.2680	−0.0460	0.032*
C21	0.30827 (14)	1.08805 (16)	−0.04408 (10)	0.0253 (3)
H21	0.3062	1.1101	−0.0956	0.030*
C22	0.36373 (14)	0.96157 (15)	0.00132 (9)	0.0215 (3)
H22	0.3981	0.8964	−0.0199	0.026*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0314 (6)	0.0195 (5)	0.0163 (5)	−0.0023 (4)	0.0106 (4)	−0.0020 (4)
N1	0.0245 (6)	0.0178 (6)	0.0170 (6)	0.0024 (5)	0.0114 (5)	0.0014 (5)
N2	0.0214 (6)	0.0161 (6)	0.0209 (6)	0.0023 (5)	0.0116 (5)	0.0027 (5)
N3	0.0206 (6)	0.0177 (6)	0.0178 (6)	0.0018 (5)	0.0100 (5)	0.0004 (5)
C1	0.0167 (7)	0.0185 (7)	0.0180 (7)	−0.0015 (5)	0.0088 (6)	0.0000 (5)
C2	0.0187 (7)	0.0183 (7)	0.0121 (6)	−0.0008 (5)	0.0058 (5)	−0.0022 (5)
C3	0.0248 (7)	0.0237 (7)	0.0183 (7)	0.0018 (6)	0.0138 (6)	0.0016 (6)
C4	0.0220 (7)	0.0248 (7)	0.0204 (7)	0.0004 (6)	0.0146 (6)	0.0042 (6)
C5	0.0268 (8)	0.0291 (8)	0.0230 (7)	0.0028 (6)	0.0138 (6)	0.0018 (6)
C6	0.0337 (9)	0.0395 (10)	0.0237 (8)	−0.0059 (7)	0.0144 (7)	−0.0034 (7)

C7	0.0232 (8)	0.0478 (11)	0.0282 (8)	−0.0051 (7)	0.0095 (7)	0.0067 (8)
C8	0.0220 (8)	0.0415 (10)	0.0406 (10)	0.0052 (7)	0.0179 (7)	0.0100 (8)
C9	0.0263 (8)	0.0306 (8)	0.0315 (8)	0.0026 (7)	0.0193 (7)	0.0026 (7)
C10	0.0271 (8)	0.0180 (7)	0.0278 (8)	0.0033 (6)	0.0160 (7)	0.0004 (6)
C11	0.0207 (7)	0.0159 (6)	0.0246 (7)	−0.0021 (5)	0.0119 (6)	−0.0013 (6)
C12	0.0235 (7)	0.0195 (7)	0.0258 (7)	−0.0014 (6)	0.0132 (6)	0.0008 (6)
C13	0.0284 (8)	0.0292 (8)	0.0339 (9)	−0.0029 (7)	0.0204 (7)	−0.0026 (7)
C14	0.0230 (8)	0.0412 (10)	0.0456 (10)	0.0030 (7)	0.0199 (8)	−0.0006 (8)
C15	0.0224 (9)	0.0616 (13)	0.0336 (9)	0.0106 (8)	0.0098 (7)	0.0099 (9)
C16	0.0244 (8)	0.0461 (10)	0.0242 (8)	0.0027 (7)	0.0108 (7)	0.0022 (7)
C17	0.0164 (7)	0.0168 (6)	0.0197 (7)	−0.0023 (5)	0.0085 (6)	−0.0005 (5)
C18	0.0297 (8)	0.0220 (7)	0.0290 (8)	0.0011 (6)	0.0196 (7)	0.0017 (6)
C19	0.0275 (8)	0.0222 (7)	0.0393 (9)	0.0049 (6)	0.0215 (7)	0.0019 (7)
C20	0.0197 (7)	0.0194 (7)	0.0324 (8)	0.0024 (6)	0.0097 (6)	0.0065 (6)
C21	0.0263 (8)	0.0240 (7)	0.0213 (7)	−0.0022 (6)	0.0105 (6)	0.0030 (6)
C22	0.0229 (7)	0.0205 (7)	0.0202 (7)	−0.0003 (6)	0.0114 (6)	−0.0010 (6)

Geometric parameters (Å, °)

O1—C1	1.2482 (17)	C10—H10B	0.9800
N1—C1	1.3419 (18)	C10—H10C	0.9800
N1—C2	1.3464 (18)	C11—C16	1.388 (2)
N2—C2	1.3541 (19)	C11—C12	1.391 (2)
N2—C11	1.417 (2)	C12—C13	1.386 (2)
N2—H2	0.891 (19)	C12—H12	0.9500
N3—C2	1.3396 (19)	C13—C14	1.379 (2)
N3—C10	1.4608 (19)	C13—H13	0.9500
N3—C3	1.4642 (19)	C14—C15	1.382 (3)
C1—C17	1.5028 (19)	C14—H14	0.9500
C3—C4	1.513 (2)	C15—C16	1.384 (3)
C3—H3A	0.9900	C15—H15	0.9500
C3—H3B	0.9900	C16—H16	0.9500
C4—C9	1.388 (2)	C17—C18	1.391 (2)
C4—C5	1.392 (2)	C17—C22	1.393 (2)
C5—C6	1.388 (2)	C18—C19	1.387 (2)
C5—H5	0.9500	C18—H18	0.9500
C6—C7	1.388 (3)	C19—C20	1.380 (2)
C6—H6	0.9500	C19—H19	0.9500
C7—C8	1.377 (3)	C20—C21	1.387 (2)
C7—H7	0.9500	C20—H20	0.9500
C8—C9	1.389 (2)	C21—C22	1.388 (2)
C8—H8	0.9500	C21—H21	0.9500
C9—H9	0.9500	C22—H22	0.9500
C10—H10A	0.9800		
C1—N1—C2	117.52 (12)	N3—C10—H10C	109.5
C2—N2—C11	125.26 (12)	H10A—C10—H10C	109.5
C2—N2—H2	118.7 (12)	H10B—C10—H10C	109.5
C11—N2—H2	114.2 (12)	C16—C11—C12	119.30 (15)
C2—N3—C10	122.87 (12)	C16—C11—N2	122.34 (14)

C2—N3—C3	120.99 (12)	C12—C11—N2	118.31 (13)
C10—N3—C3	115.60 (12)	C13—C12—C11	120.29 (14)
O1—C1—N1	125.30 (13)	C13—C12—H12	119.9
O1—C1—C17	119.27 (12)	C11—C12—H12	119.9
N1—C1—C17	115.40 (12)	C14—C13—C12	120.55 (16)
N3—C2—N1	119.53 (13)	C14—C13—H13	119.7
N3—C2—N2	116.88 (13)	C12—C13—H13	119.7
N1—C2—N2	123.36 (13)	C13—C14—C15	118.90 (16)
N3—C3—C4	111.63 (12)	C13—C14—H14	120.5
N3—C3—H3A	109.3	C15—C14—H14	120.5
C4—C3—H3A	109.3	C14—C15—C16	121.37 (16)
N3—C3—H3B	109.3	C14—C15—H15	119.3
C4—C3—H3B	109.3	C16—C15—H15	119.3
H3A—C3—H3B	108.0	C15—C16—C11	119.57 (16)
C9—C4—C5	118.97 (14)	C15—C16—H16	120.2
C9—C4—C3	120.93 (14)	C11—C16—H16	120.2
C5—C4—C3	120.08 (13)	C18—C17—C22	119.13 (13)
C6—C5—C4	120.35 (15)	C18—C17—C1	119.48 (13)
C6—C5—H5	119.8	C22—C17—C1	121.39 (13)
C4—C5—H5	119.8	C19—C18—C17	120.41 (15)
C7—C6—C5	120.05 (16)	C19—C18—H18	119.8
C7—C6—H6	120.0	C17—C18—H18	119.8
C5—C6—H6	120.0	C20—C19—C18	120.19 (15)
C8—C7—C6	119.90 (16)	C20—C19—H19	119.9
C8—C7—H7	120.0	C18—C19—H19	119.9
C6—C7—H7	120.0	C19—C20—C21	119.89 (14)
C7—C8—C9	120.09 (16)	C19—C20—H20	120.1
C7—C8—H8	120.0	C21—C20—H20	120.1
C9—C8—H8	120.0	C20—C21—C22	120.13 (15)
C4—C9—C8	120.61 (16)	C20—C21—H21	119.9
C4—C9—H9	119.7	C22—C21—H21	119.9
C8—C9—H9	119.7	C21—C22—C17	120.23 (14)
N3—C10—H10A	109.5	C21—C22—H22	119.9
N3—C10—H10B	109.5	C17—C22—H22	119.9
H10A—C10—H10B	109.5		
C2—N1—C1—O1	14.6 (2)	C2—N2—C11—C16	44.1 (2)
C2—N1—C1—C17	−167.60 (12)	C2—N2—C11—C12	−138.63 (14)
C10—N3—C2—N1	−170.01 (12)	C16—C11—C12—C13	−0.4 (2)
C3—N3—C2—N1	18.81 (19)	N2—C11—C12—C13	−177.76 (13)
C10—N3—C2—N2	4.67 (19)	C11—C12—C13—C14	−1.1 (2)
C3—N3—C2—N2	−166.52 (12)	C12—C13—C14—C15	1.2 (3)
C1—N1—C2—N3	−133.45 (14)	C13—C14—C15—C16	0.1 (3)
C1—N1—C2—N2	52.24 (19)	C14—C15—C16—C11	−1.6 (3)
C11—N2—C2—N3	−167.33 (12)	C12—C11—C16—C15	1.7 (2)
C11—N2—C2—N1	7.1 (2)	N2—C11—C16—C15	178.95 (16)
C2—N3—C3—C4	102.60 (15)	O1—C1—C17—C18	−25.3 (2)
C10—N3—C3—C4	−69.19 (15)	N1—C1—C17—C18	156.75 (13)
N3—C3—C4—C9	101.46 (16)	O1—C1—C17—C22	154.08 (14)
N3—C3—C4—C5	−76.89 (17)	N1—C1—C17—C22	−23.86 (19)

C9—C4—C5—C6	0.6 (2)	C22—C17—C18—C19	0.8 (2)
C3—C4—C5—C6	179.02 (14)	C1—C17—C18—C19	−179.80 (14)
C4—C5—C6—C7	−1.6 (2)	C17—C18—C19—C20	−1.0 (2)
C5—C6—C7—C8	1.3 (3)	C18—C19—C20—C21	0.0 (2)
C6—C7—C8—C9	0.1 (3)	C19—C20—C21—C22	1.0 (2)
C5—C4—C9—C8	0.8 (2)	C20—C21—C22—C17	−1.2 (2)
C3—C4—C9—C8	−177.61 (14)	C18—C17—C22—C21	0.3 (2)
C7—C8—C9—C4	−1.1 (3)	C1—C17—C22—C21	−179.13 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.891 (19)	1.89 (2)	2.7757 (17)	172.0 (17)

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

Fig. 1

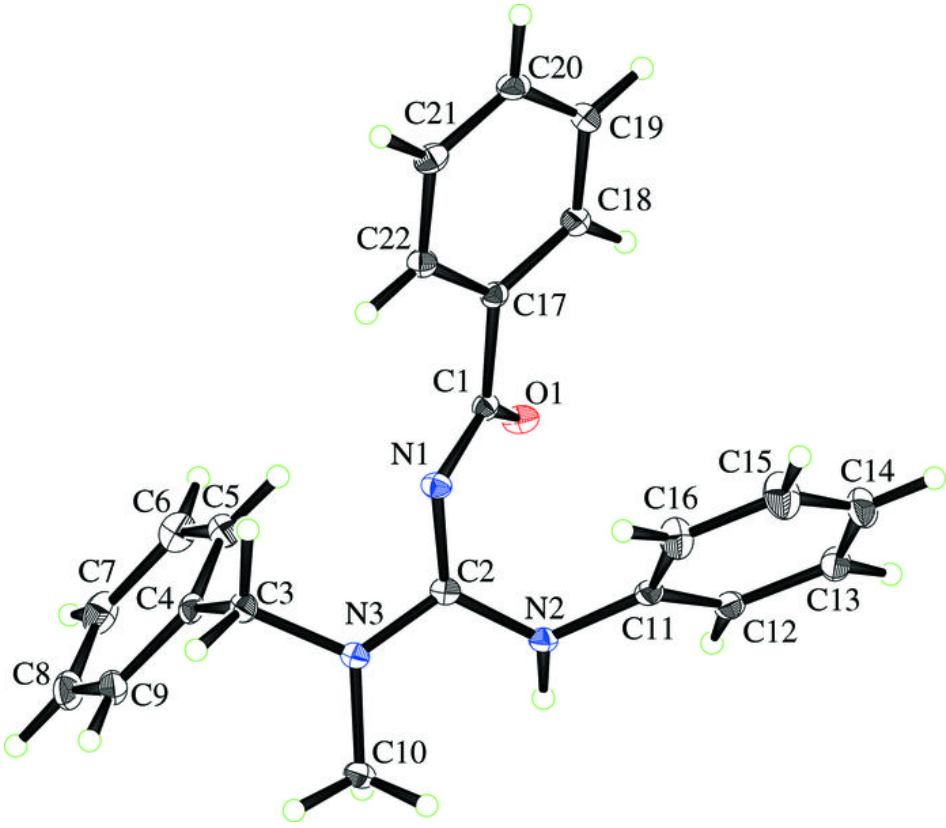
C20
C21
C19
C18
C22
C17
C1
O1
N1
C15
C14
C16
C6
C5
C7
C4
C3
C2
N3
N2
C11
C12
C13
C8
C9
C10

Fig. 2