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Crystal structure of 3-(9*H*-carbazol-9-yl)-*N*'-[(*E*)-4-chlorobenzylidene]propanohydrazide

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In the title compound, $C_{22}H_{18}ClN_3O$, the carbazole ring system is essentially planar (r.m.s deviation = 0.003 Å), and makes a dihedral angle of 9.01 (8)° with the plane of the chlorophenyl ring. In the crystal, neighbouring molecules are linked into centrosymmetric $R_2^2(8)$ dimers by pairs of N– H···O interactions and into a three-dimensional network by C–H··· π interactions. The dimers are arranged into layers parallel to (010).

Keywords: crystal structure; the carbazole ring system; bio-active molecules; hydrogen bonding.

CCDC reference: 1434700

1. Related literature

For synthesis and pharmacuetical studies of carbazole containing compounds, see: Hewlins *et al.* (1984); Kansal & Potier (1986); Haider *et al.* (1998); Hirata *et al.* (1999); Chowdhury *et al.* (1978); Sakano *et al.* (1980); Pindur (1990); Knölker & Reddy (2002); Martin & Prasad (2006); Saturnino *et al.* (2003).



2. Experimental

2.1. Crystal data

 $C_{22}H_{18}CIN_{3}O$ $M_{r} = 375.84$ Monoclinic, $P2_{1}/c$ a = 16.0126 (7) Å b = 7.4316 (3) Å c = 16.1654 (9) Å $\beta = 94.607 (4)^{\circ}$

2.2. Data collection

Agilent Xcalibur Eos Gemini diffractometer Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2014) $T_{\rm min} = 0.847, T_{\rm max} = 1.000$

2.3. Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.058$ $wR(F^2) = 0.167$ S = 1.026312 reflections Z = 4 Mo K\alpha radiation $\mu = 0.22 \text{ mm}^{-1}$ T = 293 K 0.42 × 0.36 × 0.08 mm

V = 1917.46 (16) Å³

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12277 measured reflections
6312 independent reflections
3066 reflections with I > 2\sigma(I)
R_{\text{int}} = 0.023
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244 parameters H-atom parameters constrained $\begin{array}{l} \Delta \rho_{max} = 0.20 \text{ e } \text{\AA}^{-3} \\ \Delta \rho_{min} = -0.24 \text{ e } \text{\AA}^{-3} \end{array}$

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

Cg2, Cg3 and Cg4 are the centroids of the two benzene rings (C1–C6 and C7–C12) of the carbazole ring system and the chlorophenyl ring (C17–C22), respectively.

$D - H \cdots A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$N2-H2N\cdotsO1^{i}$	0.81	2.08	2.8952 (19)	175
$C5-H5\cdots Cg4^{ii}$	0.93	2.81	3.696 (3)	160
$C21 - H21 \cdots Cg3^{iii}$	0.93	2.97	3.858 (3)	160
$C22-H22\cdots Cg2^{iii}$	0.93	2.79	3.699 (2)	166
			1 1 000	1 1

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

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

Acknowledgements

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References

- Agilent (2014). CrysAlis PRO. Agilent Technologies Ltd, Yarnton, England. Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C.,
- Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). J. Appl. Cryst. **32**, 115–119.
- Chowdhury, D. N., Basak, S. K. & Das, B. P. (1978). Curr. Sci. 47, 490–491. Farrugia, L. J. (2012). J. Appl. Cryst. 45, 849–854.
- Haider, N., Jbara, R., Khadami, F. & Wanko, R. (1998). *Heterocycles*, **48**, 1609–1622.

- Hewlins, M. J. E., Oliveira-Campos, A. & Shannon, P. V. R. (1984). *Synthesis*, pp. 289–302.
- Hirata, K., Ito, C., Furukawa, H., Itoigawa, M., Cosentino, L. M. & Lee, K. H. (1999). *Bioorg. Med. Chem. Lett.* 9, 119–122.
- Kansal, V. K. & Potier, P. (1986). Tetrahedron, 42, 2389-2408.
- Knölker, H. J. & Reddy, K. R. (2002). Chem. Rev. 102, 4303-4428.
- Martin, A. E. & Prasad, K. J. R. (2006). Acta Pharm. 56, 79-86.
- Pindur, U. (1990). Chimia, 44, 406-412.
- Sakano, K., Ishimaru, K. & Nakamura, S. (1980). J. Antibiot. 33, 683-689.
- Saturnino, C., Buonerba, M., Boatto, G., Pascale, M., Moltedo, O., de Napoli, L., Montesarchio, D., Lancelot, J. C. & de Caprariis, P. (2003). Chem. Pharm.
- Bull. **51**, 971–974.
- Sheldrick, G. M. (2015). Acta Cryst. C71, 3-8.
- Spek, A. L. (2009). Acta Cryst. D65, 148-155.

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Crystal structure of 3-(9*H*-carbazol-9-yl)-*N*'-[(*E*)-4-chlorobenzylidene]propanohydrazide

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S1. Comment

Carbazole scaffold compunds are well known for their pharmacological activities. The syntheses of carbazole derivatives in connection with the search for newer physiologically activities have been recognized in many reports (Hewlins *et al.*, 1984; Kansal & Potier 1986; Haider *et al.*, 1998; Hirata *et al.*, 1999). Carbazomycin A and carbazomycin B have been found to be useful antibacterial and antifungal agents (Chowdhury *et al.*, 1978; Sakano *et al.*, 1980). In addition pyridocarbazoles show marked anticancer and anti-HIV activities (Pindur, 1990; Knölker & Reddy, 2002; Martin & Prasad 2006; Saturnino *et al.*, 2003). Based on such facts we report in this study the synthesis and crystal structure of the title compound.

As shown in Fig. 1, the carbazole ring system (N1/C1–C12) of the title compound is essentially planar (r.m.s deviation = 0.003 Å), and makes a dihedral angle of 9.01 (8)° with the plane of the chlorophenyl ring (C17–C22). The bond lengths and angles are within normal ranges and are similar to those reported earlier for similar compounds.

In the crystal, two molecules are associated through a pair of N—H···O intermolecular hydrogen bonds, forming a centrosymmetric dimer with $R_2^2(8)$ ring motifs (Table 1), into layers parallel to (010) (Fig. 2). The dimers are connected by C—H··· π interactions, forming a three-dimensional network.

S2. Experimental

A mixture of 1.5 mmol (380 mg) of 3-(9*H*-carbazol-9-yl)propanehydrazide and 1.5 mmol (261 mg) of 4-chlorobenzaldehyde was heated in 10 ml of absolute ethanol and 3 ml of acetic acid catalyst. The reaction was monitored by TLC till completion after 3 h. The product which deposited on cooling, was collected, dried under vacuum and recrystallized from dioxan to give orange plates in 78% yield.

S3. Refinement

All H atoms were placed in calculated positions with N—H = 0.81 and C—H = 0.93 - 0.97 Å, and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C, N)$.



Figure 1

View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.





3-(9H-Carbazol-9-yl)-N'-[(E)-4-chlorobenzylidene]propanohydrazide

Crystal data

C₂₂H₁₈ClN₃O $M_r = 375.84$ Monoclinic, $P2_1/c$ Hall symbol: -P 2ybc a = 16.0126 (7) Å b = 7.4316 (3) Å c = 16.1654 (9) Å $\beta = 94.607$ (4)° V = 1917.46 (16) Å³ Z = 4

Data collection

Agilent Xcalibur Eos Gemini diffractometer	12277 measured reflections 6312 independent reflections
Radiation source: Enhance (Mo) X-ray Source	3066 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.023$
Detector resolution: 16.0416 pixels mm ⁻¹	$\theta_{\text{max}} = 32.8^{\circ}, \theta_{\text{min}} = 3.0^{\circ}$
ω scans	$h = -21 \rightarrow 24$
Absorption correction: multi-scan	$k = -5 \rightarrow 10$
(CrysAlis PRO; Agilent, 2014)	$l = -23 \rightarrow 19$
$T_{\min} = 0.847, \ T_{\max} = 1.000$	
Refinement	
Refinement on F^2	Hydrogen site location: mixed

Refinement on F^2 Hydrogen site location: mixedLeast-squares matrix: fullH-atom parameters constrained $R[F^2 > 2\sigma(F^2)] = 0.058$ $w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.350P]$ $wR(F^2) = 0.167$ where $P = (F_o^2 + 2F_c^2)/3$ S = 1.02 $(\Delta/\sigma)_{max} < 0.001$ 6312 reflections $\Delta\rho_{max} = 0.20$ e Å⁻³244 parameters $\Delta\rho_{min} = -0.24$ e Å⁻³0 restraints $\Delta\rho_{min} = -0.24$ e Å⁻³

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating *-R*-factor-obs *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.

F(000) = 784

 $\theta = 3.7 - 30.7^{\circ}$

 $\mu = 0.22 \text{ mm}^{-1}$ T = 293 K

Plate, orange

 $0.42 \times 0.36 \times 0.08 \text{ mm}$

 $D_{\rm x} = 1.302 {\rm Mg} {\rm m}^{-3}$

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 2141 reflections

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters $(Å^2)$

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Cl1	0.99666 (4)	-0.31996 (9)	0.20792 (5)	0.0942 (3)	
01	0.50960 (9)	-0.32276 (16)	0.57559 (9)	0.0624 (5)	
N1	0.66300 (10)	0.17932 (18)	0.56956 (10)	0.0547 (5)	
N2	0.60196 (9)	-0.39049 (19)	0.48394 (9)	0.0535 (5)	
N3	0.67596 (9)	-0.35405 (19)	0.44990 (10)	0.0511 (5)	

C1	0.64514 (12)	0.2806 (2)	0.63777 (12)	0.0539 (6)
C2	0.57672 (16)	0.2737 (3)	0.68399 (17)	0.0803 (9)
C3	0.5780 (2)	0.3896 (4)	0.75265 (19)	0.1108 (14)
C4	0.6440 (3)	0.5071 (4)	0.77117 (19)	0.1203 (16)
C5	0.7099 (2)	0.5122 (3)	0.72554 (17)	0.0944 (12)
C6	0.71287 (14)	0.3976 (2)	0.65793 (12)	0.0609 (7)
C7	0.77393 (13)	0.3604 (3)	0.60061 (13)	0.0649 (7)
C8	0.85479 (19)	0.4244 (4)	0.5889 (2)	0.1049 (13)
C9	0.8972 (2)	0.3490 (6)	0.5267 (3)	0.1362 (18)
C10	0.8626 (3)	0.2141 (6)	0.4766 (3)	0.1306 (17)
C11	0.78534 (18)	0.1509 (4)	0.48540 (17)	0.0887 (10)
C12	0.74149 (13)	0.2233 (2)	0.54750 (13)	0.0578 (6)
C13	0.61339 (13)	0.0290 (2)	0.53681 (13)	0.0646 (7)
C14	0.63465 (11)	-0.1461 (2)	0.58248 (12)	0.0522 (6)
C15	0.57783 (12)	-0.2941 (2)	0.54829 (12)	0.0502 (6)
C16	0.69414 (11)	-0.4544 (2)	0.39006 (12)	0.0546 (6)
C17	0.76989 (11)	-0.4242 (2)	0.34818 (11)	0.0507 (6)
C18	0.83316 (12)	-0.3082 (2)	0.37949 (12)	0.0567 (6)
C19	0.90254 (12)	-0.2777 (3)	0.33665 (14)	0.0625 (7)
C20	0.90972 (13)	-0.3622 (3)	0.26225 (14)	0.0626 (7)
C21	0.84950 (14)	-0.4801 (3)	0.23015 (14)	0.0701 (8)
C22	0.78026 (13)	-0.5105 (3)	0.27385 (13)	0.0647 (7)
H2	0.53200	0.19640	0.67050	0.0960*
H2N	0.57290	-0.47400	0.46610	0.0640*
Н3	0.53370	0.38750	0.78640	0.1330*
H4	0.64240	0.58410	0.81640	0.1450*
Н5	0.75350	0.59220	0.73900	0.1130*
H8	0.87900	0.51530	0.62240	0.1260*
H9	0.95070	0.39030	0.51840	0.1640*
H10	0.89350	0.16560	0.43560	0.1570*
H11	0.76210	0.06110	0.45070	0.1060*
H13A	0.62230	0.01380	0.47860	0.0780*
H13B	0.55450	0.05590	0.54060	0.0780*
H14A	0.69250	-0.17810	0.57610	0.0630*
H14B	0.62810	-0.13070	0.64120	0.0630*
H16	0.65840	-0.54830	0.37290	0.0660*
H18	0.82840	-0.25080	0.43000	0.0680*
H19	0.94440	-0.20000	0.35810	0.0750*
H21	0.85520	-0.53820	0.18000	0.0840*
H22	0.73950	-0.59110	0.25280	0.0780*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0802 (4)	0.0860 (4)	0.1213 (6)	0.0009 (3)	0.0377 (4)	-0.0096 (4)
01	0.0627 (8)	0.0490 (7)	0.0762 (9)	-0.0175 (6)	0.0092 (7)	-0.0065 (6)
N1	0.0572 (9)	0.0354 (7)	0.0690 (10)	-0.0128 (6)	-0.0100 (7)	-0.0014 (7)
N2	0.0576 (9)	0.0383 (7)	0.0638 (10)	-0.0184 (7)	0.0009 (7)	-0.0023 (7)

supporting information

N3	0.0525 (8)	0.0393 (7)	0.0605 (9)	-0.0101 (6)	-0.0020 (7)	0.0047 (7)
C1	0.0650 (12)	0.0325 (8)	0.0620 (11)	-0.0028 (8)	-0.0089 (9)	0.0074 (8)
C2	0.0819 (16)	0.0551 (12)	0.1050 (19)	0.0077 (11)	0.0151 (14)	0.0141 (13)
C3	0.157 (3)	0.0816 (19)	0.101 (2)	0.041 (2)	0.055 (2)	0.0206 (17)
C4	0.221 (4)	0.0656 (17)	0.074 (2)	0.013 (2)	0.010 (2)	-0.0023 (15)
C5	0.160 (3)	0.0472 (12)	0.0692 (16)	-0.0157 (15)	-0.0327 (17)	0.0001 (11)
C6	0.0858 (14)	0.0358 (9)	0.0567 (11)	-0.0128 (9)	-0.0216 (10)	0.0100 (8)
C7	0.0677 (12)	0.0478 (10)	0.0745 (14)	-0.0214 (9)	-0.0224 (11)	0.0250 (10)
C8	0.0827 (18)	0.093 (2)	0.133 (3)	-0.0414 (16)	-0.0290 (17)	0.0530 (19)
C9	0.0716 (19)	0.149 (3)	0.191 (4)	-0.016 (2)	0.029 (2)	0.094 (3)
C10	0.115 (3)	0.137 (3)	0.147 (3)	0.019 (2)	0.055 (2)	0.062 (3)
C11	0.101 (2)	0.0791 (16)	0.0881 (18)	0.0100 (15)	0.0215 (15)	0.0222 (14)
C12	0.0640 (12)	0.0444 (9)	0.0637 (12)	-0.0037 (9)	-0.0031 (9)	0.0148 (9)
C13	0.0723 (13)	0.0375 (9)	0.0786 (13)	-0.0143 (9)	-0.0275 (10)	0.0013 (9)
C14	0.0569 (10)	0.0389 (8)	0.0584 (11)	-0.0108 (8)	-0.0099 (8)	-0.0005 (8)
C15	0.0580 (11)	0.0334 (8)	0.0575 (11)	-0.0100 (8)	-0.0050 (8)	0.0058 (8)
C16	0.0560 (11)	0.0377 (9)	0.0682 (12)	-0.0101 (8)	-0.0073 (9)	-0.0006 (8)
C17	0.0524 (10)	0.0370 (8)	0.0609 (11)	-0.0019 (7)	-0.0073 (8)	-0.0011 (8)
C18	0.0584 (11)	0.0493 (10)	0.0611 (11)	-0.0056 (9)	-0.0033 (9)	-0.0079 (9)
C19	0.0538 (11)	0.0509 (10)	0.0811 (14)	-0.0078 (9)	-0.0043 (10)	-0.0045 (10)
C20	0.0579 (11)	0.0515 (10)	0.0783 (14)	0.0090 (9)	0.0054 (10)	-0.0043 (10)
C21	0.0703 (13)	0.0644 (13)	0.0750 (14)	0.0045 (11)	0.0019 (11)	-0.0212 (11)
C22	0.0606 (12)	0.0534 (11)	0.0781 (14)	-0.0052 (9)	-0.0060 (10)	-0.0178 (10)

Geometric parameters (Å, °)

Cl1—C20	1.733 (2)	C16—C17	1.453 (3)
O1—C15	1.229 (2)	C17—C22	1.384 (3)
N1—C1	1.384 (2)	C17—C18	1.394 (2)
N1-C12	1.373 (3)	C18—C19	1.374 (3)
N1—C13	1.446 (2)	C19—C20	1.370 (3)
N2—N3	1.373 (2)	C20—C21	1.374 (3)
N2—C15	1.345 (2)	C21—C22	1.380 (3)
N3—C16	1.274 (2)	C2—H2	0.9300
C1—C2	1.376 (3)	С3—Н3	0.9300
C1—C6	1.408 (3)	C4—H4	0.9300
C2—C3	1.404 (4)	С5—Н5	0.9300
N2—H2N	0.8100	C8—H8	0.9300
C3—C4	1.385 (5)	С9—Н9	0.9300
C4—C5	1.336 (5)	C10—H10	0.9300
C5—C6	1.389 (3)	C11—H11	0.9300
C6—C7	1.427 (3)	C13—H13A	0.9700
C7—C12	1.405 (3)	C13—H13B	0.9700
С7—С8	1.406 (4)	C14—H14A	0.9700
C8—C9	1.377 (5)	C14—H14B	0.9700
C9—C10	1.377 (6)	C16—H16	0.9300
C10—C11	1.342 (6)	C18—H18	0.9300
C11—C12	1.380 (3)	C19—H19	0.9300

supporting information

C13—C14	1.521 (2)	C21—H21	0.9300
C14—C15	1.504 (2)	C22—H22	0.9300
C1—N1—C12	109.24 (15)	C19—C20—C21	121.2 (2)
C1—N1—C13	124.70 (16)	C20—C21—C22	118.7 (2)
C12—N1—C13	125.17 (16)	C17—C22—C21	121.73 (19)
N3—N2—C15	121.05 (14)	C1—C2—H2	122.00
N2—N3—C16	116.50 (14)	С3—С2—Н2	122.00
N1—C1—C2	129.57 (18)	С2—С3—Н3	119.00
N1—C1—C6	108.41 (16)	С4—С3—Н3	119.00
$C_{2}-C_{1}-C_{6}$	121.98 (18)	C3—C4—H4	119.00
C1-C2-C3	1164(2)	C5-C4-H4	119.00
N3—N2—H2N	120.00	C4—C5—H5	120.00
C15— $N2$ — $H2N$	119.00	С6—С5—Н5	120.00
C_{2} C_{3} C_{4}	121 4 (3)	C7-C8-H8	121.00
C_{2}^{-} C_{3}^{-} C_{4}^{-} C_{5}^{-}	121.4(3)	C_{0} C_{8} H_{8}	121.00
C_{3}	121.4(3) 110.7(3)	C_{8} C_{9} H_{9}	110.00
$C_{4} = C_{5} = C_{6}$	119.7(3) 124.2(2)	$C_{0} = C_{0} = H_{0}$	119.00
$C_{3} = C_{0} = C_{7}$	134.3(2) 106.58(16)	$C_{10} - C_{9} - H_{9}$	119.00
C1 - C6 - C5	100.36(10) 110.1(2)	C_{11} C_{10} H_{10}	119.00
CI = CO = CS	119.1(2)	C10_C11_H11	119.00
$C_{0} - C_{1} - C_{8}$	135.1(2)		121.00
C_{0} C_{1} C_{12}	107.36 (18)	CI2—CII—HII	121.00
C8—C7—C12	117.5 (2)	NI—CI3—HI3A	109.00
C7—C8—C9	118.3 (3)	N1—C13—H13B	109.00
C8—C9—C10	121.8 (3)	С14—С13—Н13А	109.00
C9—C10—C11	121.6 (4)	C14—C13—H13B	109.00
C10-C11-C12	117.9 (3)	H13A—C13—H13B	108.00
N1—C12—C7	108.37 (17)	C13—C14—H14A	110.00
N1—C12—C11	128.76 (19)	C13—C14—H14B	110.00
C7—C12—C11	122.9 (2)	C15—C14—H14A	110.00
N1—C13—C14	112.84 (16)	C15—C14—H14B	110.00
C13—C14—C15	110.00 (15)	H14A—C14—H14B	108.00
N2-C15-C14	118.09 (16)	N3—C16—H16	120.00
O1—C15—C14	121.57 (16)	C17—C16—H16	120.00
O1—C15—N2	120.28 (16)	C17—C18—H18	120.00
N3—C16—C17	120.91 (15)	C19—C18—H18	120.00
C18—C17—C22	117.87 (17)	C18—C19—H19	120.00
C16—C17—C18	122.40 (16)	С20—С19—Н19	120.00
C16—C17—C22	119.72 (16)	C20—C21—H21	121.00
C17—C18—C19	120.82 (18)	C22—C21—H21	121.00
C18—C19—C20	119.68 (19)	С17—С22—Н22	119.00
C11—C20—C21	119.48 (17)	C21—C22—H22	119.00
C11 - C20 - C19	119.30 (16)		
	()		
C1—N1—C12—C7	-2.1(2)	C5—C6—C7—C8	-0.5(4)
$C_{12} = N_1 = C_1 = C_2$	-175.4 (2)	C6-C7-C12-N1	1.2 (2)
$C_{13} - N_{1} - C_{1} - C_{2}$	-5.7 (3)	C6—C7—C12—C11	-178.4(2)
$C_{12} = N_1 = C_1 = C_6$	2.3 (2)	C6-C7-C8-C9	177.5 (3)

C13—N1—C1—C6	171.93 (16)	C12—C7—C8—C9	-0.2(4)
C12—N1—C13—C14 C1—N1—C13—C14	84.8 (2) -83.2 (2)	C8—C7—C12—N1 C8—C7—C12—C11	-0.1(3)
C13—N1—C12—C7	-171.72 (17)	C7—C8—C9—C10	-0.1 (6)
C1—N1—C12—C11	177.4 (2)	C8—C9—C10—C11	0.8 (7)
C13—N1—C12—C11	7.8 (3)	C9—C10—C11—C12	-1.1 (6)
C15—N2—N3—C16	178.89 (16)	C10-C11-C12-C7	0.7 (4)
N3—N2—C15—C14	-0.5 (2)	C10-C11-C12-N1	-178.7 (3)
N3—N2—C15—O1	176.58 (16)	N1—C13—C14—C15	177.03 (16)
N2—N3—C16—C17	178.32 (15)	C13-C14-C15-O1	-88.0 (2)
N1-C1-C6-C5	-179.18 (18)	C13—C14—C15—N2	89.05 (19)
N1-C1-C6-C7	-1.5 (2)	N3—C16—C17—C18	11.7 (3)
C6—C1—C2—C3	-0.1 (3)	N3—C16—C17—C22	-167.34 (18)
N1—C1—C2—C3	177.3 (2)	C16—C17—C18—C19	-177.55 (17)
C2-C1-C6-C7	176.36 (19)	C22-C17-C18-C19	1.5 (3)
C2-C1-C6-C5	-1.3 (3)	C16—C17—C22—C21	177.23 (19)
C1—C2—C3—C4	1.5 (4)	C18—C17—C22—C21	-1.9 (3)
C2—C3—C4—C5	-1.5 (5)	C17—C18—C19—C20	0.0 (3)
C3—C4—C5—C6	0.0 (5)	C18—C19—C20—Cl1	178.96 (16)
C4—C5—C6—C7	-175.5 (3)	C18—C19—C20—C21	-1.3 (3)
C4—C5—C6—C1	1.4 (4)	Cl1—C20—C21—C22	-179.29 (17)
C5—C6—C7—C12	177.4 (2)	C19—C20—C21—C22	1.0 (3)
C1—C6—C7—C12	0.2 (2)	C20—C21—C22—C17	0.7 (3)
C1—C6—C7—C8	-177.6 (3)		

Hydrogen-bond geometry (Å, °)

Cg2, Cg3 and Cg4 are the centroids of the two benzene rings (C1–C6 and C7–C12) of the carbazole ring system and the chlorophenyl ring (C17–C22), respectively.

D H 4	лц	Ц Л	D <i>1</i>	D H 1
	D—II	II A	D^{-A}	$D = \Pi^{*} A$
N2—H2N····O1 ⁱ	0.81	2.08	2.8952 (19)	175
C14—H14A…N3	0.97	2.42	2.765 (2)	100
C5—H5…Cg4 ⁱⁱ	0.93	2.81	3.696 (3)	160
C21—H21···Cg3 ⁱⁱⁱ	0.93	2.97	3.858 (3)	160
C22—H22…Cg2 ⁱⁱⁱ	0.93	2.79	3.699 (2)	166

Symmetry codes: (i) -x+1, -y-1, -z+1; (ii) x, -y+1/2, z+1/2; (iii) x, -y-1/2, z-1/2.