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5-Benzoyl-2-(1*H*-indol-3-yl)-4-(naphthalen-2-yl)-1*H*-pyrrole-3-carbonitrile

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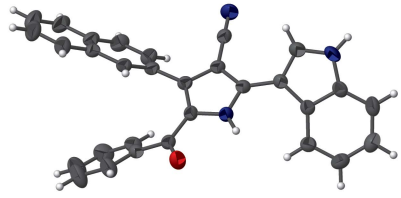
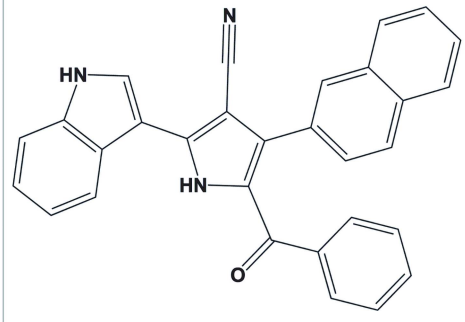
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{30}H_{19}N_3O$, the indole and the naphthalene ring systems are inclined to the central pyrrole ring (r.m.s. deviation = 0.012 Å) by 29.09 (9) and 49.92 (9)°, respectively. The naphthalene ring system and the indole ring are inclined to one another by 73.57 (6) and by 42.58 (10) and 74.12 (10)°, respectively, to the benzoyl ring. In the crystal, molecules are linked by pairs of N_p—H···O (p = pyrrole) hydrogen bonds, forming inversion dimers with $R_2^2(10)$ loops. These dimers are linked *via* pairs of N_i—H···N_c (i = indole and c = carbonitrile) hydrogen bonds, enclosing $R_2^2(16)$ loops, which leads to the formation of chains propagating in [101]. The chains are linked by C—H···π interactions, forming slabs lying parallel to $(10\overline{1})$.

3D view



Chemical scheme



Structure description

Indole derivatives exhibit antibacterial, antifungal (Singh *et al.* 2000), antitumor (Andreani *et al.*, 2001), antihepatitis B virus (Chai *et al.*, 2006) and anti-inflammatory (Rodriguez *et al.*, 1985) activities. Some of the indole alkaloids extracted from plants possess interesting cytotoxic and antiparasitic properties (Quetin-Leclercq, 1994). They are also used as bioactive drugs (Stevenson *et al.*, 2000) and have also been shown to display high aldose reductase inhibitory (Rajeswaran *et al.*, 1999) and antimicrobial activities (Amal Raj *et al.*, 2003). As part of our studies of this family of compounds, we synthesized the title indole derivative and report herein on its crystal structure.

The molecular structure of the title compound is illustrated in Fig. 1. The five-membered central pyrrole ring (N2/C2–C5; r.m.s. deviation = 0.012 Å) makes dihedral angles of 29.09 (9) and 45.92 (9)° with the indole ring (N3/C23–C30) and the naphthalene ring system (C6–C15), respectively. The naphthalene ring system and the benzoyl ring (C17–C22) are inclined to the indole ring by 73.57 (6) and 74.12 (10)°, respectively. The

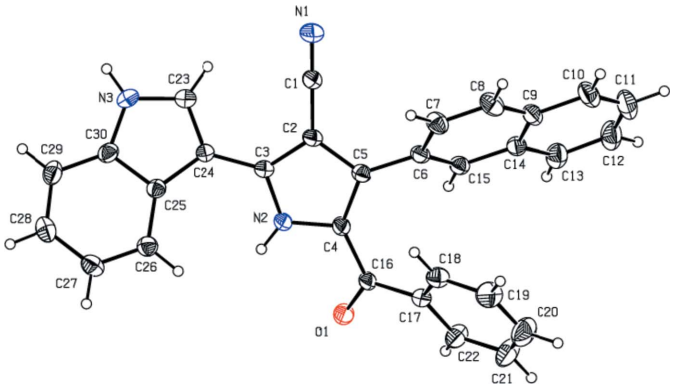


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at 30% probability level.

bond lengths and bond angles are similar to those for reported similar structures (Vimala *et al.*, 2015; Inglebert *et al.*, 2013).

In the crystal, molecules are linked by pairs of N_p—H···O (p = pyrrole) hydrogen bonds, forming inversion dimers with $R_2^2(10)$ loops (Table 1 and Fig. 2). These dimers are linked *via* pairs of N_i—H···N_c (i = indole and c = carbonitrile) hydrogen bonds, enclosing $R_2^2(16)$ loops, which leads to the formation of chains propagating in [101]; see Table 1 and Fig. 2. The chains are linked by C—H···π interactions (Table 1), forming slabs lying parallel to $(10\bar{1})$.

Synthesis and crystallization

To a stirred mixture of 2-naphthaldehyde 1 (1.0 mmol), 3-cyanoacetylindole 2 (1.0 mmol) and phenacylazide 3 (1.0 mmol) in water (3 ml), piperidine (0.25 mmol) was added at 353 K. The turbid solution slowly turned into a clear solution, followed by the formation of a solid after 2 h. After completion of the reaction, as indicated by TLC, the solid was filtered and washed with a petroleum ether–EtOAc mixture (1:1 ratio, *v*/*v*, 5 ml) to give the pure compound (as confirmed by TLC, NMR and mass spectroscopy). The compound was recrystallized from ethanol solution by slow evaporation, giving yellow block-like crystals of the title compound (yield 86%).

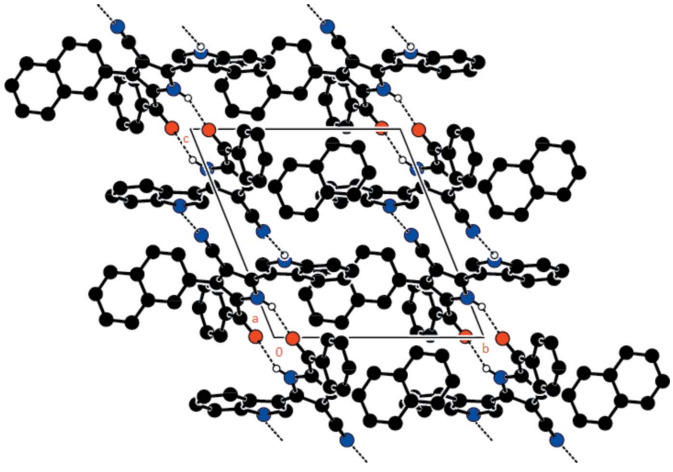


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. The hydrogen bonds are shown as dashed lines (see Table 1), and C-bound H atoms have been omitted for clarity.

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

*Cg*3, *Cg*4 and *Cg*6 are the centroids of rings C6–C9/C14/C15, C9–C14 and C25–C30, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.15	2.875 (2)	141
N3—H3···N1^{ii}	0.86	2.27	3.023 (3)	147
C22—H22···*Cg*6^{i}	0.93	2.58	3.456 (2)	158
C26—H26···*Cg*4^{iii}	0.93	2.98	3.784 (2)	146
C27—H27···*Cg*3^{iii}	0.93	2.74	3.555 (2)	147

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

Refinement

Crystal data, data collection and structure refinement details for the title compound are summarized in Table 2.

Acknowledgements

The authors thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the data collection.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{19}N_3O$
M_r	437.48
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, *b*, *c* (Å)	10.2688 (4), 10.5322 (4), 11.2934 (4)
α, β, γ (°)	111.720 (2), 93.883 (2), 91.653 (3)
V (Å^3)	1130.18 (7)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.984, 0.987
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25456, 3992, 2997
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.039, 0.129, 0.74
No. of reflections	3950
No. of parameters	307
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.20

Computer programs: *APEX2* (Bruker, 2004), *APEX2* and *SAINT* (Bruker, 2004), *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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full crystallographic data

IUCrData (2016). **1**, x160526 [doi:10.1107/S2414314616005265]

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5-Benzoyl-2-(1*H*-indol-3-yl)-4-(naphthalen-2-yl)-1*H*-pyrrole-3-carbonitrile

Crystal data

$C_{30}H_{19}N_3O$
M_r = 437.48
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 10.2688 (4) Å
b = 10.5322 (4) Å
c = 11.2934 (4) Å
α = 111.720 (2)°
β = 93.883 (2)°
γ = 91.653 (3)°
V = 1130.18 (7) Å^3
Z = 2
$F(000)$ = 456
D_x = 1.285 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2997 reflections
θ = 2.0–25.0°
μ = 0.08 mm^{-1}
T = 293 K
Block, yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.984, T_{max} = 0.987
25456 measured reflections
3992 independent reflections
2997 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −12→12
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.129
S = 0.74
3950 reflections
307 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 1.3759P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N2	0.06088 (15)	−0.00372 (16)	0.19168 (15)	0.0361 (4)
H2	0.0550	0.0483	0.1484	0.043*
C6	−0.04251 (18)	−0.29361 (19)	0.27603 (18)	0.0344 (4)
C16	−0.14783 (18)	−0.12464 (19)	0.09442 (17)	0.0341 (4)
O1	−0.14205 (14)	−0.08637 (15)	0.00453 (13)	0.0473 (4)
C15	−0.08017 (18)	−0.40765 (19)	0.17018 (18)	0.0355 (4)
H15	−0.0728	−0.4049	0.0895	0.043*
C3	0.16176 (18)	0.00371 (19)	0.27732 (17)	0.0343 (4)
C4	−0.03160 (18)	−0.10523 (19)	0.18232 (17)	0.0340 (4)
C17	−0.27269 (18)	−0.18422 (19)	0.11539 (18)	0.0360 (4)
C14	−0.12994 (18)	−0.52944 (19)	0.1799 (2)	0.0383 (5)
C5	0.01315 (18)	−0.16945 (19)	0.26318 (17)	0.0338 (4)
C24	0.27135 (18)	0.10241 (19)	0.30757 (18)	0.0363 (4)
C7	−0.0546 (2)	−0.2977 (2)	0.39845 (19)	0.0446 (5)
H7	−0.0293	−0.2208	0.4712	0.054*
C2	0.13406 (18)	−0.09886 (19)	0.32411 (18)	0.0360 (4)
C25	0.27433 (18)	0.23655 (19)	0.30202 (17)	0.0335 (4)
N3	0.47408 (17)	0.19722 (19)	0.36922 (18)	0.0511 (5)
H3	0.5558	0.2072	0.3951	0.061*
C1	0.2157 (2)	−0.1277 (2)	0.4167 (2)	0.0413 (5)
C26	0.18131 (19)	0.3171 (2)	0.27229 (19)	0.0392 (5)
H26	0.0953	0.2831	0.2456	0.047*
C9	−0.1415 (2)	−0.5319 (2)	0.3034 (2)	0.0435 (5)
C18	−0.3052 (2)	−0.1726 (2)	0.2361 (2)	0.0437 (5)
H18	−0.2481	−0.1261	0.3077	0.052*
N1	0.2814 (2)	−0.1508 (2)	0.4910 (2)	0.0592 (5)
C27	0.2193 (2)	0.4470 (2)	0.2832 (2)	0.0476 (5)
H27	0.1575	0.5017	0.2654	0.057*
C8	−0.1029 (2)	−0.4134 (2)	0.4105 (2)	0.0504 (6)
H8	−0.1106	−0.4141	0.4919	0.061*
C29	0.4423 (2)	0.4229 (2)	0.3486 (2)	0.0473 (5)
H29	0.5287	0.4571	0.3718	0.057*
C10	−0.1894 (2)	−0.6545 (2)	0.3141 (3)	0.0583 (6)
H10	−0.1973	−0.6572	0.3947	0.070*
C28	0.3479 (2)	0.4990 (2)	0.3203 (2)	0.0508 (6)
H28	0.3703	0.5874	0.3260	0.061*
C30	0.40339 (19)	0.2926 (2)	0.34107 (18)	0.0393 (5)
C13	−0.1667 (2)	−0.6492 (2)	0.0723 (2)	0.0520 (6)
H13	−0.1600	−0.6491	−0.0094	0.062*
C23	0.3952 (2)	0.0853 (2)	0.3500 (2)	0.0489 (5)

H23	0.4213	0.0076	0.3636	0.059*
C22	−0.3603 (2)	−0.2515 (2)	0.0105 (2)	0.0505 (6)
H22	−0.3404	−0.2572	−0.0704	0.061*
C12	−0.2121 (2)	−0.7655 (2)	0.0868 (3)	0.0656 (7)
H12	−0.2356	−0.8440	0.0150	0.079*
C11	−0.2235 (3)	−0.7672 (3)	0.2089 (3)	0.0685 (8)
H11	−0.2549	−0.8468	0.2176	0.082*
C20	−0.5076 (3)	−0.2994 (3)	0.1439 (3)	0.0733 (8)
H20	−0.5864	−0.3391	0.1534	0.088*
C21	−0.4763 (2)	−0.3098 (3)	0.0249 (3)	0.0678 (7)
H21	−0.5339	−0.3565	−0.0463	0.081*
C19	−0.4231 (2)	−0.2306 (3)	0.2493 (2)	0.0604 (7)
H19	−0.4451	−0.2230	0.3300	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0379 (9)	0.0380 (9)	0.0386 (9)	−0.0036 (7)	−0.0047 (7)	0.0233 (7)
C6	0.0350 (10)	0.0348 (10)	0.0377 (10)	0.0054 (8)	0.0028 (8)	0.0185 (8)
C16	0.0392 (10)	0.0321 (10)	0.0327 (10)	−0.0004 (8)	−0.0024 (8)	0.0150 (8)
O1	0.0489 (8)	0.0579 (9)	0.0435 (8)	−0.0119 (7)	−0.0089 (7)	0.0317 (7)
C15	0.0354 (10)	0.0391 (10)	0.0365 (10)	0.0043 (8)	0.0038 (8)	0.0189 (9)
C3	0.0341 (10)	0.0356 (10)	0.0354 (10)	0.0033 (8)	−0.0013 (8)	0.0164 (8)
C4	0.0376 (10)	0.0339 (10)	0.0330 (10)	−0.0030 (8)	−0.0012 (8)	0.0164 (8)
C17	0.0352 (10)	0.0365 (10)	0.0388 (11)	0.0021 (8)	−0.0003 (8)	0.0174 (8)
C14	0.0317 (10)	0.0359 (10)	0.0496 (12)	0.0060 (8)	0.0061 (8)	0.0177 (9)
C5	0.0380 (10)	0.0332 (10)	0.0319 (10)	0.0038 (8)	0.0008 (8)	0.0143 (8)
C24	0.0360 (10)	0.0366 (10)	0.0374 (10)	−0.0008 (8)	−0.0046 (8)	0.0167 (8)
C7	0.0588 (13)	0.0416 (11)	0.0358 (11)	0.0025 (10)	0.0037 (9)	0.0174 (9)
C2	0.0386 (10)	0.0357 (10)	0.0368 (10)	0.0033 (8)	−0.0032 (8)	0.0180 (8)
C25	0.0346 (10)	0.0365 (10)	0.0291 (9)	0.0001 (8)	0.0005 (8)	0.0123 (8)
N3	0.0321 (9)	0.0598 (12)	0.0661 (12)	−0.0051 (8)	−0.0136 (8)	0.0327 (10)
C1	0.0444 (11)	0.0356 (11)	0.0456 (12)	−0.0014 (9)	−0.0068 (9)	0.0193 (9)
C26	0.0372 (10)	0.0402 (11)	0.0412 (11)	0.0040 (8)	0.0034 (8)	0.0163 (9)
C9	0.0405 (11)	0.0425 (11)	0.0578 (13)	0.0087 (9)	0.0132 (10)	0.0286 (10)
C18	0.0432 (11)	0.0498 (12)	0.0406 (11)	0.0073 (9)	0.0041 (9)	0.0193 (10)
N1	0.0602 (12)	0.0602 (12)	0.0643 (13)	−0.0040 (10)	−0.0216 (10)	0.0367 (11)
C27	0.0523 (13)	0.0419 (12)	0.0541 (13)	0.0113 (10)	0.0090 (10)	0.0227 (10)
C8	0.0635 (14)	0.0553 (14)	0.0441 (12)	0.0081 (11)	0.0148 (10)	0.0300 (11)
C29	0.0466 (12)	0.0480 (12)	0.0432 (12)	−0.0134 (10)	−0.0038 (9)	0.0148 (10)
C10	0.0570 (14)	0.0509 (14)	0.0846 (18)	0.0086 (11)	0.0245 (13)	0.0420 (14)
C28	0.0644 (15)	0.0377 (11)	0.0506 (13)	−0.0038 (10)	0.0070 (11)	0.0169 (10)
C30	0.0367 (10)	0.0457 (11)	0.0343 (10)	−0.0027 (9)	−0.0044 (8)	0.0150 (9)
C13	0.0484 (13)	0.0434 (12)	0.0594 (14)	0.0002 (10)	0.0088 (11)	0.0131 (11)
C23	0.0427 (12)	0.0496 (13)	0.0610 (14)	−0.0005 (10)	−0.0097 (10)	0.0309 (11)
C22	0.0424 (12)	0.0665 (15)	0.0430 (12)	−0.0084 (10)	−0.0010 (9)	0.0225 (11)
C12	0.0572 (15)	0.0372 (13)	0.093 (2)	−0.0017 (10)	0.0140 (14)	0.0127 (13)
C11	0.0607 (16)	0.0431 (14)	0.111 (2)	0.0036 (11)	0.0278 (15)	0.0360 (15)

C20	0.0465 (14)	0.101 (2)	0.081 (2)	−0.0155 (14)	0.0082 (13)	0.0447 (17)
C21	0.0483 (14)	0.090 (2)	0.0606 (16)	−0.0231 (13)	−0.0077 (12)	0.0264 (14)
C19	0.0531 (14)	0.0819 (18)	0.0583 (15)	0.0076 (13)	0.0189 (12)	0.0376 (14)

Geometric parameters (Å, º)

N2—C3	1.348 (2)	C1—N1	1.141 (3)
N2—C4	1.378 (2)	C26—C27	1.370 (3)
N2—H2	0.8600	C26—H26	0.9300
C6—C15	1.367 (3)	C9—C8	1.402 (3)
C6—C7	1.413 (3)	C9—C10	1.417 (3)
C6—C5	1.472 (3)	C18—C19	1.381 (3)
C16—O1	1.227 (2)	C18—H18	0.9300
C16—C4	1.458 (3)	C27—C28	1.391 (3)
C16—C17	1.483 (3)	C27—H27	0.9300
C15—C14	1.412 (3)	C8—H8	0.9300
C15—H15	0.9300	C29—C28	1.370 (3)
C3—C2	1.397 (3)	C29—C30	1.389 (3)
C3—C24	1.443 (3)	C29—H29	0.9300
C4—C5	1.386 (3)	C10—C11	1.349 (4)
C17—C22	1.383 (3)	C10—H10	0.9300
C17—C18	1.388 (3)	C28—H28	0.9300
C14—C13	1.409 (3)	C13—C12	1.368 (3)
C14—C9	1.418 (3)	C13—H13	0.9300
C5—C2	1.421 (3)	C23—H23	0.9300
C24—C23	1.368 (3)	C22—C21	1.372 (3)
C24—C25	1.437 (3)	C22—H22	0.9300
C7—C8	1.360 (3)	C12—C11	1.398 (4)
C7—H7	0.9300	C12—H12	0.9300
C2—C1	1.421 (3)	C11—H11	0.9300
C25—C26	1.400 (3)	C20—C21	1.369 (4)
C25—C30	1.408 (3)	C20—C19	1.371 (4)
N3—C23	1.351 (3)	C20—H20	0.9300
N3—C30	1.372 (3)	C21—H21	0.9300
N3—H3	0.8600	C19—H19	0.9300
C3—N2—C4	111.47 (15)	C8—C9—C10	122.5 (2)
C3—N2—H2	124.3	C14—C9—C10	118.9 (2)
C4—N2—H2	124.3	C19—C18—C17	119.6 (2)
C15—C6—C7	118.99 (18)	C19—C18—H18	120.2
C15—C6—C5	120.71 (17)	C17—C18—H18	120.2
C7—C6—C5	120.28 (17)	C26—C27—C28	121.7 (2)
O1—C16—C4	118.79 (17)	C26—C27—H27	119.2
O1—C16—C17	120.14 (16)	C28—C27—H27	119.2
C4—C16—C17	121.03 (16)	C7—C8—C9	121.70 (19)
C6—C15—C14	121.82 (18)	C7—C8—H8	119.2
C6—C15—H15	119.1	C9—C8—H8	119.2
C14—C15—H15	119.1	C28—C29—C30	117.08 (19)

N2—C3—C2	105.95 (16)	C28—C29—H29	121.5
N2—C3—C24	123.18 (17)	C30—C29—H29	121.5
C2—C3—C24	130.88 (17)	C11—C10—C9	120.9 (2)
N2—C4—C5	107.75 (16)	C11—C10—H10	119.6
N2—C4—C16	117.92 (16)	C9—C10—H10	119.6
C5—C4—C16	134.31 (17)	C29—C28—C27	121.4 (2)
C22—C17—C18	119.26 (19)	C29—C28—H28	119.3
C22—C17—C16	118.33 (18)	C27—C28—H28	119.3
C18—C17—C16	122.40 (17)	N3—C30—C29	129.86 (19)
C13—C14—C15	122.87 (19)	N3—C30—C25	107.47 (17)
C13—C14—C9	118.61 (19)	C29—C30—C25	122.67 (19)
C15—C14—C9	118.52 (18)	C12—C13—C14	120.7 (2)
C4—C5—C2	105.71 (16)	C12—C13—H13	119.7
C4—C5—C6	128.48 (17)	C14—C13—H13	119.7
C2—C5—C6	125.52 (16)	N3—C23—C24	110.37 (18)
C23—C24—C25	106.17 (17)	N3—C23—H23	124.8
C23—C24—C3	125.53 (18)	C24—C23—H23	124.8
C25—C24—C3	128.29 (17)	C21—C22—C17	120.4 (2)
C8—C7—C6	120.37 (19)	C21—C22—H22	119.8
C8—C7—H7	119.8	C17—C22—H22	119.8
C6—C7—H7	119.8	C13—C12—C11	120.4 (2)
C3—C2—C1	124.81 (17)	C13—C12—H12	119.8
C3—C2—C5	109.08 (16)	C11—C12—H12	119.8
C1—C2—C5	126.10 (17)	C10—C11—C12	120.5 (2)
C26—C25—C30	118.37 (18)	C10—C11—H11	119.7
C26—C25—C24	134.94 (18)	C12—C11—H11	119.7
C30—C25—C24	106.66 (16)	C21—C20—C19	120.1 (2)
C23—N3—C30	109.33 (17)	C21—C20—H20	119.9
C23—N3—H3	125.3	C19—C20—H20	119.9
C30—N3—H3	125.3	C20—C21—C22	120.2 (2)
N1—C1—C2	179.9 (3)	C20—C21—H21	119.9
C27—C26—C25	118.76 (19)	C22—C21—H21	119.9
C27—C26—H26	120.6	C20—C19—C18	120.4 (2)
C25—C26—H26	120.6	C20—C19—H19	119.8
C8—C9—C14	118.60 (18)	C18—C19—H19	119.8

C7—C6—C15—C14	−0.4 (3)	C3—C24—C25—C30	179.78 (19)
C5—C6—C15—C14	177.95 (17)	C3—C2—C1—N1	−38 (100)
C4—N2—C3—C2	0.8 (2)	C5—C2—C1—N1	141 (100)
C4—N2—C3—C24	−179.00 (17)	C30—C25—C26—C27	−0.4 (3)
C3—N2—C4—C5	−1.7 (2)	C24—C25—C26—C27	176.9 (2)
C3—N2—C4—C16	179.21 (17)	C13—C14—C9—C8	178.97 (19)
O1—C16—C4—N2	23.7 (3)	C15—C14—C9—C8	−0.1 (3)
C17—C16—C4—N2	−153.80 (17)	C13—C14—C9—C10	0.1 (3)
O1—C16—C4—C5	−155.0 (2)	C15—C14—C9—C10	−178.97 (18)
C17—C16—C4—C5	27.5 (3)	C22—C17—C18—C19	1.3 (3)
O1—C16—C17—C22	28.7 (3)	C16—C17—C18—C19	−179.9 (2)
C4—C16—C17—C22	−153.85 (19)	C25—C26—C27—C28	1.4 (3)

O1—C16—C17—C18	−150.2 (2)	C6—C7—C8—C9	0.4 (3)
C4—C16—C17—C18	27.3 (3)	C14—C9—C8—C7	−0.3 (3)
C6—C15—C14—C13	−178.58 (19)	C10—C9—C8—C7	178.5 (2)
C6—C15—C14—C9	0.4 (3)	C8—C9—C10—C11	−178.9 (2)
N2—C4—C5—C2	1.9 (2)	C14—C9—C10—C11	0.0 (3)
C16—C4—C5—C2	−179.3 (2)	C30—C29—C28—C27	−1.3 (3)
N2—C4—C5—C6	−172.21 (18)	C26—C27—C28—C29	−0.5 (3)
C16—C4—C5—C6	6.6 (4)	C23—N3—C30—C29	178.8 (2)
C15—C6—C5—C4	46.2 (3)	C23—N3—C30—C25	−0.2 (2)
C7—C6—C5—C4	−135.5 (2)	C28—C29—C30—N3	−176.7 (2)
C15—C6—C5—C2	−126.8 (2)	C28—C29—C30—C25	2.2 (3)
C7—C6—C5—C2	51.5 (3)	C26—C25—C30—N3	177.73 (18)
N2—C3—C24—C23	−152.6 (2)	C24—C25—C30—N3	−0.3 (2)
C2—C3—C24—C23	27.7 (3)	C26—C25—C30—C29	−1.4 (3)
N2—C3—C24—C25	28.5 (3)	C24—C25—C30—C29	−179.39 (19)
C2—C3—C24—C25	−151.3 (2)	C15—C14—C13—C12	178.8 (2)
C15—C6—C7—C8	0.0 (3)	C9—C14—C13—C12	−0.3 (3)
C5—C6—C7—C8	−178.36 (19)	C30—N3—C23—C24	0.7 (3)
N2—C3—C2—C1	179.65 (19)	C25—C24—C23—N3	−0.8 (2)
C24—C3—C2—C1	−0.5 (3)	C3—C24—C23—N3	−179.97 (19)
N2—C3—C2—C5	0.4 (2)	C18—C17—C22—C21	−2.0 (4)
C24—C3—C2—C5	−179.81 (19)	C16—C17—C22—C21	179.1 (2)
C4—C5—C2—C3	−1.4 (2)	C14—C13—C12—C11	0.4 (4)
C6—C5—C2—C3	172.89 (18)	C9—C10—C11—C12	0.1 (4)
C4—C5—C2—C1	179.3 (2)	C13—C12—C11—C10	−0.3 (4)
C6—C5—C2—C1	−6.4 (3)	C19—C20—C21—C22	0.0 (5)
C23—C24—C25—C26	−176.9 (2)	C17—C22—C21—C20	1.4 (4)
C3—C24—C25—C26	2.3 (4)	C21—C20—C19—C18	−0.7 (4)
C23—C24—C25—C30	0.7 (2)	C17—C18—C19—C20	0.0 (4)

Hydrogen-bond geometry (Å, º)

Cg3, Cg4 and Cg6 are the centroids of rings C6–C9/C14/C15, C9–C14 and C25–C30, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.86	2.15	2.875 (2)	141
N3—H3···N1^{ii}	0.86	2.27	3.023 (3)	147
C22—H22···*Cg*6^{i}	0.93	2.58	3.456 (2)	158
C26—H26···*Cg*4^{iii}	0.93	2.98	3.784 (2)	146
C27—H27···*Cg*3^{iii}	0.93	2.74	3.555 (2)	147

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*, *y*+1, *z*.