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1-Benzyl-5-nitro-1*H*-indazole

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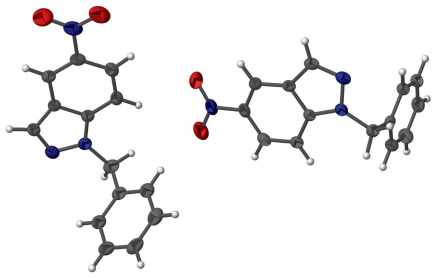
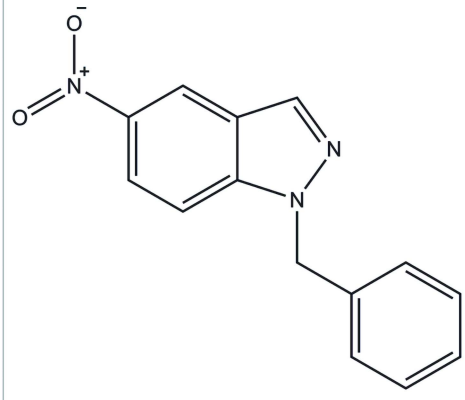
The asymmetric unit of the title compound, $C_{14}H_{11}N_3O_2$, contains two independent molecules linked by a C—H···O hydrogen bond. Pairs of neighboring dimeric units associate *via* π–π stacking interactions.

3D view



Chemical scheme



Structure description

Indazole derivatives are a versatile class of compounds that have found use in biology, catalysis, and medicinal chemistry (Schmidt *et al.*, 2008). Although rare in nature (Liu *et al.*, 2004; Ali *et al.*, 2008), indazoles exhibit a variety of biological activities such as HIV protease inhibition (Patel *et al.*, 1999), antiarrhythmic and analgesic activities (Mosti *et al.*, 2000), and antitumor activity and antihypertensive properties (Bouissane *et al.*, 2006; Abbassi *et al.*, 2012). As a continuation of our studies of indazole derivatives (Boulhaoua *et al.*, 2015) we report the synthesis and structure of the title compound.

The asymmetric unit contains two independent molecules which have slightly different orientations of the pendant phenyl groups. Thus, the C9–C14 ring in molecule 1 (Fig. 1) makes a dihedral angle of 79.26 (3)° with the mean plane of its indazole moiety while the corresponding angle in molecule 2 is 75.55 (4)°. In both molecules, the nitro groups are very slightly twisted out of the planes of the indazole ring systems. A weak C20—H20···O2 hydrogen bond links the two unique molecules in the asymmetric unit (Fig. 1, Table 1). π–π-stacking interactions occur between the C2–C7 benzene rings and the C16–C21 rings of the indazole ring systems of related molecules, Fig. 2, with $Cg1\cdots Cg6^{i}$ and $Cg1^{ii}\cdots Cg6$ distances of 3.5257 (7) Å [symmetry codes: (i) $\frac{3}{2}-x, -\frac{1}{2}+y, \frac{3}{2}-z$; (ii) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$]. These contacts form tetramers which pack without other short contacts (Fig. 3).

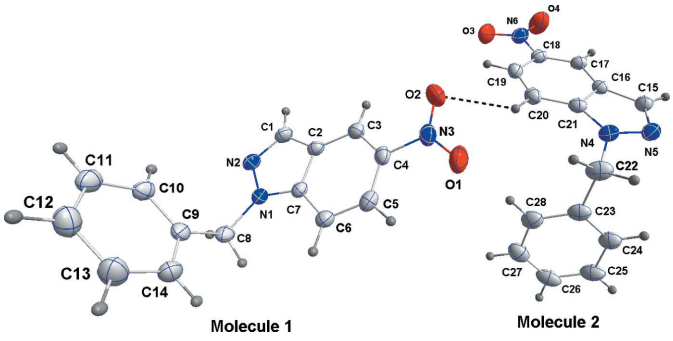


Figure 1
The title molecule with the atom- labeling scheme and 50% probability ellipsoids. The intermolecular C—H···O hydrogen bond is shown as a dotted line.

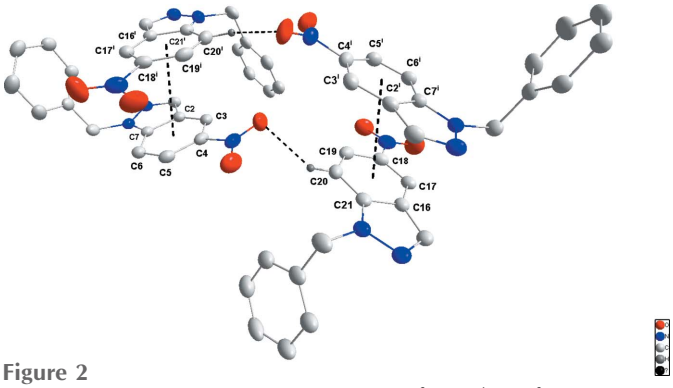


Figure 2
Detail of the π-stacking [symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$].

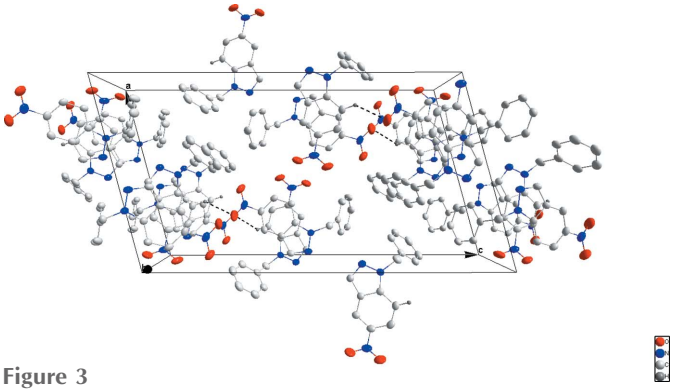


Figure 3
Packing viewed along the *b* axis with the intermolecular C—H···O hydrogen bonds shown as dotted lines.

Synthesis and crystallization

5-Nitro-1*H*-indazole (0.5 g, 3 mmol) and benzyl chloride (0.7 ml, 6 mmol) were reacted in THF (20 ml) in the presence of potassium carbonate (0.83 g, 6 mmol) and tetra-*n*-butylammonium bromide (0.11 g, 0.33 mmol). The mixture was stirred for 48 h, filtered, and the THF removed under vacuum. The product was separated by chromatography on silica gel with a hexane:ethyl acetate (8:2) solvent system. Crystals were obtained when the solvent was allowed to evaporate. The solid product was purified by recrystallization from ethyl acetate to afford colourless crystals (yield: 58%; m.p. = 393–395 K).

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

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20···O2	0.95	2.48	3.2242 (17)	135

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{11}N_3O_2$
M_r	253.26
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	14.0236 (3), 6.9976 (1), 25.3551 (5)
β (°)	105.245 (1)
V (Å^3)	2400.58 (8)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.80
Crystal size (mm)	0.24 × 0.13 × 0.05
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.86, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18022, 4833, 3995
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.094, 1.04
No. of reflections	4833
No. of parameters	344
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.16

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{14}H_{11}N_3O_2$
M_r = 253.26
Monoclinic, $P2_1/n$
a = 14.0236 (3) Å
b = 6.9976 (1) Å
c = 25.3551 (5) Å
β = 105.245 (1)°
V = 2400.58 (8) Å^3
Z = 8
$F(000)$ = 1056
D_x = 1.401 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9935 reflections
θ = 3.3–74.4°
μ = 0.80 mm^{-1}
T = 150 K
Thick plate, colourless
0.24 × 0.13 × 0.05 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.86, T_{max} = 0.96
18022 measured reflections
4833 independent reflections
3995 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 74.6°, θ_{min} = 3.3°
h = −16→17
k = −8→8
l = −31→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.04
4833 reflections
344 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
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.4746P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015a), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00186 (16)

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 $F^2 > \sigma(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 − 0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.58982 (9)	0.48868 (18)	0.69442 (5)	0.0515 (3)
O2	0.74164 (10)	0.54713 (19)	0.73731 (4)	0.0536 (3)
N1	0.81889 (8)	0.27863 (14)	0.52227 (4)	0.0249 (2)
N2	0.91894 (8)	0.29139 (15)	0.54421 (5)	0.0293 (2)
N3	0.67906 (10)	0.48846 (17)	0.69708 (5)	0.0381 (3)
C1	0.93186 (9)	0.33746 (18)	0.59595 (5)	0.0287 (3)
H1	0.9946	0.3544	0.6213	0.034*
C2	0.84003 (9)	0.35852 (17)	0.60908 (5)	0.0248 (3)
C3	0.81071 (10)	0.41041 (18)	0.65552 (5)	0.0286 (3)
H3	0.8575	0.4376	0.6892	0.034*
C4	0.71084 (10)	0.42037 (18)	0.65016 (5)	0.0295 (3)
C5	0.63849 (10)	0.37740 (18)	0.60129 (6)	0.0294 (3)
H5	0.5704	0.3836	0.6003	0.035*
C6	0.66655 (9)	0.32670 (18)	0.55531 (5)	0.0265 (3)
H6	0.6192	0.2975	0.5220	0.032*
C7	0.76849 (9)	0.31984 (16)	0.55972 (5)	0.0233 (3)
C8	0.77899 (10)	0.24803 (18)	0.46378 (5)	0.0287 (3)
H8A	0.7174	0.1721	0.4574	0.034*
H8B	0.8271	0.1741	0.4496	0.034*
C9	0.75716 (9)	0.43506 (18)	0.43307 (5)	0.0261 (3)
C10	0.83424 (9)	0.56089 (18)	0.43277 (5)	0.0270 (3)
H10	0.9003	0.5261	0.4506	0.032*
C11	0.81532 (10)	0.73627 (19)	0.40663 (5)	0.0301 (3)
H11	0.8682	0.8217	0.4071	0.036*
C12	0.71933 (11)	0.7866 (2)	0.37989 (6)	0.0368 (3)
H12	0.7062	0.9063	0.3618	0.044*
C13	0.64270 (11)	0.6621 (2)	0.37965 (6)	0.0429 (4)
H13	0.5768	0.6965	0.3612	0.051*
C14	0.66151 (10)	0.4867 (2)	0.40624 (6)	0.0359 (3)
H14	0.6084	0.4021	0.4060	0.043*
O3	0.96938 (8)	0.32608 (19)	0.92541 (6)	0.0556 (3)
O4	0.93680 (8)	0.2992 (2)	1.00357 (5)	0.0600 (4)
N4	0.51068 (8)	0.37236 (15)	0.85992 (4)	0.0286 (2)
N5	0.47236 (8)	0.33620 (16)	0.90328 (5)	0.0308 (3)

N6	0.91111 (9)	0.32284 (18)	0.95410 (6)	0.0402 (3)
C15	0.54843 (10)	0.31492 (18)	0.94615 (5)	0.0281 (3)
H15	0.5433	0.2907	0.9822	0.034*
C16	0.63952 (9)	0.33289 (17)	0.93161 (5)	0.0246 (3)
C17	0.73991 (10)	0.31849 (17)	0.95871 (5)	0.0272 (3)
H17	0.7617	0.2919	0.9967	0.033*
C18	0.80552 (9)	0.34486 (18)	0.92748 (6)	0.0292 (3)
C19	0.77729 (10)	0.38914 (19)	0.87135 (6)	0.0316 (3)
H19	0.8263	0.4096	0.8522	0.038*
C20	0.67933 (10)	0.40277 (18)	0.84434 (5)	0.0300 (3)
H20	0.6585	0.4324	0.8065	0.036*
C21	0.61093 (9)	0.37104 (17)	0.87506 (5)	0.0260 (3)
C22	0.44581 (11)	0.3748 (2)	0.80465 (6)	0.0360 (3)
H22A	0.4753	0.4575	0.7815	0.043*
H22B	0.3815	0.4311	0.8055	0.043*
C23	0.42832 (10)	0.17754 (19)	0.77920 (5)	0.0310 (3)
C24	0.35930 (10)	0.0558 (2)	0.79196 (6)	0.0345 (3)
H24	0.3238	0.0954	0.8172	0.041*
C25	0.34200 (12)	−0.1238 (2)	0.76785 (6)	0.0398 (3)
H25	0.2946	−0.2063	0.7766	0.048*
C26	0.39368 (12)	−0.1827 (2)	0.73113 (6)	0.0421 (4)
H26	0.3810	−0.3047	0.7143	0.050*
C27	0.46371 (12)	−0.0641 (2)	0.71898 (6)	0.0418 (4)
H27	0.5000	−0.1051	0.6942	0.050*
C28	0.48104 (11)	0.1157 (2)	0.74309 (6)	0.0363 (3)
H28	0.5294	0.1969	0.7348	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0513 (7)	0.0579 (7)	0.0567 (7)	−0.0026 (5)	0.0343 (6)	−0.0042 (6)
O2	0.0676 (8)	0.0640 (8)	0.0344 (6)	−0.0176 (6)	0.0224 (6)	−0.0121 (5)
N1	0.0232 (5)	0.0240 (5)	0.0279 (5)	−0.0002 (4)	0.0075 (4)	0.0024 (4)
N2	0.0224 (5)	0.0277 (5)	0.0378 (6)	−0.0004 (4)	0.0080 (5)	0.0032 (5)
N3	0.0503 (8)	0.0343 (6)	0.0366 (7)	−0.0063 (5)	0.0238 (6)	0.0004 (5)
C1	0.0226 (6)	0.0277 (6)	0.0338 (7)	−0.0020 (5)	0.0039 (5)	0.0028 (5)
C2	0.0247 (6)	0.0209 (6)	0.0274 (6)	−0.0025 (4)	0.0042 (5)	0.0030 (5)
C3	0.0343 (7)	0.0246 (6)	0.0261 (6)	−0.0056 (5)	0.0065 (5)	0.0022 (5)
C4	0.0385 (7)	0.0242 (6)	0.0300 (7)	−0.0034 (5)	0.0164 (6)	0.0018 (5)
C5	0.0263 (6)	0.0270 (6)	0.0372 (7)	−0.0006 (5)	0.0126 (5)	0.0040 (5)
C6	0.0240 (6)	0.0249 (6)	0.0297 (6)	−0.0013 (5)	0.0054 (5)	0.0026 (5)
C7	0.0254 (6)	0.0187 (5)	0.0261 (6)	−0.0020 (4)	0.0075 (5)	0.0022 (4)
C8	0.0321 (7)	0.0259 (6)	0.0288 (7)	−0.0039 (5)	0.0092 (5)	−0.0042 (5)
C9	0.0297 (7)	0.0291 (6)	0.0200 (6)	−0.0030 (5)	0.0075 (5)	−0.0030 (5)
C10	0.0239 (6)	0.0292 (6)	0.0285 (6)	−0.0003 (5)	0.0078 (5)	−0.0004 (5)
C11	0.0304 (7)	0.0312 (7)	0.0305 (7)	−0.0020 (5)	0.0109 (5)	0.0003 (5)
C12	0.0370 (8)	0.0409 (8)	0.0320 (7)	0.0050 (6)	0.0084 (6)	0.0120 (6)
C13	0.0275 (7)	0.0596 (10)	0.0376 (8)	0.0016 (7)	0.0018 (6)	0.0170 (7)

C14	0.0271 (7)	0.0485 (8)	0.0305 (7)	−0.0085 (6)	0.0047 (5)	0.0051 (6)
O3	0.0311 (6)	0.0636 (8)	0.0774 (9)	0.0013 (5)	0.0236 (6)	−0.0142 (6)
O4	0.0315 (6)	0.0854 (10)	0.0555 (8)	0.0031 (6)	−0.0023 (5)	0.0078 (7)
N4	0.0280 (6)	0.0264 (5)	0.0293 (6)	−0.0007 (4)	0.0039 (4)	0.0017 (4)
N5	0.0281 (6)	0.0279 (5)	0.0370 (6)	−0.0003 (4)	0.0099 (5)	0.0001 (5)
N6	0.0264 (6)	0.0357 (6)	0.0585 (9)	0.0013 (5)	0.0111 (6)	−0.0073 (6)
C15	0.0301 (7)	0.0243 (6)	0.0309 (6)	−0.0009 (5)	0.0098 (5)	−0.0003 (5)
C16	0.0271 (6)	0.0188 (5)	0.0279 (6)	0.0000 (5)	0.0073 (5)	−0.0020 (5)
C17	0.0281 (7)	0.0209 (6)	0.0311 (6)	−0.0002 (5)	0.0054 (5)	−0.0020 (5)
C18	0.0252 (7)	0.0223 (6)	0.0396 (7)	0.0008 (5)	0.0077 (5)	−0.0053 (5)
C19	0.0356 (7)	0.0250 (6)	0.0392 (7)	−0.0018 (5)	0.0188 (6)	−0.0056 (5)
C20	0.0388 (7)	0.0250 (6)	0.0284 (6)	−0.0020 (5)	0.0124 (6)	−0.0020 (5)
C21	0.0294 (7)	0.0183 (6)	0.0295 (6)	0.0000 (5)	0.0067 (5)	−0.0014 (5)
C22	0.0362 (8)	0.0295 (7)	0.0348 (7)	0.0020 (5)	−0.0041 (6)	0.0060 (6)
C23	0.0304 (7)	0.0291 (6)	0.0266 (6)	0.0024 (5)	−0.0047 (5)	0.0059 (5)
C24	0.0338 (7)	0.0357 (7)	0.0297 (7)	−0.0007 (6)	0.0006 (5)	0.0038 (6)
C25	0.0442 (8)	0.0353 (7)	0.0328 (7)	−0.0083 (6)	−0.0026 (6)	0.0058 (6)
C26	0.0541 (10)	0.0317 (7)	0.0304 (7)	0.0029 (6)	−0.0064 (6)	0.0015 (6)
C27	0.0451 (9)	0.0446 (8)	0.0313 (7)	0.0097 (7)	0.0024 (6)	0.0011 (6)
C28	0.0340 (7)	0.0402 (8)	0.0302 (7)	−0.0002 (6)	0.0005 (6)	0.0071 (6)

Geometric parameters (Å, º)

O1—N3	1.2355 (17)	O3—N6	1.2289 (17)
O2—N3	1.2283 (17)	O4—N6	1.2218 (18)
N1—C7	1.3555 (16)	N4—C21	1.3566 (17)
N1—N2	1.3696 (15)	N4—N5	1.3683 (16)
N1—C8	1.4566 (16)	N4—C22	1.4564 (17)
N2—C1	1.3163 (17)	N5—C15	1.3159 (17)
N3—C4	1.4560 (17)	N6—C18	1.4650 (18)
C1—C2	1.4198 (18)	C15—C16	1.4252 (18)
C1—H1	0.9500	C15—H15	0.9500
C2—C3	1.3937 (18)	C16—C17	1.3985 (18)
C2—C7	1.4091 (17)	C16—C21	1.4089 (18)
C3—C4	1.3728 (19)	C17—C18	1.3750 (19)
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.4121 (19)	C18—C19	1.408 (2)
C5—C6	1.3716 (19)	C19—C20	1.368 (2)
C5—H5	0.9500	C19—H19	0.9500
C6—C7	1.4052 (18)	C20—C21	1.4033 (18)
C6—H6	0.9500	C20—H20	0.9500
C8—C9	1.5125 (18)	C22—C23	1.5159 (19)
C8—H8A	0.9900	C22—H22A	0.9900
C8—H8B	0.9900	C22—H22B	0.9900
C9—C14	1.3830 (19)	C23—C28	1.388 (2)
C9—C10	1.3958 (18)	C23—C24	1.390 (2)
C10—C11	1.3868 (18)	C24—C25	1.391 (2)
C10—H10	0.9500	C24—H24	0.9500

C11—C12	1.384 (2)	C25—C26	1.384 (2)
C11—H11	0.9500	C25—H25	0.9500
C12—C13	1.382 (2)	C26—C27	1.381 (2)
C12—H12	0.9500	C26—H26	0.9500
C13—C14	1.392 (2)	C27—C28	1.392 (2)
C13—H13	0.9500	C27—H27	0.9500
C14—H14	0.9500	C28—H28	0.9500

C7—N1—N2	111.63 (10)	C21—N4—N5	111.59 (10)
C7—N1—C8	127.81 (11)	C21—N4—C22	127.67 (12)
N2—N1—C8	120.10 (10)	N5—N4—C22	119.83 (11)
C1—N2—N1	106.18 (10)	C15—N5—N4	106.28 (11)
O2—N3—O1	122.50 (13)	O4—N6—O3	123.21 (14)
O2—N3—C4	118.86 (13)	O4—N6—C18	118.47 (13)
O1—N3—C4	118.63 (12)	O3—N6—C18	118.31 (14)
N2—C1—C2	111.30 (11)	N5—C15—C16	111.31 (12)
N2—C1—H1	124.3	N5—C15—H15	124.3
C2—C1—H1	124.3	C16—C15—H15	124.3
C3—C2—C7	120.07 (12)	C17—C16—C21	119.61 (12)
C3—C2—C1	135.43 (12)	C17—C16—C15	136.18 (12)
C7—C2—C1	104.46 (11)	C21—C16—C15	104.20 (11)
C4—C3—C2	116.72 (12)	C18—C17—C16	116.55 (12)
C4—C3—H3	121.6	C18—C17—H17	121.7
C2—C3—H3	121.6	C16—C17—H17	121.7
C3—C4—C5	123.71 (12)	C17—C18—C19	123.98 (12)
C3—C4—N3	117.34 (12)	C17—C18—N6	117.97 (12)
C5—C4—N3	118.88 (12)	C19—C18—N6	118.05 (12)
C6—C5—C4	120.03 (12)	C20—C19—C18	119.99 (12)
C6—C5—H5	120.0	C20—C19—H19	120.0
C4—C5—H5	120.0	C18—C19—H19	120.0
C5—C6—C7	117.03 (12)	C19—C20—C21	117.02 (12)
C5—C6—H6	121.5	C19—C20—H20	121.5
C7—C6—H6	121.5	C21—C20—H20	121.5
N1—C7—C6	131.18 (12)	N4—C21—C20	130.58 (12)
N1—C7—C2	106.40 (11)	N4—C21—C16	106.61 (11)
C6—C7—C2	122.41 (12)	C20—C21—C16	122.80 (12)
N1—C8—C9	111.62 (10)	N4—C22—C23	112.91 (10)
N1—C8—H8A	109.3	N4—C22—H22A	109.0
C9—C8—H8A	109.3	C23—C22—H22A	109.0
N1—C8—H8B	109.3	N4—C22—H22B	109.0
C9—C8—H8B	109.3	C23—C22—H22B	109.0
H8A—C8—H8B	108.0	H22A—C22—H22B	107.8
C14—C9—C10	119.00 (12)	C28—C23—C24	119.11 (13)
C14—C9—C8	121.22 (12)	C28—C23—C22	120.65 (13)
C10—C9—C8	119.77 (11)	C24—C23—C22	120.24 (13)
C11—C10—C9	120.65 (12)	C23—C24—C25	120.22 (15)
C11—C10—H10	119.7	C23—C24—H24	119.9
C9—C10—H10	119.7	C25—C24—H24	119.9

C12—C11—C10	119.90 (13)	C26—C25—C24	120.18 (15)
C12—C11—H11	120.1	C26—C25—H25	119.9
C10—C11—H11	120.1	C24—C25—H25	119.9
C13—C12—C11	119.78 (13)	C27—C26—C25	119.99 (14)
C13—C12—H12	120.1	C27—C26—H26	120.0
C11—C12—H12	120.1	C25—C26—H26	120.0
C12—C13—C14	120.37 (13)	C26—C27—C28	119.83 (15)
C12—C13—H13	119.8	C26—C27—H27	120.1
C14—C13—H13	119.8	C28—C27—H27	120.1
C9—C14—C13	120.30 (13)	C23—C28—C27	120.64 (14)
C9—C14—H14	119.9	C23—C28—H28	119.7
C13—C14—H14	119.9	C27—C28—H28	119.7

C7—N1—N2—C1	1.10 (13)	C21—N4—N5—C15	0.97 (14)
C8—N1—N2—C1	173.93 (11)	C22—N4—N5—C15	170.86 (11)
N1—N2—C1—C2	−0.75 (14)	N4—N5—C15—C16	−1.21 (14)
N2—C1—C2—C3	−177.42 (14)	N5—C15—C16—C17	−177.66 (13)
N2—C1—C2—C7	0.16 (14)	N5—C15—C16—C21	1.00 (14)
C7—C2—C3—C4	0.19 (17)	C21—C16—C17—C18	0.53 (17)
C1—C2—C3—C4	177.48 (14)	C15—C16—C17—C18	179.03 (14)
C2—C3—C4—C5	1.41 (19)	C16—C17—C18—C19	1.61 (19)
C2—C3—C4—N3	−175.42 (11)	C16—C17—C18—N6	−177.49 (11)
O2—N3—C4—C3	5.49 (19)	O4—N6—C18—C17	−6.44 (19)
O1—N3—C4—C3	−176.00 (12)	O3—N6—C18—C17	172.42 (13)
O2—N3—C4—C5	−171.50 (13)	O4—N6—C18—C19	174.40 (13)
O1—N3—C4—C5	7.01 (18)	O3—N6—C18—C19	−6.74 (19)
C3—C4—C5—C6	−1.6 (2)	C17—C18—C19—C20	−1.9 (2)
N3—C4—C5—C6	175.15 (12)	N6—C18—C19—C20	177.16 (12)
C4—C5—C6—C7	0.17 (18)	C18—C19—C20—C21	0.04 (18)
N2—N1—C7—C6	179.18 (12)	N5—N4—C21—C20	−179.26 (13)
C8—N1—C7—C6	7.0 (2)	C22—N4—C21—C20	11.8 (2)
N2—N1—C7—C2	−1.00 (13)	N5—N4—C21—C16	−0.34 (13)
C8—N1—C7—C2	−173.14 (11)	C22—N4—C21—C16	−169.25 (12)
C5—C6—C7—N1	−178.80 (12)	C19—C20—C21—N4	−179.15 (12)
C5—C6—C7—C2	1.41 (18)	C19—C20—C21—C16	2.08 (18)
C3—C2—C7—N1	178.54 (11)	C17—C16—C21—N4	178.56 (11)
C1—C2—C7—N1	0.50 (13)	C15—C16—C21—N4	−0.37 (13)
C3—C2—C7—C6	−1.62 (18)	C17—C16—C21—C20	−2.42 (18)
C1—C2—C7—C6	−179.66 (11)	C15—C16—C21—C20	178.65 (12)
C7—N1—C8—C9	80.48 (15)	C21—N4—C22—C23	83.39 (17)
N2—N1—C8—C9	−91.07 (13)	N5—N4—C22—C23	−84.71 (16)
N1—C8—C9—C14	−114.90 (14)	N4—C22—C23—C28	−99.17 (15)
N1—C8—C9—C10	63.43 (15)	N4—C22—C23—C24	80.59 (16)
C14—C9—C10—C11	0.87 (19)	C28—C23—C24—C25	−1.39 (19)
C8—C9—C10—C11	−177.50 (12)	C22—C23—C24—C25	178.84 (12)
C9—C10—C11—C12	−0.9 (2)	C23—C24—C25—C26	0.2 (2)
C10—C11—C12—C13	0.4 (2)	C24—C25—C26—C27	1.0 (2)
C11—C12—C13—C14	0.2 (2)	C25—C26—C27—C28	−1.0 (2)

C10—C9—C14—C13	−0.4 (2)	C24—C23—C28—C27	1.39 (19)
C8—C9—C14—C13	177.99 (13)	C22—C23—C28—C27	−178.85 (12)
C12—C13—C14—C9	−0.2 (2)	C26—C27—C28—C23	−0.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···O2	0.95	2.48	3.2242 (17)	135