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ISSN 2414-3146

(1*E*,2*E*)-N^1,N^2-Bis(5′-methyl-[1,1′:3′,1″-terphenyl]-4′-yl)acenaphthylene-1,2-diimine unknown solvent

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Received 31 March 2016
Accepted 10 April 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

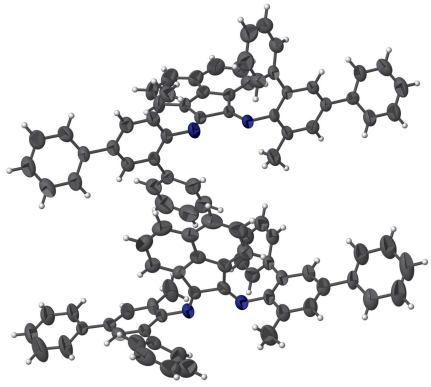
Keywords: crystal structure; acenaphthylene-1,2-dione; α-diimine catalyst; potential bidentate ligand; C—H···N hydrogen bonding; π-π interactions.

CCDC reference: 1473249

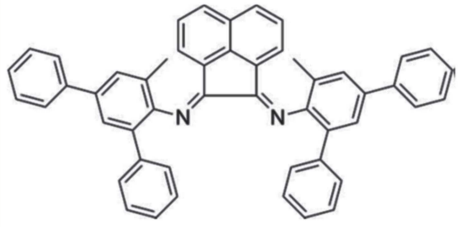
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{50}H_{36}N_2$, synthesized by the condensation reaction of 2-methyl-4,6-diphenylaniline and acenaphthylene-1,2-dione, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The two molecules differ essentially in the orientation of the phenyl ring at position 3′ of the terphenyl group with respect to the central ring of this unit. In molecule *A* this dihedral angle is 16.68 (14)°, while in molecule *B* the corresponding angle is 33.10 (16)°. The three-fused-ring 1,2-dihydroacenaphthylene units are planar in each molecule; r.m.s. deviation of 0.025 Å in molecule *A* and 0.017 Å in molecule *B*. The central rings of the terphenyl groups are almost normal to the mean plane of the three-fused-ring units with dihedral angles of 79.43 (12) and 82.66 (13)° in molecule *A* and 88.99 (13) and 87.98 (12)° in molecule *B*. In the crystal, the two molecules are linked *via* a C—H···N hydrogen bond. These *A*–*B* units are linked by a pair of C—H···π interactions, forming a four-molecule unit located about an inversion center. These four-molecule units are linked by weak π–π interactions [most significant intercentroid distance = 3.794 (2) Å], forming columns along direction [010]. A region of disordered electron density was corrected for using the SQUEEZE routine in *PLATON* [Spek (2015). *Acta Cryst*. C**71**, 9–18]. The formula mass and unit-cell characteristics of this unknown solvent were not be taken into account during the refinement.

3D view



Chemical scheme



Structure description

In the past few decades, there has been a rapid development of a series of α-diimine palladium and nickel complex catalysts [MX_2(α-diimine)] (where M = Ni, Pd; X = halide) for the polymerization of α-olefins since the original discovery of highly active α-diimine nickel catalysts (Johnson *et al.*, 1995). The catalytic activity and properties of the resulting

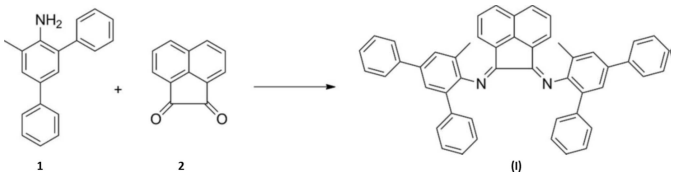


Figure 1
The condensation reaction of 2-methyl-4,6-diphenylaniline (1) and acenaphthylene-1,2-dione (2), giving the title compound.

polymers are greatly dependent on the reaction conditions (Helldörfer *et al.*, 2003) and ligand structures (Meinhard *et al.*, 2007; Popeney *et al.*, 2011; Yuan *et al.*, 2005; 2013). Nickel and palladium metal complex catalysts have a high catalytic activity for ethylene polymerization which gives high branched polyethylene, and the copolymerization of ethylene and polar monomers have also high catalytic activity. In this study, we describe the synthesis and crystal structure of the title compound, a new potential bidentate ligand prepared by the condensation reaction of 2-methyl-4,6-diphenylaniline (**1**) and acenaphthylene-1,2-dione (**2**); Fig. 1.

The title compound crystallizes with two independent molecules in the asymmetric unit. The molecular structure of molecule *A* is illustrated in Fig. 2, while that of molecule *B* is illustrated in Fig. 3. The *AutoMolFit* of molecule *B* inverted on molecule *A* gives the best fit (Fig. 4; Spek, 2009). The two molecules having weighted and unit weight r.m.s. fits of 0.317 and 0.278 Å, respectively, for the 52 non-H atoms. The two molecules differ essentially in the orientation of the phenyl ring at position 3′ of the terphenyl group with respect to the

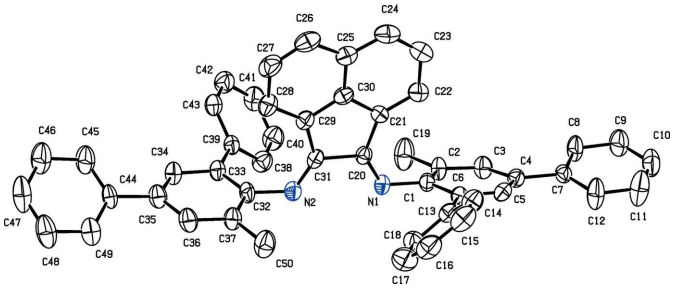


Figure 2
The molecular structure of molecule *A* of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

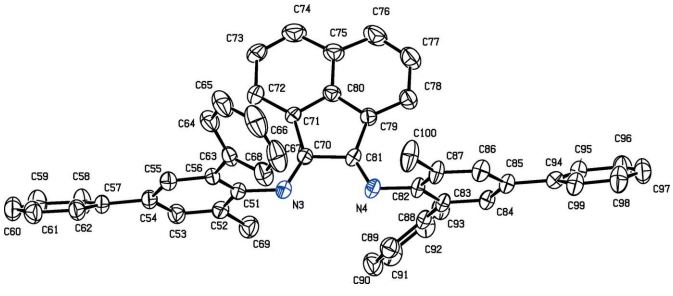


Figure 3
The molecular structure of molecule *B* of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

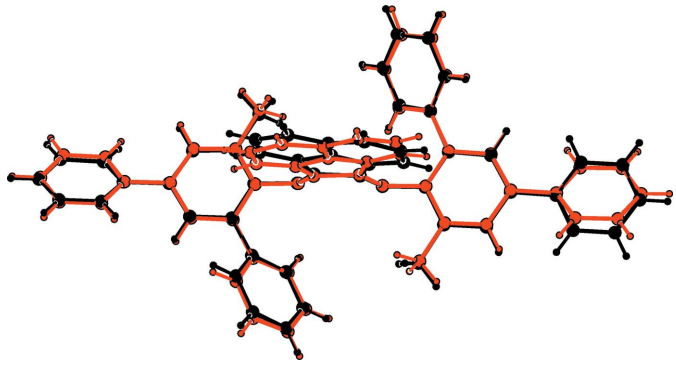


Figure 4
The *AutoMolFit* of molecule *B* (red) inverted on molecule *A* (black) gives the best fit (*PLATON*; Spek, 2009).

central ring of this unit. In molecule *A* this dihedral angle (C7–C12/C1-C6) is 16.68 (14)°, while in molecule *B* the corresponding angle (C94–C99/C82–C87) is 33.10 (16)°. The three-fused-ring 1,2-dihydroacenaphthylene units (C20–C31 in molecule *A*, and C70–C81 in molecule *B*) are planar in each molecule with r.m.s. deviation of 0.025 Å in molecule *A* and 0.017 Å in molecule *B*. The central ring of the terphenyl groups (C1–C6 and C32–C37 in molecule *A*, and C82–C88 and C51–C56 in molecule *B*) are almost normal to the mean plane of the three-fused-ring units, with dihedral angles of 79.43 (12) and 82.66 (13)°, respectively, in molecule *A*, and 88.99 (13) and 87.98 (12)°, respectively, in molecule *B*.

In the crystal, the two molecules are linked *via* a C—H···N hydrogen bond (Table 1 and Fig. 5). These *A*–*B* units are linked about a center of inversion by a pair of C—H···π interactions, forming a four-molecule unit (Table 1 and Fig. 5). These four-molecule units are linked by slipped parallel π–π interactions forming columns along the *b*-axis direction [$Cg3\cdots Cg18^{i}$ = 3.794 (2) Å, interplanar distance = 3.590 (1) Å, slippage = 0.787 Å, *Cg*3 is the centroid of ring C7–C12 in molecule *A* and *Cg*18 is the centroid of ring C71–C75/C80 in molecule *B*, symmetry code (i): $-x+1, -y+2, -z+1$].

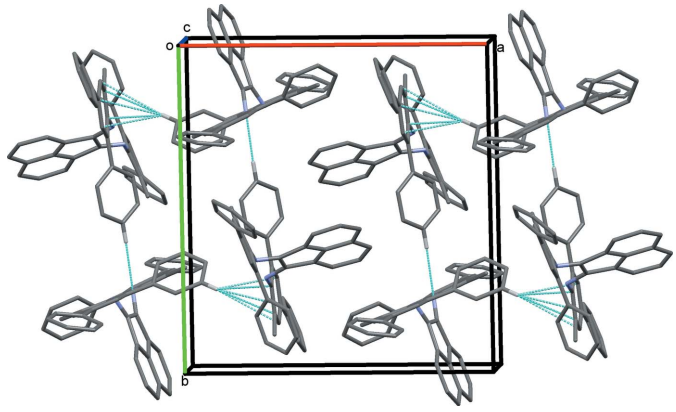


Figure 5
A view along the *c* axis of the crystal packing of the title compound. The C—H···N hydrogen bonds and C—H···π interactions are represented by dashed lines (see Table 1). H atoms not involved in these interactions have been omitted for clarity.

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

*Cg*2 is the centroid of ring C1–C6 in molecule *A*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···N3^{i}	0.93	2.60	3.517 (6)	168
C92—H92···*Cg*2^{ii}	0.93	2.95	3.789 (5)	151

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

Synthesis and crystallization

The synthesis of the title compound is illustrated in Fig. 1.

Synthesis of 2-methyl-4,6-diphenylaniline (**1**): 2-methyl-4,6-dibromo-aniline (2 mmol, 0.53 g) was dissolved in PEG-400 (10 ml) containing phenylboronic acid (0.586 g, 4.8 mmol), K_2CO_3 (0,828 g;0.6 mmol) $PdCl_2$ (50 µg). The solution was placed in a round-bottomed flask and stirred at room temperature for 12 h. After the reaction, the solution was eluted with ethyl acetate/petroleum ether (*v*/*v* = 1:15) through a column, giving compound (**1**) as a colourless liquid (yield: 0.75 g, 79%).

Synthesis of the title compound: Formic acid (0.5 ml) was added to a stirred solution of acenaphthylene-1,2-dione (**2**) [0.18 g, 1.00 mmol] and compound (**1**) [0.57 g, 2.2 mmol) in ethanol (10 ml]. The mixture was refluxed for 24 h, and then cooled and the precipitate separated by filtration. The solid was recrystallized from EtOH/CH_2Cl_2 (*v*/*v* = 10:1), washed and dried under vacuum (yield: 0.43 g, 72%). Crystals suitable for *X*–ray structure analysis were grown from a cyclohexane/dichloromethane (*v*/*v* = 1:2) solution by slow evaporation.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. A region of disordered electron density was corrected for using the SQUEEZE routine in *PLATON* (Spek, 2015): volume *ca* 690 Å^3 for two regions of 36 and 65 electron counts. The formula mass and unit-cell characteristics of this unknown solvent were not taken into account during the refinement.

Acknowledgements

We thank the Key Laboratory of Bioelectrochemical and Environmental Analysis of Gansu Province, College of Chemistry and Chemical Engineering, (Northwest Normal University), for financial support.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{50}H_{36}N_2$
M_r	664.81
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	15.579 (3), 16.799 (4), 17.332 (4)
α, β, γ (°)	72.622 (2), 73.116 (2), 84.324 (2)
V (Å^3)	4142.0 (15)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.06
Crystal size (mm)	0.23 × 0.21 × 0.16
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.986, 0.990
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29357, 14707, 5868
R_{int}	0.041
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.599
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.065, 0.144, 1.04
No. of reflections	14707
No. of parameters	930
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

IUCrData (2016). **1**, x160594 [doi:10.1107/S2414314616005940]

(1*E*,2*E*)-N^1,N^2-Bis(5′-methyl-[1,1′:3′,1″-terphenyl]-4′-yl)acenaphthylene-1,2-diimine unknown solvent

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(1*E*,2*E*)-N^1,N^2-Bis(5′-methyl-[1,1′:3′,1″-\ terphenyl]-4′-yl)acenaphthylene-1,2-diimine unknown solvent

Crystal data

$C_{50}H_{36}N_2$
M_r = 664.81
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 15.579 (3) Å
b = 16.799 (4) Å
c = 17.332 (4) Å
α = 72.622 (2)°
β = 73.116 (2)°
γ = 84.324 (2)°
V = 4142.0 (15) Å^3
Z = 4
$F(000)$ = 1400
D_x = 1.066 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3879 reflections
θ = 2.3–21.0°
μ = 0.06 mm^{-1}
T = 296 K
Block, colorless
0.23 × 0.21 × 0.16 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.986, T_{max} = 0.990
29357 measured reflections
14707 independent reflections
5868 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 25.2°, θ_{min} = 2.3°
h = −18→18
k = −20→20
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.144
S = 1.04
14707 reflections
930 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
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.3174P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0017 (2)

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}
C7	0.31195 (15)	0.84290 (16)	0.84423 (15)	0.0510 (8)
C8	0.34685 (16)	0.92224 (15)	0.82139 (13)	0.0807 (11)
H8	0.3571	0.9556	0.7661	0.097*
C9	0.36642 (16)	0.95177 (14)	0.8812 (2)	0.0916 (13)
H9	0.3898	1.0049	0.8659	0.110*
C10	0.35108 (18)	0.9020 (2)	0.96375 (17)	0.0931 (14)
H10	0.3642	0.9217	1.0037	0.112*
C11	0.3162 (2)	0.82262 (19)	0.98659 (12)	0.1235 (18)
H11	0.3059	0.7893	1.0419	0.148*
C12	0.29661 (18)	0.79309 (13)	0.92683 (18)	0.0998 (14)
H12	0.2733	0.7400	0.9421	0.120*
C1	0.26934 (19)	0.7493 (2)	0.65182 (19)	0.0488 (8)
C2	0.2781 (2)	0.8342 (2)	0.6375 (2)	0.0611 (9)
C3	0.2890 (2)	0.8636 (2)	0.7015 (2)	0.0630 (10)
H3	0.2928	0.9208	0.6922	0.076*
C4	0.29437 (19)	0.8097 (2)	0.77868 (19)	0.0521 (8)
C5	0.28410 (19)	0.7258 (2)	0.79027 (19)	0.0534 (9)
H5	0.2872	0.6884	0.8413	0.064*
C6	0.26940 (19)	0.6942 (2)	0.72966 (19)	0.0483 (8)
C13	0.2546 (2)	0.6033 (2)	0.74996 (19)	0.0557 (9)
C14	0.3040 (2)	0.5452 (2)	0.7955 (2)	0.0742 (11)
H14	0.3488	0.5632	0.8119	0.089*
C15	0.2878 (3)	0.4594 (3)	0.8174 (2)	0.0891 (13)
H15	0.3204	0.4210	0.8492	0.107*
C16	0.2237 (4)	0.4331 (3)	0.7916 (3)	0.0936 (14)
H16	0.2140	0.3763	0.8043	0.112*
C17	0.1739 (3)	0.4891 (3)	0.7474 (3)	0.1001 (14)
H17	0.1293	0.4707	0.7312	0.120*
C18	0.1896 (3)	0.5727 (3)	0.7268 (2)	0.0771 (11)
H18	0.1552	0.6102	0.6961	0.093*
C19	0.2785 (3)	0.8948 (2)	0.5528 (2)	0.1027 (14)
H19A	0.3331	0.8876	0.5119	0.154*
H19B	0.2746	0.9509	0.5569	0.154*
H19C	0.2282	0.8842	0.5361	0.154*
C20	0.3182 (2)	0.68981 (18)	0.54082 (19)	0.0470 (8)

C21	0.4137 (2)	0.67354 (19)	0.5368 (2)	0.0521 (8)
C22	0.4692 (2)	0.6909 (2)	0.5773 (2)	0.0704 (10)
H22	0.4471	0.7172	0.6195	0.084*
C23	0.5600 (3)	0.6685 (3)	0.5545 (3)	0.0869 (12)
H23	0.5978	0.6810	0.5819	0.104*
C24	0.5952 (3)	0.6293 (2)	0.4938 (3)	0.0850 (12)
H24	0.6558	0.6148	0.4811	0.102*
C25	0.5400 (3)	0.6105 (2)	0.4502 (2)	0.0668 (10)
C26	0.5655 (3)	0.5709 (2)	0.3845 (3)	0.0845 (12)
H26	0.6245	0.5527	0.3673	0.101*
C27	0.5042 (3)	0.5597 (2)	0.3468 (2)	0.0863 (12)
H27	0.5226	0.5331	0.3046	0.104*
C28	0.4146 (3)	0.5862 (2)	0.3686 (2)	0.0707 (10)
H28	0.3746	0.5785	0.3408	0.085*
C29	0.3871 (2)	0.62395 (19)	0.4323 (2)	0.0542 (9)
C30	0.4493 (2)	0.63508 (18)	0.4723 (2)	0.0532 (8)
C31	0.3009 (2)	0.65909 (18)	0.47245 (18)	0.0504 (8)
C32	0.2104 (2)	0.6412 (2)	0.3931 (2)	0.0538 (9)
C33	0.2297 (2)	0.6958 (2)	0.3117 (2)	0.0534 (9)
C34	0.2151 (2)	0.6676 (2)	0.2489 (2)	0.0624 (9)
H34	0.2279	0.7033	0.1945	0.075*
C35	0.1830 (2)	0.5901 (2)	0.2629 (2)	0.0639 (10)
C36	0.1594 (2)	0.5397 (2)	0.3458 (2)	0.0689 (10)
H36	0.1341	0.4881	0.3574	0.083*
C37	0.1723 (2)	0.5637 (2)	0.4115 (2)	0.0630 (10)
C38	0.2641 (2)	0.7811 (2)	0.2913 (2)	0.0509 (8)
C39	0.2268 (2)	0.8331 (2)	0.3420 (2)	0.0675 (10)
H39	0.1814	0.8135	0.3913	0.081*
C40	0.2569 (3)	0.9140 (2)	0.3193 (3)	0.0781 (11)
H40	0.2316	0.9480	0.3539	0.094*
C41	0.3232 (3)	0.9444 (2)	0.2471 (3)	0.0763 (11)
H41	0.3427	0.9989	0.2321	0.092*
C42	0.3601 (2)	0.8938 (2)	0.1975 (2)	0.0729 (11)
H42	0.4052	0.9138	0.1481	0.088*
C43	0.3314 (2)	0.8131 (2)	0.2199 (2)	0.0639 (10)
H43	0.3584	0.7792	0.1855	0.077*
C44	0.1732 (3)	0.5603 (2)	0.1918 (2)	0.0604 (10)
C45	0.2328 (3)	0.5863 (2)	0.1142 (3)	0.0896 (13)
H45	0.2776	0.6233	0.1055	0.108*
C46	0.2273 (4)	0.5581 (3)	0.0477 (3)	0.1095 (16)
H46	0.2688	0.5753	−0.0047	0.131*
C47	0.1602 (5)	0.5047 (3)	0.0605 (4)	0.1186 (19)
H47	0.1555	0.4865	0.0162	0.142*
C48	0.0998 (4)	0.4778 (3)	0.1380 (4)	0.1112 (17)
H48	0.0549	0.4407	0.1473	0.133*
C49	0.1077 (3)	0.5081 (2)	0.2038 (3)	0.0855 (12)
H49	0.0665	0.4915	0.2564	0.103*
C50	0.1477 (3)	0.5070 (2)	0.4999 (2)	0.0949 (13)

H50A	0.2011	0.4901	0.5180	0.142*
H50B	0.1183	0.4587	0.5016	0.142*
H50C	0.1081	0.5361	0.5366	0.142*
C51	0.8308 (2)	0.76630 (18)	0.26840 (19)	0.0506 (8)
C52	0.9136 (2)	0.72957 (19)	0.2736 (2)	0.0539 (9)
C53	0.9371 (2)	0.71489 (19)	0.3476 (2)	0.0591 (9)
H53	0.9926	0.6904	0.3509	0.071*
C54	0.8800 (2)	0.73574 (19)	0.4176 (2)	0.0538 (9)
C55	0.7973 (2)	0.77178 (18)	0.41044 (19)	0.0545 (9)
H55	0.7581	0.7857	0.4565	0.065*
C56	0.7713 (2)	0.78774 (17)	0.33696 (19)	0.0471 (8)
C57	0.9076 (2)	0.71895 (18)	0.4972 (2)	0.0527 (9)
C58	0.9928 (3)	0.7233 (2)	0.4962 (2)	0.0766 (11)
H58	1.0368	0.7340	0.4451	0.092*
C59	1.0182 (3)	0.7122 (2)	0.5705 (3)	0.0910 (13)
H59	1.0780	0.7163	0.5682	0.109*
C60	0.9536 (3)	0.6954 (2)	0.6464 (3)	0.0825 (12)
H60	0.9693	0.6886	0.6959	0.099*
C61	0.8648 (3)	0.6886 (2)	0.6488 (2)	0.0790 (11)
H61	0.8209	0.6760	0.7000	0.095*
C62	0.8416 (2)	0.70062 (19)	0.5749 (2)	0.0664 (10)
H62	0.7819	0.6965	0.5766	0.080*
C63	0.6810 (2)	0.8266 (2)	0.33531 (19)	0.0552 (9)
C64	0.6497 (3)	0.8902 (2)	0.3721 (2)	0.0710 (10)
H64	0.6874	0.9114	0.3940	0.085*
C65	0.5653 (3)	0.9229 (3)	0.3773 (2)	0.0985 (14)
H65	0.5464	0.9659	0.4020	0.118*
C66	0.5085 (3)	0.8927 (4)	0.3462 (3)	0.1140 (18)
H66	0.4505	0.9142	0.3507	0.137*
C67	0.5375 (3)	0.8304 (4)	0.3084 (3)	0.1068 (16)
H67	0.4994	0.8106	0.2860	0.128*
C68	0.6237 (3)	0.7964 (2)	0.3032 (2)	0.0784 (11)
H68	0.6425	0.7535	0.2781	0.094*
C69	0.9770 (2)	0.7041 (2)	0.1997 (2)	0.0746 (11)
H69A	1.0356	0.6932	0.2084	0.112*
H69B	0.9801	0.7484	0.1489	0.112*
H69C	0.9552	0.6547	0.1952	0.112*
C70	0.81620 (19)	0.8452 (2)	0.13499 (19)	0.0456 (8)
C71	0.8550 (2)	0.92518 (18)	0.12345 (19)	0.0486 (8)
C72	0.8870 (2)	0.9589 (2)	0.1719 (2)	0.0654 (10)
H72	0.8871	0.9283	0.2263	0.078*
C73	0.9201 (2)	1.0411 (2)	0.1382 (3)	0.0797 (11)
H73	0.9414	1.0641	0.1715	0.096*
C74	0.9218 (3)	1.0874 (2)	0.0591 (3)	0.0862 (12)
H74	0.9444	1.1411	0.0393	0.103*
C75	0.8898 (2)	1.0551 (2)	0.0065 (2)	0.0670 (10)
C76	0.8858 (3)	1.0956 (2)	−0.0769 (3)	0.0879 (12)
H76	0.9072	1.1496	−0.1029	0.105*

C77	0.8513 (3)	1.0568 (3)	−0.1192 (2)	0.0824 (12)
H77	0.8497	1.0851	−0.1738	0.099*
C78	0.8178 (2)	0.9754 (2)	−0.0835 (2)	0.0629 (9)
H78	0.7947	0.9500	−0.1139	0.075*
C79	0.82002 (19)	0.93409 (19)	−0.0025 (2)	0.0493 (8)
C80	0.8562 (2)	0.9742 (2)	0.0411 (2)	0.0502 (8)
C81	0.79069 (19)	0.8515 (2)	0.05548 (18)	0.0450 (8)
C82	0.7271 (2)	0.80212 (19)	−0.02622 (19)	0.0504 (8)
C83	0.7878 (2)	0.77977 (18)	−0.09352 (19)	0.0480 (8)
C84	0.7617 (2)	0.79215 (18)	−0.16637 (19)	0.0517 (8)
H84	0.8020	0.7784	−0.2120	0.062*
C85	0.6780 (2)	0.82414 (19)	−0.17419 (19)	0.0520 (8)
C86	0.6187 (2)	0.8422 (2)	−0.1044 (2)	0.0616 (9)
H86	0.5614	0.8619	−0.1073	0.074*
C87	0.6419 (2)	0.8317 (2)	−0.0305 (2)	0.0618 (9)
C88	0.8793 (2)	0.7470 (2)	−0.0903 (2)	0.0512 (8)
C89	0.8943 (2)	0.6866 (2)	−0.0210 (2)	0.0653 (10)
H89	0.8462	0.6673	0.0259	0.078*
C90	0.9794 (3)	0.6543 (2)	−0.0199 (3)	0.0821 (12)
H90	0.9881	0.6137	0.0272	0.099*
C91	1.0508 (3)	0.6828 (3)	−0.0891 (3)	0.0894 (13)
H91	1.1082	0.6617	−0.0887	0.107*
C92	1.0378 (3)	0.7421 (3)	−0.1585 (2)	0.0778 (11)
H92	1.0859	0.7609	−0.2056	0.093*
C93	0.9524 (3)	0.7738 (2)	−0.1581 (2)	0.0657 (10)
H93	0.9441	0.8147	−0.2052	0.079*
C94	0.6529 (2)	0.83902 (18)	−0.2551 (2)	0.0498 (8)
C95	0.7146 (2)	0.86355 (19)	−0.3299 (2)	0.0637 (10)
H95	0.7736	0.8703	−0.3313	0.076*
C96	0.6921 (3)	0.8790 (2)	−0.4048 (2)	0.0782 (11)
H96	0.7359	0.8949	−0.4560	0.094*
C97	0.6048 (3)	0.8706 (2)	−0.4028 (3)	0.0884 (13)
H97	0.5888	0.8806	−0.4525	0.106*
C98	0.5420 (3)	0.8474 (2)	−0.3274 (3)	0.0878 (12)
H98	0.4825	0.8423	−0.3256	0.105*
C99	0.5658 (3)	0.8315 (2)	−0.2534 (2)	0.0717 (10)
H99	0.5224	0.8156	−0.2020	0.086*
C100	0.5755 (2)	0.8559 (3)	0.0424 (2)	0.0992 (14)
H10A	0.5746	0.8131	0.0938	0.149*
H10B	0.5168	0.8623	0.0338	0.149*
H10C	0.5932	0.9076	0.0458	0.149*
N1	0.25457 (17)	0.72250 (15)	0.58708 (16)	0.0530 (7)
N2	0.22359 (19)	0.66608 (15)	0.46041 (15)	0.0557 (7)
N3	0.80571 (17)	0.77649 (16)	0.19320 (16)	0.0552 (7)
N4	0.74955 (16)	0.79299 (16)	0.04974 (14)	0.0514 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C7	0.048 (2)	0.060 (2)	0.054 (2)	0.0065 (18)	−0.0176 (18)	−0.0279 (19)
C8	0.110 (3)	0.089 (3)	0.063 (3)	−0.006 (2)	−0.034 (2)	−0.040 (2)
C9	0.116 (3)	0.096 (3)	0.084 (3)	−0.004 (3)	−0.035 (3)	−0.047 (3)
C10	0.103 (3)	0.122 (4)	0.086 (3)	0.032 (3)	−0.050 (3)	−0.063 (3)
C11	0.217 (6)	0.098 (4)	0.073 (3)	−0.002 (4)	−0.063 (3)	−0.027 (3)
C12	0.167 (4)	0.083 (3)	0.074 (3)	−0.003 (3)	−0.055 (3)	−0.036 (3)
C1	0.053 (2)	0.055 (2)	0.042 (2)	0.0005 (17)	−0.0165 (17)	−0.0169 (18)
C2	0.080 (3)	0.064 (3)	0.050 (2)	0.006 (2)	−0.034 (2)	−0.019 (2)
C3	0.084 (3)	0.048 (2)	0.062 (2)	−0.0010 (19)	−0.028 (2)	−0.0161 (19)
C4	0.052 (2)	0.058 (2)	0.049 (2)	0.0044 (18)	−0.0151 (17)	−0.0205 (19)
C5	0.057 (2)	0.057 (2)	0.041 (2)	0.0026 (18)	−0.0085 (17)	−0.0130 (17)
C6	0.050 (2)	0.053 (2)	0.046 (2)	−0.0001 (16)	−0.0105 (17)	−0.0227 (18)
C13	0.063 (2)	0.053 (2)	0.047 (2)	−0.001 (2)	−0.0061 (19)	−0.0175 (18)
C14	0.089 (3)	0.063 (3)	0.068 (3)	0.004 (2)	−0.016 (2)	−0.021 (2)
C15	0.116 (4)	0.060 (3)	0.072 (3)	0.007 (3)	−0.006 (3)	−0.013 (2)
C16	0.119 (4)	0.066 (3)	0.082 (3)	−0.030 (3)	0.003 (3)	−0.022 (3)
C17	0.108 (4)	0.084 (4)	0.103 (4)	−0.037 (3)	−0.015 (3)	−0.020 (3)
C18	0.083 (3)	0.071 (3)	0.080 (3)	−0.018 (2)	−0.024 (2)	−0.019 (2)
C19	0.179 (4)	0.068 (3)	0.073 (3)	−0.007 (3)	−0.059 (3)	−0.010 (2)
C20	0.058 (2)	0.042 (2)	0.040 (2)	−0.0046 (17)	−0.0121 (18)	−0.0100 (16)
C21	0.047 (2)	0.058 (2)	0.053 (2)	−0.0069 (17)	−0.0139 (18)	−0.0170 (18)
C22	0.059 (3)	0.085 (3)	0.070 (3)	−0.005 (2)	−0.013 (2)	−0.030 (2)
C23	0.063 (3)	0.106 (3)	0.097 (3)	−0.013 (2)	−0.025 (3)	−0.030 (3)
C24	0.053 (3)	0.095 (3)	0.096 (3)	0.000 (2)	−0.008 (3)	−0.023 (3)
C25	0.060 (3)	0.069 (3)	0.063 (3)	0.001 (2)	−0.008 (2)	−0.016 (2)
C26	0.067 (3)	0.086 (3)	0.084 (3)	0.015 (2)	0.002 (2)	−0.027 (2)
C27	0.082 (3)	0.097 (3)	0.078 (3)	0.010 (3)	−0.002 (3)	−0.044 (2)
C28	0.080 (3)	0.074 (3)	0.061 (2)	0.007 (2)	−0.015 (2)	−0.030 (2)
C29	0.061 (2)	0.052 (2)	0.048 (2)	−0.0013 (18)	−0.0097 (19)	−0.0166 (17)
C30	0.055 (2)	0.046 (2)	0.052 (2)	−0.0002 (17)	−0.0056 (19)	−0.0113 (17)
C31	0.065 (3)	0.046 (2)	0.038 (2)	−0.0045 (18)	−0.0092 (19)	−0.0123 (16)
C32	0.064 (2)	0.056 (2)	0.057 (2)	0.0057 (19)	−0.0253 (19)	−0.033 (2)
C33	0.064 (2)	0.054 (2)	0.051 (2)	0.0033 (18)	−0.0215 (19)	−0.0237 (19)
C34	0.083 (3)	0.058 (2)	0.055 (2)	0.001 (2)	−0.029 (2)	−0.0207 (19)
C35	0.087 (3)	0.049 (2)	0.068 (3)	0.001 (2)	−0.034 (2)	−0.021 (2)
C36	0.094 (3)	0.050 (2)	0.077 (3)	−0.004 (2)	−0.036 (2)	−0.026 (2)
C37	0.082 (3)	0.056 (2)	0.060 (3)	0.001 (2)	−0.026 (2)	−0.023 (2)
C38	0.057 (2)	0.055 (2)	0.049 (2)	0.0020 (19)	−0.0208 (19)	−0.0228 (19)
C39	0.076 (3)	0.062 (3)	0.065 (2)	−0.002 (2)	−0.013 (2)	−0.025 (2)
C40	0.099 (3)	0.064 (3)	0.079 (3)	0.001 (2)	−0.022 (3)	−0.034 (2)
C41	0.104 (3)	0.056 (3)	0.072 (3)	−0.013 (2)	−0.029 (3)	−0.014 (2)
C42	0.084 (3)	0.073 (3)	0.065 (3)	−0.013 (2)	−0.017 (2)	−0.022 (2)
C43	0.074 (3)	0.067 (3)	0.062 (3)	−0.003 (2)	−0.021 (2)	−0.033 (2)
C44	0.088 (3)	0.048 (2)	0.064 (3)	0.001 (2)	−0.042 (2)	−0.025 (2)
C45	0.138 (4)	0.069 (3)	0.080 (3)	−0.013 (3)	−0.043 (3)	−0.032 (3)

C46	0.172 (5)	0.089 (3)	0.085 (3)	−0.016 (3)	−0.050 (3)	−0.033 (3)
C47	0.214 (6)	0.078 (4)	0.102 (4)	0.002 (4)	−0.097 (4)	−0.030 (3)
C48	0.178 (5)	0.075 (3)	0.116 (4)	−0.013 (3)	−0.085 (4)	−0.030 (3)
C49	0.117 (4)	0.073 (3)	0.084 (3)	0.006 (3)	−0.051 (3)	−0.027 (2)
C50	0.142 (4)	0.073 (3)	0.072 (3)	−0.027 (3)	−0.028 (3)	−0.018 (2)
C51	0.067 (2)	0.047 (2)	0.043 (2)	−0.0067 (18)	−0.0208 (19)	−0.0126 (16)
C52	0.066 (3)	0.051 (2)	0.047 (2)	−0.0028 (18)	−0.016 (2)	−0.0160 (17)
C53	0.060 (2)	0.064 (2)	0.057 (2)	0.0094 (18)	−0.024 (2)	−0.0199 (19)
C54	0.060 (2)	0.058 (2)	0.048 (2)	0.0054 (18)	−0.0225 (19)	−0.0172 (17)
C55	0.060 (2)	0.058 (2)	0.047 (2)	−0.0003 (18)	−0.0162 (18)	−0.0149 (17)
C56	0.058 (2)	0.045 (2)	0.040 (2)	−0.0047 (17)	−0.0185 (18)	−0.0086 (16)
C57	0.063 (3)	0.056 (2)	0.046 (2)	0.0036 (18)	−0.025 (2)	−0.0168 (17)
C58	0.065 (3)	0.111 (3)	0.052 (2)	0.004 (2)	−0.017 (2)	−0.023 (2)
C59	0.077 (3)	0.129 (4)	0.078 (3)	0.015 (3)	−0.034 (3)	−0.039 (3)
C60	0.098 (3)	0.097 (3)	0.069 (3)	0.023 (3)	−0.044 (3)	−0.036 (2)
C61	0.097 (3)	0.086 (3)	0.056 (3)	0.022 (2)	−0.026 (2)	−0.027 (2)
C62	0.078 (3)	0.072 (2)	0.059 (3)	0.017 (2)	−0.035 (2)	−0.023 (2)
C63	0.059 (2)	0.061 (2)	0.044 (2)	−0.007 (2)	−0.0239 (19)	−0.0011 (18)
C64	0.073 (3)	0.075 (3)	0.062 (2)	0.018 (2)	−0.025 (2)	−0.015 (2)
C65	0.098 (4)	0.115 (4)	0.076 (3)	0.040 (3)	−0.037 (3)	−0.018 (3)
C66	0.076 (4)	0.166 (5)	0.080 (4)	0.022 (4)	−0.027 (3)	−0.009 (3)
C67	0.071 (4)	0.164 (5)	0.080 (3)	−0.014 (3)	−0.039 (3)	−0.004 (3)
C68	0.074 (3)	0.092 (3)	0.066 (3)	−0.010 (2)	−0.030 (2)	−0.005 (2)
C69	0.080 (3)	0.083 (3)	0.064 (2)	0.005 (2)	−0.018 (2)	−0.029 (2)
C70	0.051 (2)	0.045 (2)	0.042 (2)	−0.0048 (17)	−0.0136 (17)	−0.0131 (17)
C71	0.057 (2)	0.043 (2)	0.053 (2)	−0.0048 (17)	−0.0235 (18)	−0.0168 (18)
C72	0.082 (3)	0.063 (3)	0.067 (2)	−0.005 (2)	−0.038 (2)	−0.023 (2)
C73	0.101 (3)	0.060 (3)	0.101 (3)	−0.015 (2)	−0.054 (3)	−0.028 (2)
C74	0.097 (3)	0.054 (3)	0.113 (4)	−0.016 (2)	−0.042 (3)	−0.013 (3)
C75	0.071 (3)	0.051 (2)	0.080 (3)	−0.009 (2)	−0.029 (2)	−0.010 (2)
C76	0.101 (3)	0.063 (3)	0.084 (3)	−0.025 (2)	−0.030 (3)	0.013 (2)
C77	0.094 (3)	0.078 (3)	0.066 (3)	−0.008 (2)	−0.028 (2)	0.002 (2)
C78	0.069 (3)	0.064 (3)	0.051 (2)	−0.003 (2)	−0.0188 (19)	−0.0078 (19)
C79	0.051 (2)	0.051 (2)	0.046 (2)	−0.0044 (17)	−0.0161 (17)	−0.0109 (18)
C80	0.050 (2)	0.044 (2)	0.055 (2)	−0.0045 (17)	−0.0164 (18)	−0.0079 (18)
C81	0.044 (2)	0.053 (2)	0.044 (2)	−0.0024 (17)	−0.0110 (16)	−0.0239 (18)
C82	0.051 (2)	0.069 (2)	0.040 (2)	−0.0087 (18)	−0.0155 (18)	−0.0228 (17)
C83	0.053 (2)	0.058 (2)	0.043 (2)	−0.0071 (17)	−0.0157 (18)	−0.0230 (17)
C84	0.052 (2)	0.064 (2)	0.043 (2)	−0.0032 (18)	−0.0102 (18)	−0.0237 (17)
C85	0.053 (2)	0.064 (2)	0.048 (2)	−0.0019 (18)	−0.0176 (19)	−0.0242 (18)
C86	0.050 (2)	0.082 (3)	0.059 (2)	0.0000 (18)	−0.014 (2)	−0.031 (2)
C87	0.058 (2)	0.093 (3)	0.046 (2)	−0.002 (2)	−0.0128 (19)	−0.037 (2)
C88	0.058 (2)	0.061 (2)	0.044 (2)	−0.0061 (19)	−0.016 (2)	−0.0242 (18)
C89	0.065 (3)	0.072 (3)	0.058 (2)	−0.002 (2)	−0.012 (2)	−0.022 (2)
C90	0.087 (3)	0.089 (3)	0.077 (3)	0.019 (3)	−0.039 (3)	−0.024 (2)
C91	0.060 (3)	0.118 (4)	0.100 (4)	0.017 (3)	−0.029 (3)	−0.044 (3)
C92	0.059 (3)	0.103 (3)	0.069 (3)	0.000 (2)	−0.015 (2)	−0.024 (2)
C93	0.065 (3)	0.080 (3)	0.054 (2)	−0.001 (2)	−0.016 (2)	−0.023 (2)

C94	0.049 (2)	0.051 (2)	0.051 (2)	−0.0012 (17)	−0.012 (2)	−0.0198 (17)
C95	0.079 (3)	0.066 (2)	0.055 (2)	0.000 (2)	−0.028 (2)	−0.0213 (19)
C96	0.101 (4)	0.080 (3)	0.051 (3)	0.005 (2)	−0.021 (2)	−0.017 (2)
C97	0.108 (4)	0.107 (3)	0.066 (3)	0.028 (3)	−0.047 (3)	−0.035 (3)
C98	0.083 (3)	0.124 (4)	0.072 (3)	0.015 (3)	−0.037 (3)	−0.041 (3)
C99	0.076 (3)	0.091 (3)	0.061 (3)	0.003 (2)	−0.026 (2)	−0.034 (2)
C100	0.070 (3)	0.177 (4)	0.075 (3)	0.016 (3)	−0.022 (2)	−0.075 (3)
N1	0.0632 (19)	0.0567 (18)	0.0465 (17)	0.0013 (14)	−0.0177 (15)	−0.0238 (14)
N2	0.061 (2)	0.0595 (18)	0.0519 (18)	−0.0010 (15)	−0.0178 (16)	−0.0212 (14)
N3	0.072 (2)	0.0536 (19)	0.0468 (18)	−0.0049 (15)	−0.0221 (15)	−0.0173 (15)
N4	0.0555 (18)	0.0631 (19)	0.0427 (17)	−0.0100 (14)	−0.0117 (14)	−0.0243 (14)

Geometric parameters (Å, º)

C7—C8	1.3900	C51—C52	1.389 (4)
C7—C12	1.3900	C51—C56	1.397 (4)
C7—C4	1.505 (3)	C51—N3	1.425 (3)
C8—C9	1.3900	C52—C53	1.380 (4)
C8—H8	0.9300	C52—C69	1.518 (4)
C9—C10	1.3900	C53—C54	1.397 (4)
C9—H9	0.9300	C53—H53	0.9300
C10—C11	1.3900	C54—C55	1.391 (4)
C10—H10	0.9300	C54—C57	1.503 (4)
C11—C12	1.3900	C55—C56	1.390 (4)
C11—H11	0.9300	C55—H55	0.9300
C12—H12	0.9300	C56—C63	1.495 (4)
C1—C2	1.386 (4)	C57—C58	1.331 (4)
C1—C6	1.390 (4)	C57—C62	1.406 (4)
C1—N1	1.410 (3)	C58—C59	1.410 (4)
C2—C3	1.397 (4)	C58—H58	0.9300
C2—C19	1.514 (4)	C59—C60	1.374 (5)
C3—C4	1.394 (4)	C59—H59	0.9300
C3—H3	0.9300	C60—C61	1.387 (5)
C4—C5	1.383 (4)	C60—H60	0.9300
C5—C6	1.390 (4)	C61—C62	1.383 (4)
C5—H5	0.9300	C61—H61	0.9300
C6—C13	1.486 (4)	C62—H62	0.9300
C13—C14	1.384 (4)	C63—C64	1.382 (4)
C13—C18	1.384 (4)	C63—C68	1.383 (4)
C14—C15	1.405 (5)	C64—C65	1.363 (5)
C14—H14	0.9300	C64—H64	0.9300
C15—C16	1.363 (5)	C65—C66	1.363 (5)
C15—H15	0.9300	C65—H65	0.9300
C16—C17	1.357 (5)	C66—C67	1.368 (6)
C16—H16	0.9300	C66—H66	0.9300
C17—C18	1.370 (5)	C67—C68	1.395 (5)
C17—H17	0.9300	C67—H67	0.9300
C18—H18	0.9300	C68—H68	0.9300

C19—H19A	0.9600	C69—H69A	0.9600
C19—H19B	0.9600	C69—H69B	0.9600
C19—H19C	0.9600	C69—H69C	0.9600
C20—N1	1.273 (3)	C70—N3	1.274 (3)
C20—C21	1.472 (4)	C70—C71	1.463 (4)
C20—C31	1.524 (4)	C70—C81	1.514 (4)
C21—C22	1.359 (4)	C71—C72	1.363 (4)
C21—C30	1.405 (4)	C71—C80	1.414 (4)
C22—C23	1.400 (4)	C72—C73	1.413 (4)
C22—H22	0.9300	C72—H72	0.9300
C23—C24	1.359 (5)	C73—C74	1.352 (4)
C23—H23	0.9300	C73—H73	0.9300
C24—C25	1.408 (5)	C74—C75	1.410 (4)
C24—H24	0.9300	C74—H74	0.9300
C25—C30	1.407 (4)	C75—C80	1.398 (4)
C25—C26	1.427 (5)	C75—C76	1.418 (5)
C26—C27	1.359 (4)	C76—C77	1.354 (4)
C26—H26	0.9300	C76—H76	0.9300
C27—C28	1.401 (4)	C77—C78	1.405 (4)
C27—H27	0.9300	C77—H77	0.9300
C28—C29	1.376 (4)	C78—C79	1.376 (4)
C28—H28	0.9300	C78—H78	0.9300
C29—C30	1.400 (4)	C79—C80	1.404 (4)
C29—C31	1.478 (4)	C79—C81	1.473 (4)
C31—N2	1.269 (3)	C81—N4	1.267 (3)
C32—C37	1.394 (4)	C82—C87	1.385 (4)
C32—C33	1.399 (4)	C82—C83	1.395 (4)
C32—N2	1.423 (3)	C82—N4	1.420 (3)
C33—C34	1.390 (4)	C83—C84	1.388 (4)
C33—C38	1.485 (4)	C83—C88	1.488 (4)
C34—C35	1.370 (4)	C84—C85	1.387 (4)
C34—H34	0.9300	C84—H84	0.9300
C35—C36	1.394 (4)	C85—C86	1.386 (4)
C35—C44	1.511 (4)	C85—C94	1.508 (4)
C36—C37	1.388 (4)	C86—C87	1.387 (4)
C36—H36	0.9300	C86—H86	0.9300
C37—C50	1.503 (4)	C87—C100	1.515 (4)
C38—C43	1.371 (4)	C88—C93	1.374 (4)
C38—C39	1.391 (4)	C88—C89	1.383 (4)
C39—C40	1.386 (4)	C89—C90	1.384 (4)
C39—H39	0.9300	C89—H89	0.9300
C40—C41	1.367 (4)	C90—C91	1.377 (5)
C40—H40	0.9300	C90—H90	0.9300
C41—C42	1.359 (4)	C91—C92	1.366 (5)
C41—H41	0.9300	C91—H91	0.9300
C42—C43	1.377 (4)	C92—C93	1.382 (4)
C42—H42	0.9300	C92—H92	0.9300
C43—H43	0.9300	C93—H93	0.9300

C44—C49	1.341 (4)	C94—C95	1.344 (4)
C44—C45	1.365 (5)	C94—C99	1.365 (4)
C45—C46	1.397 (5)	C95—C96	1.387 (4)
C45—H45	0.9300	C95—H95	0.9300
C46—C47	1.371 (6)	C96—C97	1.370 (5)
C46—H46	0.9300	C96—H96	0.9300
C47—C48	1.372 (6)	C97—C98	1.359 (5)
C47—H47	0.9300	C97—H97	0.9300
C48—C49	1.420 (5)	C98—C99	1.381 (4)
C48—H48	0.9300	C98—H98	0.9300
C49—H49	0.9300	C99—H99	0.9300
C50—H50A	0.9600	C100—H10A	0.9600
C50—H50B	0.9600	C100—H10B	0.9600
C50—H50C	0.9600	C100—H10C	0.9600
C8—C7—C12	120.0	C56—C51—N3	120.7 (3)
C8—C7—C4	119.9 (2)	C53—C52—C51	119.1 (3)
C12—C7—C4	120.1 (2)	C53—C52—C69	120.2 (3)
C9—C8—C7	120.0	C51—C52—C69	120.7 (3)
C9—C8—H8	120.0	C52—C53—C54	121.9 (3)
C7—C8—H8	120.0	C52—C53—H53	119.0
C8—C9—C10	120.0	C54—C53—H53	119.0
C8—C9—H9	120.0	C55—C54—C53	117.4 (3)
C10—C9—H9	120.0	C55—C54—C57	121.9 (3)
C9—C10—C11	120.0	C53—C54—C57	120.6 (3)
C9—C10—H10	120.0	C56—C55—C54	122.4 (3)
C11—C10—H10	120.0	C56—C55—H55	118.8
C12—C11—C10	120.0	C54—C55—H55	118.8
C12—C11—H11	120.0	C55—C56—C51	118.2 (3)
C10—C11—H11	120.0	C55—C56—C63	118.5 (3)
C11—C12—C7	120.0	C51—C56—C63	123.3 (3)
C11—C12—H12	120.0	C58—C57—C62	118.9 (3)
C7—C12—H12	120.0	C58—C57—C54	121.8 (3)
C2—C1—C6	120.2 (3)	C62—C57—C54	119.3 (3)
C2—C1—N1	117.7 (3)	C57—C58—C59	121.9 (4)
C6—C1—N1	122.0 (3)	C57—C58—H58	119.0
C1—C2—C3	119.4 (3)	C59—C58—H58	119.0
C1—C2—C19	120.7 (3)	C60—C59—C58	119.3 (4)
C3—C2—C19	119.9 (3)	C60—C59—H59	120.3
C4—C3—C2	121.9 (3)	C58—C59—H59	120.3
C4—C3—H3	119.0	C59—C60—C61	119.5 (4)
C2—C3—H3	119.0	C59—C60—H60	120.2
C5—C4—C3	116.5 (3)	C61—C60—H60	120.2
C5—C4—C7	122.9 (3)	C62—C61—C60	120.0 (4)
C3—C4—C7	120.6 (3)	C62—C61—H61	120.0
C4—C5—C6	123.4 (3)	C60—C61—H61	120.0
C4—C5—H5	118.3	C61—C62—C57	120.4 (3)
C6—C5—H5	118.3	C61—C62—H62	119.8

C1—C6—C5	118.4 (3)	C57—C62—H62	119.8
C1—C6—C13	122.4 (3)	C64—C63—C68	117.9 (3)
C5—C6—C13	119.2 (3)	C64—C63—C56	120.3 (3)
C14—C13—C18	116.8 (3)	C68—C63—C56	121.6 (3)
C14—C13—C6	121.0 (3)	C65—C64—C63	121.9 (4)
C18—C13—C6	122.2 (3)	C65—C64—H64	119.1
C13—C14—C15	121.0 (4)	C63—C64—H64	119.1
C13—C14—H14	119.5	C66—C65—C64	120.3 (4)
C15—C14—H14	119.5	C66—C65—H65	119.8
C16—C15—C14	119.4 (4)	C64—C65—H65	119.8
C16—C15—H15	120.3	C65—C66—C67	119.4 (5)
C14—C15—H15	120.3	C65—C66—H66	120.3
C17—C16—C15	120.6 (4)	C67—C66—H66	120.3
C17—C16—H16	119.7	C66—C67—C68	120.7 (5)
C15—C16—H16	119.7	C66—C67—H67	119.7
C16—C17—C18	119.8 (4)	C68—C67—H67	119.7
C16—C17—H17	120.1	C63—C68—C67	119.8 (4)
C18—C17—H17	120.1	C63—C68—H68	120.1
C17—C18—C13	122.4 (4)	C67—C68—H68	120.1
C17—C18—H18	118.8	C52—C69—H69A	109.5
C13—C18—H18	118.8	C52—C69—H69B	109.5
C2—C19—H19A	109.5	H69A—C69—H69B	109.5
C2—C19—H19B	109.5	C52—C69—H69C	109.5
H19A—C19—H19B	109.5	H69A—C69—H69C	109.5
C2—C19—H19C	109.5	H69B—C69—H69C	109.5
H19A—C19—H19C	109.5	N3—C70—C71	133.4 (3)
H19B—C19—H19C	109.5	N3—C70—C81	119.4 (3)
N1—C20—C21	133.3 (3)	C71—C70—C81	107.0 (3)
N1—C20—C31	120.0 (3)	C72—C71—C80	118.4 (3)
C21—C20—C31	106.7 (3)	C72—C71—C70	135.3 (3)
C22—C21—C30	119.2 (3)	C80—C71—C70	106.3 (3)
C22—C21—C20	134.4 (3)	C71—C72—C73	119.0 (3)
C30—C21—C20	106.3 (3)	C71—C72—H72	120.5
C21—C22—C23	118.9 (3)	C73—C72—H72	120.5
C21—C22—H22	120.5	C74—C73—C72	122.3 (3)
C23—C22—H22	120.5	C74—C73—H73	118.8
C24—C23—C22	122.7 (4)	C72—C73—H73	118.8
C24—C23—H23	118.6	C73—C74—C75	120.8 (4)
C22—C23—H23	118.6	C73—C74—H74	119.6
C23—C24—C25	120.1 (4)	C75—C74—H74	119.6
C23—C24—H24	120.0	C80—C75—C74	116.2 (3)
C25—C24—H24	120.0	C80—C75—C76	116.0 (3)
C24—C25—C30	116.6 (3)	C74—C75—C76	127.8 (4)
C24—C25—C26	127.7 (4)	C77—C76—C75	121.0 (4)
C30—C25—C26	115.7 (4)	C77—C76—H76	119.5
C27—C26—C25	120.3 (4)	C75—C76—H76	119.5
C27—C26—H26	119.8	C76—C77—C78	122.3 (4)
C25—C26—H26	119.8	C76—C77—H77	118.8

C26—C27—C28	123.1 (4)	C78—C77—H77	118.8
C26—C27—H27	118.4	C79—C78—C77	118.5 (3)
C28—C27—H27	118.4	C79—C78—H78	120.7
C29—C28—C27	118.3 (3)	C77—C78—H78	120.7
C29—C28—H28	120.8	C78—C79—C80	119.1 (3)
C27—C28—H28	120.8	C78—C79—C81	134.4 (3)
C28—C29—C30	119.2 (3)	C80—C79—C81	106.5 (3)
C28—C29—C31	134.2 (3)	C75—C80—C79	123.0 (3)
C30—C29—C31	106.6 (3)	C75—C80—C71	123.3 (3)
C29—C30—C21	114.3 (3)	C79—C80—C71	113.7 (3)
C29—C30—C25	123.3 (3)	N4—C81—C79	132.5 (3)
C21—C30—C25	122.3 (3)	N4—C81—C70	121.1 (3)
N2—C31—C29	133.1 (3)	C79—C81—C70	106.4 (3)
N2—C31—C20	120.8 (3)	C87—C82—C83	121.0 (3)
C29—C31—C20	106.1 (3)	C87—C82—N4	117.8 (3)
C37—C32—C33	121.1 (3)	C83—C82—N4	121.2 (3)
C37—C32—N2	118.2 (3)	C84—C83—C82	117.8 (3)
C33—C32—N2	120.5 (3)	C84—C83—C88	120.0 (3)
C34—C33—C32	117.5 (3)	C82—C83—C88	122.1 (3)
C34—C33—C38	120.1 (3)	C85—C84—C83	122.9 (3)
C32—C33—C38	122.4 (3)	C85—C84—H84	118.5
C35—C34—C33	123.5 (3)	C83—C84—H84	118.5
C35—C34—H34	118.2	C86—C85—C84	117.1 (3)
C33—C34—H34	118.2	C86—C85—C94	121.4 (3)
C34—C35—C36	117.0 (3)	C84—C85—C94	121.5 (3)
C34—C35—C44	121.6 (3)	C85—C86—C87	122.1 (3)
C36—C35—C44	121.4 (3)	C85—C86—H86	118.9
C37—C36—C35	122.5 (3)	C87—C86—H86	118.9
C37—C36—H36	118.8	C82—C87—C86	118.9 (3)
C35—C36—H36	118.8	C82—C87—C100	121.3 (3)
C36—C37—C32	118.1 (3)	C86—C87—C100	119.8 (3)
C36—C37—C50	121.0 (3)	C93—C88—C89	117.3 (3)
C32—C37—C50	120.9 (3)	C93—C88—C83	120.7 (3)
C43—C38—C39	117.3 (3)	C89—C88—C83	122.0 (3)
C43—C38—C33	121.3 (3)	C90—C89—C88	121.5 (3)
C39—C38—C33	121.3 (3)	C90—C89—H89	119.2
C40—C39—C38	120.2 (3)	C88—C89—H89	119.2
C40—C39—H39	119.9	C91—C90—C89	119.4 (4)
C38—C39—H39	119.9	C91—C90—H90	120.3
C41—C40—C39	121.1 (3)	C89—C90—H90	120.3
C41—C40—H40	119.4	C92—C91—C90	120.2 (4)
C39—C40—H40	119.4	C92—C91—H91	119.9
C42—C41—C40	118.9 (4)	C90—C91—H91	119.9
C42—C41—H41	120.6	C91—C92—C93	119.4 (4)
C40—C41—H41	120.6	C91—C92—H92	120.3
C41—C42—C43	120.5 (4)	C93—C92—H92	120.3
C41—C42—H42	119.8	C88—C93—C92	122.2 (3)
C43—C42—H42	119.8	C88—C93—H93	118.9

C38—C43—C42	122.0 (3)	C92—C93—H93	118.9
C38—C43—H43	119.0	C95—C94—C99	119.0 (3)
C42—C43—H43	119.0	C95—C94—C85	120.8 (3)
C49—C44—C45	119.5 (3)	C99—C94—C85	120.1 (3)
C49—C44—C35	121.1 (4)	C94—C95—C96	121.5 (3)
C45—C44—C35	119.4 (4)	C94—C95—H95	119.3
C44—C45—C46	120.9 (4)	C96—C95—H95	119.3
C44—C45—H45	119.5	C97—C96—C95	119.3 (4)
C46—C45—H45	119.5	C97—C96—H96	120.3
C47—C46—C45	119.3 (5)	C95—C96—H96	120.3
C47—C46—H46	120.3	C98—C97—C96	119.4 (4)
C45—C46—H46	120.3	C98—C97—H97	120.3
C46—C47—C48	120.6 (5)	C96—C97—H97	120.3
C46—C47—H47	119.7	C97—C98—C99	120.4 (4)
C48—C47—H47	119.7	C97—C98—H98	119.8
C47—C48—C49	118.2 (5)	C99—C98—H98	119.8
C47—C48—H48	120.9	C94—C99—C98	120.4 (4)
C49—C48—H48	120.9	C94—C99—H99	119.8
C44—C49—C48	121.5 (4)	C98—C99—H99	119.8
C44—C49—H49	119.3	C87—C100—H10A	109.5
C48—C49—H49	119.3	C87—C100—H10B	109.5
C37—C50—H50A	109.5	H10A—C100—H10B	109.5
C37—C50—H50B	109.5	C87—C100—H10C	109.5
H50A—C50—H50B	109.5	H10A—C100—H10C	109.5
C37—C50—H50C	109.5	H10B—C100—H10C	109.5
H50A—C50—H50C	109.5	C20—N1—C1	120.5 (3)
H50B—C50—H50C	109.5	C31—N2—C32	119.7 (3)
C52—C51—C56	120.9 (3)	C70—N3—C51	121.9 (3)
C52—C51—N3	118.2 (3)	C81—N4—C82	118.8 (3)

C12—C7—C8—C9	0.0	C53—C54—C55—C56	−0.5 (4)
C4—C7—C8—C9	−177.5 (2)	C57—C54—C55—C56	179.8 (3)
C7—C8—C9—C10	0.0	C54—C55—C56—C51	0.2 (4)
C8—C9—C10—C11	0.0	C54—C55—C56—C63	179.9 (3)
C9—C10—C11—C12	0.0	C52—C51—C56—C55	0.4 (4)
C10—C11—C12—C7	0.0	N3—C51—C56—C55	176.2 (3)
C8—C7—C12—C11	0.0	C52—C51—C56—C63	−179.4 (3)
C4—C7—C12—C11	177.5 (2)	N3—C51—C56—C63	−3.6 (4)
C6—C1—C2—C3	1.4 (5)	C55—C54—C57—C58	−147.3 (3)
N1—C1—C2—C3	177.3 (3)	C53—C54—C57—C58	33.1 (5)
C6—C1—C2—C19	179.7 (3)	C55—C54—C57—C62	30.7 (4)
N1—C1—C2—C19	−4.4 (5)	C53—C54—C57—C62	−148.9 (3)
C1—C2—C3—C4	2.2 (5)	C62—C57—C58—C59	−1.7 (5)
C19—C2—C3—C4	−176.1 (3)	C54—C57—C58—C59	176.3 (3)
C2—C3—C4—C5	−3.0 (5)	C57—C58—C59—C60	0.8 (6)
C2—C3—C4—C7	176.1 (3)	C58—C59—C60—C61	0.8 (6)
C8—C7—C4—C5	161.4 (2)	C59—C60—C61—C62	−1.4 (5)
C12—C7—C4—C5	−16.1 (4)	C60—C61—C62—C57	0.6 (5)

C8—C7—C4—C3	−17.6 (3)	C58—C57—C62—C61	1.0 (5)
C12—C7—C4—C3	164.9 (2)	C54—C57—C62—C61	−177.1 (3)
C3—C4—C5—C6	0.2 (4)	C55—C56—C63—C64	41.2 (4)
C7—C4—C5—C6	−178.8 (3)	C51—C56—C63—C64	−139.1 (3)
C2—C1—C6—C5	−4.0 (4)	C55—C56—C63—C68	−133.8 (3)
N1—C1—C6—C5	−179.7 (3)	C51—C56—C63—C68	46.0 (4)
C2—C1—C6—C13	176.1 (3)	C68—C63—C64—C65	0.1 (5)
N1—C1—C6—C13	0.4 (4)	C56—C63—C64—C65	−175.1 (3)
C4—C5—C6—C1	3.2 (4)	C63—C64—C65—C66	0.5 (6)
C4—C5—C6—C13	−176.9 (3)	C64—C65—C66—C67	−1.3 (7)
C1—C6—C13—C14	139.5 (3)	C65—C66—C67—C68	1.5 (7)
C5—C6—C13—C14	−40.3 (4)	C64—C63—C68—C67	0.2 (5)
C1—C6—C13—C18	−42.4 (4)	C56—C63—C68—C67	175.3 (3)
C5—C6—C13—C18	137.7 (3)	C66—C67—C68—C63	−1.0 (6)
C18—C13—C14—C15	−0.5 (5)	N3—C70—C71—C72	−6.8 (6)
C6—C13—C14—C15	177.6 (3)	C81—C70—C71—C72	177.2 (3)
C13—C14—C15—C16	1.6 (5)	N3—C70—C71—C80	173.5 (3)
C14—C15—C16—C17	−2.1 (6)	C81—C70—C71—C80	−2.4 (3)
C15—C16—C17—C18	1.5 (6)	C80—C71—C72—C73	−0.1 (5)
C16—C17—C18—C13	−0.5 (6)	C70—C71—C72—C73	−179.7 (3)
C14—C13—C18—C17	0.0 (5)	C71—C72—C73—C74	−0.6 (5)
C6—C13—C18—C17	−178.1 (3)	C72—C73—C74—C75	0.3 (6)
N1—C20—C21—C22	−4.0 (6)	C73—C74—C75—C80	0.5 (5)
C31—C20—C21—C22	175.6 (3)	C73—C74—C75—C76	179.1 (4)
N1—C20—C21—C30	179.6 (3)	C80—C75—C76—C77	−0.1 (5)
C31—C20—C21—C30	−0.9 (3)	C74—C75—C76—C77	−178.6 (4)
C30—C21—C22—C23	−1.1 (5)	C75—C76—C77—C78	0.0 (6)
C20—C21—C22—C23	−177.2 (3)	C76—C77—C78—C79	0.3 (5)
C21—C22—C23—C24	−0.6 (6)	C77—C78—C79—C80	−0.6 (5)
C22—C23—C24—C25	0.8 (6)	C77—C78—C79—C81	178.6 (3)
C23—C24—C25—C30	0.7 (5)	C74—C75—C80—C79	178.5 (3)
C23—C24—C25—C26	179.1 (4)	C76—C75—C80—C79	−0.3 (5)
C24—C25—C26—C27	−177.8 (4)	C74—C75—C80—C71	−1.2 (5)
C30—C25—C26—C27	0.6 (5)	C76—C75—C80—C71	−179.9 (3)
C25—C26—C27—C28	0.7 (6)	C78—C79—C80—C75	0.6 (5)
C26—C27—C28—C29	−1.3 (6)	C81—C79—C80—C75	−178.8 (3)
C27—C28—C29—C30	0.5 (5)	C78—C79—C80—C71	−179.7 (3)
C27—C28—C29—C31	−179.7 (3)	C81—C79—C80—C71	0.9 (3)
C28—C29—C30—C21	−179.4 (3)	C72—C71—C80—C75	1.0 (5)
C31—C29—C30—C21	0.8 (4)	C70—C71—C80—C75	−179.3 (3)
C28—C29—C30—C25	0.9 (5)	C72—C71—C80—C79	−178.7 (3)
C31—C29—C30—C25	−179.0 (3)	C70—C71—C80—C79	1.0 (3)
C22—C21—C30—C29	−177.0 (3)	C78—C79—C81—N4	−3.9 (6)
C20—C21—C30—C29	0.1 (4)	C80—C79—C81—N4	175.4 (3)
C22—C21—C30—C25	2.7 (5)	C78—C79—C81—C70	178.4 (3)
C20—C21—C30—C25	179.9 (3)	C80—C79—C81—C70	−2.3 (3)
C24—C25—C30—C29	177.2 (3)	N3—C70—C81—N4	8.3 (4)
C26—C25—C30—C29	−1.4 (5)	C71—C70—C81—N4	−175.1 (3)

C24—C25—C30—C21	−2.5 (5)	N3—C70—C81—C79	−173.6 (3)
C26—C25—C30—C21	178.9 (3)	C71—C70—C81—C79	3.0 (3)
C28—C29—C31—N2	−0.5 (6)	C87—C82—C83—C84	3.2 (4)
C30—C29—C31—N2	179.3 (3)	N4—C82—C83—C84	−178.7 (3)
C28—C29—C31—C20	178.9 (3)	C87—C82—C83—C88	−179.3 (3)
C30—C29—C31—C20	−1.3 (3)	N4—C82—C83—C88	−1.2 (4)
N1—C20—C31—N2	0.4 (4)	C82—C83—C84—C85	−1.1 (4)
C21—C20—C31—N2	−179.1 (3)	C88—C83—C84—C85	−178.6 (3)
N1—C20—C31—C29	−179.0 (3)	C83—C84—C85—C86	−1.5 (4)
C21—C20—C31—C29	1.4 (3)	C83—C84—C85—C94	178.3 (3)
C37—C32—C33—C34	−4.4 (5)	C84—C85—C86—C87	2.1 (5)
N2—C32—C33—C34	−179.9 (3)	C94—C85—C86—C87	−177.6 (3)
C37—C32—C33—C38	175.4 (3)	C83—C82—C87—C86	−2.7 (5)
N2—C32—C33—C38	−0.1 (5)	N4—C82—C87—C86	179.2 (3)
C32—C33—C34—C35	0.2 (5)	C83—C82—C87—C100	179.9 (3)
C38—C33—C34—C35	−179.6 (3)	N4—C82—C87—C100	1.7 (5)
C33—C34—C35—C36	3.7 (5)	C85—C86—C87—C82	−0.1 (5)
C33—C34—C35—C44	−176.5 (3)	C85—C86—C87—C100	177.4 (3)
C34—C35—C36—C37	−3.8 (5)	C84—C83—C88—C93	40.2 (4)
C44—C35—C36—C37	176.4 (3)	C82—C83—C88—C93	−137.1 (3)
C35—C36—C37—C32	−0.1 (5)	C84—C83—C88—C89	−137.4 (3)
C35—C36—C37—C50	−178.7 (3)	C82—C83—C88—C89	45.2 (4)
C33—C32—C37—C36	4.3 (5)	C93—C88—C89—C90	−0.2 (5)
N2—C32—C37—C36	179.9 (3)	C83—C88—C89—C90	177.6 (3)
C33—C32—C37—C50	−177.1 (3)	C88—C89—C90—C91	0.1 (5)
N2—C32—C37—C50	−1.5 (5)	C89—C90—C91—C92	−0.4 (6)
C34—C33—C38—C43	−42.3 (4)	C90—C91—C92—C93	0.8 (6)
C32—C33—C38—C43	137.9 (3)	C89—C88—C93—C92	0.5 (5)
C34—C33—C38—C39	134.9 (3)	C83—C88—C93—C92	−177.2 (3)
C32—C33—C38—C39	−44.9 (4)	C91—C92—C93—C88	−0.9 (5)
C43—C38—C39—C40	0.7 (5)	C86—C85—C94—C95	145.4 (3)
C33—C38—C39—C40	−176.6 (3)	C84—C85—C94—C95	−34.4 (4)
C38—C39—C40—C41	0.3 (5)	C86—C85—C94—C99	−31.5 (4)
C39—C40—C41—C42	−0.6 (5)	C84—C85—C94—C99	148.8 (3)
C40—C41—C42—C43	−0.2 (5)	C99—C94—C95—C96	−1.9 (5)
C39—C38—C43—C42	−1.4 (5)	C85—C94—C95—C96	−178.8 (3)
C33—C38—C43—C42	175.9 (3)	C94—C95—C96—C97	1.2 (5)
C41—C42—C43—C38	1.2 (5)	C95—C96—C97—C98	0.1 (6)
C34—C35—C44—C49	−147.9 (3)	C96—C97—C98—C99	−0.8 (6)
C36—C35—C44—C49	32.0 (5)	C95—C94—C99—C98	1.2 (5)
C34—C35—C44—C45	32.9 (5)	C85—C94—C99—C98	178.1 (3)
C36—C35—C44—C45	−147.3 (4)	C97—C98—C99—C94	0.2 (5)
C49—C44—C45—C46	−1.2 (6)	C21—C20—N1—C1	−2.1 (5)
C35—C44—C45—C46	178.1 (3)	C31—C20—N1—C1	178.5 (3)
C44—C45—C46—C47	1.1 (6)	C2—C1—N1—C20	103.1 (3)
C45—C46—C47—C48	−1.2 (7)	C6—C1—N1—C20	−81.1 (4)
C46—C47—C48—C49	1.3 (7)	C29—C31—N2—C32	−4.2 (5)
C45—C44—C49—C48	1.3 (6)	C20—C31—N2—C32	176.4 (3)

C35—C44—C49—C48	−178.0 (3)	C37—C32—N2—C31	100.5 (4)
C47—C48—C49—C44	−1.4 (6)	C33—C32—N2—C31	−83.9 (4)
C56—C51—C52—C53	−0.5 (4)	C71—C70—N3—C51	2.7 (5)
N3—C51—C52—C53	−176.4 (3)	C81—C70—N3—C51	178.3 (3)
C56—C51—C52—C69	178.2 (3)	C52—C51—N3—C70	−97.4 (3)
N3—C51—C52—C69	2.3 (4)	C56—C51—N3—C70	86.7 (4)
C51—C52—C53—C54	0.1 (5)	C79—C81—N4—C82	2.4 (5)
C69—C52—C53—C54	−178.6 (3)	C70—C81—N4—C82	179.9 (3)
C52—C53—C54—C55	0.4 (5)	C87—C82—N4—C81	−95.6 (3)
C52—C53—C54—C57	−180.0 (3)	C83—C82—N4—C81	86.3 (4)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of ring C1–C6 in molecule *A*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···N3^{i}	0.93	2.60	3.517 (6)	168
C92—H92···*Cg*2^{ii}	0.93	2.95	3.789 (5)	151

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