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(4*Z*,5*E*,9*E*,10*Z*)-N^4,N^5,N^9,N^{10}-Tetrakis(2,6-diisopropylphenyl)pyrene-4,5,9,10-tetraimine

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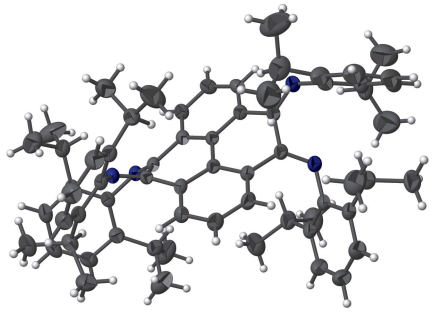
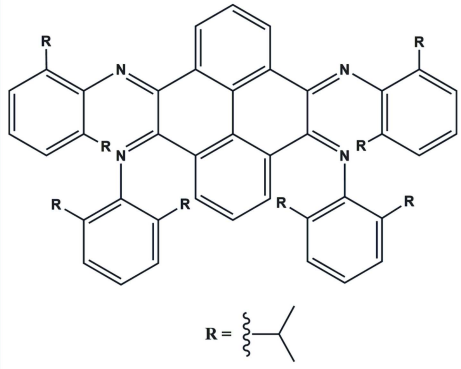
Structural data: full structural data are available from iucrdata.iucr.org

The title molecule, $C_{64}H_{74}N_4$, consists of a pyrene backbone with imine moieties located on the 4-, 5-, 9-, and 10-positions of the ring system. The aryl groups on these imines are sterically bulky 2,6-diisopropylphenyl units. As a consequence, the backbone itself is twisted, with an angle of 15.29 (6)° between the mean planes (r.m.s. deviations = 0.006 and 0.009 Å) of the phenyl units. The N=C—C=N units are significantly twisted and feature torsion angles of −48.8 (2) and −46.3 (3)°. The non-planarity of the backbone and short C—N distances [ranging from 1.281 (2) to 1.285 (2) Å] indicate the lack of conjugation in the molecule and double-bond nature of the imines. Weak intramolecular and intermolecular C—H···π interactions are observed.

3D view



Chemical scheme



Structure description

Imine–metal complexes have been widely studied as ligands in organometallic catalysts (Xing *et al.*, 2014; Song *et al.*, 2013; Zhao *et al.*, 2015; Gao *et al.*, 2012). In addition, the syntheses and structures of a variety of phenanthrene-based imine complexes have been reported (Cherkasov *et al.*, 2012) and the crystal structure of the asymmetric (*Z*)-*N*-{(*E*)-10-[(2,6-diisopropylphenyl)imino]-9,10-dihydrophenanthren-9-ylidene}-2,6-dimethylaniline complex has been reported by Li *et al.* (2012). Our lab has been active in the study of bis-imino acenaphenthene-based complexes due to the unique redox characteristics of the ligand. Herein is reported the structure of a sterically hindered diimine molecule based on the pyrene backbone (Figs. 1 and 2). The structure shows a twisted rather than planar backbone, indicating the lack of conjugation across the ring system. The imines adopt an *E*–*Z*, *E*–*Z* conformation with relatively large torsion angles across the N—C—C—N fragments.

There are three weak intramolecular C—H···π interactions observed (Table 1), one between the pyrene backbone and phenyl imine substituents, and two between isopropyl

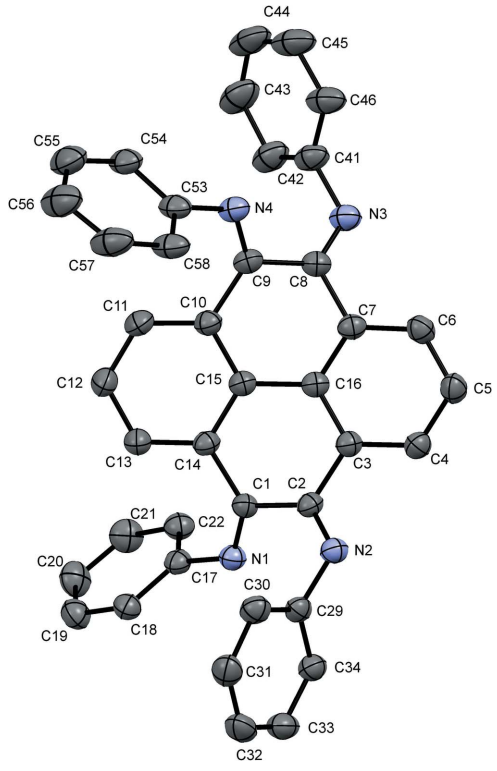


Figure 1
The molecular structure of the title compound, shown with 50% probability ellipsoids for non-H atoms. For clarity, the H atoms and the isopropyl groups have been removed.

H atoms and neighboring phenyl substituents. In the crystal, a weak C—H$\cdots\pi$ interaction links inversion-related molecules.

Synthesis and crystallization

Pyrene-4,5,9,10-tetraone was synthesized according to literature procedures (Hu *et al.*, 2005). 2,6-Diisopropylaniline was purchased from Sigma Aldrich and purified by distillation under vacuum. $TiCl_4$ was purchased as a 1 *M* solution in DCM and used as received. The tetraone (52.3 mg; 0.2 mmol) and aniline (0.4375 g; 2.5 mmol) were added to a Schlenk flask and pumped under vacuum for one h. To this, 100 ml of dry toluene was added *via* cannulation. To this, 0.4 ml of 1.0 *M* $TiCl_4$ was added *via* syringe. This exothermic reaction was allowed to continue overnight, followed by careful neutralization of excess $TiCl_4$ by hydrolysis with 20 mL of deionized water. This mixture was washed three times with toluene (50 mL) to extract the product. The resulting organic solution was then washed three times with water (50 mL) and the aqueous layers discarded. The resulting organic solution was then dried over magnesium sulfate and excess toluene solvent removed *in vacuo*, leaving a crude product with excess aniline oil. The oil was removed by additional washing in acetonitrile and crystals were produced by slow evaporation of a saturated solution of the product in dichloromethane (yield: 62.5 mg; 0.07 mmol; 35%).

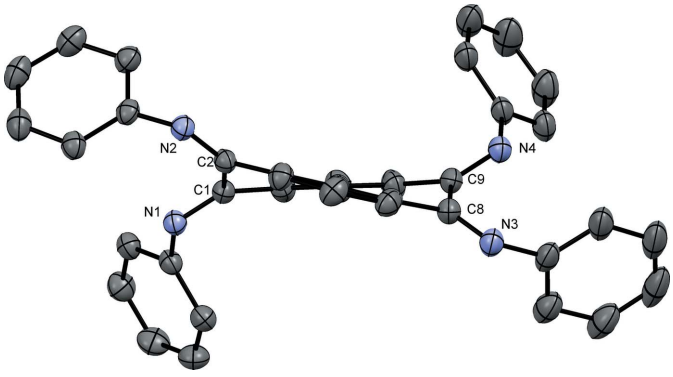


Figure 2
Alternative view of the title compound, shown with 50% probability ellipsoids for non-H atoms. For clarity, the H atoms and the isopropyl groups have been removed.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C29–C34, C53–C58 and C41–C46 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots Cg1^{i}$	0.93	2.61	3.327 (2)	134
C11—H11$\cdots Cg2$	0.93	2.93	3.469 (2)	118
C23—H23$\cdots Cg1$	0.98	2.73	3.613 (2)	149
C59—H59$\cdots Cg3$	0.98	2.64	3.571 (2)	158

Symmetry code: (i) $-x, -y, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{64}H_{74}N_4$
M_r	899.27
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	223
a, b, c (Å)	14.527 (4), 10.721 (3), 36.004 (10)
β (°)	97.459 (3)
V (Å^3)	5560 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.06
Crystal size (mm)	0.30 × 0.28 × 0.25
Data collection	
Diffractometer	Rigaku SCXMini
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 2001)
T_{min}, T_{max}	0.875, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	55003, 12755, 9576
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.175, 1.06
No. of reflections	12755
No. of parameters	630
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.26

Computer programs: *CrystalClear* (Rigaku, 2008), *SIR97* (Altomare *et al.*, 1999), *SHELXL2015* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2006), *publCIF* (Westrip, 2010) and *WinGX* (Farrugia, 2012).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160484 [doi:10.1107/S2414314616004843]

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Crystal data

$C_{64}H_{74}N_4$
M_r = 899.27
Monoclinic, $P2_1/n$
a = 14.527 (4) Å
b = 10.721 (3) Å
c = 36.004 (10) Å
β = 97.459 (3)°
V = 5560 (3) Å^3
Z = 4
$F(000)$ = 1944
D_x = 1.074 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 12747 reflections
θ = 1.5–31.8°
μ = 0.06 mm^{-1}
T = 223 K
Chip, red
0.30 × 0.28 × 0.25 mm

Data collection

Rigaku SCXMini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
dtprofit.ref scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 2001)
T_{min} = 0.875, T_{max} = 1.000
55003 measured reflections
12755 independent reflections
9576 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 1.5°
h = −18→18
k = −13→13
l = −46→46

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.175
S = 1.06
12755 reflections
630 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
$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 1.9541P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: *SHELXL2015* (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0022 (4)

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}
C1	0.49832 (11)	0.51934 (15)	0.12003 (4)	0.0277 (3)
C2	0.48073 (11)	0.50049 (16)	0.07841 (5)	0.0284 (3)
C3	0.41788 (11)	0.39395 (16)	0.06713 (4)	0.0287 (3)
C4	0.42666 (12)	0.32550 (17)	0.03492 (5)	0.0339 (4)
H4	0.4710	0.3481	0.0197	0.041*
C5	0.36908 (13)	0.22307 (17)	0.02536 (5)	0.0371 (4)
H5	0.3760	0.1766	0.0041	0.045*
C6	0.30148 (13)	0.19055 (17)	0.04757 (5)	0.0352 (4)
H6	0.2634	0.1222	0.0411	0.042*
C7	0.29020 (11)	0.25977 (16)	0.07959 (5)	0.0305 (4)
C8	0.21651 (11)	0.22783 (16)	0.10310 (5)	0.0318 (4)
C9	0.18629 (11)	0.33671 (16)	0.12526 (5)	0.0313 (4)
C10	0.26231 (11)	0.41920 (16)	0.14303 (5)	0.0314 (4)
C11	0.25731 (12)	0.48532 (18)	0.17612 (5)	0.0378 (4)
H11	0.2056	0.4761	0.1886	0.045*
C12	0.32859 (13)	0.56458 (19)	0.19062 (5)	0.0398 (4)
H12	0.3239	0.6087	0.2125	0.048*
C13	0.40675 (12)	0.57830 (17)	0.17261 (5)	0.0346 (4)
H13	0.4540	0.6321	0.1824	0.042*
C14	0.41470 (11)	0.51166 (16)	0.13989 (5)	0.0289 (3)
C15	0.34171 (11)	0.43211 (15)	0.12454 (4)	0.0282 (3)
C16	0.34973 (11)	0.36087 (15)	0.09003 (4)	0.0279 (3)
C17	0.61232 (11)	0.52544 (16)	0.17381 (5)	0.0305 (4)
C18	0.65262 (12)	0.63428 (17)	0.19052 (5)	0.0336 (4)
C19	0.68610 (13)	0.63059 (19)	0.22873 (5)	0.0410 (4)
H19	0.7121	0.7019	0.2405	0.049*
C20	0.68105 (14)	0.5223 (2)	0.24931 (5)	0.0458 (5)
H20	0.7036	0.5212	0.2747	0.055*
C21	0.64232 (14)	0.4153 (2)	0.23205 (5)	0.0433 (5)
H21	0.6394	0.3432	0.2462	0.052*
C22	0.60764 (12)	0.41313 (17)	0.19406 (5)	0.0351 (4)
C23	0.65868 (13)	0.75380 (18)	0.16818 (5)	0.0390 (4)
H23	0.6312	0.7373	0.1423	0.047*
C24	0.60355 (17)	0.8601 (2)	0.18337 (7)	0.0585 (6)
H24A	0.5399	0.8354	0.1828	0.088*

H24B	0.6069	0.9330	0.1681	0.088*
H24C	0.6294	0.8785	0.2087	0.088*
C25	0.75956 (15)	0.7927 (2)	0.16737 (6)	0.0518 (5)
H25A	0.7888	0.8069	0.1925	0.078*
H25B	0.7614	0.8680	0.1531	0.078*
H25C	0.7919	0.7278	0.1560	0.078*
C26	0.56948 (13)	0.29313 (18)	0.17513 (6)	0.0395 (4)
H26	0.5170	0.3162	0.1565	0.047*
C27	0.64194 (18)	0.2308 (2)	0.15424 (8)	0.0658 (7)
H27A	0.6646	0.2900	0.1376	0.099*
H27B	0.6143	0.1615	0.1401	0.099*
H27C	0.6926	0.2018	0.1719	0.099*
C28	0.5334 (2)	0.1993 (3)	0.20199 (8)	0.0752 (8)
H28A	0.5844	0.1679	0.2190	0.113*
H28B	0.5033	0.1314	0.1879	0.113*
H28C	0.4898	0.2399	0.2159	0.113*
C29	0.57577 (12)	0.66810 (16)	0.06262 (5)	0.0313 (4)
C30	0.53572 (13)	0.78722 (17)	0.06514 (5)	0.0380 (4)
C31	0.59601 (15)	0.89013 (19)	0.06964 (6)	0.0439 (5)
H31	0.5713	0.9696	0.0714	0.053*
C32	0.69093 (15)	0.87621 (19)	0.07145 (6)	0.0462 (5)
H32	0.7294	0.9458	0.0741	0.055*
C33	0.72863 (14)	0.7581 (2)	0.06927 (5)	0.0439 (5)
H33	0.7927	0.7494	0.0708	0.053*
C34	0.67281 (12)	0.65180 (18)	0.06483 (5)	0.0355 (4)
C35	0.71522 (14)	0.5223 (2)	0.06276 (6)	0.0447 (5)
H35	0.6664	0.4611	0.0654	0.054*
C36	0.7492 (2)	0.4998 (3)	0.02474 (7)	0.0849 (10)
H36A	0.6970	0.4998	0.0054	0.127*
H36B	0.7802	0.4206	0.0250	0.127*
H36C	0.7915	0.5648	0.0200	0.127*
C37	0.79362 (16)	0.5003 (3)	0.09455 (7)	0.0621 (6)
H37A	0.8439	0.5563	0.0919	0.093*
H37B	0.8150	0.4157	0.0936	0.093*
H37C	0.7713	0.5150	0.1181	0.093*
C38	0.43110 (14)	0.8061 (2)	0.06214 (7)	0.0497 (5)
H38	0.4031	0.7251	0.0665	0.060*
C39	0.40294 (19)	0.8972 (3)	0.09120 (8)	0.0752 (8)
H39A	0.4269	0.8688	0.1158	0.113*
H39B	0.3365	0.9019	0.0890	0.113*
H39C	0.4278	0.9783	0.0870	0.113*
C40	0.39214 (18)	0.8485 (3)	0.02283 (8)	0.0814 (9)
H40A	0.4213	0.9252	0.0171	0.122*
H40B	0.3264	0.8611	0.0216	0.122*
H40C	0.4042	0.7858	0.0050	0.122*
C41	0.11614 (14)	0.07997 (17)	0.12561 (6)	0.0431 (5)
C42	0.14708 (16)	0.0448 (2)	0.16259 (7)	0.0508 (5)
C43	0.07912 (18)	0.0067 (2)	0.18480 (8)	0.0623 (7)

H43	0.0971	−0.0157	0.2096	0.075*
C44	−0.01338 (18)	0.0019 (2)	0.17045 (9)	0.0668 (8)
H44	−0.0574	−0.0205	0.1858	0.080*
C45	−0.04085 (17)	0.0303 (2)	0.13339 (9)	0.0645 (7)
H45	−0.1033	0.0234	0.1238	0.077*
C46	0.02251 (14)	0.0690 (2)	0.10983 (7)	0.0529 (6)
C47	0.24984 (17)	0.0398 (2)	0.17811 (7)	0.0598 (6)
H47	0.2847	0.0760	0.1592	0.072*
C48	0.2740 (2)	0.1124 (4)	0.21356 (10)	0.0971 (11)
H48A	0.2531	0.1969	0.2097	0.146*
H48B	0.3400	0.1114	0.2205	0.146*
H48C	0.2442	0.0753	0.2332	0.146*
C49	0.2818 (3)	−0.0966 (3)	0.18420 (11)	0.1078 (13)
H49A	0.3479	−0.0988	0.1911	0.162*
H49B	0.2655	−0.1429	0.1615	0.162*
H49C	0.2519	−0.1329	0.2039	0.162*
C50	−0.00859 (16)	0.0977 (3)	0.06890 (8)	0.0675 (7)
H50	0.0453	0.1274	0.0576	0.081*
C51	−0.0829 (2)	0.1989 (3)	0.06418 (12)	0.1088 (13)
H51A	−0.1371	0.1702	0.0743	0.163*
H51B	−0.0988	0.2174	0.0380	0.163*
H51C	−0.0596	0.2728	0.0772	0.163*
C52	−0.0476 (3)	−0.0191 (3)	0.04723 (10)	0.0965 (10)
H52A	0.0019	−0.0769	0.0451	0.145*
H52B	−0.0758	0.0048	0.0227	0.145*
H52C	−0.0933	−0.0580	0.0605	0.145*
C53	0.06311 (12)	0.46672 (17)	0.13839 (6)	0.0380 (4)
C54	0.01332 (13)	0.45625 (19)	0.16917 (6)	0.0422 (4)
C55	−0.01907 (15)	0.5656 (2)	0.18385 (8)	0.0575 (6)
H55	−0.0503	0.5616	0.2048	0.069*
C56	−0.00538 (17)	0.6805 (2)	0.16772 (9)	0.0669 (7)
H56	−0.0261	0.7527	0.1783	0.080*
C57	0.03855 (15)	0.6884 (2)	0.13618 (8)	0.0597 (6)
H57	0.0452	0.7659	0.1252	0.072*
C58	0.07356 (13)	0.58199 (19)	0.12018 (6)	0.0449 (5)
C59	−0.00367 (13)	0.33123 (19)	0.18684 (6)	0.0434 (5)
H59	0.0224	0.2662	0.1721	0.052*
C60	0.04326 (18)	0.3211 (3)	0.22711 (7)	0.0658 (7)
H60A	0.1091	0.3306	0.2276	0.099*
H60B	0.0301	0.2410	0.2371	0.099*
H60C	0.0201	0.3855	0.2420	0.099*
C61	−0.10869 (15)	0.3066 (2)	0.18514 (7)	0.0587 (6)
H61A	−0.1358	0.3687	0.1996	0.088*
H61B	−0.1184	0.2254	0.1952	0.088*
H61C	−0.1373	0.3104	0.1596	0.088*
C62	0.11638 (14)	0.5925 (2)	0.08387 (7)	0.0504 (5)
H62	0.1510	0.5153	0.0811	0.061*
C63	0.04002 (19)	0.6008 (3)	0.05049 (8)	0.0797 (8)

H63A	0.0014	0.5279	0.0499	0.120*
H63B	0.0677	0.6058	0.0277	0.120*
H63C	0.0030	0.6738	0.0529	0.120*
C64	0.18473 (19)	0.7004 (3)	0.08374 (9)	0.0724 (8)
H64A	0.1525	0.7779	0.0855	0.109*
H64B	0.2124	0.6987	0.0609	0.109*
H64C	0.2323	0.6925	0.1047	0.109*
N1	0.58376 (9)	0.52720 (13)	0.13434 (4)	0.0301 (3)
N2	0.51647 (10)	0.56282 (13)	0.05351 (4)	0.0314 (3)
N3	0.18357 (10)	0.11668 (14)	0.10194 (4)	0.0379 (4)
N4	0.09839 (10)	0.35489 (14)	0.12354 (4)	0.0355 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0269 (8)	0.0274 (8)	0.0290 (8)	−0.0020 (6)	0.0045 (6)	0.0005 (6)
C2	0.0239 (8)	0.0328 (8)	0.0291 (8)	0.0006 (6)	0.0052 (6)	0.0013 (6)
C3	0.0272 (8)	0.0320 (9)	0.0266 (8)	−0.0004 (6)	0.0025 (6)	0.0029 (6)
C4	0.0354 (9)	0.0377 (10)	0.0294 (9)	−0.0043 (7)	0.0071 (7)	0.0006 (7)
C5	0.0465 (10)	0.0352 (9)	0.0304 (9)	−0.0041 (8)	0.0081 (8)	−0.0023 (7)
C6	0.0391 (9)	0.0303 (9)	0.0359 (9)	−0.0053 (7)	0.0035 (7)	−0.0001 (7)
C7	0.0287 (8)	0.0311 (9)	0.0318 (9)	−0.0001 (7)	0.0043 (7)	0.0044 (7)
C8	0.0279 (8)	0.0324 (9)	0.0350 (9)	−0.0025 (7)	0.0039 (7)	0.0022 (7)
C9	0.0279 (8)	0.0325 (9)	0.0343 (9)	−0.0012 (7)	0.0073 (7)	0.0045 (7)
C10	0.0267 (8)	0.0321 (9)	0.0359 (9)	0.0000 (7)	0.0063 (7)	0.0001 (7)
C11	0.0292 (9)	0.0459 (11)	0.0402 (10)	−0.0002 (8)	0.0115 (7)	−0.0034 (8)
C12	0.0361 (9)	0.0484 (11)	0.0359 (10)	0.0000 (8)	0.0090 (8)	−0.0094 (8)
C13	0.0306 (9)	0.0395 (10)	0.0341 (9)	−0.0025 (7)	0.0054 (7)	−0.0052 (7)
C14	0.0243 (8)	0.0343 (9)	0.0281 (8)	0.0005 (6)	0.0035 (6)	0.0026 (7)
C15	0.0262 (8)	0.0293 (8)	0.0291 (8)	0.0003 (6)	0.0041 (6)	0.0028 (6)
C16	0.0262 (8)	0.0285 (8)	0.0288 (8)	0.0006 (6)	0.0025 (6)	0.0037 (6)
C17	0.0241 (8)	0.0376 (9)	0.0297 (8)	0.0004 (7)	0.0031 (6)	0.0000 (7)
C18	0.0290 (8)	0.0381 (9)	0.0330 (9)	−0.0013 (7)	0.0020 (7)	−0.0017 (7)
C19	0.0404 (10)	0.0438 (11)	0.0373 (10)	−0.0033 (8)	−0.0009 (8)	−0.0052 (8)
C20	0.0488 (11)	0.0546 (12)	0.0313 (9)	0.0025 (9)	−0.0048 (8)	0.0014 (9)
C21	0.0451 (11)	0.0452 (11)	0.0382 (10)	0.0032 (9)	−0.0006 (8)	0.0097 (8)
C22	0.0301 (9)	0.0376 (10)	0.0373 (9)	0.0008 (7)	0.0027 (7)	0.0021 (7)
C23	0.0415 (10)	0.0385 (10)	0.0361 (10)	−0.0081 (8)	0.0018 (8)	−0.0013 (8)
C24	0.0597 (14)	0.0387 (11)	0.0781 (16)	0.0006 (10)	0.0125 (12)	0.0065 (11)
C25	0.0497 (12)	0.0643 (14)	0.0414 (11)	−0.0186 (11)	0.0056 (9)	−0.0056 (10)
C26	0.0365 (10)	0.0354 (10)	0.0452 (11)	−0.0004 (8)	−0.0002 (8)	0.0048 (8)
C27	0.0604 (15)	0.0536 (14)	0.0872 (19)	−0.0082 (11)	0.0236 (13)	−0.0212 (13)
C28	0.095 (2)	0.0570 (15)	0.0794 (19)	−0.0236 (14)	0.0319 (16)	−0.0015 (13)
C29	0.0337 (9)	0.0347 (9)	0.0260 (8)	−0.0053 (7)	0.0060 (7)	0.0030 (7)
C30	0.0403 (10)	0.0359 (10)	0.0392 (10)	−0.0028 (8)	0.0101 (8)	0.0045 (8)
C31	0.0550 (12)	0.0354 (10)	0.0432 (11)	−0.0054 (9)	0.0129 (9)	−0.0004 (8)
C32	0.0527 (12)	0.0428 (11)	0.0437 (11)	−0.0188 (9)	0.0090 (9)	−0.0021 (9)
C33	0.0363 (10)	0.0544 (12)	0.0413 (11)	−0.0126 (9)	0.0064 (8)	0.0006 (9)

C34	0.0324 (9)	0.0417 (10)	0.0329 (9)	−0.0041 (8)	0.0068 (7)	0.0004 (7)
C35	0.0343 (10)	0.0482 (12)	0.0518 (12)	0.0001 (8)	0.0063 (8)	0.0006 (9)
C36	0.107 (2)	0.092 (2)	0.0540 (15)	0.0527 (19)	0.0045 (15)	−0.0058 (14)
C37	0.0494 (13)	0.0716 (16)	0.0642 (15)	0.0124 (12)	0.0028 (11)	0.0099 (12)
C38	0.0418 (11)	0.0391 (11)	0.0702 (14)	0.0037 (9)	0.0143 (10)	0.0066 (10)
C39	0.0639 (16)	0.092 (2)	0.0724 (18)	0.0221 (15)	0.0203 (13)	−0.0010 (15)
C40	0.0537 (15)	0.116 (3)	0.0720 (18)	0.0201 (16)	−0.0011 (13)	−0.0130 (17)
C41	0.0406 (10)	0.0294 (9)	0.0630 (13)	−0.0035 (8)	0.0206 (9)	0.0035 (9)
C42	0.0530 (12)	0.0405 (11)	0.0640 (14)	−0.0004 (9)	0.0274 (11)	0.0076 (10)
C43	0.0716 (16)	0.0459 (13)	0.0778 (17)	−0.0033 (11)	0.0415 (14)	0.0100 (11)
C44	0.0644 (15)	0.0380 (12)	0.110 (2)	−0.0085 (11)	0.0553 (16)	−0.0005 (13)
C45	0.0450 (12)	0.0430 (12)	0.111 (2)	−0.0094 (10)	0.0317 (14)	0.0022 (13)
C46	0.0382 (11)	0.0375 (11)	0.0859 (17)	−0.0055 (9)	0.0190 (11)	0.0022 (11)
C47	0.0591 (14)	0.0753 (17)	0.0482 (13)	0.0044 (12)	0.0192 (11)	0.0159 (12)
C48	0.078 (2)	0.104 (3)	0.112 (3)	−0.0106 (19)	0.0232 (19)	−0.031 (2)
C49	0.103 (3)	0.098 (3)	0.113 (3)	0.046 (2)	−0.022 (2)	−0.023 (2)
C50	0.0380 (12)	0.0681 (16)	0.095 (2)	−0.0067 (11)	0.0022 (12)	0.0140 (14)
C51	0.095 (2)	0.079 (2)	0.140 (3)	0.0176 (19)	−0.032 (2)	−0.005 (2)
C52	0.116 (3)	0.074 (2)	0.101 (3)	−0.0035 (19)	0.022 (2)	−0.0123 (18)
C53	0.0244 (8)	0.0344 (9)	0.0555 (11)	−0.0022 (7)	0.0070 (8)	−0.0006 (8)
C54	0.0287 (9)	0.0413 (10)	0.0585 (12)	−0.0031 (8)	0.0131 (8)	−0.0022 (9)
C55	0.0453 (12)	0.0497 (13)	0.0836 (17)	−0.0031 (10)	0.0313 (12)	−0.0075 (12)
C56	0.0530 (14)	0.0407 (12)	0.114 (2)	0.0018 (10)	0.0372 (14)	−0.0095 (13)
C57	0.0443 (12)	0.0361 (11)	0.103 (2)	0.0007 (9)	0.0272 (12)	0.0060 (11)
C58	0.0283 (9)	0.0387 (10)	0.0690 (14)	−0.0016 (8)	0.0117 (9)	0.0054 (9)
C59	0.0388 (10)	0.0439 (11)	0.0500 (11)	−0.0009 (8)	0.0149 (9)	0.0027 (9)
C60	0.0584 (14)	0.0793 (18)	0.0592 (15)	0.0043 (13)	0.0055 (11)	0.0046 (13)
C61	0.0427 (12)	0.0576 (14)	0.0776 (16)	−0.0086 (10)	0.0148 (11)	0.0158 (12)
C62	0.0392 (11)	0.0470 (12)	0.0667 (14)	−0.0006 (9)	0.0128 (10)	0.0155 (10)
C63	0.0599 (16)	0.098 (2)	0.0799 (19)	−0.0061 (15)	0.0019 (14)	0.0099 (17)
C64	0.0633 (16)	0.0670 (17)	0.090 (2)	−0.0177 (13)	0.0231 (14)	0.0145 (14)
N1	0.0270 (7)	0.0328 (7)	0.0302 (7)	−0.0024 (6)	0.0030 (5)	0.0004 (6)
N2	0.0291 (7)	0.0342 (8)	0.0312 (7)	−0.0024 (6)	0.0054 (6)	0.0024 (6)
N3	0.0331 (8)	0.0346 (8)	0.0470 (9)	−0.0040 (6)	0.0094 (7)	0.0022 (7)
N4	0.0291 (7)	0.0343 (8)	0.0443 (9)	−0.0019 (6)	0.0096 (6)	0.0039 (7)

Geometric parameters (Å, º)

C1—N1	1.283 (2)	C36—H36B	0.9600
C1—C14	1.490 (2)	C36—H36C	0.9600
C1—C2	1.501 (2)	C37—H37A	0.9600
C2—N2	1.281 (2)	C37—H37B	0.9600
C2—C3	1.486 (2)	C37—H37C	0.9600
C3—C4	1.392 (2)	C38—C40	1.524 (4)
C3—C16	1.414 (2)	C38—C39	1.526 (3)
C4—C5	1.396 (2)	C38—H38	0.9800
C4—H4	0.9300	C39—H39A	0.9600
C5—C6	1.389 (3)	C39—H39B	0.9600

C5—H5	0.9300	C39—H39C	0.9600
C6—C7	1.398 (2)	C40—H40A	0.9600
C6—H6	0.9300	C40—H40B	0.9600
C7—C16	1.407 (2)	C40—H40C	0.9600
C7—C8	1.488 (2)	C41—C42	1.401 (3)
C8—N3	1.283 (2)	C41—C46	1.409 (3)
C8—C9	1.511 (2)	C41—N3	1.434 (2)
C9—N4	1.285 (2)	C42—C43	1.409 (3)
C9—C10	1.492 (2)	C42—C47	1.525 (3)
C10—C11	1.396 (2)	C43—C44	1.377 (4)
C10—C15	1.412 (2)	C43—H43	0.9300
C11—C12	1.388 (3)	C44—C45	1.376 (4)
C11—H11	0.9300	C44—H44	0.9300
C12—C13	1.386 (2)	C45—C46	1.393 (3)
C12—H12	0.9300	C45—H45	0.9300
C13—C14	1.395 (2)	C46—C50	1.516 (4)
C13—H13	0.9300	C47—C48	1.497 (4)
C14—C15	1.416 (2)	C47—C49	1.541 (4)
C15—C16	1.476 (2)	C47—H47	0.9800
C17—C18	1.405 (2)	C48—H48A	0.9600
C17—C22	1.414 (2)	C48—H48B	0.9600
C17—N1	1.428 (2)	C48—H48C	0.9600
C18—C19	1.399 (3)	C49—H49A	0.9600
C18—C23	1.522 (3)	C49—H49B	0.9600
C19—C20	1.384 (3)	C49—H49C	0.9600
C19—H19	0.9300	C50—C51	1.524 (4)
C20—C21	1.388 (3)	C50—C52	1.544 (4)
C20—H20	0.9300	C50—H50	0.9800
C21—C22	1.395 (3)	C51—H51A	0.9600
C21—H21	0.9300	C51—H51B	0.9600
C22—C26	1.526 (3)	C51—H51C	0.9600
C23—C25	1.528 (3)	C52—H52A	0.9600
C23—C24	1.534 (3)	C52—H52B	0.9600
C23—H23	0.9800	C52—H52C	0.9600
C24—H24A	0.9600	C53—C54	1.404 (3)
C24—H24B	0.9600	C53—C58	1.416 (3)
C24—H24C	0.9600	C53—N4	1.434 (2)
C25—H25A	0.9600	C54—C55	1.393 (3)
C25—H25B	0.9600	C54—C59	1.517 (3)
C25—H25C	0.9600	C55—C56	1.387 (3)
C26—C27	1.525 (3)	C55—H55	0.9300
C26—C28	1.534 (3)	C56—C57	1.376 (4)
C26—H26	0.9800	C56—H56	0.9300
C27—H27A	0.9600	C57—C58	1.403 (3)
C27—H27B	0.9600	C57—H57	0.9300
C27—H27C	0.9600	C58—C62	1.523 (3)
C28—H28A	0.9600	C59—C60	1.524 (3)
C28—H28B	0.9600	C59—C61	1.542 (3)

C28—H28C	0.9600	C59—H59	0.9800
C29—C30	1.411 (3)	C60—H60A	0.9600
C29—C34	1.412 (2)	C60—H60B	0.9600
C29—N2	1.432 (2)	C60—H60C	0.9600
C30—C31	1.405 (3)	C61—H61A	0.9600
C30—C38	1.523 (3)	C61—H61B	0.9600
C31—C32	1.380 (3)	C61—H61C	0.9600
C31—H31	0.9300	C62—C64	1.525 (3)
C32—C33	1.386 (3)	C62—C63	1.529 (4)
C32—H32	0.9300	C62—H62	0.9800
C33—C34	1.395 (3)	C63—H63A	0.9600
C33—H33	0.9300	C63—H63B	0.9600
C34—C35	1.525 (3)	C63—H63C	0.9600
C35—C37	1.524 (3)	C64—H64A	0.9600
C35—C36	1.533 (3)	C64—H64B	0.9600
C35—H35	0.9800	C64—H64C	0.9600
C36—H36A	0.9600		

N1—C1—C14	128.11 (15)	H37A—C37—H37B	109.5
N1—C1—C2	116.12 (14)	C35—C37—H37C	109.5
C14—C1—C2	115.35 (14)	H37A—C37—H37C	109.5
N2—C2—C3	120.00 (15)	H37B—C37—H37C	109.5
N2—C2—C1	126.64 (15)	C30—C38—C40	110.63 (18)
C3—C2—C1	113.30 (13)	C30—C38—C39	113.0 (2)
C4—C3—C16	120.04 (15)	C40—C38—C39	110.2 (2)
C4—C3—C2	120.91 (15)	C30—C38—H38	107.6
C16—C3—C2	119.04 (15)	C40—C38—H38	107.6
C3—C4—C5	120.21 (16)	C39—C38—H38	107.6
C3—C4—H4	119.9	C38—C39—H39A	109.5
C5—C4—H4	119.9	C38—C39—H39B	109.5
C6—C5—C4	120.08 (17)	H39A—C39—H39B	109.5
C6—C5—H5	120.0	C38—C39—H39C	109.5
C4—C5—H5	120.0	H39A—C39—H39C	109.5
C5—C6—C7	120.58 (16)	H39B—C39—H39C	109.5
C5—C6—H6	119.7	C38—C40—H40A	109.5
C7—C6—H6	119.7	C38—C40—H40B	109.5
C6—C7—C16	119.69 (15)	H40A—C40—H40B	109.5
C6—C7—C8	121.11 (15)	C38—C40—H40C	109.5
C16—C7—C8	119.20 (15)	H40A—C40—H40C	109.5
N3—C8—C7	119.21 (16)	H40B—C40—H40C	109.5
N3—C8—C9	127.02 (15)	C42—C41—C46	122.31 (19)
C7—C8—C9	113.73 (14)	C42—C41—N3	118.64 (18)
N4—C9—C10	127.31 (16)	C46—C41—N3	118.8 (2)
N4—C9—C8	116.52 (15)	C41—C42—C43	117.1 (2)
C10—C9—C8	115.76 (14)	C41—C42—C47	122.38 (18)
C11—C10—C15	119.27 (15)	C43—C42—C47	120.4 (2)
C11—C10—C9	123.30 (15)	C44—C43—C42	121.3 (3)
C15—C10—C9	117.41 (15)	C44—C43—H43	119.4

C12—C11—C10	120.86 (16)	C42—C43—H43	119.4
C12—C11—H11	119.6	C45—C44—C43	120.1 (2)
C10—C11—H11	119.6	C45—C44—H44	119.9
C13—C12—C11	120.35 (17)	C43—C44—H44	119.9
C13—C12—H12	119.8	C44—C45—C46	121.7 (2)
C11—C12—H12	119.8	C44—C45—H45	119.2
C12—C13—C14	120.20 (16)	C46—C45—H45	119.2
C12—C13—H13	119.9	C45—C46—C41	117.3 (2)
C14—C13—H13	119.9	C45—C46—C50	121.0 (2)
C13—C14—C15	119.88 (15)	C41—C46—C50	121.68 (19)
C13—C14—C1	122.62 (15)	C48—C47—C42	113.8 (2)
C15—C14—C1	117.50 (15)	C48—C47—C49	109.8 (3)
C10—C15—C14	119.42 (15)	C42—C47—C49	110.3 (2)
C10—C15—C16	120.33 (15)	C48—C47—H47	107.5
C14—C15—C16	120.23 (14)	C42—C47—H47	107.5
C7—C16—C3	119.35 (15)	C49—C47—H47	107.5
C7—C16—C15	120.71 (14)	C47—C48—H48A	109.5
C3—C16—C15	119.94 (15)	C47—C48—H48B	109.5
C18—C17—C22	122.11 (16)	H48A—C48—H48B	109.5
C18—C17—N1	117.78 (15)	C47—C48—H48C	109.5
C22—C17—N1	119.83 (15)	H48A—C48—H48C	109.5
C19—C18—C17	118.03 (17)	H48B—C48—H48C	109.5
C19—C18—C23	120.47 (16)	C47—C49—H49A	109.5
C17—C18—C23	121.50 (15)	C47—C49—H49B	109.5
C20—C19—C18	120.95 (18)	H49A—C49—H49B	109.5
C20—C19—H19	119.5	C47—C49—H49C	109.5
C18—C19—H19	119.5	H49A—C49—H49C	109.5
C19—C20—C21	119.98 (18)	H49B—C49—H49C	109.5
C19—C20—H20	120.0	C46—C50—C51	111.8 (3)
C21—C20—H20	120.0	C46—C50—C52	111.7 (2)
C20—C21—C22	121.77 (18)	C51—C50—C52	108.2 (2)
C20—C21—H21	119.1	C46—C50—H50	108.4
C22—C21—H21	119.1	C51—C50—H50	108.4
C21—C22—C17	117.13 (17)	C52—C50—H50	108.4
C21—C22—C26	121.07 (17)	C50—C51—H51A	109.5
C17—C22—C26	121.77 (16)	C50—C51—H51B	109.5
C18—C23—C25	111.20 (16)	H51A—C51—H51B	109.5
C18—C23—C24	111.62 (16)	C50—C51—H51C	109.5
C25—C23—C24	110.51 (17)	H51A—C51—H51C	109.5
C18—C23—H23	107.8	H51B—C51—H51C	109.5
C25—C23—H23	107.8	C50—C52—H52A	109.5
C24—C23—H23	107.8	C50—C52—H52B	109.5
C23—C24—H24A	109.5	H52A—C52—H52B	109.5
C23—C24—H24B	109.5	C50—C52—H52C	109.5
H24A—C24—H24B	109.5	H52A—C52—H52C	109.5
C23—C24—H24C	109.5	H52B—C52—H52C	109.5
H24A—C24—H24C	109.5	C54—C53—C58	122.16 (18)
H24B—C24—H24C	109.5	C54—C53—N4	118.22 (16)

C23—C25—H25A	109.5	C58—C53—N4	119.47 (17)
C23—C25—H25B	109.5	C55—C54—C53	117.78 (19)
H25A—C25—H25B	109.5	C55—C54—C59	120.21 (18)
C23—C25—H25C	109.5	C53—C54—C59	121.99 (17)
H25A—C25—H25C	109.5	C56—C55—C54	121.0 (2)
H25B—C25—H25C	109.5	C56—C55—H55	119.5
C27—C26—C22	110.83 (16)	C54—C55—H55	119.5
C27—C26—C28	109.8 (2)	C57—C56—C55	120.5 (2)
C22—C26—C28	113.91 (18)	C57—C56—H56	119.7
C27—C26—H26	107.3	C55—C56—H56	119.7
C22—C26—H26	107.3	C56—C57—C58	121.4 (2)
C28—C26—H26	107.3	C56—C57—H57	119.3
C26—C27—H27A	109.5	C58—C57—H57	119.3
C26—C27—H27B	109.5	C57—C58—C53	116.94 (19)
H27A—C27—H27B	109.5	C57—C58—C62	120.17 (19)
C26—C27—H27C	109.5	C53—C58—C62	122.84 (18)
H27A—C27—H27C	109.5	C54—C59—C60	112.61 (19)
H27B—C27—H27C	109.5	C54—C59—C61	110.40 (17)
C26—C28—H28A	109.5	C60—C59—C61	110.10 (18)
C26—C28—H28B	109.5	C54—C59—H59	107.9
H28A—C28—H28B	109.5	C60—C59—H59	107.9
C26—C28—H28C	109.5	C61—C59—H59	107.9
H28A—C28—H28C	109.5	C59—C60—H60A	109.5
H28B—C28—H28C	109.5	C59—C60—H60B	109.5
C30—C29—C34	121.68 (16)	H60A—C60—H60B	109.5
C30—C29—N2	119.16 (15)	C59—C60—H60C	109.5
C34—C29—N2	118.80 (16)	H60A—C60—H60C	109.5
C31—C30—C29	117.52 (17)	H60B—C60—H60C	109.5
C31—C30—C38	120.37 (18)	C59—C61—H61A	109.5
C29—C30—C38	122.10 (17)	C59—C61—H61B	109.5
C32—C31—C30	121.65 (19)	H61A—C61—H61B	109.5
C32—C31—H31	119.2	C59—C61—H61C	109.5
C30—C31—H31	119.2	H61A—C61—H61C	109.5
C31—C32—C33	119.72 (18)	H61B—C61—H61C	109.5
C31—C32—H32	120.1	C58—C62—C64	113.4 (2)
C33—C32—H32	120.1	C58—C62—C63	110.09 (18)
C32—C33—C34	121.63 (18)	C64—C62—C63	111.1 (2)
C32—C33—H33	119.2	C58—C62—H62	107.3
C34—C33—H33	119.2	C64—C62—H62	107.3
C33—C34—C29	117.80 (18)	C63—C62—H62	107.3
C33—C34—C35	121.10 (17)	C62—C63—H63A	109.5
C29—C34—C35	121.10 (16)	C62—C63—H63B	109.5
C37—C35—C34	111.79 (18)	H63A—C63—H63B	109.5
C37—C35—C36	110.53 (19)	C62—C63—H63C	109.5
C34—C35—C36	111.44 (18)	H63A—C63—H63C	109.5
C37—C35—H35	107.6	H63B—C63—H63C	109.5
C34—C35—H35	107.6	C62—C64—H64A	109.5
C36—C35—H35	107.6	C62—C64—H64B	109.5

C35—C36—H36A	109.5	H64A—C64—H64B	109.5
C35—C36—H36B	109.5	C62—C64—H64C	109.5
H36A—C36—H36B	109.5	H64A—C64—H64C	109.5
C35—C36—H36C	109.5	H64B—C64—H64C	109.5
H36A—C36—H36C	109.5	C1—N1—C17	122.66 (14)
H36B—C36—H36C	109.5	C2—N2—C29	122.49 (14)
C35—C37—H37A	109.5	C8—N3—C41	121.07 (16)
C35—C37—H37B	109.5	C9—N4—C53	120.64 (15)

N1—C1—C2—N2	−48.8 (2)	C34—C29—C30—C38	178.96 (17)
C14—C1—C2—N2	138.04 (17)	N2—C29—C30—C38	5.9 (3)
N1—C1—C2—C3	128.57 (16)	C29—C30—C31—C32	0.2 (3)
C14—C1—C2—C3	−44.60 (19)	C38—C30—C31—C32	−178.28 (19)
N2—C2—C3—C4	28.3 (2)	C30—C31—C32—C33	−0.8 (3)
C1—C2—C3—C4	−149.28 (16)	C31—C32—C33—C34	0.7 (3)
N2—C2—C3—C16	−153.03 (16)	C32—C33—C34—C29	−0.1 (3)
C1—C2—C3—C16	29.4 (2)	C32—C33—C34—C35	−179.54 (18)
C16—C3—C4—C5	−0.8 (3)	C30—C29—C34—C33	−0.6 (3)
C2—C3—C4—C5	177.87 (16)	N2—C29—C34—C33	172.46 (16)
C3—C4—C5—C6	1.3 (3)	C30—C29—C34—C35	178.89 (17)
C4—C5—C6—C7	0.1 (3)	N2—C29—C34—C35	−8.1 (2)
C5—C6—C7—C16	−2.0 (3)	C33—C34—C35—C37	49.3 (3)
C5—C6—C7—C8	178.46 (16)	C29—C34—C35—C37	−130.14 (19)
C6—C7—C8—N3	22.8 (3)	C33—C34—C35—C36	−74.9 (3)
C16—C7—C8—N3	−156.74 (16)	C29—C34—C35—C36	105.6 (2)
C6—C7—C8—C9	−155.04 (16)	C31—C30—C38—C40	79.0 (3)
C16—C7—C8—C9	25.4 (2)	C29—C30—C38—C40	−99.4 (2)
N3—C8—C9—N4	−46.3 (3)	C31—C30—C38—C39	−45.1 (3)
C7—C8—C9—N4	131.38 (16)	C29—C30—C38—C39	136.5 (2)
N3—C8—C9—C10	140.50 (18)	C46—C41—C42—C43	−5.0 (3)
C7—C8—C9—C10	−41.8 (2)	N3—C41—C42—C43	−178.65 (19)
N4—C9—C10—C11	37.2 (3)	C46—C41—C42—C47	171.5 (2)
C8—C9—C10—C11	−150.49 (17)	N3—C41—C42—C47	−2.2 (3)
N4—C9—C10—C15	−141.28 (18)	C41—C42—C43—C44	1.3 (3)
C8—C9—C10—C15	31.1 (2)	C47—C42—C43—C44	−175.3 (2)
C15—C10—C11—C12	1.0 (3)	C42—C43—C44—C45	2.4 (4)
C9—C10—C11—C12	−177.43 (17)	C43—C44—C45—C46	−2.5 (4)
C10—C11—C12—C13	−0.8 (3)	C44—C45—C46—C41	−1.0 (3)
C11—C12—C13—C14	−0.5 (3)	C44—C45—C46—C50	178.9 (2)
C12—C13—C14—C15	1.5 (3)	C42—C41—C46—C45	4.9 (3)
C12—C13—C14—C1	−177.92 (17)	N3—C41—C46—C45	178.52 (19)
N1—C1—C14—C13	37.8 (3)	C42—C41—C46—C50	−175.1 (2)
C2—C1—C14—C13	−149.99 (16)	N3—C41—C46—C50	−1.4 (3)
N1—C1—C14—C15	−141.67 (18)	C41—C42—C47—C48	127.0 (3)
C2—C1—C14—C15	30.5 (2)	C43—C42—C47—C48	−56.6 (3)
C11—C10—C15—C14	0.1 (2)	C41—C42—C47—C49	−109.0 (3)
C9—C10—C15—C14	178.56 (15)	C43—C42—C47—C49	67.3 (3)
C11—C10—C15—C16	178.48 (16)	C45—C46—C50—C51	57.7 (3)

C9—C10—C15—C16	−3.0 (2)	C41—C46—C50—C51	−122.4 (3)
C13—C14—C15—C10	−1.3 (2)	C45—C46—C50—C52	−63.7 (3)
C1—C14—C15—C10	178.19 (15)	C41—C46—C50—C52	116.2 (3)
C13—C14—C15—C16	−179.73 (15)	C58—C53—C54—C55	−5.8 (3)
C1—C14—C15—C16	−0.2 (2)	N4—C53—C54—C55	178.76 (19)
C6—C7—C16—C3	2.4 (2)	C58—C53—C54—C59	175.47 (18)
C8—C7—C16—C3	−177.99 (15)	N4—C53—C54—C59	0.0 (3)
C6—C7—C16—C15	−177.48 (15)	C53—C54—C55—C56	2.2 (3)
C8—C7—C16—C15	2.1 (2)	C59—C54—C55—C56	−179.0 (2)
C4—C3—C16—C7	−1.1 (2)	C54—C55—C56—C57	1.7 (4)
C2—C3—C16—C7	−179.76 (15)	C55—C56—C57—C58	−2.2 (4)
C4—C3—C16—C15	178.85 (15)	C56—C57—C58—C53	−1.2 (3)
C2—C3—C16—C15	0.2 (2)	C56—C57—C58—C62	176.1 (2)
C10—C15—C16—C7	−14.3 (2)	C54—C53—C58—C57	5.3 (3)
C14—C15—C16—C7	164.07 (15)	N4—C53—C58—C57	−179.36 (18)
C10—C15—C16—C3	165.74 (15)	C54—C53—C58—C62	−171.93 (18)
C14—C15—C16—C3	−15.8 (2)	N4—C53—C58—C62	3.4 (3)
C22—C17—C18—C19	−2.1 (3)	C55—C54—C59—C60	−62.9 (3)
N1—C17—C18—C19	−176.02 (15)	C53—C54—C59—C60	115.8 (2)
C22—C17—C18—C23	178.90 (16)	C55—C54—C59—C61	60.6 (3)
N1—C17—C18—C23	5.0 (2)	C53—C54—C59—C61	−120.7 (2)
C17—C18—C19—C20	1.1 (3)	C57—C58—C62—C64	46.7 (3)
C23—C18—C19—C20	−179.91 (18)	C53—C58—C62—C64	−136.2 (2)
C18—C19—C20—C21	0.0 (3)	C57—C58—C62—C63	−78.5 (3)
C19—C20—C21—C22	−0.1 (3)	C53—C58—C62—C63	98.6 (2)
C20—C21—C22—C17	−0.9 (3)	C14—C1—N1—C17	2.3 (3)
C20—C21—C22—C26	177.08 (18)	C2—C1—N1—C17	−169.90 (15)
C18—C17—C22—C21	2.0 (3)	C18—C17—N1—C1	−113.95 (19)
N1—C17—C22—C21	175.80 (16)	C22—C17—N1—C1	72.0 (2)
C18—C17—C22—C26	−175.96 (16)	C3—C2—N2—C29	178.53 (15)
N1—C17—C22—C26	−2.2 (2)	C1—C2—N2—C29	−4.3 (3)
C19—C18—C23—C25	62.7 (2)	C30—C29—N2—C2	−86.7 (2)
C17—C18—C23—C25	−118.32 (19)	C34—C29—N2—C2	100.1 (2)
C19—C18—C23—C24	−61.2 (2)	C7—C8—N3—C41	176.58 (16)
C17—C18—C23—C24	117.8 (2)	C9—C8—N3—C41	−5.9 (3)
C21—C22—C26—C27	−98.8 (2)	C42—C41—N3—C8	−82.3 (2)
C17—C22—C26—C27	79.0 (2)	C46—C41—N3—C8	103.8 (2)
C21—C22—C26—C28	25.5 (3)	C10—C9—N4—C53	2.6 (3)
C17—C22—C26—C28	−156.6 (2)	C8—C9—N4—C53	−169.70 (15)
C34—C29—C30—C31	0.5 (3)	C54—C53—N4—C9	−114.88 (19)
N2—C29—C30—C31	−172.49 (16)	C58—C53—N4—C9	69.6 (2)

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg3 are the centroids of the C29–C34, C53–C58 and C41–C46 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*1^{i}	0.93	2.61	3.327 (2)	134
C11—H11···*Cg*2	0.93	2.93	3.469 (2)	118

C23—H23···*Cg*1	0.98	2.73	3.613 (2)	149
C59—H59···*Cg*3	0.98	2.64	3.571 (2)	158

Symmetry code: (i) −*x*, −*y*, −*z*.