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2,7,10,13-Tetra-*tert*-butyl-*N*-phenylacenaphtho-[1,2-*j*]fluoranthene-4,5-dicarboximide

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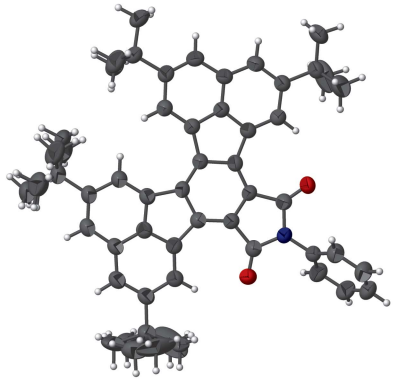
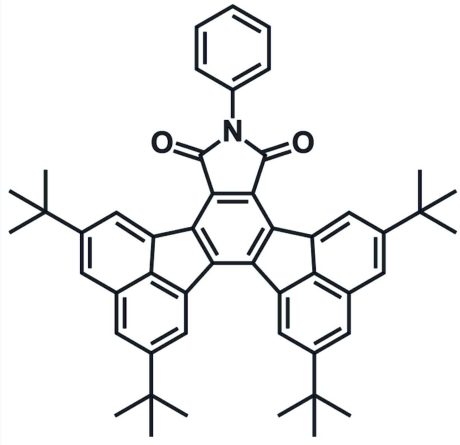
Structural data: full structural data are available from iucrdata.iucr.org

In the molecule of the title compound, $C_{50}H_{49}NO_2$, the acenaphtho[1,2-*j*]-fluoranthene-4,5-dicarboximide framework has an approximately planar structure [maximum deviation = 0.124 (3) Å] and subtends a dihedral angle of 62.94 (8)° with the pendant phenyl group. Two of the *tert*-butyl groups are disordered over two sets of sites, with occupancy ratios of 0.506 (8):0.494 (8) and 0.669 (17):0.331 (17). An intermolecular short contact between a methyl group and the aromatic ring occurs in the crystal structure.

3D view



Chemical scheme



Structure description

Imides having a polycyclic aromatic hydrocarbon skeleton are of interest as electronic devices. For example, naphthalenedimide and perylenedimide have been investigated (Weil *et al.*, 2010). Very recently, we reported a new imide preparation by the Diels–Alder reaction of diacenaphtho[1,2-*j*]thiophene (Watson *et al.*, 2000) and maleic anhydride, followed by treatment with amines to afford acenaphtho[1,2-*j*]fluoranthene-4,5-dicarboximide derivatives (Ozoe *et al.*, 2014). To improve the solubility, the introduction of four *tert*-butyl groups onto the above ring was carried out. As a part of our ongoing research on the imide derivatives, we represent here the crystal structure of the title compound.

In the molecular structure of the title compound (Fig. 1), the acenaphtho[1,2-*j*]fluoranthene-4,5-dicarboximide framework has a nearly planar structure with a maximum deviation of 0.124 (3) Å for C12. The dihedral angle between the imide ring and the peripheral phenyl ring is 62.94 (8)°.

In the crystal (Fig. 2), the molecules adopt a herringbone-like arrangement without π–π stacking due to the steric hindrance of *tert*-butyl groups. There are no classical hydrogen bonds although there are intermolecular short contacts between C21 and H45B^{i} of 2.87 (3) Å [symmetry code: (i) $1-x, -\frac{1}{2}+y, \frac{3}{2}-z$].

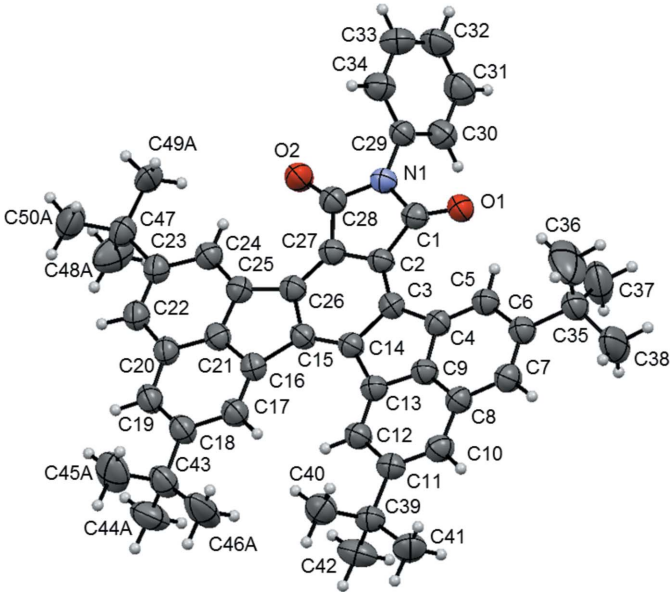


Figure 1
The molecular structure of the title compound, showing the atom-numbering with 50% probability displacement ellipsoids. Only the major occupancy disorder components are shown for clarity.

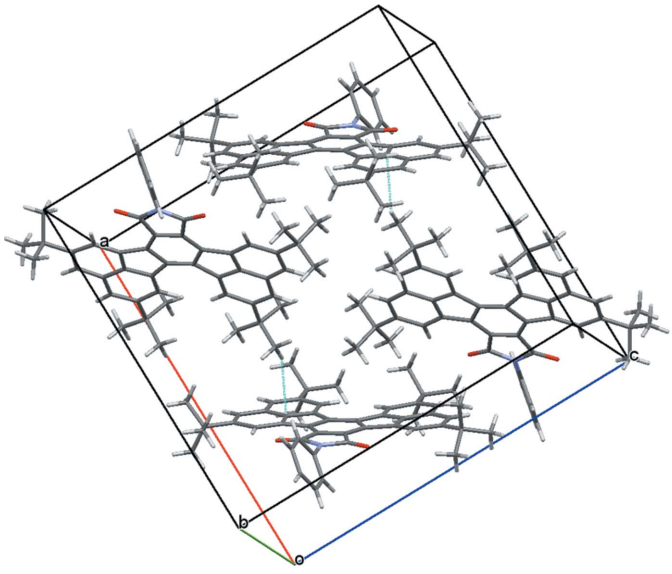


Figure 2
The crystal packing of the title compound. Only the major occupancy disorder components are shown for clarity. Intermolecular short contacts are drawn as blue lines.

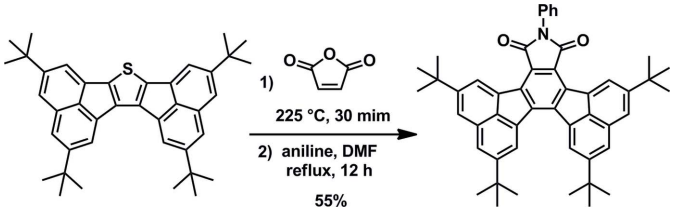


Figure 3
Reaction scheme for the synthesis of the title compound.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{50}H_{49}NO_2$
M_r	695.9
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	223
a, b, c (Å)	19.155 (3), 10.5762 (14), 19.495 (3)
β (°)	92.382 (3)
V (Å^3)	3946.0 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.50 × 0.45 × 0.18
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36876, 9011, 4306
R_{int}	0.082
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.077, 0.243, 1.06
No. of reflections	9011
No. of parameters	534
No. of restraints	60
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.25

Computer programs: *PROCESS-AUTO* (Rigaku, 1998), *SIR2004* (Burla *et al.*, 2005), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012).

Synthesis and crystallization

The Diels–Alder reaction of 2,5,9,12-tetra(*tert*-butyl)diacenaphtho[1,2-*b*:1′,2′-*d*]thiophene (Watson *et al.*, 2000) and maleic anhydride at 225°C for 30 min under neat conditions provided an anhydride, which was then heated with aniline at reflux in dimethylformamide for 12 h (Fig. 3). After cooling, the title compound was obtained as stable yellow crystals in 55% yield over the two steps. ^{1}H -NMR ($CDCl_3$, 500 MHz) δ 9.57 (*s*, 2H),9.05 (*s*, 2H), 8.05 (*s*, 2H), 8.01 (*s*, 2H), 7.63–7.62 (*m*, 4H), 7.52–7.49 (*m*,1H), 1.68 (*s*, 18H), 1.57 (*s*, 18H). MS (EI) *m*/*z* 695 (M^+,100), 680 (12), 333 (75).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. Two *tert*-butyl groups are each disordered over two sets of sites; the site occupancy factors are 0.506 (8) for C44*A*–C46*A* and 0.494 (8) for C44*B*–C46*B*, and 0.669 (17) for C48*A*–C50*A* and 0.331 (17) for C48*B*–C50*B*.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160473 [doi:10.1107/S2414314616004739]

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Crystal data

$C_{50}H_{49}NO_2$
M_r = 695.9
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 19.155 (3) Å
b = 10.5762 (14) Å
c = 19.495 (3) Å
β = 92.382 (3)°
V = 3946.0 (10) Å^3
Z = 4
$F(000)$ = 1488
D_x = 1.171 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10293 reflections
θ = 3–27.4°
μ = 0.07 mm^{-1}
T = 223 K
Prism, yellow
0.50 × 0.45 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed x-ray tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
φ and ω scans
36876 measured reflections
9011 independent reflections
4306 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −24→24
k = −13→13
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.243
S = 1.06
9011 reflections
534 parameters
60 restraints
0 constraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0978P)^2 + 1.0477P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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. To refine the structure, the *SHELX* commands, such as DELU and SADI, were used because two *tert*-butyl groups were disordered over two positions. All the H atoms were positioned geometrically and refined using a riding model.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.13806 (16)	0.0838 (3)	0.80828 (15)	0.0526 (7)	
C2	0.18062 (15)	0.2011 (2)	0.80595 (14)	0.0494 (7)	
C3	0.18331 (14)	0.3038 (3)	0.84956 (14)	0.0509 (7)	
C4	0.15047 (15)	0.3296 (3)	0.91487 (14)	0.0518 (7)	
C5	0.10657 (16)	0.2646 (3)	0.95600 (15)	0.0551 (7)	
H5	0.0911	0.1833	0.9431	0.066*	
C6	0.08416 (16)	0.3193 (3)	1.01825 (15)	0.0565 (8)	
C7	0.10950 (16)	0.4367 (3)	1.03773 (15)	0.0601 (8)	
H7	0.0955	0.4721	1.0792	0.072*	
C8	0.15568 (16)	0.5050 (3)	0.99720 (14)	0.0547 (7)	
C9	0.17466 (15)	0.4498 (3)	0.93602 (14)	0.0522 (7)	
C10	0.18541 (16)	0.6257 (3)	1.01245 (15)	0.0583 (8)	
H10	0.1753	0.6662	1.0538	0.07*	
C11	0.22873 (16)	0.6841 (3)	0.96766 (15)	0.0548 (7)	
C12	0.24549 (16)	0.6228 (3)	0.90557 (15)	0.0558 (7)	
H12	0.2747	0.6639	0.8751	0.067*	
C13	0.21992 (15)	0.5050 (3)	0.88923 (14)	0.0516 (7)	
C14	0.22796 (15)	0.4107 (3)	0.83327 (14)	0.0501 (7)	
C15	0.26736 (14)	0.4054 (3)	0.77527 (14)	0.0497 (7)	
C16	0.31842 (14)	0.4932 (3)	0.74463 (14)	0.0508 (7)	
C17	0.34844 (16)	0.6078 (3)	0.76063 (15)	0.0581 (8)	
H17	0.3354	0.6501	0.8005	0.07*	
C18	0.39867 (16)	0.6642 (3)	0.71856 (15)	0.0590 (8)	
C19	0.41857 (15)	0.6022 (3)	0.66032 (15)	0.0580 (8)	
H19	0.4518	0.6397	0.6326	0.07*	
C20	0.39002 (15)	0.4833 (3)	0.64136 (14)	0.0535 (7)	
C21	0.34122 (15)	0.4334 (3)	0.68469 (14)	0.0514 (7)	
C22	0.40672 (16)	0.4094 (3)	0.58431 (15)	0.0592 (8)	
H22	0.4395	0.4405	0.554	0.071*	
C23	0.37641 (16)	0.2922 (3)	0.57127 (15)	0.0570 (8)	
C24	0.32698 (16)	0.2448 (3)	0.61681 (15)	0.0579 (8)	
H24	0.3059	0.1657	0.6084	0.07*	
C25	0.30968 (15)	0.3147 (3)	0.67363 (15)	0.0522 (7)	
C26	0.26357 (15)	0.2958 (3)	0.73085 (14)	0.0519 (7)	
C27	0.22046 (15)	0.1962 (3)	0.74767 (14)	0.0527 (7)	
C28	0.20711 (16)	0.0730 (3)	0.71275 (15)	0.0564 (7)	
C29	0.12609 (16)	−0.1075 (3)	0.73321 (15)	0.0538 (7)	
C30	0.05538 (17)	−0.1131 (3)	0.71880 (16)	0.0650 (9)	
H30	0.0279	−0.0399	0.7222	0.078*	
C31	0.0247 (2)	−0.2257 (4)	0.69935 (18)	0.0770 (10)	
H31	−0.0237	−0.2296	0.6897	0.092*	
C32	0.0646 (2)	−0.3319 (3)	0.69411 (19)	0.0815 (11)	
H32	0.0436	−0.4087	0.6805	0.098*	
C33	0.1350 (2)	−0.3271 (3)	0.70859 (19)	0.0814 (11)	
H33	0.1621	−0.4008	0.7053	0.098*	

C34	0.16656 (19)	−0.2143 (3)	0.72803 (18)	0.0713 (9)	
H34	0.215	−0.2107	0.7376	0.086*	
C35	0.03577 (18)	0.2437 (3)	1.06289 (16)	0.0660 (9)	
C36	0.0768 (3)	0.1391 (5)	1.0968 (3)	0.142 (2)	
H36A	0.0988	0.0888	1.0621	0.213*	
H36B	0.1125	0.1746	1.1279	0.213*	
H36C	0.0459	0.086	1.1223	0.213*	
C37	−0.0240 (2)	0.1860 (5)	1.0184 (2)	0.1108 (15)	
H37A	−0.051	0.2532	0.9962	0.166*	
H37B	−0.0049	0.1317	0.9838	0.166*	
H37C	−0.054	0.1368	1.0471	0.166*	
C38	0.0006 (3)	0.3247 (4)	1.1149 (2)	0.1224 (18)	
H38A	−0.0256	0.3915	1.0914	0.184*	
H38B	−0.031	0.273	1.1406	0.184*	
H38C	0.0356	0.3617	1.1461	0.184*	
C39	0.26024 (16)	0.8157 (3)	0.98251 (16)	0.0593 (8)	
C40	0.34018 (17)	0.8035 (3)	0.98656 (19)	0.0777 (10)	
H40A	0.3559	0.7684	0.9439	0.117*	
H40B	0.3609	0.8863	0.994	0.117*	
H40C	0.3542	0.7481	1.0243	0.117*	
C41	0.2368 (2)	0.8709 (3)	1.04987 (18)	0.0803 (11)	
H41A	0.2512	0.8151	1.0874	0.121*	
H41B	0.258	0.9534	1.0571	0.121*	
H41C	0.1864	0.8792	1.0481	0.121*	
C42	0.2369 (2)	0.9054 (3)	0.9243 (2)	0.0848 (11)	
H42A	0.2514	0.8717	0.8809	0.127*	
H42B	0.1864	0.9137	0.9231	0.127*	
H42C	0.2581	0.9878	0.932	0.127*	
C43	0.43054 (17)	0.7933 (3)	0.73791 (16)	0.0719 (10)	
C44A	0.4078 (5)	0.8843 (6)	0.6781 (4)	0.097 (3)	0.506 (8)
H44A	0.4223	0.8495	0.6349	0.146*	0.506 (8)
H44B	0.3573	0.8938	0.6766	0.146*	0.506 (8)
H44C	0.4295	0.9663	0.6856	0.146*	0.506 (8)
C45A	0.5101 (3)	0.7829 (9)	0.7374 (5)	0.104 (4)	0.506 (8)
H45A	0.5234	0.7467	0.6942	0.156*	0.506 (8)
H45B	0.5306	0.8663	0.7429	0.156*	0.506 (8)
H45C	0.5266	0.729	0.7749	0.156*	0.506 (8)
C46A	0.4076 (5)	0.8490 (8)	0.8041 (4)	0.116 (5)	0.506 (8)
H46A	0.357	0.8545	0.803	0.175*	0.506 (8)
H46B	0.4235	0.7956	0.842	0.175*	0.506 (8)
H46C	0.4275	0.9329	0.81	0.175*	0.506 (8)
C44B	0.3721 (4)	0.8919 (7)	0.7425 (6)	0.117 (4)	0.494 (8)
H44D	0.3358	0.8593	0.771	0.175*	0.494 (8)
H44E	0.391	0.9691	0.7625	0.175*	0.494 (8)
H44F	0.3524	0.9094	0.6968	0.175*	0.494 (8)
C45B	0.4872 (4)	0.8431 (9)	0.6937 (4)	0.099 (4)	0.494 (8)
H45D	0.524	0.7805	0.691	0.148*	0.494 (8)
H45E	0.4677	0.8606	0.6479	0.148*	0.494 (8)

H45F	0.5064	0.9203	0.7137	0.148*	0.494 (8)
C46B	0.4629 (5)	0.7759 (10)	0.8120 (4)	0.120 (4)	0.494 (8)
H46D	0.4275	0.7439	0.8417	0.179*	0.494 (8)
H46E	0.5013	0.7164	0.8112	0.179*	0.494 (8)
H46F	0.4799	0.8567	0.8293	0.179*	0.494 (8)
C47	0.39577 (15)	0.2151 (3)	0.50786 (16)	0.0650 (9)	
C48A	0.3656 (5)	0.2781 (9)	0.4436 (4)	0.098 (3)	0.669 (17)
H48A	0.3153	0.2853	0.4464	0.147*	0.669 (17)
H48B	0.3858	0.3617	0.4393	0.147*	0.669 (17)
H48C	0.3764	0.2277	0.4038	0.147*	0.669 (17)
C49A	0.3670 (4)	0.0805 (6)	0.5102 (4)	0.079 (3)	0.669 (17)
H49A	0.3857	0.0382	0.5511	0.119*	0.669 (17)
H49B	0.3165	0.0833	0.5111	0.119*	0.669 (17)
H49C	0.3807	0.0346	0.4698	0.119*	0.669 (17)
C50A	0.4745 (3)	0.2045 (9)	0.5027 (6)	0.095 (3)	0.669 (17)
H50A	0.4943	0.1642	0.5438	0.142*	0.669 (17)
H50B	0.485	0.1543	0.4629	0.142*	0.669 (17)
H50C	0.4944	0.2883	0.4983	0.142*	0.669 (17)
C48B	0.4588 (13)	0.275 (3)	0.4776 (14)	0.198 (18)	0.331 (17)
H48D	0.4492	0.363	0.4675	0.298*	0.331 (17)
H48E	0.4984	0.2686	0.5102	0.298*	0.331 (17)
H48F	0.4696	0.2309	0.4357	0.298*	0.331 (17)
C49B	0.3336 (12)	0.227 (3)	0.4581 (13)	0.168 (15)	0.331 (17)
H49D	0.3251	0.3157	0.448	0.252*	0.331 (17)
H49E	0.3429	0.1824	0.4161	0.252*	0.331 (17)
H49F	0.2927	0.191	0.4784	0.252*	0.331 (17)
C50B	0.409 (2)	0.0784 (12)	0.5240 (13)	0.218 (18)	0.331 (17)
H50D	0.3682	0.0414	0.5434	0.327*	0.331 (17)
H50E	0.4199	0.0338	0.4822	0.327*	0.331 (17)
H50F	0.4487	0.0715	0.5568	0.327*	0.331 (17)
N1	0.15753 (12)	0.0106 (2)	0.75189 (12)	0.0543 (6)	
O1	0.09504 (10)	0.05126 (18)	0.84835 (10)	0.0586 (5)	
O2	0.23169 (12)	0.0291 (2)	0.66200 (11)	0.0686 (6)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0579 (18)	0.0469 (17)	0.0531 (17)	0.0005 (14)	0.0048 (15)	0.0011 (14)
C2	0.0566 (17)	0.0405 (15)	0.0513 (16)	−0.0050 (13)	0.0050 (13)	−0.0031 (13)
C3	0.0506 (16)	0.0475 (16)	0.0552 (16)	−0.0021 (13)	0.0076 (13)	0.0008 (14)
C4	0.0543 (17)	0.0509 (17)	0.0506 (16)	−0.0028 (14)	0.0074 (14)	−0.0036 (14)
C5	0.0603 (18)	0.0499 (17)	0.0556 (17)	−0.0053 (14)	0.0082 (14)	−0.0047 (14)
C6	0.0633 (19)	0.0526 (18)	0.0542 (17)	−0.0045 (15)	0.0114 (15)	−0.0010 (14)
C7	0.072 (2)	0.0584 (19)	0.0508 (16)	−0.0023 (16)	0.0136 (15)	−0.0039 (15)
C8	0.0625 (18)	0.0509 (17)	0.0515 (16)	−0.0003 (14)	0.0107 (14)	−0.0042 (14)
C9	0.0597 (18)	0.0464 (16)	0.0509 (16)	−0.0047 (14)	0.0061 (14)	−0.0044 (14)
C10	0.069 (2)	0.0533 (18)	0.0530 (17)	−0.0002 (15)	0.0070 (15)	−0.0070 (14)
C11	0.0584 (18)	0.0468 (17)	0.0594 (17)	−0.0019 (14)	0.0038 (15)	−0.0016 (14)

C12	0.0629 (19)	0.0491 (17)	0.0558 (17)	−0.0064 (14)	0.0086 (15)	−0.0025 (14)
C13	0.0566 (17)	0.0459 (16)	0.0527 (16)	−0.0023 (13)	0.0064 (14)	−0.0036 (14)
C14	0.0555 (17)	0.0455 (16)	0.0497 (15)	−0.0033 (13)	0.0062 (13)	−0.0007 (13)
C15	0.0515 (16)	0.0457 (16)	0.0519 (16)	−0.0063 (13)	0.0038 (13)	0.0014 (13)
C16	0.0494 (16)	0.0534 (17)	0.0499 (16)	−0.0026 (14)	0.0043 (13)	0.0013 (14)
C17	0.0596 (18)	0.0565 (18)	0.0585 (18)	−0.0089 (15)	0.0081 (15)	−0.0039 (15)
C18	0.0591 (18)	0.0581 (19)	0.0600 (18)	−0.0116 (15)	0.0068 (15)	0.0014 (15)
C19	0.0556 (18)	0.0594 (19)	0.0597 (18)	−0.0074 (15)	0.0100 (15)	0.0059 (16)
C20	0.0511 (17)	0.0572 (18)	0.0527 (16)	−0.0012 (14)	0.0090 (14)	0.0034 (14)
C21	0.0511 (16)	0.0528 (17)	0.0502 (16)	−0.0015 (14)	0.0016 (13)	0.0027 (14)
C22	0.0575 (18)	0.062 (2)	0.0588 (18)	0.0003 (15)	0.0123 (15)	0.0040 (16)
C23	0.0554 (18)	0.0608 (19)	0.0554 (17)	0.0001 (15)	0.0100 (14)	0.0014 (15)
C24	0.0634 (19)	0.0538 (18)	0.0571 (17)	−0.0024 (15)	0.0086 (15)	−0.0028 (15)
C25	0.0499 (16)	0.0509 (17)	0.0560 (17)	0.0000 (14)	0.0037 (13)	−0.0014 (14)
C26	0.0535 (17)	0.0506 (17)	0.0517 (16)	−0.0037 (14)	0.0049 (14)	−0.0026 (14)
C27	0.0594 (18)	0.0465 (17)	0.0525 (16)	−0.0033 (14)	0.0066 (14)	−0.0032 (14)
C28	0.0580 (18)	0.0539 (18)	0.0578 (18)	−0.0050 (15)	0.0070 (15)	−0.0027 (15)
C29	0.0619 (19)	0.0470 (17)	0.0531 (16)	−0.0067 (15)	0.0107 (14)	−0.0019 (14)
C30	0.063 (2)	0.059 (2)	0.073 (2)	−0.0064 (16)	0.0035 (17)	0.0001 (17)
C31	0.073 (2)	0.076 (2)	0.082 (2)	−0.023 (2)	0.0037 (19)	−0.010 (2)
C32	0.101 (3)	0.056 (2)	0.090 (3)	−0.024 (2)	0.020 (2)	−0.0182 (19)
C33	0.094 (3)	0.051 (2)	0.100 (3)	0.0001 (19)	0.015 (2)	−0.0119 (19)
C34	0.072 (2)	0.056 (2)	0.086 (2)	−0.0024 (17)	0.0043 (18)	−0.0076 (18)
C35	0.077 (2)	0.059 (2)	0.0634 (19)	−0.0109 (17)	0.0210 (17)	−0.0002 (16)
C36	0.133 (4)	0.131 (4)	0.164 (5)	0.007 (3)	0.042 (4)	0.087 (4)
C37	0.094 (3)	0.132 (4)	0.109 (3)	−0.041 (3)	0.040 (3)	−0.021 (3)
C38	0.164 (4)	0.095 (3)	0.115 (3)	−0.036 (3)	0.091 (3)	−0.021 (3)
C39	0.066 (2)	0.0483 (18)	0.0645 (18)	−0.0062 (15)	0.0067 (15)	−0.0082 (15)
C40	0.067 (2)	0.073 (2)	0.093 (3)	−0.0135 (18)	0.0037 (19)	−0.019 (2)
C41	0.087 (3)	0.063 (2)	0.092 (3)	−0.0127 (19)	0.016 (2)	−0.0286 (19)
C42	0.105 (3)	0.050 (2)	0.099 (3)	−0.0102 (19)	−0.006 (2)	0.0023 (19)
C43	0.076 (2)	0.069 (2)	0.071 (2)	−0.0269 (19)	0.0115 (18)	−0.0057 (18)
C44A	0.129 (9)	0.055 (4)	0.107 (7)	−0.021 (5)	0.011 (6)	0.006 (4)
C45A	0.077 (6)	0.115 (8)	0.120 (8)	−0.044 (5)	0.007 (5)	−0.029 (6)
C46A	0.172 (12)	0.081 (7)	0.101 (7)	−0.067 (8)	0.064 (8)	−0.038 (6)
C44B	0.129 (8)	0.058 (5)	0.164 (12)	−0.021 (5)	0.033 (8)	−0.021 (6)
C45B	0.108 (8)	0.096 (7)	0.093 (7)	−0.050 (6)	0.027 (6)	−0.011 (5)
C46B	0.149 (10)	0.117 (9)	0.092 (6)	−0.076 (8)	−0.002 (7)	−0.019 (6)
C47	0.065 (2)	0.069 (2)	0.0624 (19)	−0.0029 (17)	0.0161 (16)	−0.0084 (17)
C48A	0.132 (8)	0.101 (6)	0.061 (4)	0.025 (6)	0.004 (5)	−0.009 (4)
C49A	0.087 (5)	0.061 (4)	0.094 (4)	−0.009 (3)	0.044 (4)	−0.032 (3)
C50A	0.066 (4)	0.101 (6)	0.120 (6)	−0.005 (4)	0.028 (4)	−0.041 (5)
C48B	0.20 (3)	0.24 (3)	0.17 (3)	−0.11 (2)	0.14 (2)	−0.14 (2)
C49B	0.125 (18)	0.24 (3)	0.13 (2)	0.029 (18)	−0.053 (15)	−0.13 (2)
C50B	0.28 (4)	0.126 (17)	0.27 (3)	0.14 (2)	0.18 (3)	0.074 (18)
N1	0.0595 (15)	0.0456 (13)	0.0585 (14)	−0.0083 (12)	0.0116 (12)	−0.0074 (12)
O1	0.0627 (13)	0.0522 (12)	0.0620 (12)	−0.0076 (10)	0.0150 (11)	−0.0002 (10)
O2	0.0826 (15)	0.0606 (13)	0.0641 (13)	−0.0121 (11)	0.0223 (12)	−0.0127 (11)

Geometric parameters (Å, º)

C1—O1	1.209 (3)	C36—H36C	0.97
C1—N1	1.407 (4)	C37—H37A	0.97
C1—C2	1.487 (4)	C37—H37B	0.97
C2—C3	1.379 (4)	C37—H37C	0.97
C2—C27	1.396 (4)	C38—H38A	0.97
C3—C14	1.461 (4)	C38—H38B	0.97
C3—C4	1.469 (4)	C38—H38C	0.97
C4—C5	1.371 (4)	C39—C41	1.521 (4)
C4—C9	1.409 (4)	C39—C42	1.532 (5)
C5—C6	1.426 (4)	C39—C40	1.535 (4)
C5—H5	0.94	C40—H40A	0.97
C6—C7	1.381 (4)	C40—H40B	0.97
C6—C35	1.524 (4)	C40—H40C	0.97
C7—C8	1.409 (4)	C41—H41A	0.97
C7—H7	0.94	C41—H41B	0.97
C8—C9	1.390 (4)	C41—H41C	0.97
C8—C10	1.425 (4)	C42—H42A	0.97
C9—C13	1.411 (4)	C42—H42B	0.97
C10—C11	1.376 (4)	C42—H42C	0.97
C10—H10	0.94	C43—C46A	1.501 (6)
C11—C12	1.422 (4)	C43—C45B	1.509 (6)
C11—C39	1.539 (4)	C43—C45A	1.527 (6)
C12—C13	1.371 (4)	C43—C44B	1.535 (6)
C12—H12	0.94	C43—C46B	1.559 (6)
C13—C14	1.491 (4)	C43—C44A	1.561 (6)
C14—C15	1.386 (4)	C44A—H44A	0.97
C15—C26	1.447 (4)	C44A—H44B	0.97
C15—C16	1.491 (4)	C44A—H44C	0.97
C16—C17	1.372 (4)	C45A—H45A	0.97
C16—C21	1.414 (4)	C45A—H45B	0.97
C17—C18	1.422 (4)	C45A—H45C	0.97
C17—H17	0.94	C46A—H46A	0.97
C18—C19	1.379 (4)	C46A—H46B	0.97
C18—C43	1.536 (4)	C46A—H46C	0.97
C19—C20	1.414 (4)	C44B—H44D	0.97
C19—H19	0.94	C44B—H44E	0.97
C20—C21	1.390 (4)	C44B—H44F	0.97
C20—C22	1.407 (4)	C45B—H45D	0.97
C21—C25	1.406 (4)	C45B—H45E	0.97
C22—C23	1.388 (4)	C45B—H45F	0.97
C22—H22	0.94	C46B—H46D	0.97
C23—C24	1.417 (4)	C46B—H46E	0.97
C23—C47	1.539 (4)	C46B—H46F	0.97
C24—C25	1.384 (4)	C47—C50B	1.501 (7)
C24—H24	0.94	C47—C48B	1.504 (7)
C25—C26	1.465 (4)	C47—C49B	1.510 (7)

C26—C27	1.386 (4)	C47—C48A	1.512 (6)
C27—C28	1.488 (4)	C47—C50A	1.519 (6)
C28—O2	1.206 (3)	C47—C49A	1.528 (5)
C28—N1	1.407 (4)	C48A—H48A	0.97
C29—C30	1.373 (4)	C48A—H48B	0.97
C29—C34	1.376 (4)	C48A—H48C	0.97
C29—N1	1.427 (4)	C49A—H49A	0.97
C30—C31	1.374 (4)	C49A—H49B	0.97
C30—H30	0.94	C49A—H49C	0.97
C31—C32	1.365 (5)	C50A—H50A	0.97
C31—H31	0.94	C50A—H50B	0.97
C32—C33	1.367 (5)	C50A—H50C	0.97
C32—H32	0.94	C48B—H48D	0.97
C33—C34	1.383 (5)	C48B—H48E	0.97
C33—H33	0.94	C48B—H48F	0.97
C34—H34	0.94	C49B—H49D	0.97
C35—C36	1.495 (5)	C49B—H49E	0.97
C35—C38	1.508 (5)	C49B—H49F	0.97
C35—C37	1.535 (5)	C50B—H50D	0.97
C36—H36A	0.97	C50B—H50E	0.97
C36—H36B	0.97	C50B—H50F	0.97

O1—C1—N1	123.9 (3)	H38B—C38—H38C	109.5
O1—C1—C2	130.3 (3)	C41—C39—C42	108.4 (3)
N1—C1—C2	105.8 (2)	C41—C39—C40	108.5 (3)
C3—C2—C27	121.6 (3)	C42—C39—C40	110.5 (3)
C3—C2—C1	130.2 (3)	C41—C39—C11	112.4 (3)
C27—C2—C1	108.2 (2)	C42—C39—C11	108.7 (2)
C2—C3—C14	118.9 (3)	C40—C39—C11	108.4 (3)
C2—C3—C4	132.4 (3)	C39—C40—H40A	109.5
C14—C3—C4	108.7 (2)	C39—C40—H40B	109.5
C5—C4—C9	118.9 (3)	H40A—C40—H40B	109.5
C5—C4—C3	135.2 (3)	C39—C40—H40C	109.5
C9—C4—C3	105.9 (2)	H40A—C40—H40C	109.5
C4—C5—C6	120.5 (3)	H40B—C40—H40C	109.5
C4—C5—H5	119.7	C39—C41—H41A	109.5
C6—C5—H5	119.7	C39—C41—H41B	109.5
C7—C6—C5	118.9 (3)	H41A—C41—H41B	109.5
C7—C6—C35	122.0 (3)	C39—C41—H41C	109.5
C5—C6—C35	119.0 (3)	H41A—C41—H41C	109.5
C6—C7—C8	121.9 (3)	H41B—C41—H41C	109.5
C6—C7—H7	119.1	C39—C42—H42A	109.5
C8—C7—H7	119.1	C39—C42—H42B	109.5
C9—C8—C7	117.3 (3)	H42A—C42—H42B	109.5
C9—C8—C10	116.0 (3)	C39—C42—H42C	109.5
C7—C8—C10	126.7 (3)	H42A—C42—H42C	109.5
C8—C9—C4	122.4 (3)	H42B—C42—H42C	109.5
C8—C9—C13	124.8 (3)	C46A—C43—C45A	111.2 (4)

C4—C9—C13	112.8 (2)	C45B—C43—C44B	109.9 (4)
C11—C10—C8	121.1 (3)	C46A—C43—C18	115.6 (4)
C11—C10—H10	119.5	C45B—C43—C18	117.3 (4)
C8—C10—H10	119.5	C45A—C43—C18	108.7 (4)
C10—C11—C12	119.9 (3)	C44B—C43—C18	109.5 (4)
C10—C11—C39	121.9 (3)	C45B—C43—C46B	107.7 (4)
C12—C11—C39	118.2 (3)	C44B—C43—C46B	106.8 (4)
C13—C12—C11	121.4 (3)	C18—C43—C46B	105.1 (4)
C13—C12—H12	119.3	C46A—C43—C44A	108.5 (4)
C11—C12—H12	119.3	C45A—C43—C44A	106.7 (4)
C12—C13—C9	116.7 (3)	C18—C43—C44A	105.6 (3)
C12—C13—C14	137.0 (3)	C43—C44A—H44A	109.5
C9—C13—C14	106.3 (2)	C43—C44A—H44B	109.5
C15—C14—C3	119.3 (2)	H44A—C44A—H44B	109.5
C15—C14—C13	134.4 (3)	C43—C44A—H44C	109.5
C3—C14—C13	106.2 (2)	H44A—C44A—H44C	109.5
C14—C15—C26	120.3 (2)	H44B—C44A—H44C	109.5
C14—C15—C16	133.6 (3)	C43—C45A—H45A	109.5
C26—C15—C16	106.0 (2)	C43—C45A—H45B	109.5
C17—C16—C21	116.2 (3)	H45A—C45A—H45B	109.5
C17—C16—C15	137.3 (3)	C43—C45A—H45C	109.5
C21—C16—C15	106.4 (2)	H45A—C45A—H45C	109.5
C16—C17—C18	121.8 (3)	H45B—C45A—H45C	109.5
C16—C17—H17	119.1	C43—C46A—H46A	109.5
C18—C17—H17	119.1	C43—C46A—H46B	109.5
C19—C18—C17	119.5 (3)	H46A—C46A—H46B	109.5
C19—C18—C43	120.3 (3)	C43—C46A—H46C	109.5
C17—C18—C43	120.2 (3)	H46A—C46A—H46C	109.5
C18—C19—C20	121.4 (3)	H46B—C46A—H46C	109.5
C18—C19—H19	119.3	C43—C44B—H44D	109.5
C20—C19—H19	119.3	C43—C44B—H44E	109.5
C21—C20—C22	116.7 (3)	H44D—C44B—H44E	109.5
C21—C20—C19	116.2 (3)	C43—C44B—H44F	109.5
C22—C20—C19	127.0 (3)	H44D—C44B—H44F	109.5
C20—C21—C25	122.8 (3)	H44E—C44B—H44F	109.5
C20—C21—C16	124.8 (3)	C43—C45B—H45D	109.5
C25—C21—C16	112.4 (3)	C43—C45B—H45E	109.5
C23—C22—C20	122.3 (3)	H45D—C45B—H45E	109.5
C23—C22—H22	118.9	C43—C45B—H45F	109.5
C20—C22—H22	118.9	H45D—C45B—H45F	109.5
C22—C23—C24	119.2 (3)	H45E—C45B—H45F	109.5
C22—C23—C47	120.5 (3)	C43—C46B—H46D	109.5
C24—C23—C47	120.3 (3)	C43—C46B—H46E	109.5
C25—C24—C23	120.0 (3)	H46D—C46B—H46E	109.5
C25—C24—H24	120	C43—C46B—H46F	109.5
C23—C24—H24	120	H46D—C46B—H46F	109.5
C24—C25—C21	119.0 (3)	H46E—C46B—H46F	109.5
C24—C25—C26	135.1 (3)	C50B—C47—C48B	110.5 (6)

C21—C25—C26	105.9 (2)	C50B—C47—C49B	109.9 (7)
C27—C26—C15	118.9 (3)	C48B—C47—C49B	109.8 (6)
C27—C26—C25	131.9 (3)	C48A—C47—C50A	108.9 (4)
C15—C26—C25	109.3 (2)	C48A—C47—C49A	108.0 (4)
C26—C27—C2	121.0 (3)	C50A—C47—C49A	107.0 (4)
C26—C27—C28	130.6 (3)	C50B—C47—C23	112.8 (9)
C2—C27—C28	108.4 (2)	C48B—C47—C23	108.5 (8)
O2—C28—N1	124.1 (3)	C49B—C47—C23	105.1 (9)
O2—C28—C27	130.3 (3)	C48A—C47—C23	109.6 (5)
N1—C28—C27	105.6 (2)	C50A—C47—C23	111.4 (4)
C30—C29—C34	120.2 (3)	C49A—C47—C23	111.8 (3)
C30—C29—N1	119.5 (3)	C47—C48A—H48A	109.5
C34—C29—N1	120.3 (3)	C47—C48A—H48B	109.5
C29—C30—C31	120.0 (3)	H48A—C48A—H48B	109.5
C29—C30—H30	120	C47—C48A—H48C	109.5
C31—C30—H30	120	H48A—C48A—H48C	109.5
C32—C31—C30	120.0 (3)	H48B—C48A—H48C	109.5
C32—C31—H31	120	C47—C49A—H49A	109.5
C30—C31—H31	120	C47—C49A—H49B	109.5
C31—C32—C33	120.3 (3)	H49A—C49A—H49B	109.5
C31—C32—H32	119.8	C47—C49A—H49C	109.5
C33—C32—H32	119.8	H49A—C49A—H49C	109.5
C32—C33—C34	120.3 (3)	H49B—C49A—H49C	109.5
C32—C33—H33	119.9	C47—C50A—H50A	109.5
C34—C33—H33	119.9	C47—C50A—H50B	109.5
C29—C34—C33	119.2 (3)	H50A—C50A—H50B	109.5
C29—C34—H34	120.4	C47—C50A—H50C	109.5
C33—C34—H34	120.4	H50A—C50A—H50C	109.5
C36—C35—C38	111.4 (4)	H50B—C50A—H50C	109.5
C36—C35—C6	108.6 (3)	C47—C48B—H48D	109.5
C38—C35—C6	112.7 (3)	C47—C48B—H48E	109.5
C36—C35—C37	108.8 (4)	H48D—C48B—H48E	109.5
C38—C35—C37	105.2 (3)	C47—C48B—H48F	109.5
C6—C35—C37	110.1 (3)	H48D—C48B—H48F	109.5
C35—C36—H36A	109.5	H48E—C48B—H48F	109.5
C35—C36—H36B	109.5	C47—C49B—H49D	109.5
H36A—C36—H36B	109.5	C47—C49B—H49E	109.5
C35—C36—H36C	109.5	H49D—C49B—H49E	109.5
H36A—C36—H36C	109.5	C47—C49B—H49F	109.5
H36B—C36—H36C	109.5	H49D—C49B—H49F	109.5
C35—C37—H37A	109.5	H49E—C49B—H49F	109.5
C35—C37—H37B	109.5	C47—C50B—H50D	109.5
H37A—C37—H37B	109.5	C47—C50B—H50E	109.5
C35—C37—H37C	109.5	H50D—C50B—H50E	109.5
H37A—C37—H37C	109.5	C47—C50B—H50F	109.5
H37B—C37—H37C	109.5	H50D—C50B—H50F	109.5
C35—C38—H38A	109.5	H50E—C50B—H50F	109.5
C35—C38—H38B	109.5	C28—N1—C1	111.9 (2)

H38A—C38—H38B	109.5	C28—N1—C29	124.0 (2)
C35—C38—H38C	109.5	C1—N1—C29	123.9 (2)
H38A—C38—H38C	109.5		
O1—C1—C2—C3	1.2 (5)	C20—C21—C25—C24	−0.9 (4)
N1—C1—C2—C3	−178.7 (3)	C16—C21—C25—C24	−179.9 (3)
O1—C1—C2—C27	−177.3 (3)	C20—C21—C25—C26	178.6 (3)
N1—C1—C2—C27	2.8 (3)	C16—C21—C25—C26	−0.5 (3)
C27—C2—C3—C14	1.3 (4)	C14—C15—C26—C27	−0.5 (4)
C1—C2—C3—C14	−177.1 (3)	C16—C15—C26—C27	178.8 (3)
C27—C2—C3—C4	−176.2 (3)	C14—C15—C26—C25	179.7 (3)
C1—C2—C3—C4	5.4 (5)	C16—C15—C26—C25	−0.9 (3)
C2—C3—C4—C5	0.2 (6)	C24—C25—C26—C27	0.5 (6)
C14—C3—C4—C5	−177.5 (3)	C21—C25—C26—C27	−178.8 (3)
C2—C3—C4—C9	178.4 (3)	C24—C25—C26—C15	−179.8 (3)
C14—C3—C4—C9	0.7 (3)	C21—C25—C26—C15	0.9 (3)
C9—C4—C5—C6	1.8 (4)	C15—C26—C27—C2	0.6 (4)
C3—C4—C5—C6	179.8 (3)	C25—C26—C27—C2	−179.7 (3)
C4—C5—C6—C7	−2.4 (5)	C15—C26—C27—C28	−179.1 (3)
C4—C5—C6—C35	−179.6 (3)	C25—C26—C27—C28	0.6 (6)
C5—C6—C7—C8	1.3 (5)	C3—C2—C27—C26	−1.0 (4)
C35—C6—C7—C8	178.3 (3)	C1—C2—C27—C26	177.6 (3)
C6—C7—C8—C9	0.5 (5)	C3—C2—C27—C28	178.7 (3)
C6—C7—C8—C10	−179.4 (3)	C1—C2—C27—C28	−2.6 (3)
C7—C8—C9—C4	−1.2 (4)	C26—C27—C28—O2	1.6 (6)
C10—C8—C9—C4	178.7 (3)	C2—C27—C28—O2	−178.1 (3)
C7—C8—C9—C13	179.6 (3)	C26—C27—C28—N1	−178.8 (3)
C10—C8—C9—C13	−0.5 (4)	C2—C27—C28—N1	1.5 (3)
C5—C4—C9—C8	0.1 (4)	C34—C29—C30—C31	0.2 (5)
C3—C4—C9—C8	−178.5 (3)	N1—C29—C30—C31	178.6 (3)
C5—C4—C9—C13	179.3 (3)	C29—C30—C31—C32	−0.3 (5)
C3—C4—C9—C13	0.8 (3)	C30—C31—C32—C33	0.5 (6)
C9—C8—C10—C11	1.7 (4)	C31—C32—C33—C34	−0.7 (6)
C7—C8—C10—C11	−178.4 (3)	C30—C29—C34—C33	−0.4 (5)
C8—C10—C11—C12	−1.2 (5)	N1—C29—C34—C33	−178.8 (3)
C8—C10—C11—C39	178.8 (3)	C32—C33—C34—C29	0.6 (6)
C10—C11—C12—C13	−0.7 (5)	C7—C6—C35—C36	−104.6 (4)
C39—C11—C12—C13	179.3 (3)	C5—C6—C35—C36	72.4 (4)
C11—C12—C13—C9	1.8 (4)	C7—C6—C35—C38	19.4 (5)
C11—C12—C13—C14	−176.2 (3)	C5—C6—C35—C38	−163.6 (3)
C8—C9—C13—C12	−1.3 (5)	C7—C6—C35—C37	136.4 (3)
C4—C9—C13—C12	179.5 (3)	C5—C6—C35—C37	−46.6 (4)
C8—C9—C13—C14	177.4 (3)	C10—C11—C39—C41	−1.0 (4)
C4—C9—C13—C14	−1.9 (3)	C12—C11—C39—C41	178.9 (3)
C2—C3—C14—C15	−1.1 (4)	C10—C11—C39—C42	−121.0 (3)
C4—C3—C14—C15	176.9 (3)	C12—C11—C39—C42	59.0 (4)
C2—C3—C14—C13	−179.9 (2)	C10—C11—C39—C40	118.9 (3)
C4—C3—C14—C13	−1.8 (3)	C12—C11—C39—C40	−61.1 (4)

C12—C13—C14—C15	2.0 (6)	C19—C18—C43—C46A	−177.2 (5)
C9—C13—C14—C15	−176.2 (3)	C17—C18—C43—C46A	2.8 (6)
C12—C13—C14—C3	−179.6 (3)	C19—C18—C43—C45B	−4.2 (6)
C9—C13—C14—C3	2.2 (3)	C17—C18—C43—C45B	175.8 (5)
C3—C14—C15—C26	0.8 (4)	C19—C18—C43—C45A	−51.3 (5)
C13—C14—C15—C26	179.1 (3)	C17—C18—C43—C45A	128.6 (5)
C3—C14—C15—C16	−178.4 (3)	C19—C18—C43—C44B	121.9 (5)
C13—C14—C15—C16	−0.1 (6)	C17—C18—C43—C44B	−58.2 (6)
C14—C15—C16—C17	2.6 (6)	C19—C18—C43—C46B	−123.7 (5)
C26—C15—C16—C17	−176.6 (3)	C17—C18—C43—C46B	56.2 (6)
C14—C15—C16—C21	179.9 (3)	C19—C18—C43—C44A	62.9 (5)
C26—C15—C16—C21	0.6 (3)	C17—C18—C43—C44A	−117.2 (5)
C21—C16—C17—C18	1.1 (4)	C22—C23—C47—C50B	134.6 (17)
C15—C16—C17—C18	178.2 (3)	C24—C23—C47—C50B	−45.8 (17)
C16—C17—C18—C19	−0.6 (5)	C22—C23—C47—C48B	11.8 (17)
C16—C17—C18—C43	179.4 (3)	C24—C23—C47—C48B	−168.6 (17)
C17—C18—C19—C20	0.1 (5)	C22—C23—C47—C49B	−105.6 (16)
C43—C18—C19—C20	−180.0 (3)	C24—C23—C47—C49B	74.0 (17)
C18—C19—C20—C21	−0.1 (4)	C22—C23—C47—C48A	−70.6 (5)
C18—C19—C20—C22	−178.7 (3)	C24—C23—C47—C48A	108.9 (5)
C22—C20—C21—C25	0.5 (4)	C22—C23—C47—C50A	50.0 (5)
C19—C20—C21—C25	−178.3 (3)	C24—C23—C47—C50A	−130.5 (5)
C22—C20—C21—C16	179.4 (3)	C22—C23—C47—C49A	169.7 (4)
C19—C20—C21—C16	0.7 (4)	C24—C23—C47—C49A	−10.8 (5)
C17—C16—C21—C20	−1.2 (4)	O2—C28—N1—C1	180.0 (3)
C15—C16—C21—C20	−179.1 (3)	C27—C28—N1—C1	0.3 (3)
C17—C16—C21—C25	177.8 (3)	O2—C28—N1—C29	−5.3 (5)
C15—C16—C21—C25	−0.1 (3)	C27—C28—N1—C29	175.0 (3)
C21—C20—C22—C23	0.0 (4)	O1—C1—N1—C28	178.2 (3)
C19—C20—C22—C23	178.6 (3)	C2—C1—N1—C28	−1.9 (3)
C20—C22—C23—C24	−0.1 (5)	O1—C1—N1—C29	3.5 (4)
C20—C22—C23—C47	179.5 (3)	C2—C1—N1—C29	−176.6 (3)
C22—C23—C24—C25	−0.3 (4)	C30—C29—N1—C28	−116.0 (3)
C47—C23—C24—C25	−179.8 (3)	C34—C29—N1—C28	62.4 (4)
C23—C24—C25—C21	0.7 (4)	C30—C29—N1—C1	58.1 (4)
C23—C24—C25—C26	−178.5 (3)	C34—C29—N1—C1	−123.5 (3)