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Tris[2,5-bis(decyloxy)phenyl]-1,3,4,6,8,9,11,13,14-nonaazatetracyclo[10.3.0.0^{2,6}.0^{7,11}]pentadeca-2,4,7,9,12,14-hexaene

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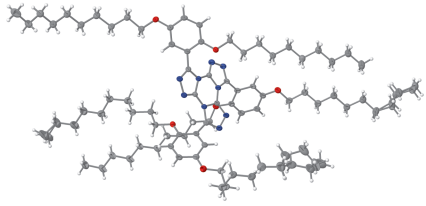
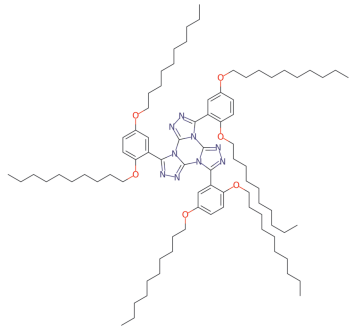
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{84}H_{135}N_9O_6$, has a nearly planar tristriazolotriazine core surrounded by three phenyl rings with torsion angles of −41.9 (3), 39.8 (3) and 58.8 (3)°. Whereas the chains in the *ortho* positions are mostly all-*trans*, several *gauche* conformations in the opposite chains inhibit linearity. Packing is dominated by decyl chain interactions.

3D view



Chemical scheme



Structure description

The title compound (Fig. 1) was prepared in a project on discotic liquid crystals based on tristriazolotriazine (Rieth *et al.*, 2014; Rieth *et al.*, 2018) as a rigid centre. The synthesis was performed *via* reaction of cyanuric chloride (Cristiano *et al.*, 2008; Cristiano *et al.*, 2012) and 2,5-didecyloxyphenyltetrazole according to Huisgen (Huisgen *et al.*, 1960; Huisgen *et al.*, 1961). Mesomorphism of tristriazolotriazines is strongly dependent on length, number and type of side chains, and also on the position (Herget *et al.*, 2013; Detert, 2018). While the 3,4-, 3,5-di- and 3,4,5-tridecyloxy substitution result in broad mesophases, the title compound with 2,5-didecyloxy groups is not mesomorphous (Rieth *et al.*, 2020). The central tristriazolotriazine is almost planar, with the largest deviations occurring for N3 [0.240 (2) Å], N5 [−0.2057 (18) Å] and C6 [0.209 (2) Å]. Due to the *ortho* substitution, the phenyl rings and central tristriazolotriazines subtend large torsion angles [N2—C1—C16—C17 = 39.8 (3)° and N7—C6—C44—C49 = −41.9 (3)°], the largest being N12—C11—C72—C73 of 58.8 (3)°. The decyl chains are mostly all-*trans*; this is true for both chains on the C44–C49 ring. But whereas the *ortho*-chain is nearly planar, the second chain is bent. The *ortho*-chain on the C72–C77 ring is also in an all-*trans* conformation and the decyloxy chain in the 5-position is too, except for a *gauche* conformation at the end. On the C16–C20 ring, the *ortho*-chain is mostly all-*trans*, except for a central *gauche* conformation: the torsion angle C36—C37—C38—C39 is −65.1°. Like the other chains on position 5, this is more distorted than its congeners. The

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sequence of torsion angles along this chain, starting with O22, is −61.9 (3), −65.5 (3), 57.6 (3), −165.6 (2), −174.8 (2), 70.1 (3), 163.3 (3) and 67.3 (3)°, with disorder on the terminal methyl C43 atom. The packing of these molecules (Fig. 2) in the crystal is controlled by van der Waals interactions between the decyl chains.

Synthesis and crystallization

Collidine (0.2 ml) was added to 250 mg 5-(2,5-didecyloxy)-phenyl-2*H*-tetrazole in 25 ml dry xylenes. After complete dissolution of the tetrazole, 1 ml of a 0.1 *M* solution of cyanuric chloride in dry xylenes was added dropwise. After 1 h stirring at ambient temperature, further cyanuric chloride solution was added until the tetrazole had completely disappeared (thin-layer chromatography, TLC). After stirring for 16 h, petroleum ether was added, filtered, concentrated and the product was purified *via* chromatography on silica gel using petroleum ether/ethyl acetate (20/1 *v*/*v*) as an eluent. The product was obtained as a colourless powder (yield 41%; m.p. 361–363 K). Recrystallization by slow evaporation of a solution in chloroform/2-propanol yielded single crystals.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.18 (*d*, *J* = 3.0 Hz, 3H, 6-H, ph), 7.12 (*dd*, *J* = 9.1 Hz, *J*′= 3.0 Hz, 3H, 4-H, ph), 6.99 (*d*, *J* = 9.1 Hz, 3H, 3-H, ph), 3.96 (*m*, 12H, OCH_2), 1.82–1.72 (*m*, 6H, CH_2), 1.47–1.40 (*m*, 6H, CH_2), 1.38–1.03 (*m*, 84H, CH_2), 0.91–0.81 (*m*, 18H, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.95, 152.38, 147.80 (C5 triazole, C-2, C-5 ph), 140.15 (C3 triazole), 119.82 (CH ph), 117.12 (CH ph), 114.19 (C-1 ph), 113.10 (CH ph), 68.89, 68.59 (OCH_2), 32.03, 31.99, 29.70, 29.54, 29.46, 29.36, 29.10, 26.19, 25.76, 22.81, 22.79 (CH_2), 14.23 (CH_3). IR (ATR): ν (cm^{-1}) 2919, 2851, 1600, 1488, 1468, 1385, 1275, 1220, 1146, 1026, 879, 793, 721; MS (FD): 1367.7 (M^+), 2733.5 (M_2^+).

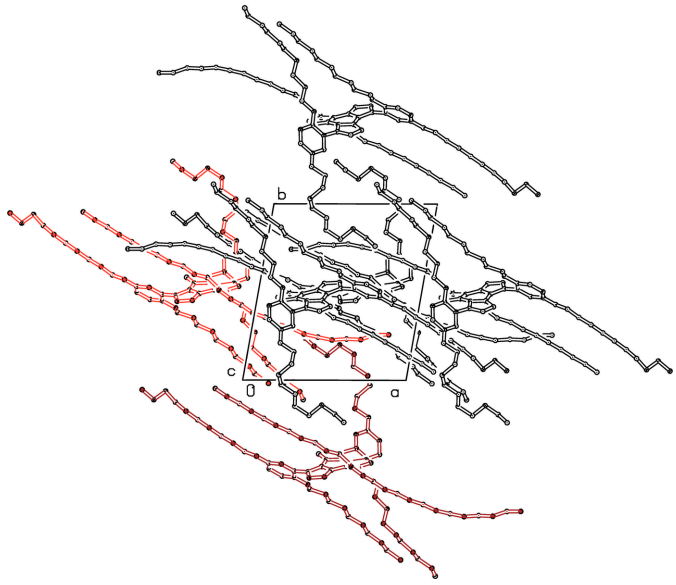

Figure 2
Part of the packing diagram, viewed along the *c*-axis direction. H atoms and disordered C atoms have been removed for clarity. Symmetry-related molecules are shown in different colours.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed at calculated positions and refined in the riding-model approximation, with aromatic C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C), methylene C—H = 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or methyl C—H = 0.98 Å, and with U_{iso}(H) = 1.5U_{eq}(C). The methyl groups were allowed to rotate but not to tip. The terminal methyl group of one decyl chain is disordered over two positions with a site-occupation factor of 0.84 (2) for the major-occupied site. In two other decyl chains, the terminal propyl moieties are

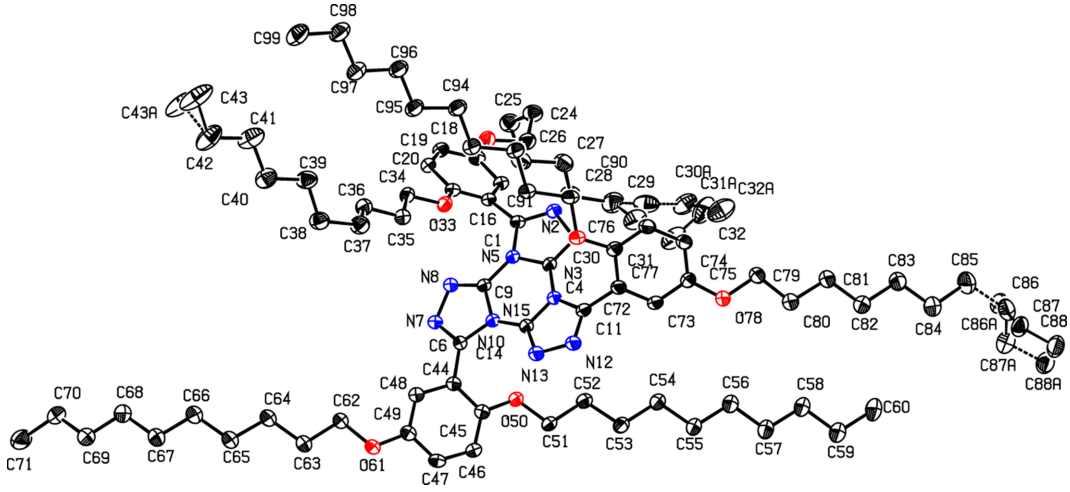

Figure 1
View of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. The minor-occupied sites of the disordered atoms are drawn with dashed bonds.

disordered over two positions with a site occupation factor of 0.751 (7) or 0.510 (6), respectively, for the major-occupied sites.

References

Cristiano, R., Eccher, J., Bechtold, I. H., Tironi, C. N., Vieira, A. A., Molin, F. & Gallardo, H. (2012). *Langmuir* **28**, 11590–11598.

Cristiano, R., Gallardo, H., Bortoluzzi, A. J., Bechtold, I. H., Campos, C. E. M. & Longo, R. L. (2008). *Chem. Commun.* pp. 5134–5136.

Detert, H. (2018). *Eur. J. Org. Chem.* **2018**, 4501–4507.

Herget, K., Schollmeyer, D. & Detert, H. (2013). *Acta Cryst.* E**69**, o365–o366.

Huisgen, R., Sauer, J., Sturm, J. H. & Markgraf, H. J. (1960). *Chem. Ber.* **93**, 2106–2124.

Huisgen, R., Sturm, H. J. & Seidel, M. (1961). *Chem. Ber.* **94**, 1555–1562.

Rieth, T., Marszalek, T., Pisula, W. & Detert, H. (2014). *Chem. A Eur. J.* **20**, 5000–5006.

Rieth, T., Röder, N., Lehmann, M. & Detert, H. (2018). *Chem. A Eur. J.* **24**, 93–96.

Rieth, T., Tober, N., Limbach, D., Haspel, T., Sperner, M., Schupp, N., Wicker, P., Glang, S., Lehmann, M. & Detert, H. (2020). *Molecules* **25**, 5761.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Stoe & Cie (2020). *WINXPOSE*, *RECIPE* and *INTEGRATE* in *X-AREA*. Stoe & Cie, Darmstadt, Germany.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{84}H_{135}N_9O_6$
M_r	1367.00
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	120
a, b, c (Å)	15.2697 (6), 16.6883 (7), 18.0255 (7)
α, β, γ (°)	73.142 (3), 72.593 (3), 75.858 (3)
V (Å^3)	4131.7 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.60 × 0.44 × 0.10
Data collection	
Diffractometer	STOE IPDS 2T
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34595, 19365, 12430
R_{int}	0.046
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.665
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.156, 1.06
No. of reflections	19365
No. of parameters	961
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.21

Computer programs: *WINXPOSE*, *RECIPE* and *INTEGRATE* in *X-AREA* (Stoe & Cie, 2020), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2019* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2020).

full crystallographic data

IUCrData (2026). **11**, x261210 [https://doi.org/10.1107/S2414314626012101]

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Tris[2,5-bis(decyloxy)phenyl]-1,3,4,6,8,9,11,13,14-nonaazatetracyclo[10.3.0.0^{2,6}.0^{7,11}]pentadeca-2,4,7,9,12,14-hexaene

Crystal data

$C_{84}H_{135}N_9O_6$
M_r = 1367.00
Triclinic, $P\overline{1}$
a = 15.2697 (6) Å
b = 16.6883 (7) Å
c = 18.0255 (7) Å
α = 73.142 (3)°
β = 72.593 (3)°
γ = 75.858 (3)°
V = 4131.7 (3) Å^3
Z = 2
$F(000)$ = 1500
D_x = 1.099 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 29541 reflections
θ = 2.4–28.6°
μ = 0.07 mm^{-1}
T = 120 K
Plate, colourless
0.60 × 0.44 × 0.10 mm

Data collection

STOE IPDS 2T diffractometer
Detector resolution: 6.67 pixels mm^{-1}
rotation method, ω scans
34595 measured reflections
19365 independent reflections
12430 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 28.2°, θ_{min} = 2.7°
h = −20→20
k = −22→22
l = −23→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.156
S = 1.06
19365 reflections
961 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 3.027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.69054 (14)	0.59087 (13)	0.52999 (11)	0.0266 (4)	
N2	0.60476 (12)	0.60849 (12)	0.52329 (10)	0.0296 (4)	
N3	0.54535 (11)	0.58175 (12)	0.59801 (10)	0.0297 (4)	
C4	0.59928 (14)	0.54820 (13)	0.64607 (11)	0.0272 (4)	
N5	0.69188 (11)	0.55075 (11)	0.60940 (9)	0.0265 (4)	
C6	0.80562 (14)	0.50957 (14)	0.76207 (12)	0.0276 (4)	
N7	0.87366 (12)	0.53127 (12)	0.69981 (10)	0.0310 (4)	
N8	0.84240 (12)	0.54838 (12)	0.63003 (10)	0.0309 (4)	
C9	0.75749 (14)	0.53671 (13)	0.65378 (11)	0.0266 (4)	
N10	0.72767 (11)	0.51142 (11)	0.73611 (9)	0.0264 (4)	
C11	0.49805 (14)	0.47959 (14)	0.77904 (12)	0.0278 (4)	
N12	0.51386 (12)	0.44557 (12)	0.84976 (10)	0.0304 (4)	
N13	0.60533 (12)	0.45143 (12)	0.84694 (10)	0.0297 (4)	
C14	0.63966 (14)	0.49006 (13)	0.77391 (12)	0.0266 (4)	
N15	0.57734 (11)	0.51006 (11)	0.72759 (9)	0.0267 (4)	
C16	0.76910 (14)	0.61279 (14)	0.46177 (11)	0.0277 (4)	
C17	0.75333 (14)	0.69204 (14)	0.40879 (12)	0.0295 (4)	
H17	0.697027	0.730641	0.421306	0.035*	
C18	0.81977 (15)	0.71411 (14)	0.33822 (12)	0.0316 (5)	
C19	0.90189 (15)	0.65730 (14)	0.32199 (12)	0.0315 (5)	
H19	0.948360	0.672756	0.274420	0.038*	
C20	0.91795 (14)	0.57879 (14)	0.37315 (12)	0.0300 (5)	
H20	0.974911	0.540977	0.360640	0.036*	
C21	0.85028 (14)	0.55494 (14)	0.44344 (12)	0.0281 (4)	
O22	0.80971 (10)	0.78911 (10)	0.28185 (9)	0.0362 (4)	
C23	0.71795 (16)	0.83939 (15)	0.28939 (13)	0.0375 (5)	
H23A	0.701268	0.864910	0.336047	0.045*	
H23B	0.671630	0.803353	0.297302	0.045*	
C24	0.71822 (18)	0.90868 (15)	0.21323 (14)	0.0401 (5)	
H24A	0.654285	0.941504	0.216353	0.048*	
H24B	0.735044	0.881629	0.167551	0.048*	
C25	0.78469 (18)	0.97014 (16)	0.19654 (14)	0.0432 (6)	
H25A	0.785837	1.008024	0.142735	0.052*	
H25B	0.848241	0.937052	0.195438	0.052*	
C26	0.76048 (18)	1.02499 (16)	0.25684 (15)	0.0431 (6)	
H26A	0.765655	0.987415	0.309643	0.052*	
H26B	0.807066	1.062939	0.240383	0.052*	
C27	0.66366 (17)	1.07920 (16)	0.26599 (15)	0.0421 (6)	
H27A	0.652051	1.106333	0.212367	0.051*	
H27B	0.616546	1.042236	0.295818	0.051*	
C28	0.65276 (19)	1.14754 (17)	0.30979 (17)	0.0500 (6)	
H28A	0.696896	1.186599	0.277193	0.060*	
H28B	0.671072	1.120060	0.360781	0.060*	
C29	0.5558 (2)	1.20005 (19)	0.32832 (18)	0.0566 (7)	
H29A	0.532216	1.221750	0.279376	0.068*	0.751 (7)

H29B	0.557995	1.249279	0.347461	0.068*	0.751 (7)
H29C	0.559769	1.231511	0.365746	0.068*	0.249 (7)
H29D	0.553474	1.243146	0.277597	0.068*	0.249 (7)
C30	0.4890 (3)	1.1421 (3)	0.3948 (3)	0.0538 (11)	0.751 (7)
H30A	0.473350	1.103108	0.370348	0.065*	0.751 (7)
H30B	0.522247	1.106949	0.436018	0.065*	0.751 (7)
C31	0.3995 (3)	1.1928 (3)	0.4348 (3)	0.0636 (15)	0.751 (7)
H31A	0.365696	1.153719	0.481112	0.076*	0.751 (7)
H31B	0.415550	1.234787	0.455464	0.076*	0.751 (7)
C32	0.3354 (4)	1.2392 (4)	0.3807 (4)	0.0712 (18)	0.751 (7)
H32A	0.365878	1.282129	0.337392	0.107*	0.751 (7)
H32B	0.277539	1.266915	0.411502	0.107*	0.751 (7)
H32C	0.321232	1.198560	0.357913	0.107*	0.751 (7)
C30A	0.4697 (10)	1.1832 (9)	0.3557 (9)	0.057 (4)	0.249 (7)
H30C	0.463232	1.151679	0.412284	0.068*	0.249 (7)
H30D	0.465133	1.143250	0.326249	0.068*	0.249 (7)
C31A	0.3847 (11)	1.2534 (8)	0.3531 (8)	0.053 (4)	0.249 (7)
H31C	0.384990	1.280402	0.296369	0.063*	0.249 (7)
H31D	0.391132	1.297178	0.377282	0.063*	0.249 (7)
C32A	0.2900 (14)	1.2259 (13)	0.3955 (11)	0.073 (5)	0.249 (7)
H32D	0.240352	1.275430	0.389592	0.109*	0.249 (7)
H32E	0.287286	1.201468	0.452386	0.109*	0.249 (7)
H32F	0.281839	1.183299	0.371586	0.109*	0.249 (7)
O33	0.85584 (10)	0.47667 (9)	0.49483 (8)	0.0308 (3)	
C34	0.94019 (14)	0.41691 (14)	0.47745 (12)	0.0315 (5)	
H34A	0.994750	0.442424	0.471490	0.038*	
H34B	0.946428	0.401651	0.426752	0.038*	
C35	0.93641 (15)	0.33882 (14)	0.54508 (13)	0.0329 (5)	
H35A	0.879758	0.315590	0.552597	0.039*	
H35B	0.932584	0.354278	0.595130	0.039*	
C36	1.02251 (16)	0.27100 (14)	0.52818 (13)	0.0360 (5)	
H36A	1.030004	0.260662	0.475064	0.043*	
H36B	1.078309	0.292511	0.526211	0.043*	
C37	1.01698 (18)	0.18770 (15)	0.59054 (14)	0.0426 (6)	
H37A	0.966732	0.162295	0.586760	0.051*	
H37B	0.999566	0.199677	0.644242	0.051*	
C38	1.10729 (18)	0.12263 (16)	0.58274 (15)	0.0438 (6)	
H38A	1.157652	0.148926	0.585023	0.053*	
H38B	1.099241	0.073791	0.629580	0.053*	
C39	1.13872 (19)	0.08906 (17)	0.50748 (15)	0.0476 (6)	
H39A	1.147480	0.137296	0.460131	0.057*	
H39B	1.089369	0.061643	0.504968	0.057*	
C40	1.22919 (19)	0.02515 (16)	0.50440 (16)	0.0490 (6)	
H40A	1.277674	0.053004	0.507829	0.059*	
H40B	1.219707	−0.022485	0.552225	0.059*	
C41	1.2655 (2)	−0.01118 (19)	0.43100 (17)	0.0645 (9)	
H41A	1.267447	0.036261	0.382785	0.077*	
H41B	1.221446	−0.046108	0.431348	0.077*	

C42	1.3617 (2)	−0.06534 (19)	0.42525 (19)	0.0698 (10)	
H42A	1.362217	−0.108755	0.476052	0.084*	0.84 (2)
H42B	1.407589	−0.028962	0.417685	0.084*	0.84 (2)
H42C	1.395776	−0.038280	0.447525	0.084*	0.16 (2)
H42D	1.352226	−0.120393	0.463627	0.084*	0.16 (2)
C43	1.3911 (8)	−0.1100 (5)	0.3555 (3)	0.089 (3)	0.84 (2)
H43A	1.392168	−0.067255	0.304946	0.133*	0.84 (2)
H43B	1.346466	−0.146880	0.363220	0.133*	0.84 (2)
H43C	1.453356	−0.144402	0.354088	0.133*	0.84 (2)
C43A	1.429 (4)	−0.087 (2)	0.3519 (19)	0.089 (3)	0.16 (2)
H43D	1.398972	−0.114483	0.326834	0.133*	0.16 (2)
H43E	1.483711	−0.126443	0.366265	0.133*	0.16 (2)
H43F	1.447999	−0.035391	0.314207	0.133*	0.16 (2)
C44	0.81366 (14)	0.49001 (14)	0.84497 (12)	0.0284 (4)	
C45	0.74519 (14)	0.52636 (14)	0.90296 (12)	0.0289 (4)	
C46	0.75854 (15)	0.50836 (14)	0.97947 (12)	0.0315 (5)	
H46	0.711204	0.530219	1.020149	0.038*	
C47	0.83997 (15)	0.45899 (15)	0.99688 (12)	0.0339 (5)	
H47	0.848296	0.447466	1.049363	0.041*	
C48	0.90973 (15)	0.42606 (14)	0.93846 (12)	0.0322 (5)	
C49	0.89672 (15)	0.44096 (14)	0.86278 (12)	0.0313 (5)	
H49	0.944015	0.417979	0.822754	0.038*	
O50	0.67172 (10)	0.58123 (9)	0.87792 (8)	0.0306 (3)	
C51	0.58856 (14)	0.59915 (15)	0.93836 (12)	0.0321 (5)	
H51A	0.598724	0.634990	0.969183	0.038*	
H51B	0.571670	0.545568	0.975802	0.038*	
C52	0.51174 (15)	0.64507 (15)	0.89723 (12)	0.0335 (5)	
H52A	0.501428	0.608088	0.867597	0.040*	
H52B	0.530850	0.696990	0.858046	0.040*	
C53	0.42106 (15)	0.66963 (15)	0.95660 (13)	0.0345 (5)	
H53A	0.405396	0.618299	0.998616	0.041*	
H53B	0.430266	0.710488	0.982765	0.041*	
C54	0.33983 (15)	0.70920 (15)	0.91787 (13)	0.0351 (5)	
H54A	0.358228	0.756527	0.871827	0.042*	
H54B	0.325989	0.666081	0.897122	0.042*	
C55	0.25219 (15)	0.74270 (16)	0.97496 (14)	0.0368 (5)	
H55A	0.233920	0.695314	1.020973	0.044*	
H55B	0.266191	0.785703	0.995745	0.044*	
C56	0.17070 (15)	0.78239 (16)	0.93692 (14)	0.0389 (5)	
H56A	0.152584	0.738015	0.920912	0.047*	
H56B	0.190732	0.826103	0.887888	0.047*	
C57	0.08623 (16)	0.82317 (17)	0.99220 (15)	0.0429 (6)	
H57A	0.064582	0.778866	1.040115	0.051*	
H57B	0.105158	0.865623	1.010190	0.051*	
C58	0.00579 (16)	0.86650 (18)	0.95340 (15)	0.0463 (6)	
H58A	−0.012654	0.824245	0.934776	0.056*	
H58B	0.027144	0.911360	0.905906	0.056*	
C59	−0.07904 (17)	0.9062 (2)	1.00928 (16)	0.0526 (7)	

H59A	−0.060441	0.947535	1.028980	0.063*
H59B	−0.101599	0.861200	1.056103	0.063*
C60	−0.1583 (2)	0.9514 (3)	0.9689 (2)	0.0800 (12)
H60A	−0.136427	0.996094	0.922457	0.120*
H60B	−0.210471	0.976771	1.006851	0.120*
H60C	−0.178876	0.910290	0.951277	0.120*
O61	0.98914 (10)	0.38031 (11)	0.96160 (9)	0.0383 (4)
C62	1.06831 (15)	0.35679 (16)	0.90077 (13)	0.0356 (5)
H62A	1.081362	0.407126	0.856492	0.043*
H62B	1.056058	0.313695	0.878978	0.043*
C63	1.15085 (15)	0.32083 (16)	0.93750 (14)	0.0374 (5)
H63A	1.137237	0.270237	0.981287	0.045*
H63B	1.161008	0.363728	0.960777	0.045*
C64	1.23888 (15)	0.29597 (15)	0.87600 (14)	0.0360 (5)
H64A	1.250625	0.346361	0.831449	0.043*
H64B	1.228582	0.252195	0.853879	0.043*
C65	1.32503 (16)	0.26167 (17)	0.90914 (14)	0.0404 (6)
H65A	1.332194	0.303334	0.935460	0.048*
H65B	1.315439	0.208432	0.950470	0.048*
C66	1.41428 (16)	0.24387 (16)	0.84635 (14)	0.0394 (5)
H66A	1.416690	0.292885	0.799454	0.047*
H66B	1.412614	0.193560	0.828560	0.047*
C67	1.50286 (16)	0.22785 (16)	0.87471 (14)	0.0405 (6)
H67A	1.509312	0.170540	0.910874	0.049*
H67B	1.496796	0.269746	0.905945	0.049*
C68	1.59095 (16)	0.23378 (17)	0.80694 (15)	0.0433 (6)
H68A	1.601826	0.186443	0.780739	0.052*
H68B	1.580622	0.287594	0.766631	0.052*
C69	1.67800 (16)	0.23061 (16)	0.83278 (14)	0.0410 (6)
H69A	1.662476	0.267868	0.870440	0.049*
H69B	1.697708	0.171823	0.861882	0.049*
C70	1.75905 (17)	0.25795 (18)	0.76405 (15)	0.0455 (6)
H70A	1.776670	0.219109	0.727608	0.055*
H70B	1.738750	0.315839	0.733485	0.055*
C71	1.84382 (19)	0.2580 (2)	0.79134 (18)	0.0654 (9)
H71A	1.893701	0.275941	0.744629	0.098*
H71B	1.865190	0.200581	0.820684	0.098*
H71C	1.827373	0.297439	0.826357	0.098*
C72	0.41433 (14)	0.48403 (14)	0.75293 (12)	0.0284 (4)
C73	0.32778 (14)	0.52365 (14)	0.78962 (12)	0.0305 (5)
H73	0.321691	0.546849	0.833571	0.037*
C74	0.24970 (14)	0.52951 (15)	0.76217 (12)	0.0327 (5)
C75	0.25917 (15)	0.49649 (15)	0.69731 (13)	0.0350 (5)
H75	0.206415	0.501746	0.677545	0.042*
C76	0.34604 (15)	0.45552 (14)	0.66094 (13)	0.0326 (5)
H76	0.351984	0.432358	0.616995	0.039*
C77	0.42326 (14)	0.44862 (14)	0.68870 (12)	0.0298 (4)
O78	0.16747 (10)	0.56832 (12)	0.80372 (9)	0.0413 (4)

C79	0.08919 (15)	0.59414 (16)	0.76894 (13)	0.0355 (5)	
H79A	0.070003	0.543773	0.763983	0.043*	
H79B	0.105736	0.631645	0.714925	0.043*	
C80	0.01078 (15)	0.64108 (16)	0.82267 (14)	0.0387 (5)	
H80A	0.033872	0.685616	0.834128	0.046*	
H80B	−0.010683	0.600936	0.874071	0.046*	
C81	−0.07088 (15)	0.68203 (16)	0.78442 (14)	0.0373 (5)	
H81A	−0.092476	0.637342	0.771794	0.045*	
H81B	−0.049072	0.722567	0.733406	0.045*	
C82	−0.15289 (16)	0.72894 (16)	0.83716 (14)	0.0395 (5)	
H82A	−0.177411	0.687787	0.886740	0.047*	
H82B	−0.130674	0.771362	0.852514	0.047*	
C83	−0.23142 (16)	0.77394 (16)	0.79617 (14)	0.0408 (6)	
H83A	−0.254319	0.731234	0.781800	0.049*	
H83B	−0.206382	0.814035	0.745946	0.049*	
C84	−0.31311 (17)	0.82270 (18)	0.84739 (16)	0.0476 (6)	
H84A	−0.289665	0.862048	0.865726	0.057*	
H84B	−0.342056	0.782045	0.895315	0.057*	
C85	−0.38697 (19)	0.87347 (19)	0.80236 (18)	0.0556 (7)	
H85A	−0.354482	0.903478	0.748938	0.067*	0.510 (6)
H85B	−0.418076	0.832488	0.793859	0.067*	0.510 (6)
H85C	−0.398852	0.838262	0.771847	0.067*	0.490 (6)
H85D	−0.364436	0.924467	0.764009	0.067*	0.490 (6)
C86	−0.4594 (4)	0.9360 (4)	0.8383 (4)	0.0444 (16)	0.510 (6)
H86A	−0.496383	0.970825	0.799768	0.053*	0.510 (6)
H86B	−0.430872	0.974351	0.853441	0.053*	0.510 (6)
C87	−0.5222 (4)	0.8875 (4)	0.9129 (3)	0.0470 (15)	0.510 (6)
H87A	−0.544595	0.845176	0.897476	0.056*	0.510 (6)
H87B	−0.484893	0.856136	0.952112	0.056*	0.510 (6)
C88	−0.6044 (4)	0.9439 (5)	0.9517 (3)	0.062 (2)	0.510 (6)
H88A	−0.644011	0.972237	0.914459	0.094*	0.510 (6)
H88B	−0.582860	0.986749	0.966159	0.094*	0.510 (6)
H88C	−0.640091	0.909773	1.000019	0.094*	0.510 (6)
C86A	−0.4851 (5)	0.9028 (5)	0.8671 (5)	0.0487 (17)	0.490 (6)
H86C	−0.535022	0.928193	0.838330	0.058*	0.490 (6)
H86D	−0.503973	0.851629	0.907826	0.058*	0.490 (6)
C87A	−0.4765 (4)	0.9646 (4)	0.9079 (4)	0.0545 (18)	0.490 (6)
H87C	−0.449464	1.012380	0.867538	0.065*	0.490 (6)
H87D	−0.433601	0.936719	0.943270	0.065*	0.490 (6)
C88A	−0.5717 (4)	0.9994 (5)	0.9580 (4)	0.0558 (18)	0.490 (6)
H88D	−0.614938	1.025349	0.923451	0.084*	0.490 (6)
H88E	−0.564170	1.042301	0.981927	0.084*	0.490 (6)
H88F	−0.596601	0.952804	1.000408	0.084*	0.490 (6)
O89	0.51095 (10)	0.40804 (10)	0.65966 (8)	0.0325 (3)	
C90	0.52872 (15)	0.38195 (15)	0.58632 (12)	0.0334 (5)	
H90A	0.507807	0.430150	0.544683	0.040*	
H90B	0.494778	0.335216	0.594928	0.040*	
C91	0.63218 (15)	0.35238 (15)	0.56074 (13)	0.0338 (5)	

H91A	0.653138	0.309952	0.606013	0.041*
H91B	0.664465	0.401351	0.547296	0.041*
C92	0.65988 (15)	0.31295 (15)	0.48872 (13)	0.0353 (5)
H92A	0.622662	0.267976	0.499762	0.042*
H92B	0.645707	0.357067	0.441586	0.042*
C93	0.76291 (16)	0.27494 (16)	0.46995 (14)	0.0393 (5)
H93A	0.777516	0.235453	0.519225	0.047*
H93B	0.799340	0.321319	0.454794	0.047*
C94	0.79489 (16)	0.22726 (16)	0.40359 (14)	0.0400 (5)
H94A	0.790926	0.268330	0.352069	0.048*
H94B	0.752367	0.186821	0.413984	0.048*
C95	0.89447 (16)	0.17850 (17)	0.39671 (14)	0.0420 (6)
H95A	0.897266	0.135679	0.447521	0.050*
H95B	0.936089	0.218696	0.389607	0.050*
C96	0.93124 (17)	0.13342 (17)	0.32800 (15)	0.0439 (6)
H96A	0.886266	0.097804	0.331560	0.053*
H96B	0.935554	0.176601	0.276649	0.053*
C97	1.02634 (17)	0.07766 (17)	0.32823 (15)	0.0440 (6)
H97A	1.021055	0.032335	0.378159	0.053*
H97B	1.070282	0.112576	0.328173	0.053*
C98	1.06616 (19)	0.03675 (19)	0.25709 (16)	0.0523 (7)
H98A	1.071596	0.081939	0.207066	0.063*
H98B	1.022478	0.001579	0.257132	0.063*
C99	1.1615 (2)	−0.01875 (19)	0.25828 (18)	0.0603 (8)
H99A	1.184192	−0.043102	0.211208	0.091*
H99B	1.156203	−0.064688	0.306893	0.091*
H99C	1.205300	0.015872	0.257501	0.091*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0277 (10)	0.0312 (11)	0.0207 (9)	−0.0030 (8)	−0.0066 (8)	−0.0071 (8)
N2	0.0262 (9)	0.0387 (10)	0.0211 (8)	−0.0057 (8)	−0.0039 (7)	−0.0051 (7)
N3	0.0244 (9)	0.0409 (10)	0.0203 (8)	−0.0044 (8)	−0.0037 (7)	−0.0048 (7)
C4	0.0229 (10)	0.0346 (11)	0.0212 (10)	−0.0023 (8)	−0.0031 (8)	−0.0066 (8)
N5	0.0225 (8)	0.0365 (10)	0.0191 (8)	−0.0026 (7)	−0.0043 (6)	−0.0071 (7)
C6	0.0224 (10)	0.0359 (11)	0.0250 (10)	−0.0010 (9)	−0.0070 (8)	−0.0104 (9)
N7	0.0262 (9)	0.0445 (11)	0.0220 (9)	−0.0020 (8)	−0.0068 (7)	−0.0102 (8)
N8	0.0255 (9)	0.0439 (11)	0.0233 (9)	−0.0024 (8)	−0.0064 (7)	−0.0102 (8)
C9	0.0242 (10)	0.0340 (11)	0.0200 (9)	−0.0002 (8)	−0.0050 (7)	−0.0083 (8)
N10	0.0223 (8)	0.0351 (9)	0.0201 (8)	−0.0017 (7)	−0.0046 (6)	−0.0073 (7)
C11	0.0270 (10)	0.0343 (11)	0.0216 (10)	−0.0060 (9)	−0.0022 (8)	−0.0092 (8)
N12	0.0285 (9)	0.0393 (10)	0.0234 (9)	−0.0074 (8)	−0.0056 (7)	−0.0070 (7)
N13	0.0278 (9)	0.0371 (10)	0.0245 (9)	−0.0071 (8)	−0.0057 (7)	−0.0070 (7)
C14	0.0240 (10)	0.0313 (11)	0.0233 (10)	−0.0012 (8)	−0.0061 (8)	−0.0072 (8)
N15	0.0230 (8)	0.0363 (10)	0.0195 (8)	−0.0042 (7)	−0.0045 (6)	−0.0064 (7)
C16	0.0256 (10)	0.0378 (12)	0.0203 (9)	−0.0037 (9)	−0.0050 (8)	−0.0098 (8)
C17	0.0283 (11)	0.0371 (12)	0.0218 (10)	−0.0023 (9)	−0.0053 (8)	−0.0087 (9)

C18	0.0333 (11)	0.0361 (12)	0.0232 (10)	−0.0044 (9)	−0.0072 (8)	−0.0050 (9)
C19	0.0299 (11)	0.0397 (12)	0.0228 (10)	−0.0078 (9)	−0.0018 (8)	−0.0073 (9)
C20	0.0257 (10)	0.0387 (12)	0.0257 (10)	−0.0033 (9)	−0.0047 (8)	−0.0110 (9)
C21	0.0285 (10)	0.0352 (11)	0.0212 (10)	−0.0038 (9)	−0.0073 (8)	−0.0075 (8)
O22	0.0337 (8)	0.0373 (9)	0.0283 (8)	−0.0020 (7)	−0.0040 (6)	−0.0011 (7)
C23	0.0394 (13)	0.0376 (12)	0.0298 (11)	0.0006 (10)	−0.0074 (9)	−0.0062 (10)
C24	0.0500 (14)	0.0345 (12)	0.0334 (12)	−0.0010 (11)	−0.0139 (10)	−0.0057 (10)
C25	0.0489 (15)	0.0410 (13)	0.0351 (13)	−0.0056 (11)	−0.0103 (11)	−0.0036 (10)
C26	0.0487 (15)	0.0431 (14)	0.0398 (13)	−0.0073 (11)	−0.0175 (11)	−0.0068 (11)
C27	0.0467 (14)	0.0410 (13)	0.0416 (13)	−0.0022 (11)	−0.0185 (11)	−0.0105 (11)
C28	0.0575 (17)	0.0440 (15)	0.0543 (16)	−0.0063 (13)	−0.0194 (13)	−0.0164 (12)
C29	0.0584 (18)	0.0559 (17)	0.0615 (18)	−0.0056 (14)	−0.0115 (14)	−0.0299 (15)
C30	0.062 (3)	0.049 (2)	0.047 (3)	−0.012 (2)	−0.0040 (19)	−0.015 (2)
C31	0.067 (3)	0.063 (3)	0.061 (3)	−0.024 (2)	0.012 (2)	−0.032 (2)
C32	0.058 (4)	0.063 (4)	0.092 (5)	−0.011 (3)	0.010 (4)	−0.047 (4)
C30A	0.081 (10)	0.054 (8)	0.048 (8)	−0.014 (7)	−0.022 (7)	−0.022 (7)
C31A	0.066 (9)	0.037 (6)	0.048 (7)	−0.010 (7)	0.002 (6)	−0.016 (5)
C32A	0.084 (13)	0.073 (11)	0.046 (8)	−0.031 (10)	0.013 (9)	−0.007 (7)
O33	0.0269 (7)	0.0352 (8)	0.0256 (7)	0.0001 (6)	−0.0042 (6)	−0.0068 (6)
C34	0.0262 (10)	0.0361 (12)	0.0282 (11)	0.0008 (9)	−0.0050 (8)	−0.0084 (9)
C35	0.0311 (11)	0.0380 (12)	0.0292 (11)	−0.0034 (9)	−0.0077 (9)	−0.0093 (9)
C36	0.0346 (12)	0.0377 (12)	0.0329 (12)	−0.0012 (10)	−0.0088 (9)	−0.0078 (10)
C37	0.0471 (14)	0.0399 (13)	0.0359 (13)	−0.0020 (11)	−0.0111 (11)	−0.0053 (10)
C38	0.0512 (15)	0.0396 (13)	0.0378 (13)	0.0027 (11)	−0.0148 (11)	−0.0094 (11)
C39	0.0601 (17)	0.0412 (14)	0.0387 (14)	0.0021 (12)	−0.0156 (12)	−0.0103 (11)
C40	0.0573 (17)	0.0372 (14)	0.0467 (15)	−0.0016 (12)	−0.0076 (12)	−0.0117 (11)
C41	0.089 (2)	0.0457 (16)	0.0416 (15)	0.0043 (16)	−0.0038 (15)	−0.0096 (13)
C42	0.081 (2)	0.0420 (16)	0.063 (2)	−0.0026 (15)	0.0127 (17)	−0.0165 (14)
C43	0.135 (6)	0.040 (3)	0.049 (2)	0.001 (3)	0.025 (3)	−0.009 (2)
C43A	0.135 (6)	0.040 (3)	0.049 (2)	0.001 (3)	0.025 (3)	−0.009 (2)
C44	0.0267 (10)	0.0357 (11)	0.0229 (10)	−0.0043 (9)	−0.0068 (8)	−0.0072 (8)
C45	0.0282 (11)	0.0329 (11)	0.0259 (10)	−0.0041 (9)	−0.0077 (8)	−0.0070 (8)
C46	0.0310 (11)	0.0390 (12)	0.0243 (10)	−0.0041 (9)	−0.0046 (8)	−0.0109 (9)
C47	0.0368 (12)	0.0435 (13)	0.0221 (10)	−0.0044 (10)	−0.0107 (9)	−0.0075 (9)
C48	0.0312 (11)	0.0381 (12)	0.0271 (11)	−0.0022 (9)	−0.0106 (9)	−0.0066 (9)
C49	0.0284 (11)	0.0396 (12)	0.0269 (11)	−0.0041 (9)	−0.0068 (8)	−0.0109 (9)
O50	0.0269 (7)	0.0381 (8)	0.0236 (7)	0.0010 (6)	−0.0054 (6)	−0.0085 (6)
C51	0.0284 (11)	0.0405 (12)	0.0245 (10)	0.0001 (9)	−0.0035 (8)	−0.0116 (9)
C52	0.0321 (11)	0.0397 (12)	0.0252 (10)	−0.0007 (10)	−0.0052 (9)	−0.0090 (9)
C53	0.0313 (11)	0.0390 (12)	0.0291 (11)	−0.0002 (10)	−0.0049 (9)	−0.0097 (9)
C54	0.0304 (11)	0.0411 (13)	0.0302 (11)	−0.0010 (10)	−0.0049 (9)	−0.0099 (10)
C55	0.0279 (11)	0.0454 (13)	0.0338 (12)	−0.0015 (10)	−0.0038 (9)	−0.0121 (10)
C56	0.0310 (12)	0.0454 (14)	0.0370 (12)	−0.0016 (10)	−0.0064 (9)	−0.0109 (10)
C57	0.0297 (12)	0.0525 (15)	0.0415 (13)	−0.0017 (11)	−0.0047 (10)	−0.0123 (11)
C58	0.0307 (12)	0.0601 (17)	0.0433 (14)	0.0020 (12)	−0.0048 (10)	−0.0173 (12)
C59	0.0349 (13)	0.0700 (19)	0.0470 (15)	0.0048 (13)	−0.0072 (11)	−0.0192 (14)
C60	0.0405 (16)	0.121 (3)	0.069 (2)	0.0270 (18)	−0.0146 (15)	−0.042 (2)
O61	0.0305 (8)	0.0548 (10)	0.0288 (8)	0.0056 (7)	−0.0134 (6)	−0.0131 (7)

C62	0.0297 (11)	0.0463 (13)	0.0306 (11)	0.0007 (10)	−0.0107 (9)	−0.0115 (10)
C63	0.0314 (12)	0.0460 (14)	0.0350 (12)	0.0003 (10)	−0.0129 (9)	−0.0105 (10)
C64	0.0334 (12)	0.0396 (13)	0.0350 (12)	−0.0011 (10)	−0.0138 (9)	−0.0078 (10)
C65	0.0346 (12)	0.0489 (14)	0.0389 (13)	0.0001 (11)	−0.0152 (10)	−0.0119 (11)
C66	0.0356 (12)	0.0432 (13)	0.0388 (13)	−0.0005 (10)	−0.0135 (10)	−0.0097 (10)
C67	0.0354 (12)	0.0458 (14)	0.0391 (13)	−0.0023 (11)	−0.0130 (10)	−0.0082 (11)
C68	0.0375 (13)	0.0507 (15)	0.0408 (13)	0.0013 (11)	−0.0114 (10)	−0.0147 (11)
C69	0.0380 (13)	0.0460 (14)	0.0374 (13)	−0.0034 (11)	−0.0092 (10)	−0.0109 (11)
C70	0.0407 (14)	0.0556 (16)	0.0404 (14)	−0.0041 (12)	−0.0046 (11)	−0.0206 (12)
C71	0.0461 (16)	0.107 (3)	0.0514 (17)	−0.0291 (17)	0.0035 (13)	−0.0332 (17)
C72	0.0277 (10)	0.0361 (11)	0.0216 (10)	−0.0094 (9)	−0.0049 (8)	−0.0053 (8)
C73	0.0290 (11)	0.0416 (12)	0.0213 (10)	−0.0075 (9)	−0.0033 (8)	−0.0098 (9)
C74	0.0260 (10)	0.0456 (13)	0.0252 (10)	−0.0079 (9)	−0.0025 (8)	−0.0088 (9)
C75	0.0299 (11)	0.0512 (14)	0.0265 (11)	−0.0108 (10)	−0.0073 (9)	−0.0097 (10)
C76	0.0346 (12)	0.0397 (12)	0.0260 (11)	−0.0084 (10)	−0.0086 (9)	−0.0087 (9)
C77	0.0302 (11)	0.0334 (11)	0.0237 (10)	−0.0074 (9)	−0.0034 (8)	−0.0052 (8)
O78	0.0255 (8)	0.0687 (12)	0.0310 (8)	−0.0022 (8)	−0.0072 (6)	−0.0184 (8)
C79	0.0295 (11)	0.0468 (14)	0.0309 (11)	−0.0070 (10)	−0.0094 (9)	−0.0077 (10)
C80	0.0316 (12)	0.0509 (14)	0.0346 (12)	−0.0060 (11)	−0.0081 (9)	−0.0125 (11)
C81	0.0312 (12)	0.0452 (13)	0.0367 (12)	−0.0067 (10)	−0.0096 (9)	−0.0098 (10)
C82	0.0342 (12)	0.0458 (14)	0.0367 (13)	−0.0050 (11)	−0.0071 (10)	−0.0102 (11)
C83	0.0353 (13)	0.0458 (14)	0.0398 (13)	−0.0049 (11)	−0.0106 (10)	−0.0083 (11)
C84	0.0387 (14)	0.0540 (16)	0.0485 (15)	0.0019 (12)	−0.0138 (11)	−0.0147 (12)
C85	0.0448 (15)	0.0572 (17)	0.0633 (18)	0.0073 (13)	−0.0216 (13)	−0.0168 (14)
C86	0.036 (3)	0.046 (4)	0.036 (3)	0.001 (3)	−0.002 (2)	−0.002 (3)
C87	0.034 (3)	0.058 (3)	0.033 (3)	−0.004 (2)	0.001 (2)	0.002 (3)
C88	0.038 (3)	0.085 (5)	0.042 (3)	0.008 (3)	−0.004 (2)	−0.004 (3)
C86A	0.036 (4)	0.052 (5)	0.056 (5)	−0.003 (3)	−0.018 (4)	−0.007 (4)
C87A	0.042 (3)	0.057 (4)	0.058 (4)	−0.004 (3)	−0.004 (3)	−0.017 (3)
C88A	0.044 (3)	0.063 (4)	0.050 (3)	0.007 (3)	−0.008 (3)	−0.013 (3)
O89	0.0327 (8)	0.0404 (9)	0.0261 (7)	−0.0012 (7)	−0.0081 (6)	−0.0137 (6)
C90	0.0382 (12)	0.0390 (12)	0.0260 (11)	−0.0041 (10)	−0.0092 (9)	−0.0129 (9)
C91	0.0361 (12)	0.0377 (12)	0.0299 (11)	−0.0042 (10)	−0.0081 (9)	−0.0133 (9)
C92	0.0363 (12)	0.0404 (13)	0.0308 (11)	−0.0058 (10)	−0.0056 (9)	−0.0141 (10)
C93	0.0375 (13)	0.0475 (14)	0.0351 (12)	−0.0066 (11)	−0.0066 (10)	−0.0160 (11)
C94	0.0378 (13)	0.0498 (14)	0.0348 (12)	−0.0110 (11)	−0.0017 (10)	−0.0182 (11)
C95	0.0389 (13)	0.0503 (15)	0.0376 (13)	−0.0076 (11)	−0.0012 (10)	−0.0202 (11)
C96	0.0413 (14)	0.0539 (15)	0.0391 (13)	−0.0102 (12)	−0.0012 (11)	−0.0221 (12)
C97	0.0428 (14)	0.0478 (15)	0.0402 (13)	−0.0082 (11)	0.0004 (11)	−0.0187 (11)
C98	0.0506 (16)	0.0573 (17)	0.0472 (15)	−0.0042 (13)	0.0000 (12)	−0.0265 (13)
C99	0.0625 (19)	0.0558 (18)	0.0542 (17)	0.0027 (15)	−0.0013 (14)	−0.0243 (14)

Geometric parameters (Å, º)

C1—N2	1.305 (3)	C54—H54B	0.9900
C1—N5	1.397 (2)	C55—C56	1.517 (3)
C1—C16	1.468 (3)	C55—H55A	0.9900
N2—N3	1.398 (2)	C55—H55B	0.9900

N3—C4	1.289 (2)	C56—C57	1.521 (3)
C4—N5	1.376 (2)	C56—H56A	0.9900
C4—N15	1.394 (2)	C56—H56B	0.9900
N5—C9	1.398 (2)	C57—C58	1.519 (3)
C6—N7	1.312 (3)	C57—H57A	0.9900
C6—N10	1.394 (3)	C57—H57B	0.9900
C6—C44	1.470 (3)	C58—C59	1.523 (3)
N7—N8	1.406 (2)	C58—H58A	0.9900
N8—C9	1.283 (3)	C58—H58B	0.9900
C9—N10	1.384 (2)	C59—C60	1.525 (4)
N10—C14	1.394 (3)	C59—H59A	0.9900
C11—N12	1.305 (3)	C59—H59B	0.9900
C11—N15	1.393 (3)	C60—H60A	0.9800
C11—C72	1.468 (3)	C60—H60B	0.9800
N12—N13	1.409 (2)	C60—H60C	0.9800
N13—C14	1.297 (3)	O61—C62	1.429 (3)
C14—N15	1.368 (2)	C62—C63	1.512 (3)
C16—C21	1.390 (3)	C62—H62A	0.9900
C16—C17	1.403 (3)	C62—H62B	0.9900
C17—C18	1.386 (3)	C63—C64	1.520 (3)
C17—H17	0.9500	C63—H63A	0.9900
C18—O22	1.373 (3)	C63—H63B	0.9900
C18—C19	1.385 (3)	C64—C65	1.523 (3)
C19—C20	1.380 (3)	C64—H64A	0.9900
C19—H19	0.9500	C64—H64B	0.9900
C20—C21	1.399 (3)	C65—C66	1.517 (3)
C20—H20	0.9500	C65—H65A	0.9900
C21—O33	1.365 (2)	C65—H65B	0.9900
O22—C23	1.436 (3)	C66—C67	1.523 (3)
C23—C24	1.517 (3)	C66—H66A	0.9900
C23—H23A	0.9900	C66—H66B	0.9900
C23—H23B	0.9900	C67—C68	1.524 (3)
C24—C25	1.523 (4)	C67—H67A	0.9900
C24—H24A	0.9900	C67—H67B	0.9900
C24—H24B	0.9900	C68—C69	1.519 (3)
C25—C26	1.525 (3)	C68—H68A	0.9900
C25—H25A	0.9900	C68—H68B	0.9900
C25—H25B	0.9900	C69—C70	1.518 (3)
C26—C27	1.523 (3)	C69—H69A	0.9900
C26—H26A	0.9900	C69—H69B	0.9900
C26—H26B	0.9900	C70—C71	1.516 (4)
C27—C28	1.517 (3)	C70—H70A	0.9900
C27—H27A	0.9900	C70—H70B	0.9900
C27—H27B	0.9900	C71—H71A	0.9800
C28—C29	1.520 (4)	C71—H71B	0.9800
C28—H28A	0.9900	C71—H71C	0.9800
C28—H28B	0.9900	C72—C73	1.387 (3)
C29—C30A	1.328 (14)	C72—C77	1.404 (3)

C29—C30	1.578 (5)	C73—C74	1.394 (3)
C29—H29A	0.9900	C73—H73	0.9500
C29—H29B	0.9900	C74—O78	1.371 (3)
C29—H29C	0.9900	C74—C75	1.387 (3)
C29—H29D	0.9900	C75—C76	1.398 (3)
C30—C31	1.517 (5)	C75—H75	0.9500
C30—H30A	0.9900	C76—C77	1.381 (3)
C30—H30B	0.9900	C76—H76	0.9500
C31—C32	1.506 (8)	C77—O89	1.367 (2)
C31—H31A	0.9900	O78—C79	1.431 (2)
C31—H31B	0.9900	C79—C80	1.508 (3)
C32—H32A	0.9800	C79—H79A	0.9900
C32—H32B	0.9800	C79—H79B	0.9900
C32—H32C	0.9800	C80—C81	1.524 (3)
C30A—C31A	1.52 (2)	C80—H80A	0.9900
C30A—H30C	0.9900	C80—H80B	0.9900
C30A—H30D	0.9900	C81—C82	1.525 (3)
C31A—C32A	1.53 (2)	C81—H81A	0.9900
C31A—H31C	0.9900	C81—H81B	0.9900
C31A—H31D	0.9900	C82—C83	1.522 (3)
C32A—H32D	0.9800	C82—H82A	0.9900
C32A—H32E	0.9800	C82—H82B	0.9900
C32A—H32F	0.9800	C83—C84	1.524 (3)
O33—C34	1.437 (2)	C83—H83A	0.9900
C34—C35	1.504 (3)	C83—H83B	0.9900
C34—H34A	0.9900	C84—C85	1.526 (3)
C34—H34B	0.9900	C84—H84A	0.9900
C35—C36	1.528 (3)	C84—H84B	0.9900
C35—H35A	0.9900	C85—C86	1.460 (7)
C35—H35B	0.9900	C85—C86A	1.665 (8)
C36—C37	1.516 (3)	C85—H85A	0.9900
C36—H36A	0.9900	C85—H85B	0.9900
C36—H36B	0.9900	C85—H85C	0.9900
C37—C38	1.530 (3)	C85—H85D	0.9900
C37—H37A	0.9900	C86—C87	1.536 (8)
C37—H37B	0.9900	C86—H86A	0.9900
C38—C39	1.518 (3)	C86—H86B	0.9900
C38—H38A	0.9900	C87—C88	1.493 (8)
C38—H38B	0.9900	C87—H87A	0.9900
C39—C40	1.522 (3)	C87—H87B	0.9900
C39—H39A	0.9900	C88—H88A	0.9800
C39—H39B	0.9900	C88—H88B	0.9800
C40—C41	1.513 (4)	C88—H88C	0.9800
C40—H40A	0.9900	C86A—C87A	1.480 (9)
C40—H40B	0.9900	C86A—H86C	0.9900
C41—C42	1.517 (4)	C86A—H86D	0.9900
C41—H41A	0.9900	C87A—C88A	1.540 (7)
C41—H41B	0.9900	C87A—H87C	0.9900

C42—C43A	1.49 (3)	C87A—H87D	0.9900
C42—C43	1.543 (7)	C88A—H88D	0.9800
C42—H42A	0.9900	C88A—H88E	0.9800
C42—H42B	0.9900	C88A—H88F	0.9800
C42—H42C	0.9900	O89—C90	1.440 (2)
C42—H42D	0.9900	C90—C91	1.506 (3)
C43—H43A	0.9800	C90—H90A	0.9900
C43—H43B	0.9800	C90—H90B	0.9900
C43—H43C	0.9800	C91—C92	1.526 (3)
C43A—H43D	0.9800	C91—H91A	0.9900
C43A—H43E	0.9800	C91—H91B	0.9900
C43A—H43F	0.9800	C92—C93	1.520 (3)
C44—C45	1.399 (3)	C92—H92A	0.9900
C44—C49	1.402 (3)	C92—H92B	0.9900
C45—O50	1.365 (2)	C93—C94	1.522 (3)
C45—C46	1.390 (3)	C93—H93A	0.9900
C46—C47	1.381 (3)	C93—H93B	0.9900
C46—H46	0.9500	C94—C95	1.527 (3)
C47—C48	1.387 (3)	C94—H94A	0.9900
C47—H47	0.9500	C94—H94B	0.9900
C48—O61	1.376 (2)	C95—C96	1.528 (3)
C48—C49	1.380 (3)	C95—H95A	0.9900
C49—H49	0.9500	C95—H95B	0.9900
O50—C51	1.437 (2)	C96—C97	1.522 (3)
C51—C52	1.505 (3)	C96—H96A	0.9900
C51—H51A	0.9900	C96—H96B	0.9900
C51—H51B	0.9900	C97—C98	1.523 (3)
C52—C53	1.523 (3)	C97—H97A	0.9900
C52—H52A	0.9900	C97—H97B	0.9900
C52—H52B	0.9900	C98—C99	1.525 (4)
C53—C54	1.521 (3)	C98—H98A	0.9900
C53—H53A	0.9900	C98—H98B	0.9900
C53—H53B	0.9900	C99—H99A	0.9800
C54—C55	1.519 (3)	C99—H99B	0.9800
C54—H54A	0.9900	C99—H99C	0.9800

N2—C1—N5	109.10 (17)	H55A—C55—H55B	107.7
N2—C1—C16	122.36 (17)	C55—C56—C57	113.1 (2)
N5—C1—C16	128.54 (18)	C55—C56—H56A	109.0
C1—N2—N3	109.46 (16)	C57—C56—H56A	109.0
C4—N3—N2	105.11 (16)	C55—C56—H56B	109.0
N3—C4—N5	113.41 (17)	C57—C56—H56B	109.0
N3—C4—N15	129.69 (18)	H56A—C56—H56B	107.8
N5—C4—N15	116.89 (17)	C58—C57—C56	113.5 (2)
C4—N5—C1	102.91 (16)	C58—C57—H57A	108.9
C4—N5—C9	121.42 (16)	C56—C57—H57A	108.9
C1—N5—C9	133.25 (18)	C58—C57—H57B	108.9
N7—C6—N10	109.25 (17)	C56—C57—H57B	108.9

N7—C6—C44	123.10 (18)	H57A—C57—H57B	107.7
N10—C6—C44	127.62 (18)	C57—C58—C59	113.3 (2)
C6—N7—N8	108.79 (16)	C57—C58—H58A	108.9
C9—N8—N7	105.78 (16)	C59—C58—H58A	108.9
N8—C9—N10	112.99 (17)	C57—C58—H58B	108.9
N8—C9—N5	129.50 (18)	C59—C58—H58B	108.9
N10—C9—N5	117.38 (17)	H58A—C58—H58B	107.7
C9—N10—C14	122.13 (17)	C58—C59—C60	112.7 (2)
C9—N10—C6	103.19 (16)	C58—C59—H59A	109.1
C14—N10—C6	134.56 (17)	C60—C59—H59A	109.1
N12—C11—N15	108.64 (18)	C58—C59—H59B	109.1
N12—C11—C72	128.24 (19)	C60—C59—H59B	109.1
N15—C11—C72	123.07 (17)	H59A—C59—H59B	107.8
C11—N12—N13	109.13 (17)	C59—C60—H60A	109.5
C14—N13—N12	105.55 (16)	C59—C60—H60B	109.5
N13—C14—N15	112.11 (18)	H60A—C60—H60B	109.5
N13—C14—N10	131.11 (18)	C59—C60—H60C	109.5
N15—C14—N10	116.75 (17)	H60A—C60—H60C	109.5
C14—N15—C11	104.56 (16)	H60B—C60—H60C	109.5
C14—N15—C4	122.96 (17)	C48—O61—C62	117.73 (16)
C11—N15—C4	132.38 (17)	O61—C62—C63	108.25 (17)
C21—C16—C17	120.58 (19)	O61—C62—H62A	110.0
C21—C16—C1	122.69 (19)	C63—C62—H62A	110.0
C17—C16—C1	116.16 (18)	O61—C62—H62B	110.0
C18—C17—C16	120.10 (19)	C63—C62—H62B	110.0
C18—C17—H17	119.9	H62A—C62—H62B	108.4
C16—C17—H17	119.9	C62—C63—C64	111.60 (18)
O22—C18—C19	116.82 (19)	C62—C63—H63A	109.3
O22—C18—C17	124.35 (19)	C64—C63—H63A	109.3
C19—C18—C17	118.8 (2)	C62—C63—H63B	109.3
C20—C19—C18	121.7 (2)	C64—C63—H63B	109.3
C20—C19—H19	119.2	H63A—C63—H63B	108.0
C18—C19—H19	119.2	C63—C64—C65	113.92 (19)
C19—C20—C21	119.93 (19)	C63—C64—H64A	108.8
C19—C20—H20	120.0	C65—C64—H64A	108.8
C21—C20—H20	120.0	C63—C64—H64B	108.8
O33—C21—C16	116.47 (18)	C65—C64—H64B	108.8
O33—C21—C20	124.68 (18)	H64A—C64—H64B	107.7
C16—C21—C20	118.79 (19)	C66—C65—C64	113.89 (19)
C18—O22—C23	116.80 (17)	C66—C65—H65A	108.8
O22—C23—C24	107.91 (18)	C64—C65—H65A	108.8
O22—C23—H23A	110.1	C66—C65—H65B	108.8
C24—C23—H23A	110.1	C64—C65—H65B	108.8
O22—C23—H23B	110.1	H65A—C65—H65B	107.7
C24—C23—H23B	110.1	C65—C66—C67	114.3 (2)
H23A—C23—H23B	108.4	C65—C66—H66A	108.7
C23—C24—C25	114.7 (2)	C67—C66—H66A	108.7
C23—C24—H24A	108.6	C65—C66—H66B	108.7

C25—C24—H24A	108.6	C67—C66—H66B	108.7
C23—C24—H24B	108.6	H66A—C66—H66B	107.6
C25—C24—H24B	108.6	C66—C67—C68	113.7 (2)
H24A—C24—H24B	107.6	C66—C67—H67A	108.8
C24—C25—C26	114.9 (2)	C68—C67—H67A	108.8
C24—C25—H25A	108.5	C66—C67—H67B	108.8
C26—C25—H25A	108.5	C68—C67—H67B	108.8
C24—C25—H25B	108.5	H67A—C67—H67B	107.7
C26—C25—H25B	108.5	C69—C68—C67	114.6 (2)
H25A—C25—H25B	107.5	C69—C68—H68A	108.6
C27—C26—C25	114.7 (2)	C67—C68—H68A	108.6
C27—C26—H26A	108.6	C69—C68—H68B	108.6
C25—C26—H26A	108.6	C67—C68—H68B	108.6
C27—C26—H26B	108.6	H68A—C68—H68B	107.6
C25—C26—H26B	108.6	C70—C69—C68	114.0 (2)
H26A—C26—H26B	107.6	C70—C69—H69A	108.8
C28—C27—C26	111.9 (2)	C68—C69—H69A	108.8
C28—C27—H27A	109.2	C70—C69—H69B	108.8
C26—C27—H27A	109.2	C68—C69—H69B	108.8
C28—C27—H27B	109.2	H69A—C69—H69B	107.7
C26—C27—H27B	109.2	C71—C70—C69	113.1 (2)
H27A—C27—H27B	107.9	C71—C70—H70A	109.0
C27—C28—C29	115.9 (2)	C69—C70—H70A	109.0
C27—C28—H28A	108.3	C71—C70—H70B	109.0
C29—C28—H28A	108.3	C69—C70—H70B	109.0
C27—C28—H28B	108.3	H70A—C70—H70B	107.8
C29—C28—H28B	108.3	C70—C71—H71A	109.5
H28A—C28—H28B	107.4	C70—C71—H71B	109.5
C30A—C29—C28	135.2 (7)	H71A—C71—H71B	109.5
C28—C29—C30	108.8 (3)	C70—C71—H71C	109.5
C28—C29—H29A	109.9	H71A—C71—H71C	109.5
C30—C29—H29A	109.9	H71B—C71—H71C	109.5
C28—C29—H29B	109.9	C73—C72—C77	120.01 (19)
C30—C29—H29B	109.9	C73—C72—C11	121.17 (18)
H29A—C29—H29B	108.3	C77—C72—C11	118.81 (18)
C30A—C29—H29C	103.4	C72—C73—C74	120.19 (19)
C28—C29—H29C	103.4	C72—C73—H73	119.9
C30A—C29—H29D	103.4	C74—C73—H73	119.9
C28—C29—H29D	103.4	O78—C74—C75	124.98 (19)
H29C—C29—H29D	105.2	O78—C74—C73	115.34 (19)
C31—C30—C29	112.9 (3)	C75—C74—C73	119.68 (19)
C31—C30—H30A	109.0	C74—C75—C76	120.2 (2)
C29—C30—H30A	109.0	C74—C75—H75	119.9
C31—C30—H30B	109.0	C76—C75—H75	119.9
C29—C30—H30B	109.0	C77—C76—C75	120.2 (2)
H30A—C30—H30B	107.8	C77—C76—H76	119.9
C32—C31—C30	114.3 (4)	C75—C76—H76	119.9
C32—C31—H31A	108.7	O89—C77—C76	125.53 (19)

C30—C31—H31A	108.7	O89—C77—C72	114.79 (18)
C32—C31—H31B	108.7	C76—C77—C72	119.67 (19)
C30—C31—H31B	108.7	C74—O78—C79	118.38 (17)
H31A—C31—H31B	107.6	O78—C79—C80	107.91 (18)
C31—C32—H32A	109.5	O78—C79—H79A	110.1
C31—C32—H32B	109.5	C80—C79—H79A	110.1
H32A—C32—H32B	109.5	O78—C79—H79B	110.1
C31—C32—H32C	109.5	C80—C79—H79B	110.1
H32A—C32—H32C	109.5	H79A—C79—H79B	108.4
H32B—C32—H32C	109.5	C79—C80—C81	111.52 (19)
C29—C30A—C31A	121.7 (12)	C79—C80—H80A	109.3
C29—C30A—H30C	106.9	C81—C80—H80A	109.3
C31A—C30A—H30C	106.9	C79—C80—H80B	109.3
C29—C30A—H30D	106.9	C81—C80—H80B	109.3
C31A—C30A—H30D	106.9	H80A—C80—H80B	108.0
H30C—C30A—H30D	106.7	C80—C81—C82	113.56 (19)
C30A—C31A—C32A	116.1 (14)	C80—C81—H81A	108.9
C30A—C31A—H31C	108.3	C82—C81—H81A	108.9
C32A—C31A—H31C	108.3	C80—C81—H81B	108.9
C30A—C31A—H31D	108.3	C82—C81—H81B	108.9
C32A—C31A—H31D	108.3	H81A—C81—H81B	107.7
H31C—C31A—H31D	107.4	C83—C82—C81	112.90 (19)
C31A—C32A—H32D	109.5	C83—C82—H82A	109.0
C31A—C32A—H32E	109.5	C81—C82—H82A	109.0
H32D—C32A—H32E	109.5	C83—C82—H82B	109.0
C31A—C32A—H32F	109.5	C81—C82—H82B	109.0
H32D—C32A—H32F	109.5	H82A—C82—H82B	107.8
H32E—C32A—H32F	109.5	C82—C83—C84	113.6 (2)
C21—O33—C34	117.00 (16)	C82—C83—H83A	108.8
O33—C34—C35	108.58 (16)	C84—C83—H83A	108.8
O33—C34—H34A	110.0	C82—C83—H83B	108.8
C35—C34—H34A	110.0	C84—C83—H83B	108.8
O33—C34—H34B	110.0	H83A—C83—H83B	107.7
C35—C34—H34B	110.0	C83—C84—C85	112.5 (2)
H34A—C34—H34B	108.4	C83—C84—H84A	109.1
C34—C35—C36	111.03 (18)	C85—C84—H84A	109.1
C34—C35—H35A	109.4	C83—C84—H84B	109.1
C36—C35—H35A	109.4	C85—C84—H84B	109.1
C34—C35—H35B	109.4	H84A—C84—H84B	107.8
C36—C35—H35B	109.4	C86—C85—C84	118.2 (3)
H35A—C35—H35B	108.0	C84—C85—C86A	109.6 (3)
C37—C36—C35	112.88 (19)	C86—C85—H85A	107.8
C37—C36—H36A	109.0	C84—C85—H85A	107.8
C35—C36—H36A	109.0	C86—C85—H85B	107.8
C37—C36—H36B	109.0	C84—C85—H85B	107.8
C35—C36—H36B	109.0	H85A—C85—H85B	107.1
H36A—C36—H36B	107.8	C84—C85—H85C	109.7
C36—C37—C38	114.4 (2)	C86A—C85—H85C	109.7

C36—C37—H37A	108.7	C84—C85—H85D	109.7
C38—C37—H37A	108.7	C86A—C85—H85D	109.7
C36—C37—H37B	108.7	H85C—C85—H85D	108.2
C38—C37—H37B	108.7	C85—C86—C87	107.7 (5)
H37A—C37—H37B	107.6	C85—C86—H86A	110.2
C39—C38—C37	115.9 (2)	C87—C86—H86A	110.2
C39—C38—H38A	108.3	C85—C86—H86B	110.2
C37—C38—H38A	108.3	C87—C86—H86B	110.2
C39—C38—H38B	108.3	H86A—C86—H86B	108.5
C37—C38—H38B	108.3	C88—C87—C86	113.3 (5)
H38A—C38—H38B	107.4	C88—C87—H87A	108.9
C38—C39—C40	112.4 (2)	C86—C87—H87A	108.9
C38—C39—H39A	109.1	C88—C87—H87B	108.9
C40—C39—H39A	109.1	C86—C87—H87B	108.9
C38—C39—H39B	109.1	H87A—C87—H87B	107.7
C40—C39—H39B	109.1	C87—C88—H88A	109.5
H39A—C39—H39B	107.9	C87—C88—H88B	109.5
C41—C40—C39	115.7 (2)	H88A—C88—H88B	109.5
C41—C40—H40A	108.3	C87—C88—H88C	109.5
C39—C40—H40A	108.3	H88A—C88—H88C	109.5
C41—C40—H40B	108.3	H88B—C88—H88C	109.5
C39—C40—H40B	108.3	C87A—C86A—C85	113.3 (5)
H40A—C40—H40B	107.4	C87A—C86A—H86C	108.9
C40—C41—C42	113.8 (3)	C85—C86A—H86C	108.9
C40—C41—H41A	108.8	C87A—C86A—H86D	108.9
C42—C41—H41A	108.8	C85—C86A—H86D	108.9
C40—C41—H41B	108.8	H86C—C86A—H86D	107.7
C42—C41—H41B	108.8	C86A—C87A—C88A	111.5 (6)
H41A—C41—H41B	107.7	C86A—C87A—H87C	109.3
C43A—C42—C41	127.0 (19)	C88A—C87A—H87C	109.3
C41—C42—C43	112.2 (5)	C86A—C87A—H87D	109.3
C41—C42—H42A	109.2	C88A—C87A—H87D	109.3
C43—C42—H42A	109.2	H87C—C87A—H87D	108.0
C41—C42—H42B	109.2	C87A—C88A—H88D	109.5
C43—C42—H42B	109.2	C87A—C88A—H88E	109.5
H42A—C42—H42B	107.9	H88D—C88A—H88E	109.5
C43A—C42—H42C	105.6	C87A—C88A—H88F	109.5
C41—C42—H42C	105.6	H88D—C88A—H88F	109.5
C43A—C42—H42D	105.6	H88E—C88A—H88F	109.5
C41—C42—H42D	105.6	C77—O89—C90	117.76 (16)
H42C—C42—H42D	106.1	O89—C90—C91	107.10 (17)
C42—C43—H43A	109.5	O89—C90—H90A	110.3
C42—C43—H43B	109.5	C91—C90—H90A	110.3
H43A—C43—H43B	109.5	O89—C90—H90B	110.3
C42—C43—H43C	109.5	C91—C90—H90B	110.3
H43A—C43—H43C	109.5	H90A—C90—H90B	108.5
H43B—C43—H43C	109.5	C90—C91—C92	112.75 (18)
C42—C43A—H43D	109.5	C90—C91—H91A	109.0

C42—C43A—H43E	109.5	C92—C91—H91A	109.0
H43D—C43A—H43E	109.5	C90—C91—H91B	109.0
C42—C43A—H43F	109.5	C92—C91—H91B	109.0
H43D—C43A—H43F	109.5	H91A—C91—H91B	107.8
H43E—C43A—H43F	109.5	C93—C92—C91	111.59 (19)
C45—C44—C49	120.15 (18)	C93—C92—H92A	109.3
C45—C44—C6	121.41 (18)	C91—C92—H92A	109.3
C49—C44—C6	118.09 (18)	C93—C92—H92B	109.3
O50—C45—C46	124.83 (19)	C91—C92—H92B	109.3
O50—C45—C44	116.26 (17)	H92A—C92—H92B	108.0
C46—C45—C44	118.82 (19)	C92—C93—C94	115.1 (2)
C47—C46—C45	120.60 (19)	C92—C93—H93A	108.5
C47—C46—H46	119.7	C94—C93—H93A	108.5
C45—C46—H46	119.7	C92—C93—H93B	108.5
C46—C47—C48	120.61 (19)	C94—C93—H93B	108.5
C46—C47—H47	119.7	H93A—C93—H93B	107.5
C48—C47—H47	119.7	C93—C94—C95	112.6 (2)
O61—C48—C49	124.55 (19)	C93—C94—H94A	109.1
O61—C48—C47	115.72 (18)	C95—C94—H94A	109.1
C49—C48—C47	119.7 (2)	C93—C94—H94B	109.1
C48—C49—C44	120.0 (2)	C95—C94—H94B	109.1
C48—C49—H49	120.0	H94A—C94—H94B	107.8
C44—C49—H49	120.0	C94—C95—C96	114.4 (2)
C45—O50—C51	117.22 (15)	C94—C95—H95A	108.7
O50—C51—C52	107.91 (16)	C96—C95—H95A	108.7
O50—C51—H51A	110.1	C94—C95—H95B	108.7
C52—C51—H51A	110.1	C96—C95—H95B	108.7
O50—C51—H51B	110.1	H95A—C95—H95B	107.6
C52—C51—H51B	110.1	C97—C96—C95	113.1 (2)
H51A—C51—H51B	108.4	C97—C96—H96A	109.0
C51—C52—C53	111.75 (17)	C95—C96—H96A	109.0
C51—C52—H52A	109.3	C97—C96—H96B	109.0
C53—C52—H52A	109.3	C95—C96—H96B	109.0
C51—C52—H52B	109.3	H96A—C96—H96B	107.8
C53—C52—H52B	109.3	C96—C97—C98	113.4 (2)
H52A—C52—H52B	107.9	C96—C97—H97A	108.9
C54—C53—C52	113.06 (18)	C98—C97—H97A	108.9
C54—C53—H53A	109.0	C96—C97—H97B	108.9
C52—C53—H53A	109.0	C98—C97—H97B	108.9
C54—C53—H53B	109.0	H97A—C97—H97B	107.7
C52—C53—H53B	109.0	C97—C98—C99	112.7 (2)
H53A—C53—H53B	107.8	C97—C98—H98A	109.1
C55—C54—C53	113.12 (18)	C99—C98—H98A	109.1
C55—C54—H54A	109.0	C97—C98—H98B	109.1
C53—C54—H54A	109.0	C99—C98—H98B	109.1
C55—C54—H54B	109.0	H98A—C98—H98B	107.8
C53—C54—H54B	109.0	C98—C99—H99A	109.5
H54A—C54—H54B	107.8	C98—C99—H99B	109.5

C56—C55—C54	113.57 (19)	H99A—C99—H99B	109.5
C56—C55—H55A	108.9	C98—C99—H99C	109.5
C54—C55—H55A	108.9	H99A—C99—H99C	109.5
C56—C55—H55B	108.9	H99B—C99—H99C	109.5
C54—C55—H55B	108.9		

N5—C1—N2—N3	0.7 (2)	C36—C37—C38—C39	−65.1 (3)
C16—C1—N2—N3	−178.82 (19)	C37—C38—C39—C40	179.7 (2)
C1—N2—N3—C4	−0.7 (2)	C38—C39—C40—C41	−179.8 (3)
N2—N3—C4—N5	0.5 (2)	C39—C40—C41—C42	172.4 (3)
N2—N3—C4—N15	−178.8 (2)	C40—C41—C42—C43A	−159 (3)
N3—C4—N5—C1	−0.1 (2)	C40—C41—C42—C43	172.9 (5)
N15—C4—N5—C1	179.28 (18)	N7—C6—C44—C45	131.4 (2)
N3—C4—N5—C9	164.40 (19)	N10—C6—C44—C45	−46.3 (3)
N15—C4—N5—C9	−16.2 (3)	N7—C6—C44—C49	−41.9 (3)
N2—C1—N5—C4	−0.3 (2)	N10—C6—C44—C49	140.5 (2)
C16—C1—N5—C4	179.1 (2)	C49—C44—C45—O50	172.4 (2)
N2—C1—N5—C9	−162.1 (2)	C6—C44—C45—O50	−0.7 (3)
C16—C1—N5—C9	17.3 (4)	C49—C44—C45—C46	−4.1 (3)
N10—C6—N7—N8	0.0 (2)	C6—C44—C45—C46	−177.2 (2)
C44—C6—N7—N8	−177.99 (19)	O50—C45—C46—C47	−173.0 (2)
C6—N7—N8—C9	0.4 (2)	C44—C45—C46—C47	3.2 (3)
N7—N8—C9—N10	−0.7 (2)	C45—C46—C47—C48	−0.4 (4)
N7—N8—C9—N5	175.0 (2)	C46—C47—C48—O61	177.8 (2)
C4—N5—C9—N8	−169.0 (2)	C46—C47—C48—C49	−1.6 (4)
C1—N5—C9—N8	−9.9 (4)	O61—C48—C49—C44	−178.7 (2)
C4—N5—C9—N10	6.6 (3)	C47—C48—C49—C44	0.7 (4)
C1—N5—C9—N10	165.7 (2)	C45—C44—C49—C48	2.2 (3)
N8—C9—N10—C14	−175.77 (19)	C6—C44—C49—C48	175.5 (2)
N5—C9—N10—C14	8.0 (3)	C46—C45—O50—C51	−22.1 (3)
N8—C9—N10—C6	0.7 (2)	C44—C45—O50—C51	161.55 (19)
N5—C9—N10—C6	−175.52 (18)	C45—O50—C51—C52	−168.23 (19)
N7—C6—N10—C9	−0.4 (2)	O50—C51—C52—C53	−178.00 (19)
C44—C6—N10—C9	177.5 (2)	C51—C52—C53—C54	−174.9 (2)
N7—C6—N10—C14	175.4 (2)	C52—C53—C54—C55	−173.6 (2)
C44—C6—N10—C14	−6.7 (4)	C53—C54—C55—C56	180.0 (2)
N15—C11—N12—N13	−0.9 (2)	C54—C55—C56—C57	−174.5 (2)
C72—C11—N12—N13	176.7 (2)	C55—C56—C57—C58	177.4 (2)
C11—N12—N13—C14	0.7 (2)	C56—C57—C58—C59	179.3 (2)
N12—N13—C14—N15	−0.3 (2)	C57—C58—C59—C60	178.6 (3)
N12—N13—C14—N10	−178.3 (2)	C49—C48—O61—C62	9.2 (3)
C9—N10—C14—N13	166.1 (2)	C47—C48—O61—C62	−170.2 (2)
C6—N10—C14—N13	−9.1 (4)	C48—O61—C62—C63	170.5 (2)
C9—N10—C14—N15	−11.8 (3)	O61—C62—C63—C64	−178.7 (2)
C6—N10—C14—N15	173.0 (2)	C62—C63—C64—C65	178.3 (2)
N13—C14—N15—C11	−0.2 (2)	C63—C64—C65—C66	−175.1 (2)
N10—C14—N15—C11	178.10 (18)	C64—C65—C66—C67	167.6 (2)
N13—C14—N15—C4	−176.90 (19)	C65—C66—C67—C68	−164.4 (2)

N10—C14—N15—C4	1.4 (3)	C66—C67—C68—C69	171.7 (2)
N12—C11—N15—C14	0.7 (2)	C67—C68—C69—C70	−165.8 (2)
C72—C11—N15—C14	−177.04 (19)	C68—C69—C70—C71	177.5 (2)
N12—C11—N15—C4	176.9 (2)	N12—C11—C72—C73	58.8 (3)
C72—C11—N15—C4	−0.8 (3)	N15—C11—C72—C73	−124.0 (2)
N3—C4—N15—C14	−168.5 (2)	N12—C11—C72—C77	−122.3 (2)
N5—C4—N15—C14	12.2 (3)	N15—C11—C72—C77	54.9 (3)
N3—C4—N15—C11	15.8 (4)	C77—C72—C73—C74	−0.9 (3)
N5—C4—N15—C11	−163.5 (2)	C11—C72—C73—C74	177.9 (2)
N2—C1—C16—C21	−131.5 (2)	C72—C73—C74—O78	178.7 (2)
N5—C1—C16—C21	49.1 (3)	C72—C73—C74—C75	−0.8 (3)
N2—C1—C16—C17	39.8 (3)	O78—C74—C75—C76	−177.8 (2)
N5—C1—C16—C17	−139.5 (2)	C73—C74—C75—C76	1.7 (4)
C21—C16—C17—C18	−1.4 (3)	C74—C75—C76—C77	−0.8 (3)
C1—C16—C17—C18	−172.93 (19)	C75—C76—C77—O89	178.0 (2)
C16—C17—C18—O22	178.3 (2)	C75—C76—C77—C72	−0.9 (3)
C16—C17—C18—C19	−1.0 (3)	C73—C72—C77—O89	−177.25 (19)
O22—C18—C19—C20	−177.7 (2)	C11—C72—C77—O89	3.9 (3)
C17—C18—C19—C20	1.7 (3)	C73—C72—C77—C76	1.8 (3)
C18—C19—C20—C21	0.0 (3)	C11—C72—C77—C76	−177.1 (2)
C17—C16—C21—O33	−174.18 (19)	C75—C74—O78—C79	−14.6 (3)
C1—C16—C21—O33	−3.2 (3)	C73—C74—O78—C79	165.9 (2)
C17—C16—C21—C20	3.1 (3)	C74—O78—C79—C80	−175.4 (2)
C1—C16—C21—C20	174.09 (19)	O78—C79—C80—C81	171.8 (2)
C19—C20—C21—O33	174.6 (2)	C79—C80—C81—C82	178.9 (2)
C19—C20—C21—C16	−2.4 (3)	C80—C81—C82—C83	176.5 (2)
C19—C18—O22—C23	166.5 (2)	C81—C82—C83—C84	−178.8 (2)
C17—C18—O22—C23	−12.8 (3)	C82—C83—C84—C85	175.0 (2)
C18—O22—C23—C24	−168.64 (19)	C83—C84—C85—C86	−168.0 (4)
O22—C23—C24—C25	−61.9 (3)	C83—C84—C85—C86A	164.6 (3)
C23—C24—C25—C26	−65.5 (3)	C84—C85—C86—C87	−69.0 (6)
C24—C25—C26—C27	−57.6 (3)	C85—C86—C87—C88	−175.1 (5)
C25—C26—C27—C28	−165.6 (2)	C84—C85—C86A—C87A	66.8 (6)
C26—C27—C28—C29	−174.8 (2)	C85—C86A—C87A—C88A	172.0 (5)
C27—C28—C29—C30A	43.4 (10)	C76—C77—O89—C90	10.6 (3)
C27—C28—C29—C30	70.1 (3)	C72—C77—O89—C90	−170.46 (19)
C28—C29—C30—C31	163.3 (3)	C77—O89—C90—C91	171.02 (18)
C29—C30—C31—C32	67.2 (5)	O89—C90—C91—C92	173.24 (19)
C28—C29—C30A—C31A	−168.3 (8)	C90—C91—C92—C93	−173.7 (2)
C29—C30A—C31A—C32A	−173.1 (13)	C91—C92—C93—C94	174.8 (2)
C16—C21—O33—C34	−178.75 (18)	C92—C93—C94—C95	−170.6 (2)
C20—C21—O33—C34	4.1 (3)	C93—C94—C95—C96	−177.0 (2)
C21—O33—C34—C35	174.17 (18)	C94—C95—C96—C97	−173.7 (2)
O33—C34—C35—C36	177.35 (18)	C95—C96—C97—C98	−176.5 (2)
C34—C35—C36—C37	−173.9 (2)	C96—C97—C98—C99	179.9 (2)
C35—C36—C37—C38	−171.5 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···N7^{i}	0.95	2.42	3.357 (3)	167
C34—H34*A*···N8^{i}	0.99	2.62	3.398 (3)	136
C47—H47···O78^{ii}	0.95	2.53	3.460 (3)	167
C76—H76···N2^{iii}	0.95	2.66	3.593 (3)	167
C90—H90*A*···N2^{iii}	0.99	2.67	3.186 (3)	113

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) −*x*+1, −*y*+1, −*z*+1.