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N,*N*,*N*′,*N*′,*N*″-Pentamethyl-*N*″-[2-(trimethylazaniumyl)ethyl]guanidinium bis(tetraphenylborate) acetone monosolvate

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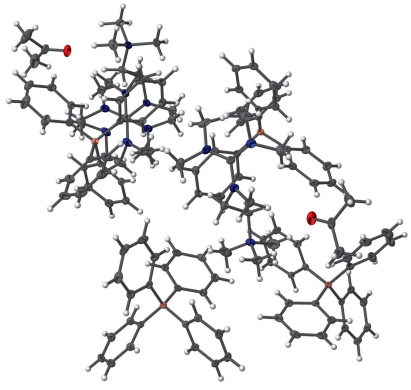
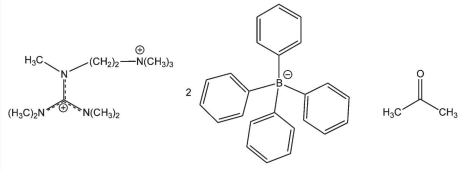
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title solvated salt, $C_{11}H_{28}N_4^{2+}\cdot 2C_{24}H_{20}B^-\cdot C_3H_6O$, comprises two cations, four tetraphenylborate anions and two acetone molecules. One cation shows an orientational disorder at the CN_3 moiety and two sets of N-atom positions were found related by a 60° rotation, with a refined occupancy ratio of 0.935 (1):0.065 (1). The respective nitrogen-bonded $-CH_2$ and $-CH_3$ groups are included in the disorder model. The C—N bond lengths in the central CN_3 units of both guanidinium ions range between 1.3329 (17) and 1.364 (16) Å, indicating a degree of double-bond character. The central C atom is bonded to the three N atoms in a nearly ideal trigonal–planar geometry and one positive charge is delocalized in the CN_3 plane. The C—N bond lengths in the terminal trimethylammonium groups have values close to a typical single bond, and the second positive charge is localized there. In the crystal, the guanidinium ions are connected by C—H···O hydrogen bonds with the acetone molecules. C—H···π interactions are present between the guanidinium and acetone hydrogen atoms and the phenyl rings of the tetraphenylborate ions, leading to the formation of a two-dimensional supramolecular pattern along the *bc* plane.

3D view



Chemical scheme



Structure description

ω-Aminoalkylguanidines such as *N*″-[2-(dimethylamino)ethyl]-*N*,*N*,*N*′,*N*′-tetramethylguanidine (Tiritiris & Kantlehner, 2012*b*) are well known in the literature. Electrophiles can attack at both the imine nitrogen of the guanidine function as well as on the nitrogen atom of the (dimethylamino)propyl group. By alkylation with two equivalents of dimethyl sulfate, a permethylated waxy guanidinium bis(methyl sulfate) salt was

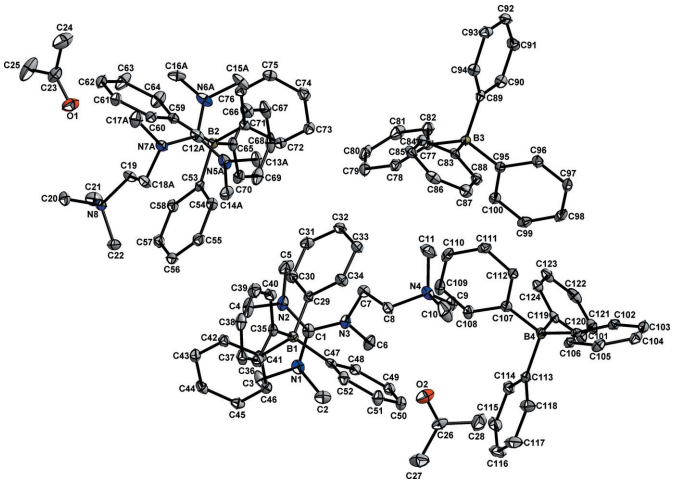


Figure 1
The structure of the title compound, with displacement ellipsoids at the 50% probability level. All H atoms have been omitted for clarity. Only the major orientation of the disordered cation II is shown.

obtained. After anion exchange with sodium tetraphenylborate and crystallization from acetone, the title compound emerged. The asymmetric unit comprises two cations, four tetraphenylborate anions and two acetone molecules (Fig. 1). Cation I is not disordered. In contrast, cation II shows an orientational disorder and two sets of N positions were found related by a 60° rotation, with an occupancy ratio of 0.935 (1):0.065 (1). The respective nitrogen bonded $-CH_2$ and $-CH_3$ groups are included in the disorder model (Fig. 2). A similar type of disorder at the CN_3 moiety has been observed in the crystal structures of salts containing the *N*,*N*,*N*′,*N*′,*N*″,*N*″-hexamethylguanidinium ion [see, for example: cyanate salt (Tiritiris & Kantlehner, 2015*a*); chloride salt (Oelkers & Sundermeyer, 2011)]. In the title salt, the central C—N bond lengths of both cations are in a range from 1.3329 (17) to 1.364 (16) Å, indicating partial double-bond character for all. The N—C1—N and N—C12—N angles range from 117.4 (17) to 120.76 (12)°, indicating that the carbon centres C1 and C12 show nearly ideal trigonal–planar environments. One of the two positive charges is completely delocalized in every CN_3 plane, while the second positive charge is localized in the terminal trimethylammonium group. The N—C bond lengths in the $[NMe_3]^+$ unit have values close to a typical single bond [*d*(N—C) = 1.4903 (16)–1.5114 (16) Å]. The crystal structure analysis reveals that the C—N and C—C bond lengths in both cations are in very good agreement with the values obtained for the cation in *N*,*N*,*N*′,*N*′,*N*″-pentamethyl-*N*″-[3-(trimethylazaniumyl)propyl]guanidinium bis(tetraphenylborate) (Tiritiris, 2013*a*). The bond lengths and angles in all four tetraphenylborate ions are in good agreement with the data from the crystal structure analysis of alkali metal tetraphenylborates (Behrens *et al.*, 2012*a*).

In the crystal, the guanidinium ions are connected by C—H···O hydrogen bonds (Fig. 3) with the acetone molecules (Table 1). C—H···π interactions between the hydrogen atoms of the $-N(CH_3)$ and $-CH_2$ groups of the guanidinium ion and and the phenyl carbon atoms of the tetraphenylborate ions are present (Table 1). The acetone molecules are involved in the C—H···π hydrogen bonding too, interacting with the hydrogen atoms of their methyl groups (Table 1). This leads to the formation of a two-dimensional supramolecular pattern along the *bc* plane (Fig. 4). Such C—H···π interactions have been also observed in *N*,*N*,*N*′,*N*′,*N*″-pentamethyl-*N*″-[3-(trimethylazaniumyl)propyl]guanidinium bis(tetraphenylborate) (Tiritiris, 2013*a*) and *N*,*N*,*N*′,*N*′-tetramethyl-*N*″-[3-(trimethylazaniumyl)propyl]guanidinium bis(tetraphenylborate) acetone disolvate (Tiritiris, 2013*b*).

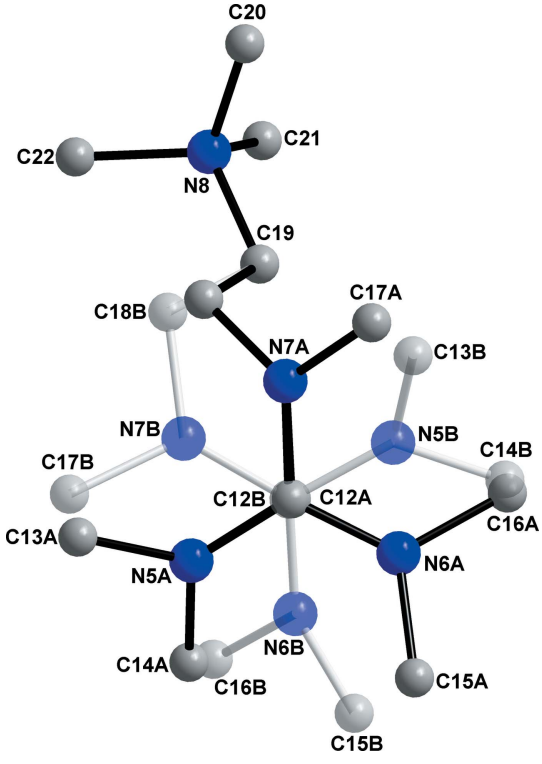


Figure 2
The structure of the orientationally disordered cation II. The N and C atoms are disordered between the opaque and dark positions. All H atoms have been omitted for clarity.

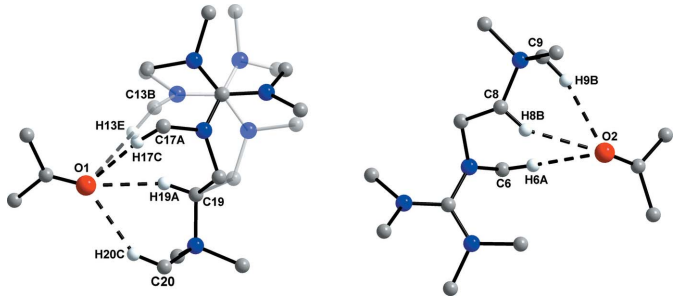


Figure 3
C—H···O hydrogen bonds (black dashed lines) between the guanidinium ions and the acetone molecules. H atoms not involved in the hydrogen bonding have been omitted. Both orientations of the disordered cation II are shown.

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

The ring centroids are defined as follows: *Cg*1 = C53–C58, *Cg*2 = C65–C70, *Cg*3 = C71–C76, *Cg*4 = C89–C94, *Cg*5 = C95–C100, *Cg*6 = C29–C34, *Cg*7 = C41–C46, *Cg*8 = C101–C106, *Cg*9 = C107–C112 and *Cg*10 = C113–C118.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13*B*—H13*E*···O1	0.98	2.61	3.513 (2)	153
C17*A*—H17*C*···O1	0.98	2.41	3.369 (2)	167
C19—H19*A*···O1	0.99	2.37	3.290 (2)	154
C20—H20*C*···O1	0.98	2.46	3.323 (2)	147
C6—H6*A*···O2	0.98	2.50	3.467 (2)	170
C8—H8*B*···O2	0.99	2.55	3.449 (2)	152
C9—H9*B*···O2	0.98	2.52	3.417 (2)	152
C4—H4*B*···*Cg*1	0.98	3.02	3.881 (2)	146
C21—H21*B*···*Cg*1	0.98	2.74	3.713 (2)	171
C3—H3*C*···*Cg*2^{i}	0.98	2.88	3.739 (2)	147
C13*A*—H13*A*···*Cg*3	0.98	2.75	3.587 (2)	144
C27—H27*C*···*Cg*3^{ii}	0.98	2.94	3.629 (2)	128
C28—H28*B*···*Cg*4^{ii}	0.98	2.84	3.554 (2)	130
C6—H6*B*···*Cg*5^{iii}	0.98	2.67	3.614 (2)	162
C8—H8*A*···*Cg*6	0.99	2.93	3.854 (2)	155
C4—H4*C*···*Cg*7	0.98	2.76	3.669 (2)	154
C24—H24*B*···*Cg*8	0.98	3.05	3.681 (2)	124
C18*A*—H18*A*···*Cg*9^{iv}	0.99	2.71	3.512 (2)	139
C18*B*—H18*C*···*Cg*9^{iv}	0.99	2.87	3.662 (2)	138
C25—H25*C*···*Cg*10^{v}	0.98	2.68	3.653 (2)	175

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x+1, y, z$; (iii) $-x+1, -y+2, -z$; (iv) $-x+1, -y+1, -z+1$; (v) $x-1, y-1, z$.

Synthesis and crystallization

The title compound was obtained by reaction of *N*′′-[2-(dimethylamino)ethyl]-*N*,*N*,*N*′,*N*′-tetramethylguanidine (Tiritiris & Kantlehner, 2012*b*) with two equivalents of dimethyl sulfate in acetonitrile at room temperature. After evaporation of the solvent, the crude *N*,*N*,*N*′,*N*′,*N*′′-pentamethyl-*N*′′-[2-(trimethylazaniumyl)ethyl]guanidinium bis(methyl sulfate) (I) was washed with diethylether and dried *in vacuo*. 1.01 g (2.3 mmol) of (I) was dissolved in 20 ml acetonitrile and 1.57 g (4.6 mmol) of sodium tetraphenylborate in 20 ml acetonitrile was added. After stirring for one h at room temperature, the precipitated sodium methyl sulfate was filtered off. The title compound crystallized from a saturated acetone solution after several days at 273 K, forming colorless single crystals. Yield: 1.36 g (70%).

Dimethyl sulfate is carcinogenic, mutagenic and highly poisonous. During the use appropriate precautions must be taken.

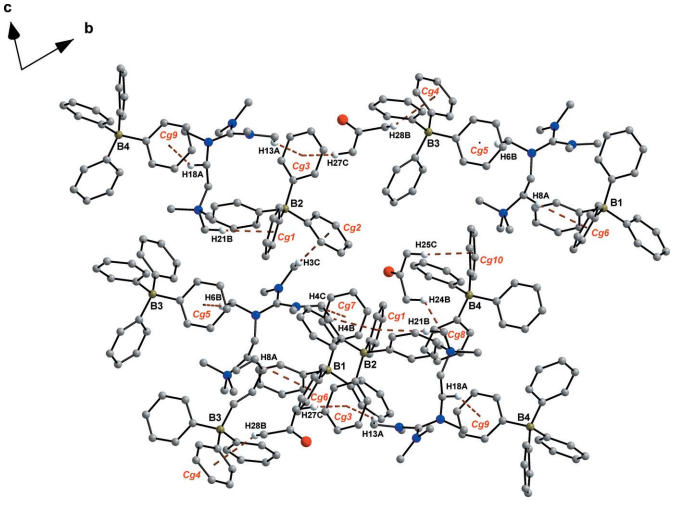


Figure 4
C—H···π interactions (brown dashed lines) between the H atoms of the guanidinium ions, the acetone molecules and the phenyl rings (centroids) of the tetraphenylborate ions (viewed along *bc*). Only the major orientation of the disordered cation II is shown.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{28}N_4{\cdot}2(C_{24}H_{20}B){\cdot}C_3H_6O$
M_r	912.87
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	14.1885 (5), 17.5801 (7), 22.2543 (9)
α, β, γ (°)	72.911 (5), 86.243 (6), 80.123 (6)
V (Å^3)	5226.6 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.35 × 0.25 × 0.10
Data collection	
Diffractometer	Bruker–Nonius KappaCCD
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	50000, 25738, 19692
R_{int}	0.028
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.046, 0.109, 1.03
No. of reflections	25738
No. of parameters	1299
No. of restraints	21
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.25

Computer programs: *COLLECT* (Hooft, 2004), *DENZO-SMN* (Otwinowski & Minor, 1997), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg & Putz, 2005).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms C12–C18 and N5–N7 of one cation (cation II) are disordered over two sets of sites (C12*A*/C12*B*–C18*A*/C18*B* and N5*A*/N5*B*–N7*A*/N7*B*) with refined occupancies of 0.935 (1):0.065 (1). They were constrained to have identical anisotropic displacement parameters. The major and minor disordered components were each restrained to have similar geometries.

Acknowledgements

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full crystallographic data

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N,*N*,*N*′,*N*′,*N*′′-Pentamethyl-*N*′′-[2-(trimethylazaniumyl)ethyl]guanidinium bis(tetraphenylborate) acetone monosolvate

Ioannis Tiritiris and Willi Kantlehner

_N_,_N_,_N_′,_N_′,_N_′′-pentamethyl-_N_′′- [2-(trimethylazaniumyl)ethyl]guanidinium bis(tetraphenylborate) acetone monosolvate

Crystal data

$C_{11}H_{28}N_4 \cdot 2(C_{24}H_{20}B) \cdot C_3H_6O$
M_r = 912.87
Triclinic, $P\overline{1}$
a = 14.1885 (5) Å
b = 17.5801 (7) Å
c = 22.2543 (9) Å
α = 72.911 (5)°
β = 86.243 (6)°
γ = 80.123 (6)°
V = 5226.6 (4) Å^3
Z = 4
$F(000)$ = 1968
D_x = 1.160 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 25414 reflections
θ = 0.4–28.3°
μ = 0.07 mm^{-1}
T = 100 K
Block, colorless
0.35 × 0.25 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ scans, and ω scans
50000 measured reflections
25738 independent reflections
19692 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 28.3°, θ_{min} = 1.3°
h = −18→18
k = −23→23
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.109
S = 1.03
25738 reflections
1299 parameters
21 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
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 2.6221P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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.

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}	Occ. (<1)
N1	0.82487 (8)	0.57886 (7)	0.09708 (5)	0.0210 (2)	
N2	0.66238 (8)	0.57289 (7)	0.10053 (5)	0.0221 (2)	
N3	0.71391 (8)	0.69638 (6)	0.08244 (5)	0.0190 (2)	
N4	0.64058 (8)	0.84798 (6)	0.16732 (5)	0.0206 (2)	
C1	0.73409 (9)	0.61530 (7)	0.09380 (6)	0.0176 (2)	
C2	0.90111 (10)	0.61008 (9)	0.11925 (7)	0.0272 (3)	
H2A	0.9387	0.6371	0.0832	0.041*	
H2B	0.9429	0.5654	0.1474	0.041*	
H2C	0.8728	0.6487	0.1420	0.041*	
C3	0.85562 (12)	0.50601 (9)	0.07669 (7)	0.0290 (3)	
H3A	0.8661	0.4588	0.1137	0.044*	
H3B	0.9153	0.5110	0.0521	0.044*	
H3C	0.8060	0.4997	0.0507	0.044*	
C4	0.66930 (12)	0.48963 (8)	0.14116 (7)	0.0288 (3)	
H4A	0.6850	0.4523	0.1155	0.043*	
H4B	0.6080	0.4817	0.1631	0.043*	
H4C	0.7196	0.4792	0.1720	0.043*	
C5	0.57415 (11)	0.60457 (10)	0.06484 (8)	0.0319 (3)	
H5A	0.5796	0.6573	0.0352	0.048*	
H5B	0.5201	0.6103	0.0938	0.048*	
H5C	0.5636	0.5673	0.0416	0.048*	
C6	0.77106 (10)	0.74951 (8)	0.03749 (6)	0.0233 (3)	
H6A	0.8121	0.7708	0.0603	0.035*	
H6B	0.7285	0.7943	0.0101	0.035*	
H6C	0.8109	0.7191	0.0120	0.035*	
C7	0.63600 (9)	0.73577 (8)	0.11471 (6)	0.0214 (3)	
H7A	0.5905	0.6980	0.1334	0.026*	
H7B	0.6010	0.7835	0.0841	0.026*	
C8	0.67607 (10)	0.76210 (7)	0.16664 (6)	0.0200 (3)	
H8A	0.6602	0.7256	0.2079	0.024*	
H8B	0.7467	0.7548	0.1622	0.024*	
C9	0.67268 (11)	0.90746 (8)	0.10968 (7)	0.0262 (3)	
H9A	0.6441	0.9021	0.0725	0.039*	
H9B	0.7426	0.8969	0.1058	0.039*	
H9C	0.6523	0.9622	0.1130	0.039*	

C10	0.68387 (14)	0.85863 (10)	0.22370 (8)	0.0406 (4)	
H10A	0.6639	0.9141	0.2255	0.061*	
H10B	0.7538	0.8474	0.2203	0.061*	
H10C	0.6621	0.8212	0.2620	0.061*	
C11	0.53426 (11)	0.86399 (9)	0.17301 (8)	0.0336 (4)	
H11A	0.5137	0.9192	0.1754	0.050*	
H11B	0.5132	0.8259	0.2112	0.050*	
H11C	0.5059	0.8574	0.1362	0.050*	
N8	0.38823 (7)	0.17506 (6)	0.34383 (5)	0.0159 (2)	
C12A	0.21387 (14)	0.37260 (11)	0.42126 (16)	0.0189 (4)	0.9346 (13)
N5A	0.28056 (9)	0.41857 (7)	0.41886 (6)	0.0228 (3)	0.9346 (13)
N6A	0.12393 (9)	0.40661 (8)	0.40406 (6)	0.0242 (3)	0.9346 (13)
N7A	0.23556 (8)	0.29141 (7)	0.44257 (6)	0.0196 (3)	0.9346 (13)
C13A	0.35642 (12)	0.39696 (10)	0.46513 (8)	0.0256 (4)	0.9346 (13)
H13A	0.4184	0.3855	0.4447	0.038*	0.9346 (13)
H13B	0.3450	0.3490	0.4989	0.038*	0.9346 (13)
H13C	0.3568	0.4419	0.4828	0.038*	0.9346 (13)
C14A	0.28006 (16)	0.49709 (14)	0.37137 (8)	0.0282 (5)	0.9346 (13)
H14A	0.3451	0.5018	0.3546	0.042*	0.9346 (13)
H14B	0.2572	0.5404	0.3908	0.042*	0.9346 (13)
H14C	0.2375	0.5014	0.3371	0.042*	0.9346 (13)
C15A	0.07899 (14)	0.48276 (10)	0.41545 (8)	0.0332 (4)	0.9346 (13)
H15A	0.0162	0.4766	0.4356	0.050*	0.9346 (13)
H15B	0.0712	0.5253	0.3754	0.050*	0.9346 (13)
H15C	0.1195	0.4973	0.4430	0.050*	0.9346 (13)
C16A	0.0642 (3)	0.3705 (3)	0.3723 (2)	0.0315 (5)	0.9346 (13)
H16A	0.1019	0.3226	0.3636	0.047*	0.9346 (13)
H16B	0.0415	0.4097	0.3327	0.047*	0.9346 (13)
H16C	0.0092	0.3550	0.3994	0.047*	0.9346 (13)
C17A	0.16544 (12)	0.23986 (10)	0.47681 (7)	0.0237 (3)	0.9346 (13)
H17A	0.1082	0.2738	0.4872	0.036*	0.9346 (13)
H17B	0.1940	0.2026	0.5156	0.036*	0.9346 (13)
H17C	0.1477	0.2090	0.4503	0.036*	0.9346 (13)
C18A	0.32576 (12)	0.24767 (10)	0.42601 (7)	0.0201 (4)	0.9346 (13)
H18A	0.3394	0.1935	0.4566	0.024*	0.9346 (13)
H18B	0.3789	0.2772	0.4268	0.024*	0.9346 (13)
C12B	0.2131 (15)	0.3729 (11)	0.426 (2)	0.0189 (4)	0.0654 (13)
N5B	0.1439 (11)	0.3299 (9)	0.4250 (7)	0.0228 (3)	0.0654 (13)
N6B	0.1950 (11)	0.4530 (9)	0.3979 (8)	0.0242 (3)	0.0654 (13)
N7B	0.3051 (10)	0.3351 (9)	0.4381 (8)	0.0196 (3)	0.0654 (13)
C13B	0.1249 (19)	0.2587 (13)	0.4773 (10)	0.0237 (3)	0.0654 (13)
H13D	0.1734	0.2464	0.5096	0.036*	0.0654 (13)
H13E	0.1274	0.2122	0.4611	0.036*	0.0654 (13)
H13F	0.0613	0.2706	0.4956	0.036*	0.0654 (13)
C14B	0.066 (5)	0.361 (5)	0.379 (3)	0.0315 (5)	0.0654 (13)
H14D	0.0387	0.4158	0.3789	0.047*	0.0654 (13)
H14E	0.0167	0.3262	0.3910	0.047*	0.0654 (13)
H14F	0.0919	0.3604	0.3373	0.047*	0.0654 (13)

C15B	0.1186 (18)	0.5088 (14)	0.4165 (12)	0.0332 (4)	0.0654 (13)
H15D	0.0850	0.4796	0.4537	0.050*	0.0654 (13)
H15E	0.0734	0.5331	0.3819	0.050*	0.0654 (13)
H15F	0.1460	0.5513	0.4262	0.050*	0.0654 (13)
C16B	0.267 (2)	0.497 (2)	0.3580 (16)	0.0282 (5)	0.0654 (13)
H16D	0.2850	0.5357	0.3778	0.042*	0.0654 (13)
H16E	0.2405	0.5265	0.3165	0.042*	0.0654 (13)
H16F	0.3242	0.4590	0.3533	0.042*	0.0654 (13)
C17B	0.3706 (19)	0.3667 (15)	0.4709 (14)	0.0256 (4)	0.0654 (13)
H17D	0.4178	0.3221	0.4943	0.038*	0.0654 (13)
H17E	0.3336	0.3929	0.5002	0.038*	0.0654 (13)
H17F	0.4037	0.4060	0.4399	0.038*	0.0654 (13)
C18B	0.341 (2)	0.2618 (15)	0.4187 (10)	0.0201 (4)	0.0654 (13)
H18C	0.3267	0.2165	0.4548	0.024*	0.0654 (13)
H18D	0.4117	0.2580	0.4172	0.024*	0.0654 (13)
C19	0.31651 (9)	0.24013 (8)	0.35999 (6)	0.0186 (3)	
H19A	0.2514	0.2293	0.3558	0.022*	
H19B	0.3234	0.2924	0.3290	0.022*	
C20	0.36799 (10)	0.09339 (8)	0.38122 (7)	0.0229 (3)	
H20A	0.3750	0.0867	0.4261	0.034*	
H20B	0.4132	0.0518	0.3686	0.034*	
H20C	0.3025	0.0882	0.3734	0.034*	
C21	0.37749 (10)	0.18370 (9)	0.27524 (6)	0.0247 (3)	
H21A	0.4238	0.1424	0.2630	0.037*	
H21B	0.3893	0.2373	0.2501	0.037*	
H21C	0.3125	0.1770	0.2679	0.037*	
C22	0.48842 (9)	0.18242 (8)	0.35574 (6)	0.0206 (3)	
H22A	0.4968	0.1719	0.4010	0.031*	
H22B	0.5005	0.2370	0.3336	0.031*	
H22C	0.5335	0.1432	0.3404	0.031*	
O1	0.13203 (7)	0.14615 (7)	0.36965 (5)	0.0334 (2)	
C23	0.05544 (11)	0.12979 (9)	0.36045 (7)	0.0263 (3)	
C24	−0.03168 (13)	0.14734 (13)	0.39853 (9)	0.0472 (5)	
H24A	−0.0136	0.1640	0.4339	0.071*	
H24B	−0.0615	0.0988	0.4145	0.071*	
H24C	−0.0771	0.1908	0.3721	0.071*	
C25	0.04366 (15)	0.09457 (12)	0.30869 (8)	0.0465 (5)	
H25A	0.1064	0.0806	0.2901	0.070*	
H25B	0.0026	0.1340	0.2764	0.070*	
H25C	0.0142	0.0459	0.3255	0.070*	
O2	0.90315 (8)	0.81071 (7)	0.13537 (6)	0.0373 (3)	
C26	0.97511 (10)	0.83664 (9)	0.11052 (7)	0.0256 (3)	
C27	1.06708 (11)	0.78230 (10)	0.10691 (8)	0.0354 (4)	
H27A	1.1153	0.7927	0.1318	0.053*	
H27B	1.0890	0.7925	0.0630	0.053*	
H27C	1.0573	0.7260	0.1236	0.053*	
C28	0.97528 (13)	0.92445 (10)	0.08092 (9)	0.0392 (4)	
H28A	0.9790	0.9357	0.0351	0.059*	

H28B	1.0307	0.9403	0.0954	0.059*
H28C	0.9163	0.9551	0.0928	0.059*
B1	0.73124 (10)	0.50461 (8)	0.35535 (6)	0.0145 (3)
C29	0.63251 (9)	0.56156 (7)	0.32308 (6)	0.0150 (2)
C30	0.58480 (9)	0.55070 (8)	0.27418 (6)	0.0199 (3)
H30	0.6093	0.5065	0.2583	0.024*
C31	0.50251 (10)	0.60210 (8)	0.24754 (7)	0.0249 (3)
H31	0.4721	0.5922	0.2144	0.030*
C32	0.46503 (9)	0.66747 (8)	0.26921 (7)	0.0232 (3)
H32	0.4095	0.7031	0.2509	0.028*
C33	0.51005 (10)	0.67986 (8)	0.31820 (7)	0.0222 (3)
H33	0.4851	0.7241	0.3339	0.027*
C34	0.59141 (9)	0.62778 (8)	0.34428 (6)	0.0200 (3)
H34	0.6207	0.6373	0.3780	0.024*
C35	0.70822 (9)	0.44652 (7)	0.42565 (6)	0.0154 (2)
C36	0.78258 (10)	0.39271 (8)	0.46173 (6)	0.0200 (3)
H36	0.8451	0.3886	0.4436	0.024*
C37	0.76879 (10)	0.34518 (8)	0.52270 (6)	0.0227 (3)
H37	0.8215	0.3105	0.5457	0.027*
C38	0.67795 (11)	0.34853 (8)	0.54986 (6)	0.0237 (3)
H38	0.6680	0.3169	0.5917	0.028*
C39	0.60202 (10)	0.39841 (8)	0.51533 (6)	0.0236 (3)
H39	0.5392	0.4001	0.5331	0.028*
C40	0.61746 (9)	0.44649 (8)	0.45430 (6)	0.0192 (3)
H40	0.5643	0.4804	0.4314	0.023*
C41	0.78052 (9)	0.44510 (7)	0.31305 (5)	0.0147 (2)
C42	0.73995 (9)	0.37708 (7)	0.31401 (6)	0.0174 (2)
H42	0.6837	0.3674	0.3388	0.021*
C43	0.77838 (10)	0.32334 (8)	0.28041 (6)	0.0197 (3)
H43	0.7479	0.2786	0.2822	0.024*
C44	0.86123 (10)	0.33495 (8)	0.24428 (6)	0.0203 (3)
H44	0.8881	0.2983	0.2215	0.024*
C45	0.90389 (9)	0.40097 (8)	0.24213 (6)	0.0196 (3)
H45	0.9607	0.4097	0.2178	0.023*
C46	0.86353 (9)	0.45484 (8)	0.27571 (6)	0.0171 (2)
H46	0.8937	0.5000	0.2731	0.021*
C47	0.80014 (9)	0.56870 (7)	0.36063 (6)	0.0152 (2)
C48	0.82057 (9)	0.63030 (7)	0.30710 (6)	0.0186 (3)
H48	0.7987	0.6308	0.2675	0.022*
C49	0.87125 (10)	0.69042 (8)	0.30944 (7)	0.0229 (3)
H49	0.8832	0.7308	0.2720	0.027*
C50	0.90441 (10)	0.69138 (8)	0.36650 (7)	0.0254 (3)
H50	0.9389	0.7322	0.3687	0.030*
C51	0.88612 (10)	0.63170 (8)	0.42001 (7)	0.0250 (3)
H51	0.9088	0.6312	0.4594	0.030*
C52	0.83471 (10)	0.57201 (8)	0.41695 (6)	0.0198 (3)
H52	0.8228	0.5321	0.4547	0.024*
B2	0.25154 (10)	0.48260 (8)	0.14556 (6)	0.0143 (3)

C53	0.35673 (9)	0.43199 (7)	0.17107 (6)	0.0151 (2)
C54	0.39992 (9)	0.43296 (7)	0.22558 (6)	0.0181 (2)
H54	0.3683	0.4672	0.2492	0.022*
C55	0.48748 (10)	0.38577 (8)	0.24654 (6)	0.0216 (3)
H55	0.5142	0.3883	0.2838	0.026*
C56	0.53581 (9)	0.33514 (8)	0.21329 (7)	0.0227 (3)
H56	0.5957	0.3032	0.2273	0.027*
C57	0.49517 (9)	0.33187 (8)	0.15917 (6)	0.0210 (3)
H57	0.5270	0.2972	0.1360	0.025*
C58	0.40797 (9)	0.37934 (7)	0.13895 (6)	0.0182 (3)
H58	0.3816	0.3762	0.1018	0.022*
C59	0.18616 (9)	0.41291 (7)	0.14802 (6)	0.0163 (2)
C60	0.17790 (9)	0.35183 (8)	0.20447 (6)	0.0201 (3)
H60	0.2059	0.3549	0.2411	0.024*
C61	0.13078 (10)	0.28712 (8)	0.20928 (7)	0.0245 (3)
H61	0.1274	0.2473	0.2485	0.029*
C62	0.08871 (10)	0.28067 (9)	0.15679 (7)	0.0271 (3)
H62	0.0575	0.2361	0.1594	0.032*
C63	0.09326 (11)	0.34039 (10)	0.10076 (7)	0.0323 (3)
H63	0.0637	0.3376	0.0645	0.039*
C64	0.14105 (11)	0.40498 (9)	0.09687 (6)	0.0263 (3)
H64	0.1429	0.4452	0.0577	0.032*
C65	0.25935 (9)	0.54335 (7)	0.07414 (6)	0.0167 (2)
C66	0.17740 (10)	0.59419 (8)	0.04480 (6)	0.0225 (3)
H66	0.1177	0.5911	0.0666	0.027*
C67	0.17972 (11)	0.64881 (8)	−0.01465 (7)	0.0270 (3)
H67	0.1223	0.6814	−0.0328	0.032*
C68	0.26575 (12)	0.65573 (8)	−0.04738 (6)	0.0266 (3)
H68	0.2679	0.6928	−0.0881	0.032*
C69	0.34830 (11)	0.60797 (8)	−0.01988 (6)	0.0257 (3)
H69	0.4079	0.6127	−0.0416	0.031*
C70	0.34470 (10)	0.55272 (8)	0.03959 (6)	0.0200 (3)
H70	0.4025	0.5202	0.0573	0.024*
C71	0.20511 (9)	0.54107 (7)	0.18889 (6)	0.0149 (2)
C72	0.25152 (9)	0.60399 (8)	0.19299 (6)	0.0183 (3)
H72	0.3112	0.6100	0.1717	0.022*
C73	0.21409 (10)	0.65752 (8)	0.22673 (6)	0.0217 (3)
H73	0.2490	0.6980	0.2292	0.026*
C74	0.12553 (10)	0.65194 (8)	0.25693 (6)	0.0224 (3)
H74	0.0992	0.6886	0.2799	0.027*
C75	0.07637 (9)	0.59213 (8)	0.25294 (6)	0.0203 (3)
H75	0.0151	0.5883	0.2725	0.024*
C76	0.11633 (9)	0.53736 (7)	0.22030 (6)	0.0168 (2)
H76	0.0820	0.4959	0.2193	0.020*
B3	0.25906 (10)	0.99580 (8)	0.12831 (6)	0.0134 (3)
C77	0.27088 (9)	0.93178 (7)	0.08536 (6)	0.0151 (2)
C78	0.31932 (9)	0.85227 (8)	0.10491 (6)	0.0191 (3)
H78	0.3461	0.8329	0.1457	0.023*

C79	0.32999 (10)	0.80033 (8)	0.06712 (7)	0.0250 (3)
H79	0.3631	0.7468	0.0826	0.030*
C80	0.29283 (10)	0.82617 (9)	0.00744 (7)	0.0264 (3)
H80	0.2997	0.7909	−0.0183	0.032*
C81	0.24530 (10)	0.90448 (9)	−0.01421 (7)	0.0259 (3)
H81	0.2197	0.9235	−0.0553	0.031*
C82	0.23489 (10)	0.95547 (8)	0.02409 (6)	0.0211 (3)
H82	0.2019	1.0089	0.0081	0.025*
C83	0.28744 (8)	0.94719 (7)	0.20161 (6)	0.0143 (2)
C84	0.24970 (9)	0.87692 (7)	0.23391 (6)	0.0167 (2)
H84	0.2053	0.8592	0.2130	0.020*
C85	0.27460 (9)	0.83237 (8)	0.29507 (6)	0.0187 (3)
H85	0.2479	0.7849	0.3148	0.022*
C86	0.33842 (9)	0.85702 (8)	0.32745 (6)	0.0202 (3)
H86	0.3560	0.8266	0.3692	0.024*
C87	0.37598 (10)	0.92650 (8)	0.29794 (6)	0.0204 (3)
H87	0.4192	0.9444	0.3196	0.025*
C88	0.35058 (9)	0.97033 (8)	0.23640 (6)	0.0171 (2)
H88	0.3772	1.0179	0.2172	0.020*
C89	0.14791 (9)	1.04397 (7)	0.12482 (6)	0.0144 (2)
C90	0.11600 (9)	1.10691 (8)	0.07111 (6)	0.0181 (2)
H90	0.1604	1.1218	0.0376	0.022*
C91	0.02294 (10)	1.14836 (8)	0.06457 (6)	0.0207 (3)
H91	0.0051	1.1903	0.0272	0.025*
C92	−0.04398 (9)	1.12862 (8)	0.11255 (6)	0.0211 (3)
H92	−0.1080	1.1562	0.1083	0.025*
C93	−0.01551 (9)	1.06792 (8)	0.16684 (6)	0.0206 (3)
H93	−0.0602	1.0539	0.2003	0.025*
C94	0.07857 (9)	1.02723 (8)	0.17261 (6)	0.0174 (2)
H94	0.0963	0.9864	0.2106	0.021*
C95	0.33082 (9)	1.06264 (7)	0.10002 (5)	0.0144 (2)
C96	0.31729 (9)	1.13486 (7)	0.11712 (6)	0.0180 (2)
H96	0.2633	1.1457	0.1427	0.022*
C97	0.37946 (10)	1.19096 (8)	0.09825 (6)	0.0211 (3)
H97	0.3678	1.2387	0.1112	0.025*
C98	0.45864 (10)	1.17713 (8)	0.06044 (6)	0.0215 (3)
H98	0.5015	1.2152	0.0474	0.026*
C99	0.47446 (9)	1.10714 (8)	0.04191 (6)	0.0202 (3)
H99	0.5281	1.0971	0.0159	0.024*
C100	0.41121 (9)	1.05129 (7)	0.06164 (6)	0.0166 (2)
H100	0.4233	1.0037	0.0485	0.020*
B4	0.73431 (10)	0.99633 (8)	0.37926 (6)	0.0139 (3)
C101	0.73191 (8)	1.05294 (7)	0.42675 (6)	0.0144 (2)
C102	0.71416 (9)	1.13735 (7)	0.40836 (6)	0.0169 (2)
H102	0.6978	1.1649	0.3659	0.020*
C103	0.71942 (9)	1.18296 (8)	0.44961 (6)	0.0203 (3)
H103	0.7069	1.2402	0.4349	0.024*
C104	0.74287 (9)	1.14494 (8)	0.51182 (6)	0.0207 (3)

H104	0.7485	1.1756	0.5398	0.025*
C105	0.75813 (9)	1.06126 (8)	0.53281 (6)	0.0199 (3)
H105	0.7729	1.0342	0.5756	0.024*
C106	0.75168 (9)	1.01714 (8)	0.49108 (6)	0.0168 (2)
H106	0.7611	0.9600	0.5067	0.020*
C107	0.66263 (9)	0.92926 (7)	0.40695 (5)	0.0146 (2)
C108	0.67618 (9)	0.85512 (7)	0.39293 (6)	0.0181 (2)
H108	0.7327	0.8406	0.3708	0.022*
C109	0.61016 (10)	0.80235 (8)	0.41024 (6)	0.0219 (3)
H109	0.6221	0.7530	0.3996	0.026*
C110	0.52682 (10)	0.82079 (8)	0.44300 (6)	0.0211 (3)
H110	0.4817	0.7846	0.4548	0.025*
C111	0.51070 (9)	0.89320 (8)	0.45813 (6)	0.0186 (3)
H111	0.4541	0.9070	0.4804	0.022*
C112	0.57788 (9)	0.94569 (7)	0.44047 (6)	0.0153 (2)
H112	0.5657	0.9947	0.4516	0.018*
C113	0.84502 (9)	0.95046 (7)	0.37163 (6)	0.0171 (2)
C114	0.87449 (10)	0.92849 (8)	0.31665 (6)	0.0215 (3)
H114	0.8299	0.9411	0.2837	0.026*
C115	0.96626 (10)	0.88903 (8)	0.30825 (7)	0.0284 (3)
H115	0.9831	0.8758	0.2701	0.034*
C116	1.03263 (11)	0.86919 (9)	0.35537 (8)	0.0346 (4)
H116	1.0953	0.8423	0.3500	0.042*
C117	1.00659 (10)	0.88896 (10)	0.41035 (8)	0.0341 (4)
H117	1.0513	0.8751	0.4433	0.041*
C118	0.91482 (10)	0.92922 (9)	0.41785 (7)	0.0247 (3)
H118	0.8991	0.9428	0.4560	0.030*
C119	0.69929 (9)	1.04997 (7)	0.30787 (6)	0.0146 (2)
C120	0.75272 (9)	1.10808 (7)	0.27122 (6)	0.0177 (2)
H120	0.8059	1.1184	0.2897	0.021*
C121	0.73128 (10)	1.15105 (8)	0.20929 (6)	0.0211 (3)
H121	0.7689	1.1903	0.1866	0.025*
C122	0.65482 (10)	1.13683 (8)	0.18036 (6)	0.0222 (3)
H122	0.6407	1.1652	0.1377	0.027*
C123	0.59957 (10)	1.08066 (8)	0.21476 (6)	0.0208 (3)
H123	0.5466	1.0707	0.1958	0.025*
C124	0.62159 (9)	1.03844 (7)	0.27750 (6)	0.0174 (2)
H124	0.5824	1.0006	0.3003	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0251 (6)	0.0208 (5)	0.0171 (5)	−0.0025 (5)	0.0011 (4)	−0.0064 (4)
N2	0.0278 (6)	0.0184 (5)	0.0221 (6)	−0.0080 (5)	−0.0022 (5)	−0.0064 (4)
N3	0.0231 (6)	0.0154 (5)	0.0182 (5)	−0.0052 (4)	0.0002 (4)	−0.0034 (4)
N4	0.0225 (6)	0.0168 (5)	0.0207 (5)	0.0019 (4)	−0.0002 (4)	−0.0055 (4)
C1	0.0246 (7)	0.0168 (6)	0.0114 (5)	−0.0041 (5)	−0.0013 (5)	−0.0035 (5)
C2	0.0215 (7)	0.0324 (8)	0.0271 (7)	−0.0030 (6)	−0.0024 (6)	−0.0081 (6)

C3	0.0408 (9)	0.0237 (7)	0.0206 (7)	0.0041 (6)	0.0017 (6)	−0.0090 (6)
C4	0.0474 (9)	0.0179 (7)	0.0242 (7)	−0.0136 (6)	0.0063 (6)	−0.0076 (6)
C5	0.0302 (8)	0.0336 (8)	0.0373 (8)	−0.0108 (6)	−0.0075 (6)	−0.0138 (7)
C6	0.0287 (7)	0.0217 (7)	0.0187 (6)	−0.0098 (6)	0.0006 (5)	−0.0015 (5)
C7	0.0188 (6)	0.0185 (6)	0.0273 (7)	−0.0018 (5)	−0.0027 (5)	−0.0071 (5)
C8	0.0209 (7)	0.0142 (6)	0.0231 (6)	0.0022 (5)	−0.0035 (5)	−0.0050 (5)
C9	0.0274 (7)	0.0183 (6)	0.0303 (7)	−0.0052 (6)	0.0009 (6)	−0.0023 (6)
C10	0.0591 (11)	0.0331 (9)	0.0331 (9)	0.0091 (8)	−0.0145 (8)	−0.0211 (7)
C11	0.0235 (8)	0.0273 (8)	0.0407 (9)	0.0039 (6)	0.0098 (6)	−0.0019 (7)
N8	0.0138 (5)	0.0164 (5)	0.0157 (5)	−0.0012 (4)	0.0005 (4)	−0.0025 (4)
C12A	0.0209 (6)	0.0232 (6)	0.0127 (9)	0.0042 (5)	−0.0032 (5)	−0.0091 (5)
N5A	0.0298 (7)	0.0191 (6)	0.0191 (6)	0.0016 (5)	−0.0070 (5)	−0.0065 (5)
N6A	0.0227 (6)	0.0269 (7)	0.0199 (6)	0.0082 (5)	−0.0025 (5)	−0.0081 (5)
N7A	0.0174 (6)	0.0205 (6)	0.0217 (6)	0.0030 (5)	−0.0037 (5)	−0.0100 (5)
C13A	0.0317 (9)	0.0231 (8)	0.0243 (8)	−0.0031 (7)	−0.0118 (6)	−0.0085 (8)
C14A	0.0419 (11)	0.0206 (7)	0.0211 (10)	−0.0025 (7)	−0.0050 (8)	−0.0050 (8)
C15A	0.0366 (10)	0.0297 (9)	0.0265 (8)	0.0157 (7)	−0.0019 (7)	−0.0091 (7)
C16A	0.0205 (7)	0.0447 (19)	0.0267 (16)	0.0012 (10)	−0.0069 (8)	−0.0082 (9)
C17A	0.0261 (8)	0.0235 (8)	0.0229 (7)	−0.0033 (6)	−0.0024 (7)	−0.0089 (6)
C18A	0.0181 (9)	0.0184 (8)	0.0237 (8)	0.0042 (6)	−0.0052 (6)	−0.0091 (6)
C12B	0.0209 (6)	0.0232 (6)	0.0127 (9)	0.0042 (5)	−0.0032 (5)	−0.0091 (5)
N5B	0.0298 (7)	0.0191 (6)	0.0191 (6)	0.0016 (5)	−0.0070 (5)	−0.0065 (5)
N6B	0.0227 (6)	0.0269 (7)	0.0199 (6)	0.0082 (5)	−0.0025 (5)	−0.0081 (5)
N7B	0.0174 (6)	0.0205 (6)	0.0217 (6)	0.0030 (5)	−0.0037 (5)	−0.0100 (5)
C13B	0.0261 (8)	0.0235 (8)	0.0229 (7)	−0.0033 (6)	−0.0024 (7)	−0.0089 (6)
C14B	0.0205 (7)	0.0447 (19)	0.0267 (16)	0.0012 (10)	−0.0069 (8)	−0.0082 (9)
C15B	0.0366 (10)	0.0297 (9)	0.0265 (8)	0.0157 (7)	−0.0019 (7)	−0.0091 (7)
C16B	0.0419 (11)	0.0206 (7)	0.0211 (10)	−0.0025 (7)	−0.0050 (8)	−0.0050 (8)
C17B	0.0317 (9)	0.0231 (8)	0.0243 (8)	−0.0031 (7)	−0.0118 (6)	−0.0085 (8)
C18B	0.0181 (9)	0.0184 (8)	0.0237 (8)	0.0042 (6)	−0.0052 (6)	−0.0091 (6)
C19	0.0161 (6)	0.0173 (6)	0.0196 (6)	0.0033 (5)	−0.0019 (5)	−0.0038 (5)
C20	0.0249 (7)	0.0153 (6)	0.0266 (7)	−0.0037 (5)	−0.0021 (5)	−0.0023 (5)
C21	0.0231 (7)	0.0341 (8)	0.0164 (6)	−0.0017 (6)	0.0002 (5)	−0.0080 (6)
C22	0.0133 (6)	0.0244 (7)	0.0235 (7)	−0.0025 (5)	−0.0002 (5)	−0.0061 (5)
O1	0.0240 (5)	0.0442 (6)	0.0384 (6)	−0.0120 (5)	−0.0031 (4)	−0.0174 (5)
C23	0.0293 (8)	0.0269 (7)	0.0239 (7)	−0.0132 (6)	−0.0046 (6)	−0.0031 (6)
C24	0.0319 (9)	0.0654 (13)	0.0527 (11)	−0.0209 (9)	0.0061 (8)	−0.0240 (10)
C25	0.0659 (13)	0.0535 (11)	0.0334 (9)	−0.0408 (10)	0.0058 (8)	−0.0164 (8)
O2	0.0245 (6)	0.0459 (7)	0.0441 (7)	−0.0139 (5)	0.0031 (5)	−0.0129 (5)
C26	0.0210 (7)	0.0336 (8)	0.0246 (7)	−0.0077 (6)	−0.0054 (5)	−0.0090 (6)
C27	0.0239 (8)	0.0430 (9)	0.0333 (8)	−0.0017 (7)	−0.0047 (6)	−0.0028 (7)
C28	0.0417 (10)	0.0335 (9)	0.0477 (10)	−0.0122 (7)	−0.0101 (8)	−0.0142 (8)
B1	0.0152 (6)	0.0135 (6)	0.0148 (6)	−0.0010 (5)	−0.0009 (5)	−0.0044 (5)
C29	0.0159 (6)	0.0134 (5)	0.0146 (6)	−0.0035 (5)	0.0020 (4)	−0.0023 (4)
C30	0.0202 (6)	0.0181 (6)	0.0226 (6)	−0.0017 (5)	−0.0023 (5)	−0.0080 (5)
C31	0.0223 (7)	0.0244 (7)	0.0287 (7)	−0.0031 (6)	−0.0096 (6)	−0.0072 (6)
C32	0.0143 (6)	0.0188 (6)	0.0319 (7)	−0.0007 (5)	−0.0037 (5)	−0.0008 (5)
C33	0.0203 (7)	0.0169 (6)	0.0280 (7)	0.0008 (5)	0.0019 (5)	−0.0068 (5)

C34	0.0214 (7)	0.0187 (6)	0.0196 (6)	0.0001 (5)	−0.0014 (5)	−0.0067 (5)
C35	0.0190 (6)	0.0127 (5)	0.0157 (6)	−0.0027 (5)	−0.0004 (5)	−0.0059 (5)
C36	0.0204 (6)	0.0175 (6)	0.0209 (6)	−0.0024 (5)	−0.0002 (5)	−0.0044 (5)
C37	0.0299 (7)	0.0153 (6)	0.0211 (7)	−0.0019 (5)	−0.0067 (5)	−0.0020 (5)
C38	0.0368 (8)	0.0176 (6)	0.0160 (6)	−0.0086 (6)	0.0014 (5)	−0.0017 (5)
C39	0.0264 (7)	0.0221 (7)	0.0219 (7)	−0.0070 (5)	0.0061 (5)	−0.0051 (5)
C40	0.0200 (6)	0.0171 (6)	0.0194 (6)	−0.0019 (5)	0.0008 (5)	−0.0042 (5)
C41	0.0155 (6)	0.0141 (6)	0.0130 (5)	0.0009 (4)	−0.0036 (4)	−0.0026 (4)
C42	0.0180 (6)	0.0149 (6)	0.0174 (6)	−0.0017 (5)	0.0005 (5)	−0.0024 (5)
C43	0.0241 (7)	0.0139 (6)	0.0210 (6)	−0.0032 (5)	−0.0024 (5)	−0.0043 (5)
C44	0.0236 (7)	0.0175 (6)	0.0199 (6)	0.0023 (5)	−0.0019 (5)	−0.0086 (5)
C45	0.0173 (6)	0.0228 (6)	0.0185 (6)	−0.0011 (5)	0.0015 (5)	−0.0073 (5)
C46	0.0166 (6)	0.0172 (6)	0.0184 (6)	−0.0034 (5)	−0.0007 (5)	−0.0060 (5)
C47	0.0131 (6)	0.0139 (6)	0.0184 (6)	0.0012 (4)	0.0012 (5)	−0.0063 (5)
C48	0.0183 (6)	0.0164 (6)	0.0201 (6)	−0.0010 (5)	0.0005 (5)	−0.0047 (5)
C49	0.0209 (7)	0.0142 (6)	0.0300 (7)	−0.0018 (5)	0.0047 (5)	−0.0026 (5)
C50	0.0230 (7)	0.0172 (6)	0.0396 (8)	−0.0057 (5)	0.0020 (6)	−0.0129 (6)
C51	0.0285 (7)	0.0239 (7)	0.0276 (7)	−0.0058 (6)	−0.0011 (6)	−0.0140 (6)
C52	0.0234 (7)	0.0184 (6)	0.0186 (6)	−0.0038 (5)	0.0013 (5)	−0.0070 (5)
B2	0.0143 (6)	0.0142 (6)	0.0147 (6)	−0.0031 (5)	−0.0001 (5)	−0.0042 (5)
C53	0.0155 (6)	0.0123 (5)	0.0165 (6)	−0.0051 (4)	0.0024 (5)	−0.0015 (4)
C54	0.0192 (6)	0.0159 (6)	0.0194 (6)	−0.0040 (5)	−0.0001 (5)	−0.0048 (5)
C55	0.0207 (7)	0.0191 (6)	0.0240 (7)	−0.0053 (5)	−0.0056 (5)	−0.0021 (5)
C56	0.0151 (6)	0.0160 (6)	0.0321 (7)	−0.0027 (5)	−0.0007 (5)	0.0009 (5)
C57	0.0204 (7)	0.0142 (6)	0.0261 (7)	−0.0029 (5)	0.0069 (5)	−0.0037 (5)
C58	0.0205 (6)	0.0155 (6)	0.0185 (6)	−0.0043 (5)	0.0017 (5)	−0.0046 (5)
C59	0.0140 (6)	0.0169 (6)	0.0191 (6)	−0.0026 (5)	0.0018 (5)	−0.0072 (5)
C60	0.0182 (6)	0.0178 (6)	0.0234 (7)	−0.0043 (5)	−0.0036 (5)	−0.0029 (5)
C61	0.0212 (7)	0.0163 (6)	0.0332 (8)	−0.0041 (5)	0.0022 (6)	−0.0026 (5)
C62	0.0233 (7)	0.0249 (7)	0.0408 (8)	−0.0115 (6)	0.0090 (6)	−0.0191 (6)
C63	0.0369 (9)	0.0450 (9)	0.0275 (8)	−0.0220 (7)	0.0051 (6)	−0.0219 (7)
C64	0.0326 (8)	0.0331 (8)	0.0179 (6)	−0.0155 (6)	0.0029 (6)	−0.0095 (6)
C65	0.0223 (6)	0.0135 (6)	0.0157 (6)	−0.0039 (5)	−0.0010 (5)	−0.0058 (5)
C66	0.0250 (7)	0.0205 (6)	0.0207 (6)	0.0008 (5)	−0.0018 (5)	−0.0060 (5)
C67	0.0387 (8)	0.0175 (6)	0.0226 (7)	0.0039 (6)	−0.0098 (6)	−0.0052 (5)
C68	0.0506 (9)	0.0152 (6)	0.0144 (6)	−0.0079 (6)	−0.0022 (6)	−0.0030 (5)
C69	0.0366 (8)	0.0223 (7)	0.0191 (7)	−0.0123 (6)	0.0054 (6)	−0.0046 (5)
C70	0.0233 (7)	0.0181 (6)	0.0185 (6)	−0.0060 (5)	−0.0006 (5)	−0.0036 (5)
C71	0.0152 (6)	0.0143 (6)	0.0139 (6)	−0.0010 (5)	−0.0028 (4)	−0.0019 (4)
C72	0.0145 (6)	0.0176 (6)	0.0228 (6)	−0.0027 (5)	−0.0018 (5)	−0.0055 (5)
C73	0.0204 (7)	0.0174 (6)	0.0293 (7)	−0.0025 (5)	−0.0062 (5)	−0.0091 (5)
C74	0.0234 (7)	0.0207 (6)	0.0246 (7)	0.0014 (5)	−0.0030 (5)	−0.0114 (5)
C75	0.0159 (6)	0.0235 (6)	0.0209 (6)	−0.0004 (5)	0.0010 (5)	−0.0073 (5)
C76	0.0160 (6)	0.0169 (6)	0.0181 (6)	−0.0035 (5)	−0.0020 (5)	−0.0052 (5)
B3	0.0139 (6)	0.0124 (6)	0.0139 (6)	−0.0022 (5)	−0.0003 (5)	−0.0039 (5)
C77	0.0131 (6)	0.0164 (6)	0.0174 (6)	−0.0063 (5)	0.0028 (4)	−0.0058 (5)
C78	0.0197 (6)	0.0176 (6)	0.0212 (6)	−0.0064 (5)	0.0042 (5)	−0.0063 (5)
C79	0.0268 (7)	0.0174 (6)	0.0333 (8)	−0.0077 (5)	0.0113 (6)	−0.0111 (6)

C80	0.0273 (7)	0.0303 (7)	0.0326 (8)	−0.0160 (6)	0.0124 (6)	−0.0221 (6)
C81	0.0261 (7)	0.0360 (8)	0.0222 (7)	−0.0106 (6)	0.0012 (5)	−0.0156 (6)
C82	0.0218 (7)	0.0222 (6)	0.0210 (6)	−0.0042 (5)	−0.0009 (5)	−0.0086 (5)
C83	0.0130 (6)	0.0136 (5)	0.0154 (6)	0.0006 (4)	0.0012 (4)	−0.0047 (5)
C84	0.0141 (6)	0.0174 (6)	0.0175 (6)	−0.0015 (5)	−0.0004 (5)	−0.0040 (5)
C85	0.0177 (6)	0.0164 (6)	0.0183 (6)	0.0006 (5)	0.0037 (5)	−0.0019 (5)
C86	0.0207 (6)	0.0226 (6)	0.0139 (6)	0.0054 (5)	−0.0008 (5)	−0.0047 (5)
C87	0.0216 (7)	0.0232 (7)	0.0181 (6)	0.0000 (5)	−0.0040 (5)	−0.0097 (5)
C88	0.0178 (6)	0.0167 (6)	0.0175 (6)	−0.0019 (5)	−0.0009 (5)	−0.0067 (5)
C89	0.0162 (6)	0.0137 (5)	0.0157 (6)	−0.0034 (5)	−0.0010 (4)	−0.0069 (5)
C90	0.0197 (6)	0.0189 (6)	0.0161 (6)	−0.0045 (5)	0.0002 (5)	−0.0051 (5)
C91	0.0228 (7)	0.0193 (6)	0.0188 (6)	0.0000 (5)	−0.0052 (5)	−0.0044 (5)
C92	0.0154 (6)	0.0236 (7)	0.0257 (7)	0.0017 (5)	−0.0040 (5)	−0.0112 (5)
C93	0.0174 (6)	0.0247 (7)	0.0203 (6)	−0.0036 (5)	0.0024 (5)	−0.0081 (5)
C94	0.0179 (6)	0.0181 (6)	0.0162 (6)	−0.0027 (5)	−0.0006 (5)	−0.0049 (5)
C95	0.0164 (6)	0.0132 (5)	0.0132 (5)	−0.0026 (5)	−0.0032 (4)	−0.0026 (4)
C96	0.0200 (6)	0.0163 (6)	0.0185 (6)	−0.0031 (5)	−0.0014 (5)	−0.0057 (5)
C97	0.0262 (7)	0.0141 (6)	0.0244 (7)	−0.0059 (5)	−0.0076 (5)	−0.0047 (5)
C98	0.0224 (7)	0.0199 (6)	0.0211 (6)	−0.0109 (5)	−0.0055 (5)	0.0012 (5)
C99	0.0169 (6)	0.0248 (7)	0.0177 (6)	−0.0065 (5)	−0.0001 (5)	−0.0027 (5)
C100	0.0180 (6)	0.0164 (6)	0.0155 (6)	−0.0038 (5)	−0.0015 (5)	−0.0037 (5)
B4	0.0149 (6)	0.0133 (6)	0.0128 (6)	−0.0023 (5)	−0.0005 (5)	−0.0025 (5)
C101	0.0114 (6)	0.0159 (6)	0.0165 (6)	−0.0044 (4)	0.0012 (4)	−0.0047 (5)
C102	0.0165 (6)	0.0178 (6)	0.0164 (6)	−0.0047 (5)	0.0002 (5)	−0.0037 (5)
C103	0.0224 (7)	0.0152 (6)	0.0248 (7)	−0.0068 (5)	0.0029 (5)	−0.0065 (5)
C104	0.0218 (7)	0.0241 (7)	0.0212 (6)	−0.0097 (5)	0.0026 (5)	−0.0112 (5)
C105	0.0212 (7)	0.0244 (7)	0.0153 (6)	−0.0092 (5)	0.0007 (5)	−0.0047 (5)
C106	0.0166 (6)	0.0166 (6)	0.0170 (6)	−0.0058 (5)	0.0008 (5)	−0.0030 (5)
C107	0.0163 (6)	0.0143 (6)	0.0121 (5)	−0.0024 (5)	−0.0037 (4)	−0.0015 (4)
C108	0.0221 (7)	0.0163 (6)	0.0161 (6)	−0.0030 (5)	−0.0015 (5)	−0.0048 (5)
C109	0.0321 (7)	0.0146 (6)	0.0202 (6)	−0.0062 (5)	−0.0063 (5)	−0.0043 (5)
C110	0.0238 (7)	0.0199 (6)	0.0193 (6)	−0.0113 (5)	−0.0072 (5)	0.0008 (5)
C111	0.0156 (6)	0.0207 (6)	0.0167 (6)	−0.0049 (5)	−0.0030 (5)	0.0005 (5)
C112	0.0159 (6)	0.0137 (6)	0.0157 (6)	−0.0026 (5)	−0.0030 (4)	−0.0024 (5)
C113	0.0160 (6)	0.0132 (6)	0.0192 (6)	−0.0035 (5)	0.0024 (5)	−0.0002 (5)
C114	0.0224 (7)	0.0162 (6)	0.0241 (7)	−0.0038 (5)	0.0053 (5)	−0.0038 (5)
C115	0.0271 (8)	0.0197 (7)	0.0339 (8)	−0.0027 (6)	0.0143 (6)	−0.0044 (6)
C116	0.0171 (7)	0.0272 (8)	0.0485 (10)	0.0018 (6)	0.0117 (7)	0.0004 (7)
C117	0.0160 (7)	0.0384 (9)	0.0387 (9)	−0.0007 (6)	−0.0028 (6)	0.0013 (7)
C118	0.0178 (7)	0.0282 (7)	0.0239 (7)	−0.0031 (5)	0.0002 (5)	−0.0012 (6)
C119	0.0163 (6)	0.0129 (5)	0.0144 (6)	0.0008 (4)	0.0012 (4)	−0.0057 (4)
C120	0.0180 (6)	0.0158 (6)	0.0183 (6)	−0.0011 (5)	0.0015 (5)	−0.0045 (5)
C121	0.0253 (7)	0.0160 (6)	0.0180 (6)	−0.0002 (5)	0.0050 (5)	−0.0019 (5)
C122	0.0288 (7)	0.0202 (6)	0.0128 (6)	0.0069 (5)	−0.0017 (5)	−0.0034 (5)
C123	0.0228 (7)	0.0214 (6)	0.0188 (6)	0.0037 (5)	−0.0049 (5)	−0.0096 (5)
C124	0.0191 (6)	0.0163 (6)	0.0172 (6)	−0.0007 (5)	0.0006 (5)	−0.0069 (5)

Geometric parameters (Å, º)

N1—C1	1.3329 (17)	C44—C45	1.3858 (18)
N1—C2	1.4654 (18)	C44—H44	0.9500
N1—C3	1.4698 (17)	C45—C46	1.3991 (17)
N2—C1	1.3371 (17)	C45—H45	0.9500
N2—C5	1.4626 (19)	C46—H46	0.9500
N2—C4	1.4677 (17)	C47—C52	1.3957 (18)
N3—C1	1.3548 (16)	C47—C48	1.4072 (17)
N3—C6	1.4611 (16)	C48—C49	1.3911 (18)
N3—C7	1.4639 (17)	C48—H48	0.9500
N4—C11	1.4903 (18)	C49—C50	1.388 (2)
N4—C9	1.4983 (17)	C49—H49	0.9500
N4—C10	1.5052 (19)	C50—C51	1.380 (2)
N4—C8	1.5114 (16)	C50—H50	0.9500
C2—H2A	0.9800	C51—C52	1.3960 (18)
C2—H2B	0.9800	C51—H51	0.9500
C2—H2C	0.9800	C52—H52	0.9500
C3—H3A	0.9800	B2—C71	1.6394 (18)
C3—H3B	0.9800	B2—C53	1.6431 (18)
C3—H3C	0.9800	B2—C65	1.6430 (18)
C4—H4A	0.9800	B2—C59	1.6457 (18)
C4—H4B	0.9800	C53—C54	1.4003 (17)
C4—H4C	0.9800	C53—C58	1.4092 (17)
C5—H5A	0.9800	C54—C55	1.3945 (18)
C5—H5B	0.9800	C54—H54	0.9500
C5—H5C	0.9800	C55—C56	1.386 (2)
C6—H6A	0.9800	C55—H55	0.9500
C6—H6B	0.9800	C56—C57	1.389 (2)
C6—H6C	0.9800	C56—H56	0.9500
C7—C8	1.5376 (18)	C57—C58	1.3883 (18)
C7—H7A	0.9900	C57—H57	0.9500
C7—H7B	0.9900	C58—H58	0.9500
C8—H8A	0.9900	C59—C64	1.3944 (18)
C8—H8B	0.9900	C59—C60	1.4058 (18)
C9—H9A	0.9800	C60—C61	1.3901 (18)
C9—H9B	0.9800	C60—H60	0.9500
C9—H9C	0.9800	C61—C62	1.388 (2)
C10—H10A	0.9800	C61—H61	0.9500
C10—H10B	0.9800	C62—C63	1.380 (2)
C10—H10C	0.9800	C62—H62	0.9500
C11—H11A	0.9800	C63—C64	1.398 (2)
C11—H11B	0.9800	C63—H63	0.9500
C11—H11C	0.9800	C64—H64	0.9500
N8—C22	1.4969 (16)	C65—C70	1.3988 (18)
N8—C20	1.4980 (16)	C65—C66	1.4060 (18)
N8—C21	1.5043 (16)	C66—C67	1.3901 (19)
N8—C19	1.5060 (16)	C66—H66	0.9500

C12A—N5A	1.335 (2)	C67—C68	1.385 (2)
C12A—N6A	1.342 (2)	C67—H67	0.9500
C12A—N7A	1.352 (2)	C68—C69	1.381 (2)
N5A—C13A	1.4623 (19)	C68—H68	0.9500
N5A—C14A	1.471 (2)	C69—C70	1.3966 (18)
N6A—C16A	1.466 (4)	C69—H69	0.9500
N6A—C15A	1.4657 (19)	C70—H70	0.9500
N7A—C18A	1.460 (2)	C71—C76	1.4020 (17)
N7A—C17A	1.4818 (19)	C71—C72	1.4079 (17)
C13A—H13A	0.9800	C72—C73	1.3868 (18)
C13A—H13B	0.9800	C72—H72	0.9500
C13A—H13C	0.9800	C73—C74	1.3903 (19)
C14A—H14A	0.9800	C73—H73	0.9500
C14A—H14B	0.9800	C74—C75	1.3839 (19)
C14A—H14C	0.9800	C74—H74	0.9500
C15A—H15A	0.9800	C75—C76	1.3949 (18)
C15A—H15B	0.9800	C75—H75	0.9500
C15A—H15C	0.9800	C76—H76	0.9500
C16A—H16A	0.9800	B3—C83	1.6439 (18)
C16A—H16B	0.9800	B3—C95	1.6448 (18)
C16A—H16C	0.9800	B3—C89	1.6521 (18)
C17A—H17A	0.9800	B3—C77	1.6598 (18)
C17A—H17B	0.9800	C77—C78	1.4028 (18)
C17A—H17C	0.9800	C77—C82	1.4064 (18)
C18A—C19	1.530 (2)	C78—C79	1.3969 (18)
C18A—H18A	0.9900	C78—H78	0.9500
C18A—H18B	0.9900	C79—C80	1.380 (2)
C12B—N5B	1.341 (18)	C79—H79	0.9500
C12B—N6B	1.349 (16)	C80—C81	1.384 (2)
C12B—N7B	1.364 (16)	C80—H80	0.9500
N5B—C14B	1.469 (18)	C81—C82	1.3925 (18)
N5B—C13B	1.488 (16)	C81—H81	0.9500
N6B—C15B	1.457 (16)	C82—H82	0.9500
N6B—C16B	1.482 (18)	C83—C88	1.4030 (17)
N7B—C18B	1.476 (16)	C83—C84	1.4085 (17)
N7B—C17B	1.488 (16)	C84—C85	1.3900 (17)
C13B—H13D	0.9800	C84—H84	0.9500
C13B—H13E	0.9800	C85—C86	1.3894 (19)
C13B—H13F	0.9800	C85—H85	0.9500
C14B—H14D	0.9800	C86—C87	1.3832 (19)
C14B—H14E	0.9800	C86—H86	0.9500
C14B—H14F	0.9800	C87—C88	1.3959 (18)
C15B—H15D	0.9800	C87—H87	0.9500
C15B—H15E	0.9800	C88—H88	0.9500
C15B—H15F	0.9800	C89—C94	1.4014 (17)
C16B—H16D	0.9800	C89—C90	1.4071 (17)
C16B—H16E	0.9800	C90—C91	1.3886 (18)
C16B—H16F	0.9800	C90—H90	0.9500

C17B—H17D	0.9800	C91—C92	1.3872 (19)
C17B—H17E	0.9800	C91—H91	0.9500
C17B—H17F	0.9800	C92—C93	1.3857 (19)
C18B—C19	1.542 (10)	C92—H92	0.9500
C18B—H18C	0.9900	C93—C94	1.3967 (18)
C18B—H18D	0.9900	C93—H93	0.9500
C19—H19A	0.9900	C94—H94	0.9500
C19—H19B	0.9900	C95—C100	1.4018 (17)
C20—H20A	0.9800	C95—C96	1.4086 (17)
C20—H20B	0.9800	C96—C97	1.3907 (18)
C20—H20C	0.9800	C96—H96	0.9500
C21—H21A	0.9800	C97—C98	1.390 (2)
C21—H21B	0.9800	C97—H97	0.9500
C21—H21C	0.9800	C98—C99	1.3878 (19)
C22—H22A	0.9800	C98—H98	0.9500
C22—H22B	0.9800	C99—C100	1.3997 (17)
C22—H22C	0.9800	C99—H99	0.9500
O1—C23	1.2152 (17)	C100—H100	0.9500
C23—C25	1.489 (2)	B4—C107	1.6451 (18)
C23—C24	1.492 (2)	B4—C101	1.6464 (18)
C24—H24A	0.9800	B4—C119	1.6501 (17)
C24—H24B	0.9800	B4—C113	1.6607 (18)
C24—H24C	0.9800	C101—C102	1.4005 (17)
C25—H25A	0.9800	C101—C106	1.4094 (17)
C25—H25B	0.9800	C102—C103	1.3976 (18)
C25—H25C	0.9800	C102—H102	0.9500
O2—C26	1.2221 (17)	C103—C104	1.3836 (19)
C26—C28	1.490 (2)	C103—H103	0.9500
C26—C27	1.492 (2)	C104—C105	1.3890 (19)
C27—H27A	0.9800	C104—H104	0.9500
C27—H27B	0.9800	C105—C106	1.3897 (18)
C27—H27C	0.9800	C105—H105	0.9500
C28—H28A	0.9800	C106—H106	0.9500
C28—H28B	0.9800	C107—C112	1.4056 (17)
C28—H28C	0.9800	C107—C108	1.4066 (17)
B1—C35	1.6449 (18)	C108—C109	1.3883 (18)
B1—C29	1.6457 (18)	C108—H108	0.9500
B1—C47	1.6463 (18)	C109—C110	1.389 (2)
B1—C41	1.6465 (18)	C109—H109	0.9500
C29—C30	1.3934 (18)	C110—C111	1.3885 (19)
C29—C34	1.4042 (17)	C110—H110	0.9500
C30—C31	1.3947 (19)	C111—C112	1.3979 (17)
C30—H30	0.9500	C111—H111	0.9500
C31—C32	1.385 (2)	C112—H112	0.9500
C31—H31	0.9500	C113—C118	1.3998 (19)
C32—C33	1.387 (2)	C113—C114	1.4058 (18)
C32—H32	0.9500	C114—C115	1.3949 (19)
C33—C34	1.3859 (18)	C114—H114	0.9500

C33—H33	0.9500	C115—C116	1.382 (2)
C34—H34	0.9500	C115—H115	0.9500
C35—C40	1.3991 (17)	C116—C117	1.379 (2)
C35—C36	1.4054 (18)	C116—H116	0.9500
C36—C37	1.3901 (18)	C117—C118	1.396 (2)
C36—H36	0.9500	C117—H117	0.9500
C37—C38	1.387 (2)	C118—H118	0.9500
C37—H37	0.9500	C119—C124	1.4028 (17)
C38—C39	1.381 (2)	C119—C120	1.4066 (17)
C38—H38	0.9500	C120—C121	1.3882 (18)
C39—C40	1.3990 (18)	C120—H120	0.9500
C39—H39	0.9500	C121—C122	1.390 (2)
C40—H40	0.9500	C121—H121	0.9500
C41—C46	1.4014 (17)	C122—C123	1.385 (2)
C41—C42	1.4076 (17)	C122—H122	0.9500
C42—C43	1.3908 (18)	C123—C124	1.4022 (18)
C42—H42	0.9500	C123—H123	0.9500
C43—C44	1.3899 (19)	C124—H124	0.9500
C43—H43	0.9500		

C1—N1—C2	122.38 (11)	C39—C40—C35	122.55 (12)
C1—N1—C3	122.06 (12)	C39—C40—H40	118.7
C2—N1—C3	115.53 (12)	C35—C40—H40	118.7
C1—N2—C5	122.18 (11)	C46—C41—C42	114.98 (11)
C1—N2—C4	122.27 (12)	C46—C41—B1	125.29 (11)
C5—N2—C4	115.44 (12)	C42—C41—B1	119.71 (11)
C1—N3—C6	121.06 (11)	C43—C42—C41	123.03 (12)
C1—N3—C7	122.72 (11)	C43—C42—H42	118.5
C6—N3—C7	116.21 (10)	C41—C42—H42	118.5
C11—N4—C9	109.37 (11)	C44—C43—C42	120.11 (12)
C11—N4—C10	109.31 (12)	C44—C43—H43	119.9
C9—N4—C10	108.30 (12)	C42—C43—H43	119.9
C11—N4—C8	111.44 (11)	C45—C44—C43	118.86 (12)
C9—N4—C8	111.66 (10)	C45—C44—H44	120.6
C10—N4—C8	106.65 (10)	C43—C44—H44	120.6
N1—C1—N2	120.76 (12)	C44—C45—C46	120.16 (12)
N1—C1—N3	119.84 (12)	C44—C45—H45	119.9
N2—C1—N3	119.40 (12)	C46—C45—H45	119.9
N1—C2—H2A	109.5	C45—C46—C41	122.85 (12)
N1—C2—H2B	109.5	C45—C46—H46	118.6
H2A—C2—H2B	109.5	C41—C46—H46	118.6
N1—C2—H2C	109.5	C52—C47—C48	115.01 (11)
H2A—C2—H2C	109.5	C52—C47—B1	124.40 (11)
H2B—C2—H2C	109.5	C48—C47—B1	120.32 (11)
N1—C3—H3A	109.5	C49—C48—C47	123.07 (12)
N1—C3—H3B	109.5	C49—C48—H48	118.5
H3A—C3—H3B	109.5	C47—C48—H48	118.5
N1—C3—H3C	109.5	C50—C49—C48	120.01 (12)

H3A—C3—H3C	109.5	C50—C49—H49	120.0
H3B—C3—H3C	109.5	C48—C49—H49	120.0
N2—C4—H4A	109.5	C51—C50—C49	118.56 (12)
N2—C4—H4B	109.5	C51—C50—H50	120.7
H4A—C4—H4B	109.5	C49—C50—H50	120.7
N2—C4—H4C	109.5	C50—C51—C52	120.76 (13)
H4A—C4—H4C	109.5	C50—C51—H51	119.6
H4B—C4—H4C	109.5	C52—C51—H51	119.6
N2—C5—H5A	109.5	C47—C52—C51	122.58 (12)
N2—C5—H5B	109.5	C47—C52—H52	118.7
H5A—C5—H5B	109.5	C51—C52—H52	118.7
N2—C5—H5C	109.5	C71—B2—C53	111.74 (10)
H5A—C5—H5C	109.5	C71—B2—C65	105.30 (10)
H5B—C5—H5C	109.5	C53—B2—C65	111.48 (10)
N3—C6—H6A	109.5	C71—B2—C59	112.03 (10)
N3—C6—H6B	109.5	C53—B2—C59	104.64 (10)
H6A—C6—H6B	109.5	C65—B2—C59	111.82 (10)
N3—C6—H6C	109.5	C54—C53—C58	115.10 (11)
H6A—C6—H6C	109.5	C54—C53—B2	125.19 (11)
H6B—C6—H6C	109.5	C58—C53—B2	119.63 (11)
N3—C7—C8	110.22 (11)	C55—C54—C53	122.65 (12)
N3—C7—H7A	109.6	C55—C54—H54	118.7
C8—C7—H7A	109.6	C53—C54—H54	118.7
N3—C7—H7B	109.6	C56—C55—C54	120.36 (13)
C8—C7—H7B	109.6	C56—C55—H55	119.8
H7A—C7—H7B	108.1	C54—C55—H55	119.8
N4—C8—C7	115.88 (10)	C55—C56—C57	118.88 (12)
N4—C8—H8A	108.3	C55—C56—H56	120.6
C7—C8—H8A	108.3	C57—C56—H56	120.6
N4—C8—H8B	108.3	C58—C57—C56	119.98 (12)
C7—C8—H8B	108.3	C58—C57—H57	120.0
H8A—C8—H8B	107.4	C56—C57—H57	120.0
N4—C9—H9A	109.5	C57—C58—C53	123.03 (12)
N4—C9—H9B	109.5	C57—C58—H58	118.5
H9A—C9—H9B	109.5	C53—C58—H58	118.5
N4—C9—H9C	109.5	C64—C59—C60	114.76 (12)
H9A—C9—H9C	109.5	C64—C59—B2	125.53 (11)
H9B—C9—H9C	109.5	C60—C59—B2	119.58 (11)
N4—C10—H10A	109.5	C61—C60—C59	123.23 (13)
N4—C10—H10B	109.5	C61—C60—H60	118.4
H10A—C10—H10B	109.5	C59—C60—H60	118.4
N4—C10—H10C	109.5	C62—C61—C60	120.06 (13)
H10A—C10—H10C	109.5	C62—C61—H61	120.0
H10B—C10—H10C	109.5	C60—C61—H61	120.0
N4—C11—H11A	109.5	C63—C62—C61	118.54 (12)
N4—C11—H11B	109.5	C63—C62—H62	120.7
H11A—C11—H11B	109.5	C61—C62—H62	120.7
N4—C11—H11C	109.5	C62—C63—C64	120.53 (14)

H11A—C11—H11C	109.5	C62—C63—H63	119.7
H11B—C11—H11C	109.5	C64—C63—H63	119.7
C22—N8—C20	109.21 (10)	C59—C64—C63	122.85 (13)
C22—N8—C21	109.69 (10)	C59—C64—H64	118.6
C20—N8—C21	108.45 (10)	C63—C64—H64	118.6
C22—N8—C19	111.56 (10)	C70—C65—C66	115.06 (12)
C20—N8—C19	110.53 (10)	C70—C65—B2	124.66 (11)
C21—N8—C19	107.34 (10)	C66—C65—B2	120.18 (11)
N5A—C12A—N6A	120.29 (15)	C67—C66—C65	123.01 (13)
N5A—C12A—N7A	120.41 (15)	C67—C66—H66	118.5
N6A—C12A—N7A	119.28 (17)	C65—C66—H66	118.5
C12A—N5A—C13A	122.70 (15)	C68—C67—C66	119.99 (13)
C12A—N5A—C14A	122.35 (15)	C68—C67—H67	120.0
C13A—N5A—C14A	114.87 (13)	C66—C67—H67	120.0
C12A—N6A—C16A	122.3 (3)	C69—C68—C67	118.95 (12)
C12A—N6A—C15A	122.18 (17)	C69—C68—H68	120.5
C16A—N6A—C15A	115.5 (3)	C67—C68—H68	120.5
C12A—N7A—C18A	121.87 (15)	C68—C69—C70	120.41 (13)
C12A—N7A—C17A	122.73 (15)	C68—C69—H69	119.8
C18A—N7A—C17A	114.90 (12)	C70—C69—H69	119.8
N5A—C13A—H13A	109.5	C69—C70—C65	122.56 (13)
N5A—C13A—H13B	109.5	C69—C70—H70	118.7
H13A—C13A—H13B	109.5	C65—C70—H70	118.7
N5A—C13A—H13C	109.5	C76—C71—C72	115.06 (11)
H13A—C13A—H13C	109.5	C76—C71—B2	124.59 (11)
H13B—C13A—H13C	109.5	C72—C71—B2	120.20 (11)
N5A—C14A—H14A	109.5	C73—C72—C71	123.01 (12)
N5A—C14A—H14B	109.5	C73—C72—H72	118.5
H14A—C14A—H14B	109.5	C71—C72—H72	118.5
N5A—C14A—H14C	109.5	C72—C73—C74	120.02 (12)
H14A—C14A—H14C	109.5	C72—C73—H73	120.0
H14B—C14A—H14C	109.5	C74—C73—H73	120.0
N6A—C15A—H15A	109.5	C75—C74—C73	118.90 (12)
N6A—C15A—H15B	109.5	C75—C74—H74	120.6
H15A—C15A—H15B	109.5	C73—C74—H74	120.6
N6A—C15A—H15C	109.5	C74—C75—C76	120.30 (12)
H15A—C15A—H15C	109.5	C74—C75—H75	119.9
H15B—C15A—H15C	109.5	C76—C75—H75	119.9
N6A—C16A—H16A	109.5	C75—C76—C71	122.66 (12)
N6A—C16A—H16B	109.5	C75—C76—H76	118.7
H16A—C16A—H16B	109.5	C71—C76—H76	118.7
N6A—C16A—H16C	109.5	C83—B3—C95	108.90 (10)
H16A—C16A—H16C	109.5	C83—B3—C89	110.27 (10)
H16B—C16A—H16C	109.5	C95—B3—C89	108.35 (9)
N7A—C17A—H17A	109.5	C83—B3—C77	110.13 (10)
N7A—C17A—H17B	109.5	C95—B3—C77	109.37 (9)
H17A—C17A—H17B	109.5	C89—B3—C77	109.79 (10)
N7A—C17A—H17C	109.5	C78—C77—C82	114.48 (11)

H17A—C17A—H17C	109.5	C78—C77—B3	124.24 (11)
H17B—C17A—H17C	109.5	C82—C77—B3	121.23 (11)
N7A—C18A—C19	107.99 (12)	C79—C78—C77	122.95 (13)
N7A—C18A—H18A	110.1	C79—C78—H78	118.5
C19—C18A—H18A	110.1	C77—C78—H78	118.5
N7A—C18A—H18B	110.1	C80—C79—C78	120.45 (13)
C19—C18A—H18B	110.1	C80—C79—H79	119.8
H18A—C18A—H18B	108.4	C78—C79—H79	119.8
N5B—C12B—N6B	117.4 (17)	C79—C80—C81	118.71 (12)
N5B—C12B—N7B	120.1 (17)	C79—C80—H80	120.6
N6B—C12B—N7B	119.9 (17)	C81—C80—H80	120.6
C12B—N5B—C14B	122 (2)	C80—C81—C82	120.19 (13)
C12B—N5B—C13B	124 (2)	C80—C81—H81	119.9
C14B—N5B—C13B	113 (2)	C82—C81—H81	119.9
C12B—N6B—C15B	125 (2)	C81—C82—C77	123.21 (13)
C12B—N6B—C16B	122 (2)	C81—C82—H82	118.4
C15B—N6B—C16B	110.5 (19)	C77—C82—H82	118.4
C12B—N7B—C18B	120.3 (19)	C88—C83—C84	114.93 (11)
C12B—N7B—C17B	120.9 (19)	C88—C83—B3	123.99 (11)
C18B—N7B—C17B	118.8 (15)	C84—C83—B3	121.07 (11)
N5B—C13B—H13D	109.5	C85—C84—C83	122.89 (12)
N5B—C13B—H13E	109.5	C85—C84—H84	118.6
H13D—C13B—H13E	109.5	C83—C84—H84	118.6
N5B—C13B—H13F	109.5	C86—C85—C84	120.18 (12)
H13D—C13B—H13F	109.5	C86—C85—H85	119.9
H13E—C13B—H13F	109.5	C84—C85—H85	119.9
N5B—C14B—H14D	109.5	C87—C86—C85	118.91 (12)
N5B—C14B—H14E	109.5	C87—C86—H86	120.5
H14D—C14B—H14E	109.5	C85—C86—H86	120.5
N5B—C14B—H14F	109.5	C86—C87—C88	120.19 (12)
H14D—C14B—H14F	109.5	C86—C87—H87	119.9
H14E—C14B—H14F	109.5	C88—C87—H87	119.9
N6B—C15B—H15D	109.5	C87—C88—C83	122.89 (12)
N6B—C15B—H15E	109.5	C87—C88—H88	118.6
H15D—C15B—H15E	109.5	C83—C88—H88	118.6
N6B—C15B—H15F	109.5	C94—C89—C90	114.58 (11)
H15D—C15B—H15F	109.5	C94—C89—B3	124.85 (11)
H15E—C15B—H15F	109.5	C90—C89—B3	120.56 (11)
N6B—C16B—H16D	109.5	C91—C90—C89	123.40 (12)
N6B—C16B—H16E	109.5	C91—C90—H90	118.3
H16D—C16B—H16E	109.5	C89—C90—H90	118.3
N6B—C16B—H16F	109.5	C92—C91—C90	120.08 (12)
H16D—C16B—H16F	109.5	C92—C91—H91	120.0
H16E—C16B—H16F	109.5	C90—C91—H91	120.0
N7B—C17B—H17D	109.5	C93—C92—C91	118.65 (12)
N7B—C17B—H17E	109.4	C93—C92—H92	120.7
H17D—C17B—H17E	109.5	C91—C92—H92	120.7
N7B—C17B—H17F	109.5	C92—C93—C94	120.37 (12)

H17D—C17B—H17F	109.5	C92—C93—H93	119.8
H17E—C17B—H17F	109.5	C94—C93—H93	119.8
N7B—C18B—C19	128.8 (17)	C93—C94—C89	122.89 (12)
N7B—C18B—H18C	105.1	C93—C94—H94	118.6
C19—C18B—H18C	105.2	C89—C94—H94	118.6
N7B—C18B—H18D	105.0	C100—C95—C96	115.32 (11)
C19—C18B—H18D	105.0	C100—C95—B3	124.25 (11)
H18C—C18B—H18D	105.9	C96—C95—B3	120.32 (11)
N8—C19—C18A	114.69 (11)	C97—C96—C95	122.88 (12)
N8—C19—C18B	114.2 (10)	C97—C96—H96	118.6
N8—C19—H19A	108.6	C95—C96—H96	118.6
C18A—C19—H19A	108.6	C98—C97—C96	119.93 (12)
N8—C19—H19B	108.6	C98—C97—H97	120.0
C18A—C19—H19B	108.6	C96—C97—H97	120.0
H19A—C19—H19B	107.6	C99—C98—C97	119.26 (12)
N8—C20—H20A	109.5	C99—C98—H98	120.4
N8—C20—H20B	109.5	C97—C98—H98	120.4
H20A—C20—H20B	109.5	C98—C99—C100	119.89 (12)
N8—C20—H20C	109.5	C98—C99—H99	120.1
H20A—C20—H20C	109.5	C100—C99—H99	120.1
H20B—C20—H20C	109.5	C99—C100—C95	122.71 (12)
N8—C21—H21A	109.5	C99—C100—H100	118.6
N8—C21—H21B	109.5	C95—C100—H100	118.6
H21A—C21—H21B	109.5	C107—B4—C101	109.69 (9)
N8—C21—H21C	109.5	C107—B4—C119	108.08 (10)
H21A—C21—H21C	109.5	C101—B4—C119	111.98 (10)
H21B—C21—H21C	109.5	C107—B4—C113	110.14 (10)
N8—C22—H22A	109.5	C101—B4—C113	110.41 (10)
N8—C22—H22B	109.5	C119—B4—C113	106.46 (9)
H22A—C22—H22B	109.5	C102—C101—C106	114.65 (11)
N8—C22—H22C	109.5	C102—C101—B4	125.10 (11)
H22A—C22—H22C	109.5	C106—C101—B4	120.21 (11)
H22B—C22—H22C	109.5	C103—C102—C101	123.01 (12)
O1—C23—C25	121.22 (15)	C103—C102—H102	118.5
O1—C23—C24	121.62 (14)	C101—C102—H102	118.5
C25—C23—C24	117.11 (14)	C104—C103—C102	120.09 (12)
C23—C24—H24A	109.5	C104—C103—H103	120.0
C23—C24—H24B	109.5	C102—C103—H103	120.0
H24A—C24—H24B	109.5	C103—C104—C105	119.04 (12)
C23—C24—H24C	109.5	C103—C104—H104	120.5
H24A—C24—H24C	109.5	C105—C104—H104	120.5
H24B—C24—H24C	109.5	C104—C105—C106	119.85 (12)
C23—C25—H25A	109.5	C104—C105—H105	120.1
C23—C25—H25B	109.5	C106—C105—H105	120.1
H25A—C25—H25B	109.5	C105—C106—C101	123.27 (12)
C23—C25—H25C	109.5	C105—C106—H106	118.4
H25A—C25—H25C	109.5	C101—C106—H106	118.4
H25B—C25—H25C	109.5	C112—C107—C108	115.15 (11)

O2—C26—C28	121.72 (15)	C112—C107—B4	122.14 (11)
O2—C26—C27	122.07 (14)	C108—C107—B4	122.36 (11)
C28—C26—C27	116.19 (13)	C109—C108—C107	122.50 (12)
C26—C27—H27A	109.5	C109—C108—H108	118.7
C26—C27—H27B	109.5	C107—C108—H108	118.7
H27A—C27—H27B	109.5	C108—C109—C110	120.80 (12)
C26—C27—H27C	109.5	C108—C109—H109	119.6
H27A—C27—H27C	109.5	C110—C109—H109	119.6
H27B—C27—H27C	109.5	C111—C110—C109	118.67 (12)
C26—C28—H28A	109.5	C111—C110—H110	120.7
C26—C28—H28B	109.5	C109—C110—H110	120.7
H28A—C28—H28B	109.5	C110—C111—C112	119.90 (12)
C26—C28—H28C	109.5	C110—C111—H111	120.0
H28A—C28—H28C	109.5	C112—C111—H111	120.0
H28B—C28—H28C	109.5	C111—C112—C107	122.97 (12)
C35—B1—C29	110.58 (10)	C111—C112—H112	118.5
C35—B1—C47	110.31 (10)	C107—C112—H112	118.5
C29—B1—C47	104.72 (9)	C118—C113—C114	114.84 (12)
C35—B1—C41	107.25 (9)	C118—C113—B4	124.42 (11)
C29—B1—C41	111.25 (10)	C114—C113—B4	120.73 (11)
C47—B1—C41	112.77 (10)	C115—C114—C113	122.93 (14)
C30—C29—C34	115.26 (11)	C115—C114—H114	118.5
C30—C29—B1	125.14 (11)	C113—C114—H114	118.5
C34—C29—B1	119.59 (11)	C116—C115—C114	120.06 (14)
C29—C30—C31	122.71 (12)	C116—C115—H115	120.0
C29—C30—H30	118.6	C114—C115—H115	120.0
C31—C30—H30	118.6	C117—C116—C115	119.00 (13)
C32—C31—C30	120.22 (13)	C117—C116—H116	120.5
C32—C31—H31	119.9	C115—C116—H116	120.5
C30—C31—H31	119.9	C116—C117—C118	120.33 (15)
C31—C32—C33	118.75 (12)	C116—C117—H117	119.8
C31—C32—H32	120.6	C118—C117—H117	119.8
C33—C32—H32	120.6	C117—C118—C113	122.83 (14)
C34—C33—C32	120.11 (12)	C117—C118—H118	118.6
C34—C33—H33	119.9	C113—C118—H118	118.6
C32—C33—H33	119.9	C124—C119—C120	115.20 (11)
C33—C34—C29	122.94 (12)	C124—C119—B4	124.58 (11)
C33—C34—H34	118.5	C120—C119—B4	120.06 (11)
C29—C34—H34	118.5	C121—C120—C119	122.98 (12)
C40—C35—C36	115.24 (11)	C121—C120—H120	118.5
C40—C35—B1	124.61 (11)	C119—C120—H120	118.5
C36—C35—B1	120.15 (11)	C120—C121—C122	120.17 (12)
C37—C36—C35	122.97 (12)	C120—C121—H121	119.9
C37—C36—H36	118.5	C122—C121—H121	119.9
C35—C36—H36	118.5	C123—C122—C121	118.91 (12)
C38—C37—C36	119.82 (13)	C123—C122—H122	120.5
C38—C37—H37	120.1	C121—C122—H122	120.5
C36—C37—H37	120.1	C122—C123—C124	120.16 (12)

C39—C38—C37	119.24 (12)	C122—C123—H123	119.9
C39—C38—H38	120.4	C124—C123—H123	119.9
C37—C38—H38	120.4	C123—C124—C119	122.56 (12)
C38—C39—C40	120.11 (13)	C123—C124—H124	118.7
C38—C39—H39	119.9	C119—C124—H124	118.7
C40—C39—H39	119.9		

C2—N1—C1—N2	−150.64 (12)	C53—B2—C65—C70	−1.46 (16)
C3—N1—C1—N2	31.40 (18)	C59—B2—C65—C70	−118.21 (13)
C2—N1—C1—N3	30.51 (18)	C71—B2—C65—C66	−56.32 (14)
C3—N1—C1—N3	−147.45 (12)	C53—B2—C65—C66	−177.67 (11)
C5—N2—C1—N1	−144.00 (13)	C59—B2—C65—C66	65.58 (14)
C4—N2—C1—N1	32.01 (18)	C70—C65—C66—C67	1.27 (19)
C5—N2—C1—N3	34.86 (18)	B2—C65—C66—C67	177.83 (12)
C4—N2—C1—N3	−149.13 (12)	C65—C66—C67—C68	−0.9 (2)
C6—N3—C1—N1	39.40 (17)	C66—C67—C68—C69	−0.3 (2)
C7—N3—C1—N1	−139.38 (12)	C67—C68—C69—C70	1.0 (2)
C6—N3—C1—N2	−139.47 (12)	C68—C69—C70—C65	−0.6 (2)
C7—N3—C1—N2	41.75 (17)	C66—C65—C70—C69	−0.53 (18)
C1—N3—C7—C8	102.31 (14)	B2—C65—C70—C69	−176.91 (12)
C6—N3—C7—C8	−76.52 (14)	C53—B2—C71—C76	−122.14 (12)
C11—N4—C8—C7	57.35 (15)	C65—B2—C71—C76	116.68 (13)
C9—N4—C8—C7	−65.30 (15)	C59—B2—C71—C76	−5.09 (17)
C10—N4—C8—C7	176.57 (13)	C53—B2—C71—C72	62.48 (14)
N3—C7—C8—N4	131.18 (11)	C65—B2—C71—C72	−58.70 (14)
N6A—C12A—N5A—C13A	144.2 (2)	C59—B2—C71—C72	179.54 (11)
N7A—C12A—N5A—C13A	−34.1 (4)	C76—C71—C72—C73	1.53 (18)
N6A—C12A—N5A—C14A	−32.3 (4)	B2—C71—C72—C73	177.33 (12)
N7A—C12A—N5A—C14A	149.4 (2)	C71—C72—C73—C74	−2.0 (2)
N5A—C12A—N6A—C16A	145.0 (3)	C72—C73—C74—C75	0.4 (2)
N7A—C12A—N6A—C16A	−36.7 (4)	C73—C74—C75—C76	1.4 (2)
N5A—C12A—N6A—C15A	−34.6 (4)	C74—C75—C76—C71	−1.9 (2)
N7A—C12A—N6A—C15A	143.7 (2)	C72—C71—C76—C75	0.38 (18)
N5A—C12A—N7A—C18A	−40.8 (4)	B2—C71—C76—C75	−175.20 (12)
N6A—C12A—N7A—C18A	140.9 (2)	C83—B3—C77—C78	−14.10 (16)
N5A—C12A—N7A—C17A	147.7 (2)	C95—B3—C77—C78	105.54 (13)
N6A—C12A—N7A—C17A	−30.6 (4)	C89—B3—C77—C78	−135.70 (12)
C12A—N7A—C18A—C19	−79.8 (2)	C83—B3—C77—C82	168.40 (11)
C17A—N7A—C18A—C19	92.35 (14)	C95—B3—C77—C82	−71.96 (14)
N6B—C12B—N5B—C14B	20 (8)	C89—B3—C77—C82	46.80 (15)
N7B—C12B—N5B—C14B	−142 (6)	C82—C77—C78—C79	−0.82 (18)
N6B—C12B—N5B—C13B	−145 (3)	B3—C77—C78—C79	−178.48 (11)
N7B—C12B—N5B—C13B	53 (6)	C77—C78—C79—C80	0.4 (2)
N5B—C12B—N6B—C15B	61 (5)	C78—C79—C80—C81	0.3 (2)
N7B—C12B—N6B—C15B	−137 (3)	C79—C80—C81—C82	−0.5 (2)
N5B—C12B—N6B—C16B	−138 (3)	C80—C81—C82—C77	0.1 (2)
N7B—C12B—N6B—C16B	24 (6)	C78—C77—C82—C81	0.56 (18)
N5B—C12B—N7B—C18B	32 (6)	B3—C77—C82—C81	178.30 (12)

N6B—C12B—N7B—C18B	−130 (3)	C95—B3—C83—C88	10.63 (16)
N5B—C12B—N7B—C17B	−148 (3)	C89—B3—C83—C88	−108.13 (13)
N6B—C12B—N7B—C17B	50 (5)	C77—B3—C83—C88	130.55 (12)
C12B—N7B—C18B—C19	35 (5)	C95—B3—C83—C84	−168.36 (11)
C17B—N7B—C18B—C19	−145 (3)	C89—B3—C83—C84	72.88 (14)
C22—N8—C19—C18A	−52.23 (14)	C77—B3—C83—C84	−48.44 (14)
C20—N8—C19—C18A	69.49 (14)	C88—C83—C84—C85	−1.55 (18)
C21—N8—C19—C18A	−172.42 (11)	B3—C83—C84—C85	177.53 (11)
C22—N8—C19—C18B	−37.6 (14)	C83—C84—C85—C86	0.81 (19)
C20—N8—C19—C18B	84.1 (14)	C84—C85—C86—C87	0.34 (19)
C21—N8—C19—C18B	−157.8 (14)	C85—C86—C87—C88	−0.65 (19)
N7A—C18A—C19—N8	−160.91 (11)	C86—C87—C88—C83	−0.17 (19)
N7B—C18B—C19—N8	161 (2)	C84—C83—C88—C87	1.23 (18)
C35—B1—C29—C30	−106.58 (13)	B3—C83—C88—C87	−177.82 (11)
C47—B1—C29—C30	134.61 (12)	C83—B3—C89—C94	−18.18 (16)
C41—B1—C29—C30	12.50 (16)	C95—B3—C89—C94	−137.27 (12)
C35—B1—C29—C34	74.54 (14)	C77—B3—C89—C94	103.34 (13)
C47—B1—C29—C34	−44.28 (14)	C83—B3—C89—C90	161.99 (11)
C41—B1—C29—C34	−166.39 (11)	C95—B3—C89—C90	42.90 (14)
C34—C29—C30—C31	0.55 (19)	C77—B3—C89—C90	−76.49 (13)
B1—C29—C30—C31	−178.37 (12)	C94—C89—C90—C91	−1.55 (18)
C29—C30—C31—C32	0.4 (2)	B3—C89—C90—C91	178.30 (11)
C30—C31—C32—C33	−0.9 (2)	C89—C90—C91—C92	0.3 (2)
C31—C32—C33—C34	0.5 (2)	C90—C91—C92—C93	0.84 (19)
C32—C33—C34—C29	0.5 (2)	C91—C92—C93—C94	−0.54 (19)
C30—C29—C34—C33	−0.97 (19)	C92—C93—C94—C89	−0.9 (2)
B1—C29—C34—C33	178.02 (12)	C90—C89—C94—C93	1.86 (18)
C29—B1—C35—C40	−0.87 (16)	B3—C89—C94—C93	−177.98 (11)
C47—B1—C35—C40	114.50 (13)	C83—B3—C95—C100	99.79 (13)
C41—B1—C35—C40	−122.34 (12)	C89—B3—C95—C100	−140.25 (11)
C29—B1—C35—C36	179.91 (11)	C77—B3—C95—C100	−20.60 (16)
C47—B1—C35—C36	−64.72 (14)	C83—B3—C95—C96	−76.06 (14)
C41—B1—C35—C36	58.44 (14)	C89—B3—C95—C96	43.89 (14)
C40—C35—C36—C37	−2.85 (18)	C77—B3—C95—C96	163.54 (11)
B1—C35—C36—C37	176.44 (12)	C100—C95—C96—C97	−0.81 (18)
C35—C36—C37—C38	1.4 (2)	B3—C95—C96—C97	175.40 (12)
C36—C37—C38—C39	1.0 (2)	C95—C96—C97—C98	0.5 (2)
C37—C38—C39—C40	−1.7 (2)	C96—C97—C98—C99	0.09 (19)
C38—C39—C40—C35	0.2 (2)	C97—C98—C99—C100	−0.35 (19)
C36—C35—C40—C39	2.06 (18)	C98—C99—C100—C95	0.02 (19)
B1—C35—C40—C39	−177.19 (12)	C96—C95—C100—C99	0.54 (18)
C35—B1—C41—C46	−132.49 (12)	B3—C95—C100—C99	−175.50 (11)
C29—B1—C41—C46	106.47 (13)	C107—B4—C101—C102	−127.47 (12)
C47—B1—C41—C46	−10.85 (17)	C119—B4—C101—C102	−7.48 (16)
C35—B1—C41—C42	45.94 (14)	C113—B4—C101—C102	110.97 (13)
C29—B1—C41—C42	−75.10 (14)	C107—B4—C101—C106	54.67 (14)
C47—B1—C41—C42	167.58 (11)	C119—B4—C101—C106	174.66 (10)
C46—C41—C42—C43	−0.31 (18)	C113—B4—C101—C106	−66.90 (14)

B1—C41—C42—C43	−178.89 (11)	C106—C101—C102—C103	2.56 (18)
C41—C42—C43—C44	0.8 (2)	B4—C101—C102—C103	−175.40 (12)
C42—C43—C44—C45	−0.48 (19)	C101—C102—C103—C104	−0.1 (2)
C43—C44—C45—C46	−0.24 (19)	C102—C103—C104—C105	−1.92 (19)
C44—C45—C46—C41	0.7 (2)	C103—C104—C105—C106	1.35 (19)
C42—C41—C46—C45	−0.44 (18)	C104—C105—C106—C101	1.3 (2)
B1—C41—C46—C45	178.06 (12)	C102—C101—C106—C105	−3.16 (18)
C35—B1—C47—C52	0.78 (16)	B4—C101—C106—C105	174.92 (11)
C29—B1—C47—C52	119.78 (12)	C101—B4—C107—C112	32.99 (15)
C41—B1—C47—C52	−119.10 (13)	C119—B4—C107—C112	−89.35 (13)
C35—B1—C47—C48	−172.97 (11)	C113—B4—C107—C112	154.72 (11)
C29—B1—C47—C48	−53.97 (14)	C101—B4—C107—C108	−154.15 (11)
C41—B1—C47—C48	67.14 (14)	C119—B4—C107—C108	83.50 (13)
C52—C47—C48—C49	−0.08 (18)	C113—B4—C107—C108	−32.43 (15)
B1—C47—C48—C49	174.24 (12)	C112—C107—C108—C109	0.75 (18)
C47—C48—C49—C50	0.1 (2)	B4—C107—C108—C109	−172.57 (12)
C48—C49—C50—C51	0.2 (2)	C107—C108—C109—C110	−0.4 (2)
C49—C50—C51—C52	−0.5 (2)	C108—C109—C110—C111	0.03 (19)
C48—C47—C52—C51	−0.28 (18)	C109—C110—C111—C112	−0.12 (18)
B1—C47—C52—C51	−174.33 (12)	C110—C111—C112—C107	0.56 (19)
C50—C51—C52—C47	0.6 (2)	C108—C107—C112—C111	−0.85 (17)
C71—B2—C53—C54	4.45 (16)	B4—C107—C112—C111	172.48 (11)
C65—B2—C53—C54	121.97 (12)	C107—B4—C113—C118	−92.34 (14)
C59—B2—C53—C54	−116.99 (12)	C101—B4—C113—C118	28.96 (16)
C71—B2—C53—C58	−179.16 (10)	C119—B4—C113—C118	150.72 (12)
C65—B2—C53—C58	−61.64 (14)	C107—B4—C113—C114	86.36 (13)
C59—B2—C53—C58	59.40 (13)	C101—B4—C113—C114	−152.35 (11)
C58—C53—C54—C55	0.36 (17)	C119—B4—C113—C114	−30.58 (15)
B2—C53—C54—C55	176.90 (11)	C118—C113—C114—C115	−0.40 (19)
C53—C54—C55—C56	0.01 (19)	B4—C113—C114—C115	−179.21 (12)
C54—C55—C56—C57	−0.47 (19)	C113—C114—C115—C116	0.5 (2)
C55—C56—C57—C58	0.54 (19)	C114—C115—C116—C117	0.0 (2)
C56—C57—C58—C53	−0.14 (19)	C115—C116—C117—C118	−0.7 (2)
C54—C53—C58—C57	−0.30 (17)	C116—C117—C118—C113	0.9 (2)
B2—C53—C58—C57	−177.05 (11)	C114—C113—C118—C117	−0.31 (19)
C71—B2—C59—C64	117.37 (14)	B4—C113—C118—C117	178.45 (13)
C53—B2—C59—C64	−121.39 (13)	C107—B4—C119—C124	−0.16 (16)
C65—B2—C59—C64	−0.58 (18)	C101—B4—C119—C124	−121.09 (12)
C71—B2—C59—C60	−67.00 (15)	C113—B4—C119—C124	118.15 (12)
C53—B2—C59—C60	54.24 (14)	C107—B4—C119—C120	−175.25 (10)
C65—B2—C59—C60	175.05 (11)	C101—B4—C119—C120	63.82 (14)
C64—C59—C60—C61	1.57 (19)	C113—B4—C119—C120	−56.94 (14)
B2—C59—C60—C61	−174.51 (12)	C124—C119—C120—C121	−0.35 (18)
C59—C60—C61—C62	−0.2 (2)	B4—C119—C120—C121	175.18 (11)
C60—C61—C62—C63	−1.3 (2)	C119—C120—C121—C122	−0.92 (19)
C61—C62—C63—C64	1.3 (2)	C120—C121—C122—C123	1.45 (19)
C60—C59—C64—C63	−1.5 (2)	C121—C122—C123—C124	−0.73 (19)
B2—C59—C64—C63	174.30 (13)	C122—C123—C124—C119	−0.58 (19)

C62—C63—C64—C59	0.1 (2)	C120—C119—C124—C123	1.09 (17)
C71—B2—C65—C70	119.89 (13)	B4—C119—C124—C123	−174.21 (11)

Hydrogen-bond geometry (Å, º)

The ring centroids are defined as follows: Cg1 = C53–C58, Cg2 = C65–C70, Cg3 = C71–C76, Cg4 = C89–C94, Cg5 = C95–C100, Cg6 = C29–C34, Cg7 = C41–C46, Cg8 = C101–C106, Cg9 = C107–C112 and Cg10 = C113–C118.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13*B*—H13*E*···O1	0.98	2.61	3.513 (2)	153
C17*A*—H17*C*···O1	0.98	2.41	3.369 (2)	167
C19—H19*A*···O1	0.99	2.37	3.290 (2)	154
C20—H20*C*···O1	0.98	2.46	3.323 (2)	147
C6—H6*A*···O2	0.98	2.50	3.467 (2)	170
C8—H8*B*···O2	0.99	2.55	3.449 (2)	152
C9—H9*B*···O2	0.98	2.52	3.417 (2)	152
C4—H4*B*···*Cg*1	0.98	3.02	3.881 (2)	146
C21—H21*B*···*Cg*1	0.98	2.74	3.713 (2)	171
C3—H3*C*···*Cg*2^{i}	0.98	2.88	3.739 (2)	147
C13*A*—H13*A*···*Cg*3	0.98	2.75	3.587 (2)	144
C27—H27*C*···*Cg*3^{ii}	0.98	2.94	3.629 (2)	128
C28—H28*B*···*Cg*4^{ii}	0.98	2.84	3.554 (2)	130
C6—H6*B*···*Cg*5^{iii}	0.98	2.67	3.614 (2)	162
C8—H8*A*···*Cg*6	0.99	2.93	3.854 (2)	155
C4—H4*C*···*Cg*7	0.98	2.76	3.669 (2)	154
C24—H24*B*···*Cg*8	0.98	3.05	3.681 (2)	124
C18*A*—H18*A*···*Cg*9^{iv}	0.99	2.71	3.512 (2)	139
C18*B*—H18*C*···*Cg*9^{iv}	0.99	2.87	3.662 (2)	138
C25—H25*C*···*Cg*10^{v}	0.98	2.68	3.653 (2)	175

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