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Bis(tetrabutylammonium) isophthalate 1-phenyl-3-[2,4,5-tris(3-phenylureido)-phenyl]urea: a synchrotron study

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Key indicators

Single-crystal synchrotron study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.149
Data-to-parameter ratio = 17.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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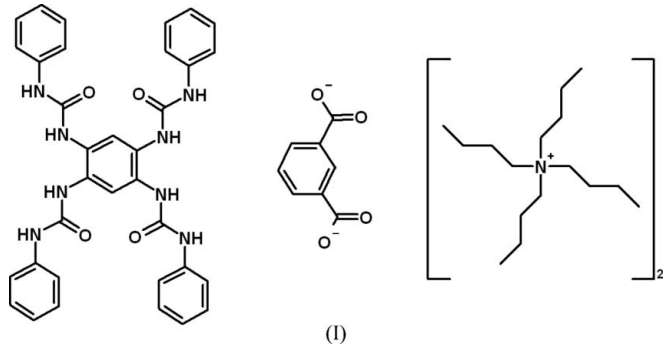
The structure of $2C_{16}H_{36}N^+\cdot C_8H_4O_4^{2-}\cdot C_{34}H_{30}N_8O_4$, comprises tapes of encapsulated hydrogen-bonded isophthalate anions which are arranged into parallel sheets interleaved with tetrabutylammonium layers; each of the two independent neutral molecules is disposed about a centre of inversion.

Comment

The title complex, (I) (Fig. 1), was prepared as part of an ongoing study into the carboxylate-binding properties of urea-based anion receptors (Brooks *et al.*, 2005*a*,*b*, 2006). The receptor of the title compound, (I), exists as two independent molecules each disposed about an inversion centre. Each of these has a similar, but not identical, conformation with the four phenyl urea arms forming a cross-like arrangement. In both cases, the least-squares planes through the pendant phenyl rings of opposing arms are parallel, from symmetry, but the arms are twisted out of the plane defined by the central aromatic ring. Constructing the least-squares planes through the rings of the symmetry-related arms and calculating the angle between them, we obtain values of 59.63 (4) (molecule 1) and 49.09 (4)° (molecule 2); it is this difference that best describes the disparity between the two independent molecules. The geometry of the isophthalate anion is unremarkable, the least-squares plane through both carboxylate groups being tilted away from the ring by 16.6 (3)°.



(I)

The guest isophthalate anions link the hosts into tapes *via* N—H···O hydrogen bonds (Fig. 2 and Table 1), each carboxylate group interacting with an adjacent receptor so that atom O5 forms three hydrogen bonds and atom O6 two; the corresponding atoms of the second independent molecule are O7 and O8, respectively. This implies that the N7—H and N2—H hydrogen bonds are bifurcated. The donor–acceptor distances range from 2.7455 (16) to 3.3616 (16) Å. Within the tapes, the two independent host molecules alternate, and these tapes interdigitate to form sheets in the $(1\bar{1}1)$ plane. The

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supramolecular structure is completed by a parallel arrangement of these sheets interleaved with layers of the tetrabutylammonium counterion.

Experimental

The receptor was prepared according to a literature procedure (Mataka *et al.*, 1993). Crystals of the tetrabutylammonium isophthalate complex were obtained by slow evaporation of a solution of the receptor in acetonitrile in the presence of excess tetrabutylammonium isophthalate.

Crystal data

$2C_{16}H_{36}N^+\cdot C_8H_4O_4^-\cdot C_{34}H_{30}N_8O_4$
$M_r = 1263.69$
Triclinic, $P\overline{1}$
$a = 12.7319\ (3)$ Å
$b = 16.0019\ (4)$ Å
$c = 19.3005\ (5)$ Å
$\alpha = 96.512\ (1)^\circ$
$\beta = 108.754\ (1)^\circ$
$\gamma = 103.554\ (1)^\circ$
$V = 3542.79\ (15)$ Å^3
$Z = 2$
$D_x = 1.185$ Mg m^{-3}
Synchrotron radiation
$\lambda = 0.6727$ Å
Cell parameters from 9807 reflections
$\theta = 2.2$–28.3°
$\mu = 0.08$ mm^{-1}
$T = 120\ (2)$ K
Plate, colourless
$0.15 \times 0.10 \times 0.03$ mm

Data collection

Bruker SMART APEX2 CCD diffractometer
Fine-slice ω scans
32925 measured reflections
16104 independent reflections
12499 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.8^\circ$
$h = -16 \rightarrow 16$
$k = -20 \rightarrow 20$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.149$
$S = 1.02$
16104 reflections
935 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0838P)^2 + 0.6824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O8^{i}	0.88	1.98	2.8316 (16)	164
N2—H2A···O7^{i}	0.88	2.25	3.0983 (16)	161
N2—H2A···O8^{i}	0.88	2.62	3.3616 (16)	143
N3—H3A···O7^{i}	0.88	1.98	2.7455 (16)	145
N4—H4A···O7^{i}	0.88	2.26	3.0052 (17)	142
N5—H5A···O5	0.88	2.23	3.0208 (18)	149
N6—H6···O5	0.88	1.90	2.7393 (17)	158
N7—H7···O5	0.88	2.43	3.2615 (18)	157
N8—H8···O6	0.88	1.87	2.7474 (16)	171

Symmetry code: (i) $-x+1, -y+1, -z+1$.

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 (aromatic), 0.96 (methylene) or 0.98 Å (methyl), N—H = 0.88 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$ and $1.5U_{eq}$(methyl C).

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

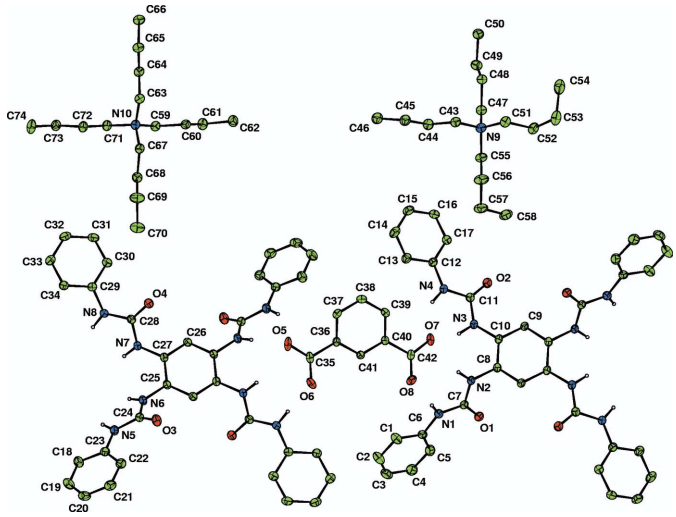

Figure 1
View of the components of (I), with the atoms of the asymmetric unit labelled; non-acidic H atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 30% probability level. In the left-hand neutral molecule unlabelled atoms are related to labelled atoms by $1-x, -y, -z$. In the right-hand neutral molecule unlabelled atoms are related to labelled atoms by $-x, -y, 1-z$.

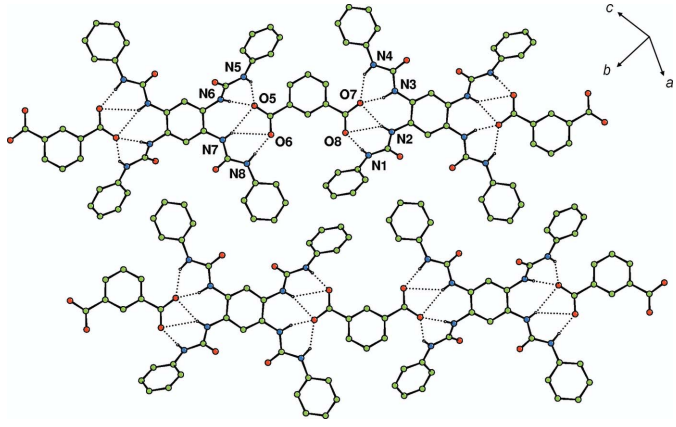

Figure 2
View of the hydrogen-bonded (dashed lines) tapes interdigitated into sheets in the $(1\overline{1}1)$ plane; non-acidic H atoms have been omitted for clarity.

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Synchrotron radiation, $\lambda = 0.6727$ Å
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32925 measured reflections
16104 independent reflections
12499 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.8°$, $\theta_{min} = 2.8°$
$h = -16\rightarrow16$
$k = -20\rightarrow20$
$l = -25\rightarrow25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.149$
$S = 1.02$
16104 reflections
935 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0838P)^2 + 0.6824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

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

Refinement. 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 $F^2 > \sigma(F^2)$ 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}
O1	0.31583 (9)	0.14432 (7)	0.54143 (6)	0.0343 (2)
O2	−0.06953 (10)	0.00678 (7)	0.68958 (6)	0.0400 (3)
N1	0.31146 (11)	0.28565 (8)	0.57725 (7)	0.0319 (3)
H1A	0.2619	0.3159	0.5771	0.048 (5)*
N2	0.15421 (10)	0.17056 (8)	0.55583 (7)	0.0290 (3)
H2A	0.1276	0.2111	0.5732	0.043 (5)*
N3	0.01571 (11)	0.10454 (8)	0.63201 (7)	0.0320 (3)
H3A	0.0549	0.1600	0.6398	0.069 (7)*
N4	−0.02380 (11)	0.15599 (8)	0.73206 (7)	0.0327 (3)
H4A	0.0147	0.2066	0.7266	0.060 (6)*
C1	0.45301 (16)	0.42587 (12)	0.62102 (11)	0.0469 (4)
H1	0.3922	0.4511	0.6201	0.052 (6)*
C2	0.56578 (17)	0.47934 (13)	0.64490 (13)	0.0569 (5)
H2	0.5821	0.5409	0.6608	0.062 (6)*
C3	0.65496 (16)	0.44338 (14)	0.64571 (11)	0.0536 (5)
H3	0.7323	0.4800	0.6612	0.072 (7)*
C4	0.63031 (16)	0.35482 (15)	0.62400 (12)	0.0568 (5)
H4	0.6916	0.3299	0.6254	0.085 (8)*
C5	0.51755 (15)	0.29989 (13)	0.59978 (11)	0.0483 (4)
H5	0.5024	0.2383	0.5844	0.069 (7)*
C6	0.42789 (13)	0.33504 (10)	0.59818 (8)	0.0332 (3)
C7	0.26580 (12)	0.19588 (9)	0.55704 (8)	0.0284 (3)
C8	0.07893 (12)	0.08373 (9)	0.52853 (8)	0.0265 (3)
C9	0.07095 (12)	0.03395 (9)	0.46199 (8)	0.0273 (3)
H9	0.1193	0.0572	0.4360	0.027 (4)*
C10	0.00757 (12)	0.04979 (9)	0.56693 (8)	0.0271 (3)
C11	−0.03008 (12)	0.08169 (9)	0.68442 (8)	0.0301 (3)
C12	−0.07210 (13)	0.15947 (10)	0.78820 (8)	0.0338 (3)
C13	−0.06457 (14)	0.24334 (11)	0.82356 (9)	0.0391 (4)
H13	−0.0262	0.2940	0.8104	0.043 (5)*
C14	−0.11310 (17)	0.25226 (13)	0.87783 (10)	0.0491 (4)
H14	−0.1104	0.3091	0.9003	0.063 (6)*
C15	−0.16465 (17)	0.18014 (15)	0.89936 (11)	0.0570 (5)
H15	−0.1961	0.1868	0.9374	0.063 (6)*
C16	−0.17077 (17)	0.09771 (14)	0.86568 (11)	0.0544 (5)
H16	−0.2069	0.0477	0.8807	0.064 (6)*
C17	−0.12512 (15)	0.08640 (12)	0.81006 (10)	0.0442 (4)
H17	−0.1301	0.0291	0.7872	0.051 (5)*
O3	0.55521 (10)	0.20580 (7)	−0.08722 (6)	0.0422 (3)
O4	0.36393 (9)	0.07163 (8)	0.13909 (6)	0.0401 (3)

N5	0.70832 (11)	0.30849 (8)	0.00552 (7)	0.0338 (3)
H5A	0.7485	0.3194	0.0538	0.049 (5)*
N6	0.63553 (12)	0.17431 (8)	0.02682 (7)	0.0353 (3)
H6	0.6885	0.1958	0.0718	0.067 (7)*
N7	0.54246 (11)	0.12028 (8)	0.13142 (7)	0.0306 (3)
H7	0.6117	0.1582	0.1526	0.051 (6)*
N8	0.50045 (11)	0.19040 (8)	0.22426 (7)	0.0302 (3)
H8	0.5648	0.2309	0.2307	0.045 (5)*
C18	0.82226 (16)	0.45197 (11)	0.00938 (10)	0.0440 (4)
H18	0.8580	0.4581	0.0619	0.064 (6)*
C19	0.85739 (17)	0.51868 (12)	−0.02504 (12)	0.0509 (4)
H19	0.9177	0.5701	0.0040	0.061 (6)*
C20	0.80624 (17)	0.51176 (12)	−0.10091 (12)	0.0488 (4)
H20	0.8314	0.5574	−0.1245	0.061 (6)*
C21	0.71772 (17)	0.43720 (12)	−0.14204 (11)	0.0470 (4)
H21	0.6805	0.4326	−0.1942	0.059 (6)*
C22	0.68175 (15)	0.36879 (11)	−0.10902 (9)	0.0410 (4)
H22	0.6214	0.3176	−0.1384	0.048 (5)*
C23	0.73489 (13)	0.37584 (10)	−0.03243 (9)	0.0328 (3)
C24	0.62686 (13)	0.22744 (9)	−0.02381 (8)	0.0307 (3)
C25	0.56495 (12)	0.08690 (9)	0.01184 (8)	0.0300 (3)
C26	0.54437 (13)	0.02792 (9)	−0.05304 (8)	0.0315 (3)
H26	0.5746	0.0473	−0.0894	0.036 (4)*
C27	0.52004 (12)	0.05923 (9)	0.06536 (8)	0.0294 (3)
C28	0.46143 (12)	0.12323 (9)	0.16398 (8)	0.0298 (3)
C29	0.44762 (12)	0.20144 (10)	0.27749 (8)	0.0297 (3)
C30	0.36617 (15)	0.13353 (12)	0.28737 (10)	0.0422 (4)
H30	0.3377	0.0779	0.2544	0.052 (6)*
C31	0.32680 (16)	0.14762 (13)	0.34578 (11)	0.0501 (4)
H31	0.2715	0.1011	0.3526	0.055 (6)*
C32	0.36704 (16)	0.22827 (13)	0.39406 (10)	0.0464 (4)
H32	0.3400	0.2371	0.4341	0.052 (5)*
C33	0.44673 (14)	0.29602 (12)	0.38382 (9)	0.0402 (4)
H33	0.4746	0.3517	0.4168	0.041 (5)*
C34	0.48633 (13)	0.28310 (10)	0.32537 (8)	0.0338 (3)
H34	0.5401	0.3303	0.3181	0.039 (5)*
N9	0.74129 (12)	0.78442 (9)	0.02404 (7)	0.0364 (3)
C43	0.72364 (14)	0.87173 (11)	0.04947 (9)	0.0377 (3)
H43A	0.6499	0.8598	0.0587	0.040 (5)*
H43B	0.7151	0.9039	0.0080	0.032 (4)*
C44	0.81849 (15)	0.93120 (11)	0.11893 (10)	0.0432 (4)
H44A	0.8230	0.9032	0.1626	0.045 (5)*
H44B	0.8941	0.9415	0.1123	0.042 (5)*
C45	0.79135 (16)	1.01849 (12)	0.13220 (11)	0.0458 (4)
H45A	0.7107	1.0063	0.1309	0.059 (6)*
H45B	0.7963	1.0488	0.0909	0.054 (6)*
C46	0.87073 (18)	1.07841 (13)	0.20488 (11)	0.0523 (5)
H46A	0.9507	1.0913	0.2065	0.068 (7)*

H46B	0.8495	1.1332	0.2095	0.084 (8)*
H46C	0.8640	1.0499	0.2462	0.063 (6)*
C47	0.76356 (14)	0.73441 (11)	0.08711 (9)	0.0362 (3)
H47A	0.8352	0.7702	0.1284	0.042 (5)*
H47B	0.7784	0.6796	0.0689	0.040 (5)*
C48	0.66856 (14)	0.71042 (11)	0.11877 (9)	0.0369 (3)
H48A	0.6427	0.7625	0.1296	0.042 (5)*
H48B	0.6013	0.6641	0.0819	0.042 (5)*
C49	0.71507 (15)	0.67750 (13)	0.19039 (10)	0.0441 (4)
H49A	0.7802	0.7252	0.2274	0.058 (6)*
H49B	0.7456	0.6281	0.1794	0.051 (5)*
C50	0.62400 (16)	0.64706 (13)	0.22428 (10)	0.0467 (4)
H50A	0.5570	0.6024	0.1869	0.047 (5)*
H50B	0.6566	0.6219	0.2674	0.068 (7)*
H50C	0.5996	0.6972	0.2405	0.058 (6)*
C51	0.63150 (15)	0.73435 (11)	−0.04096 (9)	0.0406 (4)
H51A	0.6161	0.7722	−0.0780	0.038 (5)*
H51B	0.5665	0.7238	−0.0224	0.039 (5)*
C52	0.63132 (17)	0.64712 (12)	−0.08070 (10)	0.0478 (4)
H52A	0.6882	0.6571	−0.1060	0.052 (5)*
H52B	0.6545	0.6105	−0.0437	0.057 (6)*
C53	0.5109 (2)	0.59911 (13)	−0.13827 (11)	0.0579 (5)
H53A	0.5171	0.5511	−0.1726	0.065 (6)*
H53B	0.4817	0.6406	−0.1683	0.071 (7)*
C54	0.42419 (19)	0.56076 (16)	−0.10340 (14)	0.0696 (7)
H54A	0.4164	0.6080	−0.0701	0.103 (9)*
H54B	0.3489	0.5311	−0.1429	0.085 (8)*
H54C	0.4514	0.5183	−0.0747	0.078 (8)*
C55	0.84758 (16)	0.79751 (12)	0.00160 (10)	0.0430 (4)
H55A	0.8571	0.7391	−0.0126	0.037 (4)*
H55B	0.9166	0.8306	0.0459	0.045 (5)*
C56	0.8454 (2)	0.84543 (15)	−0.06201 (13)	0.0592 (5)
H56A	0.7788	0.8119	−0.1076	0.062 (7)*
H56B	0.8354	0.9040	−0.0490	0.074 (7)*
C57	0.9580 (2)	0.85609 (15)	−0.07746 (14)	0.0612 (6)
H57A	1.0237	0.8895	−0.0314	0.076 (8)*
H57B	0.9565	0.8912	−0.1166	0.088 (8)*
C58	0.9791 (2)	0.77027 (15)	−0.10240 (13)	0.0613 (5)
H58A	0.9115	0.7342	−0.1453	0.092 (9)*
H58B	1.0475	0.7824	−0.1168	0.062 (6)*
H58C	0.9921	0.7387	−0.0612	0.059 (6)*
N10	0.79044 (11)	0.19232 (8)	0.43407 (7)	0.0321 (3)
C59	0.75728 (14)	0.27724 (10)	0.43364 (9)	0.0346 (3)
H59A	0.6778	0.2654	0.4345	0.035 (4)*
H59B	0.7551	0.2954	0.3860	0.037 (5)*
C60	0.83565 (14)	0.35338 (10)	0.49721 (9)	0.0352 (3)
H60A	0.8334	0.3389	0.5453	0.038 (5)*
H60B	0.9164	0.3648	0.4990	0.037 (4)*

C61	0.79488 (17)	0.43463 (11)	0.48513 (10)	0.0458 (4)
H61A	0.7151	0.4231	0.4853	0.050 (5)*
H61B	0.7928	0.4462	0.4355	0.053 (6)*
C62	0.87212 (19)	0.51533 (12)	0.54435 (11)	0.0500 (4)
H62A	0.9511	0.5277	0.5440	0.080 (8)*
H62B	0.8426	0.5657	0.5339	0.073 (7)*
H62C	0.8728	0.5050	0.5935	0.060 (6)*
C63	0.91331 (13)	0.20643 (11)	0.43464 (9)	0.0345 (3)
H63A	0.9289	0.1486	0.4307	0.039 (5)*
H63B	0.9676	0.2430	0.4837	0.039 (5)*
C64	0.94058 (14)	0.24938 (11)	0.37370 (9)	0.0369 (3)
H64A	0.8801	0.2194	0.3244	0.044 (5)*
H64B	0.9413	0.3117	0.3826	0.047 (5)*
C65	1.05911 (15)	0.24357 (12)	0.37368 (10)	0.0414 (4)
H65A	1.0567	0.1810	0.3630	0.046 (5)*
H65B	1.1184	0.2710	0.4239	0.044 (5)*
C66	1.09355 (16)	0.28919 (13)	0.31583 (10)	0.0461 (4)
H66A	1.1027	0.3522	0.3288	0.049 (5)*
H66B	1.1669	0.2805	0.3151	0.064 (6)*
H66C	1.0332	0.2642	0.2663	0.054 (6)*
C67	0.78886 (13)	0.15726 (10)	0.50369 (8)	0.0338 (3)
H67A	0.8113	0.1021	0.5011	0.038 (5)*
H67B	0.8492	0.2001	0.5476	0.037 (4)*
C68	0.67551 (14)	0.13882 (11)	0.51765 (9)	0.0395 (4)
H68A	0.6112	0.1028	0.4719	0.067 (6)*
H68B	0.6589	0.1947	0.5305	0.052 (5)*
C69	0.68527 (18)	0.09005 (17)	0.58158 (12)	0.0592 (5)
H69A	0.7557	0.1238	0.6247	0.089 (8)*
H69B	0.6959	0.0325	0.5659	0.101 (10)*
C70	0.5841 (2)	0.07476 (17)	0.60689 (14)	0.0636 (6)
H70A	0.5119	0.0545	0.5632	0.139 (13)*
H70B	0.5877	0.0301	0.6377	0.107 (10)*
H70C	0.5864	0.1297	0.6364	0.125 (12)*
C71	0.70345 (13)	0.12833 (10)	0.36407 (8)	0.0349 (3)
H71A	0.7117	0.1519	0.3202	0.030 (4)*
H71B	0.6247	0.1261	0.3633	0.033 (4)*
C72	0.71241 (15)	0.03530 (11)	0.35475 (9)	0.0386 (4)
H72A	0.7917	0.0360	0.3577	0.043 (5)*
H72B	0.6970	0.0083	0.3955	0.043 (5)*
C73	0.62480 (15)	−0.01867 (11)	0.27929 (9)	0.0416 (4)
H73A	0.6406	0.0089	0.2389	0.045 (5)*
H73B	0.5459	−0.0184	0.2766	0.037 (4)*
C74	0.6294 (2)	−0.11249 (13)	0.26694 (11)	0.0576 (5)
H74A	0.6117	−0.1406	0.3060	0.086 (8)*
H74B	0.5725	−0.1446	0.2179	0.070 (7)*
H74C	0.7071	−0.1131	0.2689	0.080 (8)*
O5	0.77812 (12)	0.27760 (7)	0.16339 (7)	0.0496 (3)
O6	0.71297 (10)	0.30807 (7)	0.25484 (7)	0.0428 (3)

O7	0.95609 (10)	0.71897 (7)	0.36162 (6)	0.0399 (3)
O8	0.83607 (10)	0.61897 (7)	0.39321 (6)	0.0394 (3)
C35	0.77741 (14)	0.32767 (9)	0.21837 (8)	0.0335 (3)
C36	0.86114 (12)	0.41895 (9)	0.24206 (7)	0.0267 (3)
C37	0.95254 (13)	0.43941 (10)	0.21612 (8)	0.0320 (3)
H37	0.9624	0.3956	0.1832	0.041 (5)*
C38	1.02890 (13)	0.52313 (10)	0.23789 (9)	0.0346 (3)
H38	1.0921	0.5363	0.2210	0.043 (5)*
C39	1.01301 (12)	0.58753 (9)	0.28433 (8)	0.0308 (3)
H39	1.0651	0.6451	0.2988	0.035 (4)*
C40	0.92153 (12)	0.56898 (9)	0.31013 (7)	0.0255 (3)
C41	0.84685 (11)	0.48409 (9)	0.28944 (7)	0.0248 (3)
H41	0.7854	0.4705	0.3079	0.027 (4)*
C42	0.90222 (13)	0.64053 (9)	0.35908 (8)	0.0299 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0348 (5)	0.0327 (5)	0.0392 (6)	0.0134 (4)	0.0166 (5)	0.0048 (4)
O2	0.0526 (7)	0.0298 (6)	0.0397 (6)	0.0085 (5)	0.0222 (5)	0.0060 (5)
N1	0.0311 (6)	0.0295 (6)	0.0354 (7)	0.0079 (5)	0.0141 (5)	0.0036 (5)
N2	0.0305 (6)	0.0240 (6)	0.0334 (6)	0.0091 (5)	0.0137 (5)	0.0010 (5)
N3	0.0393 (7)	0.0247 (6)	0.0319 (6)	0.0069 (5)	0.0159 (5)	0.0013 (5)
N4	0.0372 (7)	0.0278 (6)	0.0314 (6)	0.0049 (5)	0.0151 (5)	0.0011 (5)
C1	0.0412 (9)	0.0375 (9)	0.0587 (11)	0.0068 (7)	0.0153 (8)	0.0146 (8)
C2	0.0492 (11)	0.0401 (10)	0.0704 (13)	0.0001 (8)	0.0146 (10)	0.0165 (9)
C3	0.0386 (9)	0.0581 (12)	0.0536 (11)	−0.0039 (8)	0.0157 (8)	0.0109 (9)
C4	0.0352 (9)	0.0669 (13)	0.0615 (12)	0.0082 (9)	0.0190 (9)	−0.0049 (10)
C5	0.0366 (9)	0.0469 (10)	0.0558 (11)	0.0087 (7)	0.0171 (8)	−0.0051 (8)
C6	0.0331 (7)	0.0367 (8)	0.0282 (7)	0.0052 (6)	0.0123 (6)	0.0070 (6)
C7	0.0316 (7)	0.0302 (7)	0.0238 (6)	0.0096 (6)	0.0102 (6)	0.0050 (5)
C8	0.0282 (7)	0.0221 (6)	0.0291 (7)	0.0104 (5)	0.0081 (5)	0.0045 (5)
C9	0.0314 (7)	0.0237 (7)	0.0292 (7)	0.0109 (5)	0.0121 (6)	0.0051 (5)
C10	0.0320 (7)	0.0238 (7)	0.0264 (7)	0.0125 (5)	0.0088 (6)	0.0038 (5)
C11	0.0289 (7)	0.0293 (7)	0.0308 (7)	0.0087 (6)	0.0091 (6)	0.0047 (6)
C12	0.0279 (7)	0.0392 (8)	0.0309 (7)	0.0071 (6)	0.0102 (6)	0.0000 (6)
C13	0.0376 (8)	0.0414 (9)	0.0394 (8)	0.0154 (7)	0.0142 (7)	0.0036 (7)
C14	0.0517 (10)	0.0557 (11)	0.0454 (10)	0.0238 (9)	0.0225 (8)	−0.0004 (8)
C15	0.0431 (10)	0.0729 (14)	0.0516 (11)	0.0057 (9)	0.0279 (9)	−0.0092 (10)
C16	0.0487 (10)	0.0558 (11)	0.0512 (11)	−0.0080 (9)	0.0289 (9)	−0.0019 (9)
C17	0.0410 (9)	0.0431 (9)	0.0416 (9)	−0.0021 (7)	0.0197 (7)	−0.0032 (7)
O3	0.0420 (6)	0.0367 (6)	0.0364 (6)	0.0070 (5)	0.0023 (5)	0.0073 (5)
O4	0.0316 (6)	0.0418 (6)	0.0383 (6)	0.0003 (5)	0.0118 (5)	−0.0011 (5)
N5	0.0403 (7)	0.0283 (6)	0.0286 (6)	0.0053 (5)	0.0106 (5)	0.0046 (5)
N6	0.0407 (7)	0.0274 (6)	0.0294 (6)	−0.0008 (5)	0.0101 (6)	0.0029 (5)
N7	0.0314 (6)	0.0262 (6)	0.0290 (6)	0.0022 (5)	0.0104 (5)	0.0006 (5)
N8	0.0308 (6)	0.0275 (6)	0.0313 (6)	0.0038 (5)	0.0135 (5)	0.0048 (5)
C18	0.0469 (9)	0.0350 (9)	0.0457 (10)	0.0078 (7)	0.0132 (8)	0.0101 (7)

C19	0.0498 (10)	0.0355 (9)	0.0664 (12)	0.0067 (8)	0.0217 (9)	0.0161 (9)
C20	0.0588 (11)	0.0419 (10)	0.0667 (12)	0.0228 (8)	0.0391 (10)	0.0267 (9)
C21	0.0615 (11)	0.0485 (10)	0.0444 (10)	0.0246 (9)	0.0265 (9)	0.0209 (8)
C22	0.0468 (9)	0.0403 (9)	0.0385 (9)	0.0134 (7)	0.0170 (7)	0.0112 (7)
C23	0.0357 (8)	0.0293 (7)	0.0388 (8)	0.0118 (6)	0.0179 (6)	0.0091 (6)
C24	0.0317 (7)	0.0284 (7)	0.0317 (7)	0.0085 (6)	0.0120 (6)	0.0037 (6)
C25	0.0302 (7)	0.0249 (7)	0.0298 (7)	0.0027 (5)	0.0084 (6)	0.0042 (6)
C26	0.0329 (7)	0.0288 (7)	0.0300 (7)	0.0037 (6)	0.0116 (6)	0.0056 (6)
C27	0.0290 (7)	0.0272 (7)	0.0276 (7)	0.0053 (5)	0.0074 (6)	0.0023 (5)
C28	0.0299 (7)	0.0280 (7)	0.0300 (7)	0.0065 (6)	0.0097 (6)	0.0082 (6)
C29	0.0296 (7)	0.0329 (7)	0.0282 (7)	0.0108 (6)	0.0099 (6)	0.0095 (6)
C30	0.0437 (9)	0.0399 (9)	0.0405 (9)	0.0032 (7)	0.0188 (7)	0.0067 (7)
C31	0.0469 (10)	0.0552 (11)	0.0483 (10)	0.0014 (8)	0.0267 (8)	0.0112 (9)
C32	0.0453 (9)	0.0628 (12)	0.0386 (9)	0.0168 (9)	0.0236 (8)	0.0110 (8)
C33	0.0413 (9)	0.0465 (9)	0.0339 (8)	0.0157 (7)	0.0142 (7)	0.0038 (7)
C34	0.0329 (7)	0.0346 (8)	0.0336 (8)	0.0090 (6)	0.0121 (6)	0.0077 (6)
N9	0.0389 (7)	0.0398 (7)	0.0375 (7)	0.0185 (6)	0.0161 (6)	0.0134 (6)
C43	0.0406 (8)	0.0379 (8)	0.0409 (9)	0.0179 (7)	0.0169 (7)	0.0120 (7)
C44	0.0443 (9)	0.0417 (9)	0.0449 (9)	0.0168 (7)	0.0144 (8)	0.0096 (7)
C45	0.0506 (10)	0.0418 (9)	0.0512 (10)	0.0188 (8)	0.0225 (8)	0.0099 (8)
C46	0.0597 (12)	0.0462 (10)	0.0561 (11)	0.0174 (9)	0.0262 (10)	0.0092 (9)
C47	0.0358 (8)	0.0408 (9)	0.0360 (8)	0.0166 (7)	0.0123 (7)	0.0143 (7)
C48	0.0351 (8)	0.0412 (9)	0.0358 (8)	0.0123 (7)	0.0125 (7)	0.0107 (7)
C49	0.0393 (9)	0.0529 (10)	0.0370 (9)	0.0091 (8)	0.0102 (7)	0.0161 (8)
C50	0.0525 (10)	0.0477 (10)	0.0377 (9)	0.0081 (8)	0.0169 (8)	0.0110 (8)
C51	0.0458 (9)	0.0427 (9)	0.0353 (8)	0.0196 (7)	0.0112 (7)	0.0111 (7)
C52	0.0588 (11)	0.0463 (10)	0.0437 (10)	0.0229 (9)	0.0204 (9)	0.0077 (8)
C53	0.0795 (14)	0.0445 (10)	0.0410 (10)	0.0255 (10)	0.0068 (10)	0.0037 (8)
C54	0.0514 (12)	0.0651 (14)	0.0763 (15)	0.0208 (11)	0.0092 (11)	−0.0154 (12)
C55	0.0489 (10)	0.0476 (10)	0.0479 (10)	0.0234 (8)	0.0276 (8)	0.0189 (8)
C56	0.0738 (14)	0.0675 (13)	0.0666 (13)	0.0370 (12)	0.0451 (12)	0.0371 (11)
C57	0.0783 (15)	0.0616 (13)	0.0711 (14)	0.0287 (11)	0.0511 (13)	0.0308 (11)
C58	0.0770 (15)	0.0662 (13)	0.0591 (13)	0.0248 (12)	0.0443 (12)	0.0166 (11)
N10	0.0340 (6)	0.0329 (7)	0.0281 (6)	0.0124 (5)	0.0074 (5)	0.0071 (5)
C59	0.0382 (8)	0.0354 (8)	0.0337 (8)	0.0169 (7)	0.0120 (6)	0.0104 (6)
C60	0.0382 (8)	0.0365 (8)	0.0324 (8)	0.0111 (7)	0.0138 (6)	0.0087 (6)
C61	0.0592 (11)	0.0370 (9)	0.0393 (9)	0.0156 (8)	0.0134 (8)	0.0103 (7)
C62	0.0691 (13)	0.0343 (9)	0.0457 (10)	0.0107 (8)	0.0223 (9)	0.0091 (7)
C63	0.0334 (8)	0.0393 (8)	0.0321 (8)	0.0148 (6)	0.0098 (6)	0.0098 (6)
C64	0.0407 (8)	0.0398 (9)	0.0340 (8)	0.0164 (7)	0.0137 (7)	0.0107 (7)
C65	0.0426 (9)	0.0479 (10)	0.0413 (9)	0.0193 (8)	0.0185 (7)	0.0158 (7)
C66	0.0503 (10)	0.0512 (11)	0.0451 (10)	0.0185 (8)	0.0232 (8)	0.0161 (8)
C67	0.0366 (8)	0.0357 (8)	0.0269 (7)	0.0113 (6)	0.0079 (6)	0.0070 (6)
C68	0.0375 (8)	0.0408 (9)	0.0390 (9)	0.0111 (7)	0.0122 (7)	0.0086 (7)
C69	0.0501 (11)	0.0826 (16)	0.0590 (12)	0.0256 (11)	0.0259 (10)	0.0370 (11)
C70	0.0603 (13)	0.0738 (15)	0.0734 (15)	0.0243 (11)	0.0355 (12)	0.0348 (13)
C71	0.0351 (8)	0.0368 (8)	0.0282 (7)	0.0115 (6)	0.0050 (6)	0.0052 (6)
C72	0.0445 (9)	0.0369 (8)	0.0305 (8)	0.0132 (7)	0.0079 (7)	0.0052 (6)

C73	0.0465 (9)	0.0420 (9)	0.0313 (8)	0.0103 (7)	0.0099 (7)	0.0055 (7)
C74	0.0775 (15)	0.0445 (10)	0.0368 (10)	0.0162 (10)	0.0070 (9)	−0.0027 (8)
O5	0.0701 (8)	0.0279 (6)	0.0343 (6)	0.0105 (6)	0.0037 (6)	−0.0062 (5)
O6	0.0381 (6)	0.0312 (6)	0.0456 (7)	−0.0041 (5)	0.0072 (5)	0.0090 (5)
O7	0.0491 (7)	0.0215 (5)	0.0402 (6)	0.0077 (5)	0.0084 (5)	−0.0008 (4)
O8	0.0518 (7)	0.0375 (6)	0.0390 (6)	0.0217 (5)	0.0236 (5)	0.0070 (5)
C35	0.0381 (8)	0.0225 (7)	0.0282 (7)	0.0060 (6)	−0.0005 (6)	0.0029 (6)
C36	0.0308 (7)	0.0238 (7)	0.0221 (6)	0.0074 (5)	0.0056 (5)	0.0041 (5)
C37	0.0399 (8)	0.0331 (8)	0.0268 (7)	0.0159 (6)	0.0136 (6)	0.0050 (6)
C38	0.0326 (7)	0.0394 (8)	0.0374 (8)	0.0108 (6)	0.0181 (6)	0.0119 (7)
C39	0.0286 (7)	0.0266 (7)	0.0337 (7)	0.0031 (6)	0.0093 (6)	0.0081 (6)
C40	0.0268 (6)	0.0233 (6)	0.0234 (6)	0.0080 (5)	0.0050 (5)	0.0039 (5)
C41	0.0252 (6)	0.0251 (6)	0.0228 (6)	0.0065 (5)	0.0075 (5)	0.0052 (5)
C42	0.0336 (7)	0.0250 (7)	0.0259 (7)	0.0109 (6)	0.0033 (6)	0.0021 (5)

Geometric parameters (Å, º)

O1—C7	1.2210 (17)	C48—C49	1.524 (2)
O2—C11	1.2150 (18)	C48—H48A	0.9900
N1—C7	1.3745 (19)	C48—H48B	0.9900
N1—C6	1.4067 (19)	C49—C50	1.518 (2)
N1—H1A	0.8800	C49—H49A	0.9899
N2—C7	1.3747 (18)	C49—H49B	0.9900
N2—C8	1.4184 (18)	C50—H50A	0.9800
N2—H2A	0.8800	C50—H50B	0.9801
N3—C11	1.3638 (19)	C50—H50C	0.9798
N3—C10	1.4072 (18)	C51—C52	1.514 (2)
N3—H3A	0.8800	C51—H51A	0.9901
N4—C11	1.3876 (19)	C51—H51B	0.9900
N4—C12	1.4093 (19)	C52—C53	1.528 (3)
N4—H4A	0.8801	C52—H52A	0.9900
C1—C2	1.384 (3)	C52—H52B	0.9900
C1—C6	1.398 (2)	C53—C54	1.517 (3)
C1—H1	0.9500	C53—H53A	0.9901
C2—C3	1.385 (3)	C53—H53B	0.9899
C2—H2	0.9500	C54—H54A	0.9800
C3—C4	1.362 (3)	C54—H54B	0.9801
C3—H3	0.9500	C54—H54C	0.9799
C4—C5	1.391 (3)	C55—C56	1.516 (2)
C4—H4	0.9500	C55—H55A	0.9900
C5—C6	1.379 (2)	C55—H55B	0.9900
C5—H5	0.9501	C56—C57	1.532 (3)
C8—C9	1.3928 (19)	C56—H56A	0.9900
C8—C10	1.401 (2)	C56—H56B	0.9899
C9—C10^{i}	1.3965 (19)	C57—C58	1.515 (3)
C9—H9	0.9500	C57—H57A	0.9900
C10—C9^{i}	1.3965 (19)	C57—H57B	0.9900
C12—C17	1.388 (2)	C58—H58A	0.9800

C12—C13	1.402 (2)	C58—H58B	0.9800
C13—C14	1.387 (2)	C58—H58C	0.9800
C13—H13	0.9500	N10—C71	1.5142 (19)
C14—C15	1.365 (3)	N10—C59	1.5146 (19)
C14—H14	0.9501	N10—C67	1.5179 (19)
C15—C16	1.376 (3)	N10—C63	1.5236 (19)
C15—H15	0.9501	C59—C60	1.513 (2)
C16—C17	1.389 (2)	C59—H59A	0.9901
C16—H16	0.9500	C59—H59B	0.9899
C17—H17	0.9501	C60—C61	1.524 (2)
O3—C24	1.2198 (18)	C60—H60A	0.9901
O4—C28	1.2245 (18)	C60—H60B	0.9899
N5—C24	1.3798 (19)	C61—C62	1.513 (3)
N5—C23	1.4071 (19)	C61—H61A	0.9899
N5—H5A	0.8801	C61—H61B	0.9901
N6—C24	1.3612 (19)	C62—H62A	0.9801
N6—C25	1.4141 (18)	C62—H62B	0.9801
N6—H6	0.8800	C62—H62C	0.9800
N7—C28	1.3764 (19)	C63—C64	1.520 (2)
N7—C27	1.4193 (18)	C63—H63A	0.9901
N7—H7	0.8799	C63—H63B	0.9900
N8—C28	1.3601 (19)	C64—C65	1.534 (2)
N8—C29	1.4136 (19)	C64—H64A	0.9899
N8—H8	0.8801	C64—H64B	0.9901
C18—C19	1.382 (2)	C65—C66	1.524 (2)
C18—C23	1.392 (2)	C65—H65A	0.9900
C18—H18	0.9501	C65—H65B	0.9899
C19—C20	1.377 (3)	C66—H66A	0.9800
C19—H19	0.9501	C66—H66B	0.9801
C20—C21	1.380 (3)	C66—H66C	0.9800
C20—H20	0.9500	C67—C68	1.520 (2)
C21—C22	1.388 (2)	C67—H67A	0.9901
C21—H21	0.9501	C67—H67B	0.9899
C22—C23	1.392 (2)	C68—C69	1.520 (2)
C22—H22	0.9500	C68—H68A	0.9900
C25—C26	1.390 (2)	C68—H68B	0.9900
C25—C27	1.398 (2)	C69—C70	1.498 (3)
C26—C27^{ii}	1.392 (2)	C69—H69A	0.9899
C26—H26	0.9500	C69—H69B	0.9901
C27—C26^{ii}	1.392 (2)	C70—H70A	0.9799
C29—C34	1.391 (2)	C70—H70B	0.9801
C29—C30	1.392 (2)	C70—H70C	0.9800
C30—C31	1.390 (2)	C71—C72	1.514 (2)
C30—H30	0.9500	C71—H71A	0.9900
C31—C32	1.381 (3)	C71—H71B	0.9899
C31—H31	0.9499	C72—C73	1.526 (2)
C32—C33	1.381 (3)	C72—H72A	0.9900
C32—H32	0.9500	C72—H72B	0.9901

C33—C34	1.390 (2)	C73—C74	1.511 (3)
C33—H33	0.9499	C73—H73A	0.9900
C34—H34	0.9499	C73—H73B	0.9901
N9—C51	1.513 (2)	C74—H74A	0.9800
N9—C43	1.519 (2)	C74—H74B	0.9800
N9—C47	1.5194 (19)	C74—H74C	0.9800
N9—C55	1.525 (2)	O5—C35	1.2589 (19)
C43—C44	1.514 (2)	O6—C35	1.252 (2)
C43—H43A	0.9900	O7—C42	1.2685 (18)
C43—H43B	0.9900	O8—C42	1.2386 (19)
C44—C45	1.529 (2)	C35—C36	1.5114 (19)
C44—H44A	0.9900	C36—C41	1.3912 (19)
C44—H44B	0.9900	C36—C37	1.395 (2)
C45—C46	1.496 (3)	C37—C38	1.384 (2)
C45—H45A	0.9900	C37—H37	0.9501
C45—H45B	0.9901	C38—C39	1.382 (2)
C46—H46A	0.9800	C38—H38	0.9500
C46—H46B	0.9799	C39—C40	1.392 (2)
C46—H46C	0.9799	C39—H39	0.9500
C47—C48	1.515 (2)	C40—C41	1.3915 (18)
C47—H47A	0.9900	C40—C42	1.5164 (19)
C47—H47B	0.9900	C41—H41	0.9500

C7—N1—C6	127.82 (13)	C49—C50—H50C	109.5
C7—N1—H1A	116.1	H50A—C50—H50C	109.5
C6—N1—H1A	116.1	H50B—C50—H50C	109.5
C7—N2—C8	124.61 (12)	N9—C51—C52	116.23 (14)
C7—N2—H2A	117.7	N9—C51—H51A	108.2
C8—N2—H2A	117.7	C52—C51—H51A	108.2
C11—N3—C10	127.63 (13)	N9—C51—H51B	108.2
C11—N3—H3A	116.2	C52—C51—H51B	108.2
C10—N3—H3A	116.2	H51A—C51—H51B	107.4
C11—N4—C12	127.33 (13)	C51—C52—C53	110.35 (15)
C11—N4—H4A	116.3	C51—C52—H52A	109.6
C12—N4—H4A	116.3	C53—C52—H52A	109.6
C2—C1—C6	120.54 (18)	C51—C52—H52B	109.6
C2—C1—H1	119.7	C53—C52—H52B	109.6
C6—C1—H1	119.8	H52A—C52—H52B	108.1
C1—C2—C3	120.20 (19)	C54—C53—C52	113.26 (17)
C1—C2—H2	119.9	C54—C53—H53A	109.0
C3—C2—H2	119.9	C52—C53—H53A	108.9
C4—C3—C2	119.09 (17)	C54—C53—H53B	108.9
C4—C3—H3	120.4	C52—C53—H53B	108.9
C2—C3—H3	120.5	H53A—C53—H53B	107.8
C3—C4—C5	121.62 (19)	C53—C54—H54A	109.5
C3—C4—H4	119.2	C53—C54—H54B	109.5
C5—C4—H4	119.2	H54A—C54—H54B	109.5
C6—C5—C4	119.80 (18)	C53—C54—H54C	109.4

C6—C5—H5	120.1	H54A—C54—H54C	109.5
C4—C5—H5	120.1	H54B—C54—H54C	109.5
C5—C6—C1	118.74 (15)	C56—C55—N9	115.88 (14)
C5—C6—N1	124.69 (15)	C56—C55—H55A	108.3
C1—C6—N1	116.54 (15)	N9—C55—H55A	108.3
O1—C7—N1	125.41 (13)	C56—C55—H55B	108.3
O1—C7—N2	123.52 (13)	N9—C55—H55B	108.3
N1—C7—N2	111.07 (12)	H55A—C55—H55B	107.4
C9—C8—C10	119.89 (13)	C55—C56—C57	110.49 (17)
C9—C8—N2	120.61 (13)	C55—C56—H56A	109.5
C10—C8—N2	119.41 (12)	C57—C56—H56A	109.5
C8—C9—C10^{i}	120.63 (13)	C55—C56—H56B	109.6
C8—C9—H9	119.7	C57—C56—H56B	109.6
C10^{i}—C9—H9	119.7	H56A—C56—H56B	108.1
C9^{i}—C10—C8	119.49 (13)	C58—C57—C56	114.34 (19)
C9^{i}—C10—N3	123.07 (13)	C58—C57—H57A	108.7
C8—C10—N3	117.38 (12)	C56—C57—H57A	108.6
O2—C11—N3	124.92 (14)	C58—C57—H57B	108.7
O2—C11—N4	124.46 (14)	C56—C57—H57B	108.7
N3—C11—N4	110.61 (12)	H57A—C57—H57B	107.6
C17—C12—C13	119.09 (15)	C57—C58—H58A	109.5
C17—C12—N4	124.46 (14)	C57—C58—H58B	109.5
C13—C12—N4	116.44 (14)	H58A—C58—H58B	109.5
C14—C13—C12	119.97 (17)	C57—C58—H58C	109.5
C14—C13—H13	120.0	H58A—C58—H58C	109.5
C12—C13—H13	120.0	H58B—C58—H58C	109.5
C15—C14—C13	120.63 (17)	C71—N10—C59	106.21 (11)
C15—C14—H14	119.7	C71—N10—C67	111.15 (12)
C13—C14—H14	119.7	C59—N10—C67	111.42 (11)
C14—C15—C16	119.65 (17)	C71—N10—C63	110.96 (12)
C14—C15—H15	120.2	C59—N10—C63	110.95 (12)
C16—C15—H15	120.2	C67—N10—C63	106.23 (11)
C15—C16—C17	121.14 (18)	C60—C59—N10	116.10 (12)
C15—C16—H16	119.4	C60—C59—H59A	108.3
C17—C16—H16	119.4	N10—C59—H59A	108.2
C12—C17—C16	119.47 (17)	C60—C59—H59B	108.3
C12—C17—H17	120.3	N10—C59—H59B	108.3
C16—C17—H17	120.3	H59A—C59—H59B	107.4
C24—N5—C23	127.82 (13)	C59—C60—C61	109.13 (13)
C24—N5—H5A	116.1	C59—C60—H60A	109.9
C23—N5—H5A	116.1	C61—C60—H60A	109.9
C24—N6—C25	124.28 (13)	C59—C60—H60B	109.9
C24—N6—H6	117.9	C61—C60—H60B	109.8
C25—N6—H6	117.8	H60A—C60—H60B	108.3
C28—N7—C27	123.38 (12)	C62—C61—C60	112.71 (15)
C28—N7—H7	118.3	C62—C61—H61A	109.1
C27—N7—H7	118.3	C60—C61—H61A	109.0
C28—N8—C29	126.32 (12)	C62—C61—H61B	109.0

C28—N8—H8	116.8	C60—C61—H61B	109.1
C29—N8—H8	116.8	H61A—C61—H61B	107.8
C19—C18—C23	120.34 (17)	C61—C62—H62A	109.5
C19—C18—H18	119.8	C61—C62—H62B	109.5
C23—C18—H18	119.8	H62A—C62—H62B	109.5
C20—C19—C18	120.94 (18)	C61—C62—H62C	109.5
C20—C19—H19	119.5	H62A—C62—H62C	109.5
C18—C19—H19	119.5	H62B—C62—H62C	109.5
C19—C20—C21	118.70 (16)	C64—C63—N10	116.54 (12)
C19—C20—H20	120.7	C64—C63—H63A	108.1
C21—C20—H20	120.6	N10—C63—H63A	108.2
C20—C21—C22	121.52 (18)	C64—C63—H63B	108.2
C20—C21—H21	119.2	N10—C63—H63B	108.2
C22—C21—H21	119.2	H63A—C63—H63B	107.3
C21—C22—C23	119.41 (17)	C63—C64—C65	109.63 (13)
C21—C22—H22	120.3	C63—C64—H64A	109.7
C23—C22—H22	120.3	C65—C64—H64A	109.8
C18—C23—C22	119.07 (15)	C63—C64—H64B	109.7
C18—C23—N5	117.26 (14)	C65—C64—H64B	109.7
C22—C23—N5	123.62 (14)	H64A—C64—H64B	108.2
O3—C24—N6	123.85 (14)	C66—C65—C64	112.01 (14)
O3—C24—N5	124.37 (14)	C66—C65—H65A	109.2
N6—C24—N5	111.78 (13)	C64—C65—H65A	109.2
C26—C25—C27	120.11 (13)	C66—C65—H65B	109.2
C26—C25—N6	121.17 (13)	C64—C65—H65B	109.2
C27—C25—N6	118.66 (13)	H65A—C65—H65B	107.9
C25—C26—C27^{ii}	120.71 (13)	C65—C66—H66A	109.5
C25—C26—H26	119.7	C65—C66—H66B	109.5
C27^{ii}—C26—H26	119.6	H66A—C66—H66B	109.5
C26^{ii}—C27—C25	119.18 (13)	C65—C66—H66C	109.5
C26^{ii}—C27—N7	121.52 (13)	H66A—C66—H66C	109.5
C25—C27—N7	119.29 (13)	H66B—C66—H66C	109.5
O4—C28—N8	124.60 (14)	N10—C67—C68	117.15 (12)
O4—C28—N7	122.54 (14)	N10—C67—H67A	108.0
N8—C28—N7	112.83 (12)	C68—C67—H67A	108.0
C34—C29—C30	119.31 (14)	N10—C67—H67B	108.0
C34—C29—N8	117.26 (13)	C68—C67—H67B	108.0
C30—C29—N8	123.27 (14)	H67A—C67—H67B	107.2
C31—C30—C29	119.66 (16)	C67—C68—C69	109.06 (14)
C31—C30—H30	120.2	C67—C68—H68A	109.9
C29—C30—H30	120.2	C69—C68—H68A	109.9
C32—C31—C30	120.87 (16)	C67—C68—H68B	109.9
C32—C31—H31	119.6	C69—C68—H68B	109.9
C30—C31—H31	119.6	H68A—C68—H68B	108.3
C33—C32—C31	119.57 (16)	C70—C69—C68	115.33 (17)
C33—C32—H32	120.2	C70—C69—H69A	108.4
C31—C32—H32	120.2	C68—C69—H69A	108.4
C32—C33—C34	120.22 (16)	C70—C69—H69B	108.5

C32—C33—H33	119.9	C68—C69—H69B	108.4
C34—C33—H33	119.9	H69A—C69—H69B	107.5
C33—C34—C29	120.35 (15)	C69—C70—H70A	109.5
C33—C34—H34	119.8	C69—C70—H70B	109.4
C29—C34—H34	119.8	H70A—C70—H70B	109.5
C51—N9—C43	105.98 (12)	C69—C70—H70C	109.5
C51—N9—C47	111.24 (13)	H70A—C70—H70C	109.5
C43—N9—C47	110.93 (12)	H70B—C70—H70C	109.5
C51—N9—C55	111.66 (13)	N10—C71—C72	116.37 (12)
C43—N9—C55	111.37 (13)	N10—C71—H71A	108.2
C47—N9—C55	105.76 (12)	C72—C71—H71A	108.2
C44—C43—N9	116.11 (13)	N10—C71—H71B	108.2
C44—C43—H43A	108.2	C72—C71—H71B	108.2
N9—C43—H43A	108.3	H71A—C71—H71B	107.3
C44—C43—H43B	108.3	C71—C72—C73	109.72 (13)
N9—C43—H43B	108.3	C71—C72—H72A	109.7
H43A—C43—H43B	107.4	C73—C72—H72A	109.7
C43—C44—C45	108.81 (14)	C71—C72—H72B	109.7
C43—C44—H44A	109.9	C73—C72—H72B	109.7
C45—C44—H44A	109.9	H72A—C72—H72B	108.2
C43—C44—H44B	109.9	C74—C73—C72	112.11 (15)
C45—C44—H44B	109.9	C74—C73—H73A	109.2
H44A—C44—H44B	108.3	C72—C73—H73A	109.2
C46—C45—C44	113.68 (16)	C74—C73—H73B	109.2
C46—C45—H45A	108.8	C72—C73—H73B	109.2
C44—C45—H45A	108.8	H73A—C73—H73B	107.9
C46—C45—H45B	108.8	C73—C74—H74A	109.5
C44—C45—H45B	108.8	C73—C74—H74B	109.5
H45A—C45—H45B	107.7	H74A—C74—H74B	109.5
C45—C46—H46A	109.5	C73—C74—H74C	109.5
C45—C46—H46B	109.5	H74A—C74—H74C	109.5
H46A—C46—H46B	109.5	H74B—C74—H74C	109.5
C45—C46—H46C	109.4	O6—C35—O5	125.35 (14)
H46A—C46—H46C	109.5	O6—C35—C36	117.46 (13)
H46B—C46—H46C	109.5	O5—C35—C36	117.19 (14)
C48—C47—N9	116.67 (12)	C41—C36—C37	119.14 (13)
C48—C47—H47A	108.1	C41—C36—C35	120.16 (13)
N9—C47—H47A	108.1	C37—C36—C35	120.70 (13)
C48—C47—H47B	108.1	C38—C37—C36	120.49 (13)
N9—C47—H47B	108.1	C38—C37—H37	119.8
H47A—C47—H47B	107.3	C36—C37—H37	119.7
C47—C48—C49	109.01 (13)	C39—C38—C37	119.80 (13)
C47—C48—H48A	109.9	C39—C38—H38	120.1
C49—C48—H48A	109.9	C37—C38—H38	120.1
C47—C48—H48B	109.9	C38—C39—C40	120.74 (13)
C49—C48—H48B	109.9	C38—C39—H39	119.6
H48A—C48—H48B	108.3	C40—C39—H39	119.6
C50—C49—C48	113.01 (14)	C41—C40—C39	119.06 (13)

C50—C49—H49A	109.0	C41—C40—C42	120.39 (12)
C48—C49—H49A	109.0	C39—C40—C42	120.55 (12)
C50—C49—H49B	109.0	C36—C41—C40	120.74 (13)
C48—C49—H49B	109.0	C36—C41—H41	119.6
H49A—C49—H49B	107.8	C40—C41—H41	119.6
C49—C50—H50A	109.5	O8—C42—O7	124.90 (14)
C49—C50—H50B	109.5	O8—C42—C40	118.62 (13)
H50A—C50—H50B	109.5	O7—C42—C40	116.48 (13)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O8^{iii}	0.88	1.98	2.8316 (16)	164
N2—H2*A*···O7^{iii}	0.88	2.25	3.0983 (16)	161
N2—H2*A*···O8^{iii}	0.88	2.62	3.3616 (16)	143
N3—H3*A*···O7^{iii}	0.88	1.98	2.7455 (16)	145
N4—H4*A*···O7^{iii}	0.88	2.26	3.0052 (17)	142
N5—H5*A*···O5	0.88	2.23	3.0208 (18)	149
N6—H6···O5	0.88	1.90	2.7393 (17)	158
N7—H7···O5	0.88	2.43	3.2615 (18)	157
N8—H8···O6	0.88	1.87	2.7474 (16)	171

Symmetry code: (iii) −*x*+1, −*y*+1, −*z*+1.