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Structure of the White-Line-Inducing Principle Isolated from Pseudomonas Reactans

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Abstract. $C_{54}H_{93}N_9O_{16}H_2O$, $M_r = 1142.40$, orthorhombic, $P2_{1}2_{1}2_{1}$, a = 14.230 (1), b = 24.370 (5), c = 18.780 (2) Å, V = 6512.6 (11) Å³, Z = 4, $D_x = 1.16$ g cm⁻³, λ (Cu $K\alpha$) = 1.5418 Å, $\mu = 6.8$ cm⁻¹, F(000) = 2472, T = 158 (2) K, R = 0.073 for 6299 unique reflections. The structure of this cycle peptide is that of β -hydroxydecanoyl-L-Leu-D-Glu-D-allo-Thr-D-Val-D-Leu-D-Ser-D-Ser-L-Ile. Ring closure is through an ester linkage between the carboxyl of L-Ile and the hydroxyl of D-allo-Thr, leaving the γ -carboxyl of D-Glu free. The stereochemistry of the β -hydroxy acid is shown to be R.

Introduction. Members of the genus *Pseudomonas* characteristically produce a wide variety of extracellular compounds including siderophores, antibiotics, toxins and enzymes. A range of fluorescent *Pseudomonas* species are commonly found in association with the sporophore of the edible mushroom, *Agaricus bisporus* (Lange) Imbach (Olivier, Guillames &

Martin, 1978; Zarkower, Wuest, Royse & Myers, 1983; Goor, Vantomme, Swings, Gillis, Kersters & deLey, 1986). Of particular interest is the taxonomically diverse group of saprophytic Pseudomonas species, collectively referred to as Pseudomonas reactans (Wong & Preece, 1979), which are capable of forming a white line in agar when grown in association with Pseudomonas tolaasii Paine, the causal organism of the economically significant brown blotch disease of A. bisporus (Tolaas, 1915). This white-line reaction is a rapid and reliable means of identifying P. tolaasii isolates (Zarkower, Wuest, Royse & Myers, 1983; Wong & Preece, 1979) and is the result of a specific interaction between a diffusible peptide (Mortishire-Smith, Nutkins, Packman, Brodey, Rainey, Johnstone & Williams, 1991) produced by P. reactans (called the 'white-line-inducing principle' or WLIP) and the water-soluble peptide toxin (tolaasin) produced by P. tolaasii (Peng, 1986; Nutkins. Mortishire-Smith, Packman, Brodev. Rainey, Johnstone & Williams, 1991; Mortishire-Smith, Drake, Nutkins & Williams, 1991). Neither the mechanism whereby the two peptides give rise to

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O(2L) C(2M)

C(2N)

C(20)

C(2P) C(2Q)

N(2R) C(3) O(3A)

N(4) C(5)

C(5A)

C(5B) C(5C) C(6) O(6A)

N(7)

C(8) C(8A)

C(8*B*) C(8*C*)

C(8*D*) C(9)

O(9A)

N(10)

C(11) C(11A) O(11B)

C(12) O(12A)

N(13)

C(14) C(14A)

C(14B) C(14C)

C(14D)

C(15) O(15A)

N(16) C(17)

C(17A)

O(17B)

C(18) O(18A)

N(19) C(20) C(20A)

C(20*B*) C(20*C*)

C(20D)

C(21) O(21A)

O(22)

C(A) O(A1)

C(B)

C(C) O(C1)

C(D) C(E) C(F)

C(G) C(H)

C(I)

C(J) O(W1)

O(W2)

the white line nor the biological significance (if any) of the interaction are understood.





We have recently determined the primary structure of WLIP (1) by a combination of degradative and spectroscopic techniques (Mortishire-Smith, Nutkins, Packman, Prodey, Rainey, Johnstone & Williams, 1991) and report here the crystal structure of WLIP. Crystals of sufficient quality for an X-ray structure determination were obtained by the diffusion of water into a saturated solution of WLIP in methanol.

Experimental. A clear chunky crystal, $0.18 \times 0.18 \times$ 0.21 mm, was used for data collection on a Nicolet $P2_1$ diffractometer controlled by a Harris computer. All 6299 measured reflections were unique (5613 had intensities > 2σ) and were collected using graphitemonochromated Cu K α radiation at low temperature (~158 K) to $2\theta_{\text{max}} = 138^{\circ}$ at 4° min⁻¹ using $\theta/2\theta$ -step scans with scan widths > 3.4°. Ten periodically monitored reflections showed no trend towards deterioration. $\sigma^2(I)$ was approximated by $\sigma^2(I)$ from counting statistics plus $(0.012I)^2$, where the coefficient of I was calculated from the variations in intensities of the monitored reflections. Accurate cell parameters were determined by least-squares fit of $K\alpha_1 \ 2\theta$ values $[\lambda(K\alpha_1) = 1.5402 \text{ Å}]$ for 25 high 2θ reflections (Duchamp, 1977). Lorentz and polarization corrections appropriate for a monochromator with 50% perfect character were made; however, there was no absorption correction. A partial structure from NMR, as a randomly positioned fragment, was used as input to the direct methods program RANTAN81 (Yao, 1980); this was carried out in order to optimize the structure factor normalization procedure. The best figure of merit trial solution set from RANTAN yielded a 41-atom partial structure containing the frame of the ring. The successive Fourier syntheses located the remaining 38 non-H atoms as well as two partially occupied water molecules. H atoms were found in difference maps very close to positions generated using planar or tetrahedral geometry. Least-squares refinement included coordinates and anisotropic thermal parameters for the non-H atoms; H-atom parameters were included

$B_{\rm eq} = (4/3)(a^2 B_{11})$	$+ b^2 B_{22}$	+	$c^2 B_{33}$).
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x	У	Ζ	B_{eq}
4849 (3)	3158 (2)	485 (3)	2.0 (2
4687 (5)	2546 (2)	567 (3)	3.3 (3
5162 (3)	3133 (2)	- 792 (2)	1.8 (2
4959 (3)	3221 (2)	- 1484 (3)	1.9 (2
4243 (2)	3446 (1)	- 1678 (2)	2.2 (2
5024 (3)	2980 (2)	-2037(3) -2266(3)	1.9 (2
5872 (4)	2174 (2)	-2880(3)	2.5 (2
5705 (4)	1570 (2)	- 2998 (3)	2.9 (3
6170 (4) 5224 (3)	1386 (2)	- 3554 (3)	5.4 (3)
6584 (3)	2959 (2)	- 1791 (2)	1.8 (2)
6997 (3)	3416 (2)	- 1551 (3)	2.1 (2
6601 (2)	3873 (1)	- 1549 (2)	2.1 (2)
8657 (4)	3679 (2)	-1309(3) -1789(3)	2.0 (2)
8632 (4)	3513 (2)	-2573(3)	2.8 (3
9170 (5)	3921 (3)	- 3036 (4)	4.6 (3
8984 (6)	2929 (3)	- 2689 (4)	5.0 (3)
4493 (3)	3995 (2)	-281(3)	2.3 (2
3757 (2)	4235 (1)	- 182 (2)	2.4 (2
5309 (3) 5204 (4)	4249 (2)	- 400 (2)	2.0 (2
6298 (4)	4840 (2) 5075 (2)	-513(3) -532(3)	2.2 (2
6297 (5)	5670 (3)	- 767 (4)	4.7 (3
6768 (5)	5008 (3)	193 (4)	4.5 (3
4130 (3)	4989 (2)	-11/6(3) -1173(2)	2.3 (2
4915 (3)	4687 (2)	- 1764 (2)	2.0 (2
4462 (4)	4823 (2)	- 2441 (3)	2.4 (2
4890 (4)	4467 (2) 4518 (3)	-3037(3) -3127(3)	2.4 (2)
6273 (4)	5105 (3)	- 3235 (4)	3.7 (3
6264 (4)	4162 (3)	- 3756 (4)	4.3 (3
3399 (4) 2902 (2)	4/58 (2) 5040 (2)	- 2427 (3) - 2802 (2)	2.0 (2)
3046 (3)	4345 (2)	- 2003 (2)	1.9 (2)
2047 (3)	4246 (2)	- 1962 (3)	2.2 (2)
1826 (4)	3634 (2)	- 1957 (3)	2.4 (2)
1571 (4)	4512 (2)	- 1315 (3)	2.2 (2)
725 (3)	4452 (2)	- 1224 (2)	3.7 (2)
2113 (3) 1748 (4)	4814 (2)	- 885 (2)	2.5 (2)
2511 (4)	5464 (2)	33 (3)	2.3 (2)
2277 (5)	5804 (3)	693 (3)	3.4 (3)
1527 (5)	6234 (2) 6069 (3)	539 (4)	4.0 (3)
1353 (4)	4709 (2)	309 (3)	4.3 (3) 2.3 (2)
575 (2)	4773 (2)	568 (2)	2.8 (2)
1916 (3)	4282 (2)	498 (2)	2.5 (2)
1054 (4)	3422 (2)	493 (3)	2.4 (2)
1670 (3)	3201 (2)	- 36 (2)	3.2 (2)
2316 (4)	3590 (2)	1407 (3)	2.3 (2)
2920 (3)	3940 (2)	1704 (2)	2.3 (2)
3733 (4)	3755 (3)	2103 (3)	3.0 (3)
4161 (5)	4242 (3)	2502 (4)	4.3 (3)
4379 (0) 4880 (7)	4043 (3)	3068 (5)	6./(4) 7.8(5)
4527 (10)	3720 (5)	3619 (5)	11.9 (8)
4445 (4)	3454 (2)	1657 (3)	2.7 (2)
4240 (2)	3230 (2)	1894 (2) 961 (2)	3.9 (2)
7615 (4)	3288 (2)	- 56 (3)	2.4 (2)
7041 (2)	2916 (2)	- 193 (2)	2.4 (2)
7 / 81 (4) 7606 (4)	3495 (2) 3039 (2)	703 (3)	2.2 (2)
8294 (2)	2622 (1)	1152 (2)	2.4 (2)
7663 (4)	3280 (2)	2007 (3)	2.5 (2)
7388 (4) 7414 (6)	2869 (2) 3125 (3)	2584 (3)	2.7 (3)
7006 (7)	2733 (3)	3896 (4)	4.1 (3) 6.2 (4)
6971 (9)	2971 (3)	4619 (4)	7.9 (5)
6513 (9) 5477 (11)	2601 (5)	5176 (5)	9.5 (7)
- 890 (3)	4529 (2)	- 368 (3)	11.8 (8) 3 9 (7)
-1141 (23)	5036 (14)	-729(18)	20(6)

Table 2. Bond lengths (Å) and angles (°)

$C(1) \rightarrow C(1A)$		N(10) = C(11) = 1	AAA (6)
	1.516 (8)	N(10) - C(11) = 1	.444 (0)
C(1) - C(2)	1.537 (7)	C(11) - C(11A) 1	.523 (8)
$\vec{c}(\vec{u}) = \vec{0}(\vec{z})$	1 446 (6)	$\dot{c}\dot{u}\dot{u}$	536 (7)
C(2) = N(2 4)	1 467 (6)	C(11,4) = O(11,B) = 1	417 (7)
C(2) = C(2)	1.407 (0)	C(12) - O(124) = 1	225 (6)
$C(2) \rightarrow C(3)$	1.337 (8)	C(12) = O(12A) 1	.223 (0)
$N(2A) \rightarrow C(2B)$	1.349 (7)	C(12) = N(13) 1	.330 (7)
C(2B)O(2C)	1.213 (6)	N(13)—C(14) I	.452 (7)
C(2B) - C(2D)	1.522 (7)	C(14)—C(14A) 1	.518 (8)
C(2D) - C(2E)	1.530 (7)	C(14)—C(15) 1	.524 (8)
C(2D) = N(2D)	1 443 (6)	$C(14A) \rightarrow C(14B) = 1$	527 (8)
	1.579 (7)	C(14R) - C(14C)	523 (9)
C(2E) = C(2F)	1.526 (7)	C(14B) = C(14C) = 1	519 (10)
C(2F) - C(2G)	1.507 (8)	C(14B) - C(14D) = 1	.518 (10)
$C(2G) \rightarrow O(2H)$	1.316 (8)	C(15) - O(15A) = 1	.220 (6)
C(2G)O(2I)	1.188 (7)	C(15)—N(16) 1	.360 (7)
N(2,)C(2K)	1.388 (7)	N(16)—C(17) 1	.467 (7)
cirk - 0iri)	1 247 (6)	$C(17) \rightarrow C(17A) = 1$	506 (8)
C(2R) = O(2L)	1.524 (0)	C(17) - C(18) = 1	529 (8)
C(2K) = C(2M)	1.524 (7)	C(17) = C(18) 1	.329 (0)
C(2M) - C(2N)	1.500 (7)	C(1/A) = O(1/B) 1	.430 (7)
C(2M) - N(2R)	1.464 (7)	C(18)O(18A) 1	.233 (6)
C(2N)C(20)	1.527 (8)	C(18)—N(19) 1	.334 (7)
C(20C(2P)	1.527 (9)	N(19)—C(20) 1	.451 (7)
C(20) - C(20)	1 524 (10)	C(20) - C(20A) = 1	.532 (9)
N(2P) - C(A)	1 247 (7)	C(20) - C(21) 1	505 (8)
N(2R) - C(R)	1.347 (7)	C(20, 4) = C(20, B) = 1	497 (11)
C(3) = O(3A)	1.213 (6)	C(20A) - C(20B) 1	.467 (11)
C(3)—N(4)	1.334 (6)	C(20A) - C(20C) 1	.514 (12)
N(4)C(5)	1.457 (7)	C(20C)—C(20D) 1	.480 (14)
C(5) - C(5A)	1.539 (8)	C(21) - O(21A) = 1	.206 (7)
$C(5) \rightarrow C(6)$	1 523 (7)	$\vec{C}(21) = O(22)$ 1	341 (6)
C(5) $C(5)$	1.517 (0)	C(4) = O(41)	248 (7)
$C(3A) \rightarrow C(3B)$	1.517 (9)	C(A) = O(A1)	.240 (7)
C(5A) - C(5C)	1.525 (9)	C(A) - C(B)	.530 (8)
C(6)O(6A)	1.231 (6)	$C(B) \rightarrow C(C)$ 1	.545 (8)
C(6)—N(7)	1.351 (7)	$C(C) \rightarrow O(C1)$ 1	.426 (6)
$N(7) \rightarrow C(8)$	1 465 (7)	C(C) - C(D) 1	.526 (8)
C(R) = C(R, 4)	1 543 (8)	C(D) = C(E)	526 (8)
	1.545 (8)	C(D) C(D)	577 (9)
C(8) - C(9)	1.522 (7)	$C(E) \rightarrow C(F)$.527 (6)
C(8A) - C(8B)	1.551 (8)	$C(F) \rightarrow C(G)$ 1	.547 (10)
C(8B)C(8C)	1.508 (9)	$C(G) \rightarrow C(H)$ 1	.478 (11)
C(8B) - C(8D)	1.525 (9)	$C(H) \rightarrow C(I)$ 1	.527 (14)
C(9) - O(9.4)	1211 (6)	C(h-C(h)) = 1	.500 (20)
C(0) = N(10)	1 278 (6)		()
	1.570 (0)		
C(1A) - C(1) - C(2)	111.8 (4)	O(9A) - C(9) - N(10)	122.5 (5)
C(14) - C(1) - O(22)	110 3 (4)	$C(9) \rightarrow N(10) \rightarrow C(11)$	120.8 (4)
C(1A) - C(1) - O(22)	103.3 (4)		1116(4)
C(2) - C(1) - O(22)	102.5 (4)	N(10) = C(11) = C(11A)	111.0 (4)
			11411(4)
C(1) - C(2) - N(2A)	108.6 (4)	N(10) - C(11) - C(12)	114.0 (4)
C(1) - C(2) - N(2A) C(1) - C(2) - C(3)	108.6 (4) 112.0 (4)	C(11A) - C(11) - C(12)	108.6 (4)
C(1) - C(2) - N(2A) C(1) - C(2) - C(3) N(2A) - C(2) - C(3)	108.6 (4) 112.0 (4) 112.6 (4)	N(10) - C(11) - C(12) C(11A) - C(11) - C(12) C(11) - C(11A) - O(11B)	108.6 (4) 113.7 (4)
C(1) - C(2) - N(2A) C(1) - C(2) - C(3) N(2A) - C(2) - C(3) C(2) - N(2A) - C(2B)	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4)	N(10) - C(11) - C(12) C(11A) - C(11) - C(12) C(11) - C(11A) - O(11B) C(11) - C(12) - O(12A)	108.6 (4) 113.7 (4) 119.5 (5)
C(1) - C(2) - N(2A) $C(1) - C(2) - C(3)$ $N(2A) - C(2) - C(3)$ $C(2) - N(2A) - C(2B)$ $N(2A) - C(2B) - O(2C)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4)	$\begin{array}{c} N(10) - C(11) - C(12) \\ C(11A) - C(11) - C(12) \\ C(11) - C(11A) - O(11B) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \end{array}$	114.0 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4)
C(1) - C(2) - N(2A) $C(1) - C(2) - C(3)$ $N(2A) - C(2) - C(3)$ $C(2) - N(2A) - C(2B)$ $N(2A) - C(2B) - O(2C)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5)	$\begin{array}{c} N(10) - C(11) - C(12) \\ C(114) - C(11) - C(12) \\ C(11) - C(114) - O(11B) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12A) \\ C(11) - C(1$	108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4)
C(1) - C(2) - N(2A) $C(1) - C(2) - C(3)$ $N(2A) - C(2) - C(3)$ $C(2) - N(2A) - C(2B)$ $N(2A) - C(2B) - O(2C)$ $N(2A) - C(2B) - O(2C)$ $N(2A) - C(2B) - C(2D)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(114) - C(11) - C(12) \\ C(11) - C(114) - O(11B) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \\ O(12A) - C(12A) \\ O(12A) \\ O(12A$	108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5)
C(1) - C(2) - N(2A) $C(1) - C(2) - C(3)$ $N(2A) - C(2) - C(3)$ $C(2) - N(2A) - C(2B)$ $N(2A) - C(2B) - O(2C)$ $N(2A) - C(2B) - C(2D)$ $O(2C) - C(2B) - C(2D)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(11) - C(11) - C(12) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - N(13) \\ O(124) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ \end{array} $	113.6 (4) 118.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4)
$\begin{array}{l} C(1)-C(2)-N(2A)\\ C(1)-C(2)-C(3)\\ N(2A)-C(2)-C(3)\\ C(2)-N(2A)-C(2B)-O(2C)\\ N(2A)-C(2B)-O(2C)\\ N(2A)-C(2B)-C(2D)\\ O(2C)-C(2B)-C(2D)\\ O(2C)-C(2E)-C(2D)\\ \end{array}$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(11) - C(11) - C(12) \\ C(11) - C(11A) - O(11B) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \\ O(12A) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(14A) \\ \end{array} $	113.7 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4)
$\begin{array}{l} C(1)-C(2)-N(2A)\\ C(1)-C(2)-C(3)\\ N(2A)-C(2)-C(3)\\ C(2)-N(2A)-C(2B)\\ N(2A)-C(2B)-O(2C)\\ N(2A)-C(2B)-O(2C)\\ N(2A)-C(2B)-C(2D)\\ C(2B)-C(2D)-C(2E)\\ C(2B)-C(2D)-C(2E)\\ C(2B)-C(2D)-N(2J)\\ \end{array}$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4)	$\begin{array}{c} N(10)-C(11)-C(12)\\ C(11)-C(11)-C(12)-C(12)\\ C(11)-C(12)-O(124)\\ C(11)-C(12)-O(124)\\ C(11)-C(12)-N(13)\\ C(12)-C(12)-N(13)\\ C(12)-C(14)-C(14)\\ N(13)-C(14)-C(14)\\ N(13)-C(14)-C(15)\\ \end{array}$	113.7 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) \\ N(2A) - C(2B) - C(2C) \\ N(2A) - C(2B) - C(2C) \\ N(2A) - C(2B) - C(2C) \\ C(2B) - C(2D) - C(2E) \\ C(2B) - C(2D) - N(2A) \\ C(2E) - C(2D) - N(2A) \\ C(2E) - C(2D) - N(2A) \\ \end{array}$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 110.3 (4)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(11) - C(11) - C(12) - C(12) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \\ C(12A) - C(12) - N(13) \\ C(12A) - C(14) - C(14) \\ N(13) - C(14) - C(14) \\ N(13) - C(14) - C(15) \\ C(14A) - C(14) - C(15) \\ \end{array} $	113.7 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - C(2E) \\ C(2B) - C(2D) - N(2A) \\ C(2D) - C(2E) - C(2D) \\ C(2E) - C(2D) - N(2A) \\ C(2D) - C(2E) - C(2E) \\ C(2E) - C(2D) - N(2A) \\ C(2E) - C(2E) - C(2E) \\ C(2E) \\ C(2E) - C(2E) \\ C(2E) \\ C(2E) - C(2E) \\ C(2E) \\$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.9 (4)	$\begin{array}{c} N(10)-C(11)-C(12)\\ C(11)-C(11)-C(12)-C(12)\\ C(11)-C(12)-O(124)\\ C(11)-C(12)-N(13)\\ C(11)-C(12)-N(13)\\ C(12)-N(13)-C(14)\\ N(13)-C(14)-C(14)\\ N(13)-C(14)-C(14)\\ N(13)-C(14)-C(15)\\ C(14)-C(14)-C(15)\\ C(14)-C(14)-C(14)\\ \end{array}$	108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5)
C(1) - C(2) - N(2A) $C(1) - C(2) - C(3)$ $N(2A) - C(2) - C(3)$ $N(2A) - C(2B) - O(2C)$ $N(2A) - C(2B) - C(2B)$ $O(2C) - C(2B) - C(2D)$ $O(2C) - C(2B) - C(2D)$ $C(2B) - C(2D) - N(2A)$ $C(2B) - C(2D) - N(2A)$ $C(2D) - C(2E) - C(2E)$ $C(2D) - C(2E) - C(2E)$ $C(2D) - C(2E) - C(2E)$	108.6 (4) 112.0 (4) 112.5 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 110.3 (4) 112.9 (4) 113.1 (5)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(11) - C(11) - C(12) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(144) \\ N(13) - C(14) - C(144) \\ N(13) - C(14) - C(15) \\ C(144) - C(144) - C(154) \\ C(144) - C(144) - C(144) - C(144) \\ C(144) - C(144) - C(144) \\ C(144) - C(144) - C(144) - C(144) \\ C(144) - C(144) - C(144) - C(144) + C(144) \\ C(144) - C(144) - C(144) + C(144)$	113.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) \\ N(2A) - C(2B) - C(2C) \\ N(2A) - C(2B) - C(2C) \\ N(2A) - C(2B) - C(2C) \\ C(2B) - C(2D) - C(2E) \\ C(2B) - C(2D) - C(2C) \\ C(2D) - C(2D) - N(2D) \\ C(2D) - C(2D) - N(2D) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2E) - C(2E) - C(2F) \\ C(2E) - C(2E) - C(2E) \\ C(2E) \\ C(2E) - C(2E) \\ C(2E) \\$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 110.3 (4) 112.9 (4) 113.1 (5)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(11) - C(11) - C(12) \\ C(11) - C(12) - C(12) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(14) \\ N(13) - C(14) - C(15) \\ C(144) - C(144) - C(15) \\ C(144) - C(144) - C(14B) \\ C(144) - C(144) - C(14B) \\ C(144) - C(14B) - C(14B) \\ C(14B) C(14B) \\ C(14B) - C(14B) \\ C(14B) \\ C(14B) - C(14B) \\ C(14B) - C(14B) \\ C(14B) $	113.7 (4) 119.5 (5) 117.1 (4) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5)
$\begin{array}{c} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - C(2E) \\ C(2B) - C(2D) - N(2A) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2E) - C(2F) - C(2F) \\ C(2F) C(2F) \\ C(2F) - C(2F) \\ C(2F) \\ C(2F) - C(2F) \\ C(2F)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.9 (4) 113.1 (5) 111.7 (5)	$\begin{array}{c} N(10) - C(11) - C(12) \\ C(11A) - C(11) - C(12) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(14) \\ N(13) - C(14) - C(14A) \\ N(13) - C(14) - C(15) \\ C(14A) - C(14A) - C(14B) \\ C(14A) - C(14B) \\ C(14A) - C(14B) \\ C(14A) - C(14B) \\ C(14A) $	113.7 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 112.0 (4) 112.0 (4) 117.5 (5) (7) 111.9 (5) (9) 108.4 (5) 112.0 (4) 117.5 (5) (11.9 (5)) (10.8 (4)) (11.9 (5)) (11.9 (5))
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2E) - C(2D) - N(2A) \\ C(2E) - C(2E) - C(2F) \\ C(2E) - C(2E) - C(2F) \\ C(2E) - C(2C) - O(2F) \\ C(2E) - C(2E) \\ C(2E) \\ C(2E) - C(2E) \\ C(2E) \\$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.9 (4) 113.1 (5) 111.7 (5) 123.8 (5)	$ \begin{array}{c} N(10) = C(11) = C(12) \\ C(11) = C(11) = C(12) \\ C(11) = C(12) = O(124) \\ C(11) = C(12) = O(124) \\ C(11) = C(12) = N(13) \\ C(12) = N(13) = C(14) \\ N(13) = C(14) = C(15) \\ C(144) = C(144) = C(144) = C(144) \\ C(144) \\ C(144) \\ C(144) \\ $	111.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 117.5 (5) 111.9 (5) 108.4 (5) 112.6 (4) 114.9 (5) 117.5 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2D) \\ C(2B) - C(2D) - O(2E) \\ C(2B) - C(2D) - O(2E) \\ C(2B) - C(2D) - O(2E) \\ C(2D) - C(2E) - C(2E) \\ C(2D) - C(2E) - C(2E) \\ C(2E) - C(2G) - O(2E) \\ C(2F) - C(2G) - C(2E) \\ C(2F) - C(2E) - C(2E) \\ C(2F) - C(2E) - C(2E) \\ C(2E) \\ C(2E) - C(2E) - C(2E) \\ C(2E) \\ C(2E) \\ C(2E) - C(2E) - C(2E) \\ C(2E) \\ C(2E) - C(2E) \\ C(2E) \\ C(2E) - C(2E) \\ C(2E) \\ C(2E) \\ C(2E) \\ C(2E) \\ C(2E) \\$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 118.5 (4) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 110.3 (4) 112.9 (4) 112.9 (4) 113.1 (5) 111.7 (5) 123.8 (5) 124.5 (6)	$\begin{array}{c} N(10) = -C(11) = C(12) \\ C(11A) = C(11) = C(12) \\ C(11) = C(12) = O(12A) \\ C(11) = C(12) = O(12A) \\ C(11) = C(12) = N(13) \\ O(12A) = C(14) = C(14) \\ N(13) = C(14A) = C(14A) \\ N(13) = C(14A) = C(14A) \\ C(14A) = C(14B) = C(14C) \\ C(14A) = C(15A) \\ C(15A) \\ C(15A) = O(15A) \\ C(15A) \\ $	113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 0) 108.4 (5) 112.0 (2) 111.2 (5) 0) 101.2 (5) 122.4 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ Q(2) - N(2A) - C(2B) - Q(2C) \\ N(2A) - C(2B) - Q(2C) \\ Q(2B) - C(2B) - C(2D) \\ Q(2B) - C(2D) - N(2A) \\ Q(2B) - C(2B) - Q(2A) \\ Q(2B) - C(2B) - Q(2A) \\ Q(2B) - C(2G) - Q(2A) \\ Q(2D) - C(2G) - Q(2A) \\ Q(2D) - C(2A) - C(2A) \\ Q(2A) \\ Q(2A) \\ Q(2A) - C(2A) \\ Q(2A) \\ Q(2A) \\$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.6 (4) 113.1 (5) 111.7 (5) 123.8 (5) 124.5 (6) 119.6 (4)	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{N}(13) \\ &C(12) - \mathbb{N}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(144) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(144) \\ &N(14) - \mathbb{C}(144) - \mathbb{C}(144) \\ &C(144) - \mathbb{C}(145) - \mathbb{C}(144) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(154) \\ &C(14) - \mathbb{C}(15) - \mathbb{N}(16) \end{split} $	108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 0 108.4 (5) 0 108.4 (5) 111.2 (4) 112.7 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ O(2D) - C(2D) - N(2J) \\ O(2D) - C(2D) - N(2J) \\ O(2D) - C(2E) - C(2F) \\ O(2E) - C(2D) - N(2J) \\ O(2E) - C(2C) - O(2E) \\ O(2F) - C(2G) - O(2I) \\ O(2F) - C(2K) - O(2I) \\ O(2F) - O(2K) \\ O(2F) \\ O(2F) - O(2K) \\ O(2F) \\ O(2F) - O(2K) $	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 110.3 (4) 112.9 (4) 112.9 (4) 113.1 (5) 123.8 (5) 124.5 (6) 119.6 (4) 123.0 (4)	$ \begin{array}{c} N(10) = C(11) = C(12) \\ C(11) = C(11) = C(12) \\ C(11) = C(12) = O(124) \\ C(11) = C(12) = O(124) \\ C(11) = C(12) = N(13) \\ C(12) = N(13) = C(14) \\ N(13) = C(14) = C(14) \\ N(13) = C(14) = C(14) \\ N(13) = C(14) = C(15) \\ C(144) = C(144) = C(15) \\ C(144) = C(144) = C(146) \\ C(144) = C(146) = C(142) \\ C(144) = C(146) = C(142) \\ C(144) = C(146) = C(142) \\ C(144) = C(15) = O(154) \\ C(14) = C(15) = O(154) \\ C(14) = C(15) = O(154) \\ C(14) = C(15) = O(154) \\ C(15) = O(154) \\ C(15) = O(156) \\ O(154) = C(15) = N(16) \\ \end{array} $	108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 112.0 (4) 117.5 (5) (7) 111.9 (5) (7) 108.4 (5) 112.2 (4) 112.2 (5) 112.2 (5) 115.7 (4) 121.8 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2C) \\ O(2B) - C(2D) - N(2A) \\ C(2B) - C(2C) - O(2C) \\ O(2B) - O(2C) - O(2C) \\ O(2D) - N(2A) - C(2C) \\ O(2L) - C(2C) - O(2L) \\ N(2A) - C(2C) - O(2L) \\ O(2L) - C(2L) \\ O(2L) - C(2L) - O(2L) \\ O(2L) - O(2L) \\ O(2L) - O(2L) \\ O(2L) - O(2L) \\ O(2L)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.6 (4) 113.1 (5) 124.5 (6) 119.6 (4) 123.0 (4) 113.0 (4)	$\begin{array}{c} N(10) - C(11) - C(12) \\ C(11A) - C(11) - C(12) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(14) \\ N(13) - C(14) - C(14A) \\ N(13) - C(14) - C(14B) \\ C(14A) - C(14B) - C(14B) \\ C(14A) - C(15) - N(16) \\ C(15) - N(16) \\ C(15) - N(16) \\ C(17) - N(16) \\ C(17) \end{array}$	113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 117.5 (5) 111.9 (5) 111.2 (5) 111.2 (5) 111.2 (5) 111.2 (5) 112.2 (4) 115.7 (4) 121.8 (5) 119.7 (4)
C(1)-C(2)-N(2A) C(1)-C(2)-C(3) N(2A)-C(2)-C(3) N(2A)-C(2B)-C(2C) N(2A)-C(2B)-C(2C) N(2A)-C(2B)-C(2C) O(2C)-C(2B)-C(2D) C(2B)-C(2D)-N(2A) C(2B)-C(2D)-N(2A) C(2D)-C(2E)-C(2F) C(2E)-C(2F)-C(2G) C(2F)-C(2G)-O(2H) C(2F)-C(2G)-O(2H) C(2F)-C(2G)-O(2H) C(2D)-N(2A)-C(2K) N(2A)-C(2K)-O(2L) N(2A)-C(2K)-C(2M) N(2A)-C(2K)	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.9 (4) 113.1 (5) 123.8 (5) 124.5 (6) 119.6 (4) 123.0 (4) 116.3 (4)	$ \begin{split} &N(10) - C(11) - C(12) \\ &C(11) - C(11) - C(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - N(13) \\ &C(12) - N(13) - C(14) \\ &N(13) - C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &N(13) - C(14) - C(15) \\ &C(144) - C(144) - C(15) \\ &C(144) - C(144) - C(144) \\ &C(144) - C(144) - C(144) \\ &C(144) - C(144) - C(144) \\ &C(144) - C(145) - C(144) \\ &C(14) - C(15) - N(16) \\ &C(15) - N(16) - C(17) \\ &N(16) - C(17) \\ &N(16) - C(174) \\ \end{split} $	108.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 114.4 (5) 111.9 (5) 0 108.4 (5) 0 108.4 (5) 0 111.2 (5) 122.4 (5) 115.7 (4) 121.8 (5) 115.7 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2D) \\ C(2B) - C(2D) - O(2E) \\ C(2B) - C(2D) - O(2E) \\ C(2D) - C(2E) - C(2C) \\ O(2E) - C(2D) - O(2E) \\ C(2E) - C(2C) - O(2E) \\ C(2E) - C(2C) - O(2E) \\ O(2E) - C(2E) - C(2E) \\ O(2E) \\ O(2E) - C(2E) \\ O(2E) \\ O(2E) \\ O(2E) \\ O(2E) \\ O(2E)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 118.5 (4) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.9 (4) 112.9 (4) 113.1 (5) 123.8 (5) 124.5 (6) 119.6 (4) 123.0 (4) 112.6 (4) 112.6 (5) 124.5 (6) 119.6 (4) 123.0 (4) 123.0 (4) 110.5 (4) 120.6 (5) 120.6 (5) 120.7 (4) 120.6 (5) 120.7 (4) 120.6 (5) 120.7 (4) 120.6 (5) 120.7 (4) 120.6 (5) 120.7 (4) 120.6 (5) 120.7 (4) 120.6 (5) 120.7 (4) 120.7 (5) 120.7 (5)	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{N}(13) \\ &C(12) - \mathbb{N}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(144) - \mathbb{C}(144) - \mathbb{C}(15) \\ &C(144) - \mathbb{C}(14B) - \mathbb{C}(144) \\ &C(144) - \mathbb{C}(14B) - \mathbb{C}(144) \\ &C(144) - \mathbb{C}(15) - \mathbb{N}(16) \\ &C(15) - \mathbb{N}(16) \\ &C(17) - \mathbb{C}(17) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(17) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \end{split} $	113.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 117.5 (5) 111.2 (4) 117.5 (5) 111.9 (5) 111.2 (5) 122.4 (5) 112.7 (4) 123.8 (5) 119.7 (4) 109.6 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2C) - O(2C) \\ N(2A) - C(2K) - O(2A) \\ N(2A) - C(2M) - C(2M) \\ C(2B) - C(2M) - C(2M) \\ C(2D) - N(2M) - N(2M) \\ C(2D) \\ C(2D) - N(2M) \\ C(2D) - N(2M) \\ C(2D) \\ C(2D) - N(2M) \\ C(2D) \\ C(2D) \\ C(2D) - N(2M) \\ C(2D) \\$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.6 (4) 113.1 (5) 111.7 (5) 123.8 (5) 124.5 (6) 119.6 (4) 123.0 (4) 123.0 (4) 123.0 (4) 120.6 (5) 110.7 (4)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(11A) - C(11) - C(12) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(14A) \\ N(13) - C(14) - C(14A) \\ N(13) - C(14) - C(14A) \\ N(13) - C(14) - C(14B) \\ C(14A) - C(14B) - C(14E) \\ C(14A) - C(14B) - C(14E) \\ C(14A) - C(14B) - C(14E) \\ C(14A) - C(15) - N(16) \\ C(15) - N(16) - C(17) \\ N(16) - C(17) - C(17A) \\ N(16) - C(17) - C(18) \\ C(18) - C(17) - C(18) \\ C(18) \\ C(18) - C(18) \\ C(18) \\ C(18) - C(18) \\ C(18) \\ C(18) \\ C(18) - C(18) \\ C(18$	1108.6 (4) 1108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.2 (5) 111.2 (5) 111.2 (5) 112.2 (4 (5) 115.7 (4) 122.8 (5) 115.7 (4) 121.8 (5) 119.7 (4) 109.6 (4) 110.8 (4) 112.1 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ O(2D) - C(2B) - C(2D) \\ O(2D) - C(2D) - N(2D) \\ O(2E) - C(2D) - N(2D) \\ O(2E) - C(2D) - N(2D) \\ O(2E) - C(2C) - O(2E) \\ O(2E) - C(2E) - O(2E) \\ O(2E) - O(2E) O(2E) \\ O(2E) - O(2E) \\ O(2E) \\ O(2E) - O(2E) \\ O(2E) $	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.6 (4) 113.1 (5) 123.8 (5) 124.5 (6) 19.6 (4) 123.0 (4) 116.3 (4) 120.6 (5) 110.7 (4) 110.2 (4)	$ \begin{split} &N(10)C(11) - C(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &C(144) - C(144) - C(144) \\ &C(144) - C(144) - C(144) \\ &C(144) - C(144) - C(144) \\ &C(142) - C(144) - C(144) \\ &C(14) - C(15) - N(16) \\ &C(15) - N(16) - C(17) \\ &N(16) - C(17) - C(18) \\ &C(174) - C(17) - C(17) \\ &C(174) - C(17) \\ &C(1$	113.6 (4) 108.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 112.1 (4) 123.3 (5) 122.6 (4) 112.0 (4) 112.0 (4) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (5) 122.4 (5) 115.7 (4) 109.6 (4) 110.8 (4) 111.7 (4) 108.8 (4) 111.7 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2C) \\ O(2B) - C(2D) - N(2D) \\ C(2B) - C(2D) - N(2D) \\ C(2B) - C(2D) - N(2D) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2E) - C(2D) - O(2F) \\ C(2E) - C(2G) - O(2F) \\ O(2F) - C(2K) - C(2K) \\ O(2F) - C(2M) - N(2F) \\ O(2F) - C(2F) - C(2F) \\ O(2F) - C(2F) \\ O(2F) - C(2F) - C(2F) \\ O(2F) \\ O(2F) - C(2F) \\ O(2F) \\ O(2F) \\ O(2F) - C(2F) \\ O(2F) \\ O(2F)$	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 117.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.6 (4) 112.6 (4) 112.6 (4) 113.1 (5) 111.7 (5) 123.8 (5) 122.6 (6) 1196 (4) 123.0 (4) 120.6 (5)) 120.6 (5)) 110.7 (4)) 120.6 (5)) 110.2 (4)) 110.9 (4)	$ \begin{array}{c} N(10) - C(11) - C(12) \\ C(11A) - C(11) - C(12) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - O(12A) \\ C(11) - C(12) - N(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(14) \\ N(13) - C(14) - C(14A) \\ N(13) - C(14) - C(14B) \\ C(14A) - C(14B) - C(14C) \\ C(14A) - C(14B) - C(14B) \\ C(14A) - C(14B) - C(14B) \\ C(14A) - C(15) - N(16) \\ C(15) - N(16) - C(17) \\ C(14) - C(17) - N(16) - C(17) \\ N(16) - C(17) - C(18) \\ C(17) - C(17) - C(17) \\ N(16) - C(17) - C(18) \\ C(17) - C(17) - C(18) \\ C(17) - C(17) - C(17) \\ C(17A) - C(17) - C(18) \\ C(17) - C(17A) - C(17) \\ C(17A) - C(17) - C(18) \\ C(17) - C(17A) - C(17) \\ C(17A) - C(17) - C(18) \\ C(17) - C(17A) - C(17) \\ C(17A) - C(17) - C(18) \\ C(17) - C(17) - C(18) \\ C(17) - C(17) \\ C(17A) \\ C(17A) \\ C(17A) - C(17) \\ C(17A) \\ C(17A$	113.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.7 (5) 111.7 (4) 121.8 (5) 119.7 (4) 119.7 (5) 119.7 (4) 119.7 (4) 119.7 (4) 119.7 (5) 119.7 (4) 119.7 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ O(2D) - C(2D) - N(2A) \\ O(2E) - C(2C) - O(2A) \\ O(2E) - C(2C) - O(2A) \\ O(2B) - C(2C) - O(2A) \\ O(2A) - C(2A) - O(2A) \\ O(2A) - C(2A) - C(2A) \\ O(2A) - C(2A) - C(2A) \\ O(2A) - C(2A) - N(2B) \\ O(2A) - C(2A) - C(2A) \\ O(2A) \\ O(2A) - C(2A) \\ O(2A) $	108.6 (4) 112.0 (4) 112.6 (4) 118.5 (4) 122.8 (5) 107.6 (4) 119.4 (5) 110.7 (4) 112.6 (4) 112.6 (4) 112.6 (4) 112.6 (4) 112.6 (4) 112.6 (4) 113.1 (5) 123.8 (5) 124.5 (6) 119.6 (4) 123.0 (4) 120.6 (5) 110.7 (4) 120.6 (5) 110.7 (4) 120.6 (5) 110.7 (4) 120.6 (5) 110.7 (4) 120.6 (5) 110.7 (4) 120.6 (5) 110.7 (4) 110.9 (4) 110.4 (5)	$ \begin{split} &N(10) - C(11) - C(12) \\ &C(11) - C(11) - C(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - N(13) \\ &C(12) - N(13) - C(14) \\ &N(13) - C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &C(144) - C(144) - C(145) \\ &C(144) - C(144) - C(144) \\ &C(144) - C(15) - N(16) \\ &O(154) - O(154) \\ &C(17) - C(15) - N(16) \\ &C(17) - C(174) \\ &N(16) - C(17) - C(18) \\ &C(17) - C(174) - O(174) \\ &C(17) - C(18) - O(174) \\ \\ &C(17) - C(18) - O(174) \\ \\ &C(17) - C(18) - O(184) \\ \end{split}$	108.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.9 (5) 122.4 (5) 115.7 (4) 121.8 (5) 119.7 (4) 109.6 (4) 110.8 (4) 110.8 (4) 110.8 (4) 111.7 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2D) \\ O(2C) - C(2B) - O(2E) \\ O(2B) - C(2D) - N(2D) \\ C(2B) - C(2D) - N(2D) \\ C(2B) - C(2D) - N(2D) \\ C(2D) - C(2E) - C(2E) \\ O(2D) - C(2C) - O(2E) \\ O(2D) - C(2M) - N(2E) \\ O(2M) - C(2M) - N(2E) \\ O(2M) - C(2M) - N(2E) \\ O(2M) - C(2M) - C(2M) \\ O(2M) - C(2M) \\ O(2M) - C(2M) \\ O(2M) - C(2M) - C(2M) \\ O(2M) \\ O(2M) - C(2M) \\ O(2M) \\ O(2M)$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 119.4 (5)\\ 117.6 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 112.6 (4)\\ 110.3 (4)\\ 112.6 (4)\\ 112.9 (4)\\ 113.1 (5)\\ 123.8 (5)\\ 124.5 (6)\\ 119.6 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.2 (4)\\ 110.7 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 115.4 (5)\\ 111.$	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{N}(13) \\ &C(12) - \mathbb{N}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14) - \mathbb{C}(148) \\ &C(14) - \mathbb{C}(148) - \mathbb{C}(144) \\ &C(144) - \mathbb{C}(148) - \mathbb{C}(144) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(154) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(154) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(154) \\ &C(15) - \mathbb{N}(16) \\ &C(15) - \mathbb{N}(16) - \mathbb{C}(17) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(184) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ \end{split} $	113.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (5) 122.4 (5) 115.7 (4) 109.6 (4) 110.8 (4) 110.8 (5) 111.7 (5) 121.7 (5) 111.7 (5) 121.7 (5) 111.7 (5) 121.7 (5) 111.7 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2C) - N(2A) \\ C(2B) - C(2C) - O(2C) \\ O(2B) - C(2C) - C(2C) \\ O(2B) - C(2M) - O(2E) \\ C(2M) - C(2D) - C(2D) \\ C(2M) \\ C(2M$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 123.8 (5) \\ 124.5 (6) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 110.7 (4) \\ 110.2 (4) \\$	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{N}(13) \\ &C(12) - \mathbb{N}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(144) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(15) - \mathbb{N}(16) \\ &C(15) - \mathbb{N}(16) - \mathbb{C}(17) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(174) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(174) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(1844) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(18) \\ \\ &C(17)$	108.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.2 (5) 111.2 (5) 112.4 (5) 112.7 (4) 121.8 (5) 119.7 (4) 121.8 (4) 119.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 121.7 (5) 121.7 (5) 121.7 (5) 122.7 (5) 122.1 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2A) \\ C(2B) - O(2D) - O(2E) \\ C(2B) - C(2D) - O(2E) \\ C(2B) - C(2D) - C(2E) \\ C(2D) - C(2E) - C(2C) \\ C(2D) - C(2E) - C(2C) \\ C(2D) - C(2E) - C(2C) \\ C(2D) - C(2C) - O(2A) \\ C(2D) - C(2C) - O(2A) \\ C(2D) - C(2C) - O(2A) \\ C(2D) - O(2A) - O(2A) \\ C(2D) - O(2A) - O(2A) \\ C(2D) - O(2A) - O(2A) \\ C(2A) - C(2A) - C(2A) \\ C(2A) - C(2A) \\ C(2A) - C(2A) - C(2A) \\ C(2A) - C(2A) \\ C(2A) - C(2A)$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 112.6 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 122.0 (5)\\ 123.8 (5)\\ 124.5 (6)\\ 119.6 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 110.7 (4)\\ 110.2 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 111.4 (5)\\ 111.4 (5)\\ 111.4 (5)\\ 111.2 (5)\\ 111.4 (5)\\ 111.2 (5)\\ 111.3 (5)\\ 111.$	$ \begin{split} &N(10) - C(11) - C(12) \\ &C(11) - C(12) - O(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - O(13) \\ &O(124) - C(14) - C(15) \\ &C(144) - C(144) - C(15) \\ &C(144) - C(14B) - C(14L) \\ &C(14C) - C(14B) - C(14E) \\ &C(15) - N(16) - C(17) \\ &N(16) - C(17) - C(18) \\ &C(17) - C(18) - C(17) \\ &C(17) - C(18) \\ &C(17) - C(18) - N(19) \\ &C(17) - C(18) - N(19) \\ &C(18) - C(18) \\ &C(18) \\ &C(18) - C(18) \\ &C(18) \\ &\mathsf$	113.6 (4) 108.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (4) 122.4 (5) 112.7 (4) 108.4 (4) 112.1 (4) 112.1 (4) 112.1 (4) 112.1 (5) 122.1 (5) 122.1 (5) 122.2 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - C(3) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2C) \\ O(2D) - C(2B) - O(2D) \\ O(2D) - C(2D) - N(2D) \\ C(2D) - C(2D) - O(2D) \\ O(2D) - O(2D) O(2D) \\ O(2D) - O(2D) \\ O(2D) $	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 120.6 (5) \\ 110.7 (4) \\ 120.6 (5) \\ 110.7 (4) \\$	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{N}(13) \\ &C(11) - \mathbb{C}(12) - \mathbb{N}(13) \\ &C(12) - \mathbb{N}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14d) \\ &C(14) - \mathbb{C}(15) - \mathbb{N}(16) \\ &C(15) - \mathbb{N}(16) - \mathbb{C}(17) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(17d) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(18d) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ &C(18) - \mathbb{N}(19) - \mathbb{C}(20d) \\ &N(19) - \mathbb{C}(20d) \\ &N(18) - \mathbb{C}(19d) \\ &N(18) - \mathbb{C}(18d) \\ &N(18) - \mathbb{C}(18d) \\ &N(18) - \mathbb{C}(18d) \\ &N(18d) - \mathbb{C}(18d) \\ &N(18d) \\ &N(18d) - \mathbb{C}(18d) \\ &N(18d) \\ \\ &N(18d) \\ &N(18d) \\ &N(18d) \\ \\ &N(18d) \\ &N(18d) \\ \\ \\ \\ &N(18d) \\ \\ \\ \\ \\ &N(18d) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	113.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 108.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) (111.9 (5) 0) 108.4 (5) 112.7 (4) 122.4 (5) 119.7 (4) 121.8 (5) 119.7 (4) 122.4 (5) 119.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 122.4 (5) 119.7 (4) 121.8 (5) 119.7 (4) 122.4 (5) 119.7 (4) 122.4 (5) 119.6 (4) 110.8 (4) 112.1 (4) 111.7 (5) 121.7 (5) 122.1 (5) 122.0 (5) 122.0 (5) 122.0 (5) 109.1 (
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2C) \\ N(2A) - C(2B) - C(2C) \\ O(2B) - C(2D) - N(2A) \\ C(2B) - C(2C) - O(2A) \\ O(2B) - C(2G) - O(2A) \\ O(2A) - C(2A) - C(2A) \\ O(2A) - C(2A) - C(2A) \\ C(2A) C(2A) \\ C(2A) \\ C(2A) - C(2A) \\ C(2A) \\$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (5) \\ 110.6 (4) \\ 123.0 (5) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (5) \\ 111.4 (5) \\$	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(12) - \mathbb{O}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(144) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14E) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14E) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14E) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(15A) \\ &C(14) - \mathbb{C}(15) - \mathbb{N}(16) \\ &O(15A) - \mathbb{C}(15) - \mathbb{N}(16) \\ &O(15A) - \mathbb{C}(15) - \mathbb{N}(16) \\ &C(17) - \mathbb{C}(15) - \mathbb{N}(16) \\ &C(17) - \mathbb{C}(17A) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(17A) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ &O(18A) - \mathbb{C}(18) - \mathbb{N}(19) \\ &O(18A) - \mathbb{C}(20) - \mathbb{C}(20) \\ \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(20) \\ \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(20) \\ \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(21) \\ \end{split}$	110.6 (4) 110.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 123.3 (5) 122.6 (4) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.9 (5) 111.2 (5) 122.4 (5) 115.7 (4) 109.6 (4) 110.8 (4) 111.8 (5) 119.7 (4) 109.6 (4) 111.7 (5) 110.8 (4) 112.1 (4) 111.7 (5) 112.1 (4) 111.7 (5) 112.2 (5) 112.1 (4) 112.1 (4) 112.1 (4) 112.1 (5) 112.1 (5) 112.2 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2A) \\ O(2C) - C(2B) - O(2B) \\ O(2C) - C(2B) - O(2E) \\ O(2B) - C(2D) - N(2A) \\ O(2B) - C(2D) - N(2A) \\ O(2B) - C(2D) - N(2A) \\ O(2B) - C(2D) - O(2E) \\ O(2B) - C(2C) - O(2E) \\ O(2B) - C(2A) - O(2A) \\ O(2A) - C(2A) - N(2B) \\ C(2A) - C(2O) - C(2E) \\ O(2B) - O(2C) - O(2E) \\ O(2B) - O(2E) \\ O(2B) - O(2E) \\ O(2B) \\ O(2B)$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 112.6 (4)\\ 119.4 (5)\\ 117.6 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 112.6 (4)\\ 110.3 (4)\\ 112.6 (4)\\ 112.9 (4)\\ 113.1 (5)\\ 123.8 (5)\\ 124.5 (6)\\ 119.6 (4)\\ 123.0 (4)\\ 110.2 (4)\\ 110.2 (4)\\ 110.9 (4)\\ 113.4 (5)\\ 111.3 (5)\\ 111.4 (5)\\ 111.3 (5)\\ 111.3 (5)\\ 112.4 (5)\\ 111.3 (5)\\ 111.3 (5)\\ 112.4 (5)\\ 111.3 (5)\\ 112.4 (5)\\ 111.3 (5)\\ 112.4 (5)\\ 111.3 (5)\\ 112.4 (5)\\ 112.$	$\begin{split} N(10) &= C(11) = C(12) \\ C(11A) &= C(11) = C(12) \\ C(11) &= C(12) = O(12A) \\ C(11) &= C(12) = O(12A) \\ C(11) &= C(12) = O(13) \\ C(12) &= O(13) = C(14A) \\ N(13) &= C(14) = C(14A) \\ N(13) &= C(14) = C(14A) \\ N(13) &= C(14) = C(14A) \\ C(14A) = C(14B) = C(14C) \\ C(14A) = C(14B) = C(14C) \\ C(14A) = C(14B) = C(14C) \\ C(14A) = C(15) = O(15A) \\ C(14) = C(15) = O(15A) \\ C(14) = C(15) = O(15A) \\ C(14) = C(15) = O(16A) \\ C(15) = N(16) = C(17) \\ C(16) = C(17) = C(17) \\ N(16) = C(17) = C(18) \\ C(17) = C(18) = O(18A) \\ C(17) = C(18) = N(19) \\ O(18A) = C(18) = N(19) \\ O(18) = C(20) = C(20A) \\ N(19) = C(20) = C(20A) \\ N(19) = C(20) = C(20A) \\ N(19) = C(20) = C(21) \\ N(15) = C(15) = C(15) \\ N(15) = C(15) = C(15) \\ N(15) = C(20) = C(20A) \\ N(19) = C(20) = C(20A) \\ N(19) = C(20) = C(21) \\ N(15) = C(15) = C(15) \\ N(15) = C(15) = C(15) \\ N(15) = C(15) = N(19) \\ C(15) = N(16) = C(17) \\ N(16) = C(17) = C(18A) \\ C(17) = C(18) = N(19) \\ C(18) = N(19) = C(20) = C(20A) \\ N(19) = C(20) = C(20A) \\ N(19) = C(20) = C(20A) \\ N(15) = C(15) = C(15) \\ C(15) = C(15) \\ C(15) = C(15) \\ C(15) = C(15) = C(15) \\ C(15) \\$	113.6 (4) 113.7 (4) 113.7 (4) 117.1 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 117.5 (5) 112.7 (4) 117.5 (5) 111.9 (5) 111.7 (4) 108.4 (4) 111.7 (5) 111.7 (4) 109.6 (4) 112.1 (4) 111.7 (5) 111.7 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2C) - O(2C) \\ O(2E) - C(2C) - O(2C) \\ O(2E) - C(2G) - O(2A) \\ O(2E) - C(2G) - O(2A) \\ O(2B) - C(2A) - C(2A) \\ O(2A) - C(2O) - C(2Q) \\ O(2B) - O(2O) - O(2Q) \\ O(2B) - O(2D) - O(2Q) \\ O(2B) - O(2B) - O(2B) \\ O(2B) - O(2B) - O(2B) \\ O(2B) \\ O(2B) - O(2B) \\ O(2B$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 122.8 (5)\\ 117.6 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 112.6 (4)\\ 112.6 (4)\\ 113.1 (5)\\ 111.7 (5)\\ 123.8 (5)\\ 124.5 (6)\\ 123.6 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 113.6 (4)\\ 123.0 (4)\\ 113.6 (4)\\ 123.0 (4)\\ 110.7 (4)\\ 110.2 (4)\\ 110.2 (4)\\ 110.2 (4)\\ 110.2 (4)\\ 110.2 (4)\\ 110.2 (4)\\ 111.4 (5)\\ 111.$	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(12) - \mathbb{O}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14) - \mathbb{C}(14B) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(15) - \mathbb{N}(16) \\ &O(15A) - \mathbb{C}(15) - \mathbb{N}(16) \\ &O(15A) - \mathbb{C}(15) - \mathbb{N}(16) \\ &O(15A) - \mathbb{C}(15) - \mathbb{N}(16) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(17A) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(17B) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ &C(18) - \mathbb{N}(19) - \mathbb{C}(20) \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(21) \\ &C(204) - \mathbb{C}(20) - \mathbb{C}(21) \\ \\ &C(20) - \mathbb{C}(21) \\ \\ \\ \\ \\ &C(21) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	111.7 (4) 1108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.2 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.2 (5) 112.2 (4) 115.7 (4) 122.4 (5) 115.7 (4) 122.4 (5) 119.7 (4) 109.6 (4) 110.8 (4) 112.7 (5) 112.7 (5) 112.7 (5) 122.7 (5) 122.0 (5) 109.1 (5) 113.7 (4) 122.5 (5) 113.7 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2B) \\ O(2C) - C(2B) - O(2D) \\ C(2B) - C(2D) - C(2E) \\ C(2B) - C(2D) - C(2E) \\ C(2D) - C(2E) - C(2C) \\ O(2D) - C(2C) - O(2D) \\ O(2D) - C(2D) - C(2D) \\ O(2D) \\ O(2D) - C(2D) \\ O(2D) \\ O(2D) - C(2D) \\ O(2D) \\ O(2D)$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 122.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 110.7 (4)\\ 110.9 (4)\\ 110.9 (4)\\ 120.6 (4)\\ 112.7 (5)\\ 124.8 (5)\\ 124.8 (5)\\ 111.$	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(11) - \mathbb{C}(12) - \mathbb{N}(13) \\ &C(12) - \mathbb{N}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(13) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14A) - \mathbb{C}(14A) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14C) - \mathbb{C}(14B) - \mathbb{C}(14E) \\ &C(14C) - \mathbb{C}(14B) - \mathbb{C}(14E) \\ &C(15) - \mathbb{N}(16) - \mathbb{C}(17) \\ &C(15) - \mathbb{N}(16) - \mathbb{C}(17) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(16) \\ &C(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ &C(18) - \mathbb{N}(19) - \mathbb{C}(20) \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(204) \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(21) \\ &C(20A) - \mathbb{C}(20) - \mathbb{C}(21) \\ \\ &C(20A) - \mathbb{C}(20) - \mathbb{C}(21) \\ \\ &C(20B) - \mathbb{C}(20B) - \mathbb{C}(20B) \\ \end{split}$	113.6 (4) 108.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 117.5 (5) 117.1 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (4) 122.4 (5) 122.4 (5) 122.4 (5) 115.7 (4) 108.4 (4) 112.1 (4) 111.7 (5) 121.7 (5) 121.7 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.2 (5) 109.1 (5) 113.7 (4) 112.5 (4) 121.7 (5) 121.7 (5) 122.1 (5) 122.7 (5) 122.1 (5) 122.7 (5) 122.1 (5) 122.7 (5) 123.7 (4) 125.7 (4) 125.7 (4) 125.7 (4) 125.7 (4) 125.7 (5) 125.7 (4) 125.7 (4) 125.7 (5) 125.7 (4) 125.7 (5) 125.7 (4) 125.7 (5) 125.7 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2A) \\ O(2B) - C(2D) - C(2B) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2F) - C(2G) \\ O(2F) - C(2G) - O(2F) \\ C(2F) - C(2G) - C(2F) \\ C(2F) - C(2O) - C(2F) \\ C(2F) \\ C(2F) \\ C(2F) \\ C(2F) - C(2F) \\ C(2F)$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (5) \\ 110.7 (4) \\ 123.0 (5) \\ 110.7 (4) \\ 120.6 (5) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.5 (7) \\ 111.5 (7) \\ 111.7 (5) \\ 112.7 (5) \\ 117.9 (4) \\$	$\begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(12) - \mathbb{O}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14) - \mathbb{C}(144) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(144) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(144) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(141) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(141) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(15.4) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(15.4) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(15.4) \\ &C(17) - \mathbb{C}(15) - \mathbb{O}(16) \\ &C(15) - \mathbb{O}(16) \\ &C(17) - \mathbb{C}(18) \\ &O(17) \\ &C(18) - \mathbb{O}(18) \\ &N(19) - \mathbb{C}(20) \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(21) \\ \\ &C(20) - \mathbb{C}(204) - \mathbb{C}(20B) \\ \\ \\ \\ &C(10) - \mathbb{C}(10) - \mathbb{C}(10) \\ \\ \\ \\ &C(10) - \mathbb{C}(10) - \mathbb{C}(10) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.7 (4) 123.3 (5) 122.6 (4) 118.7 (4) 123.3 (5) 122.6 (4) 117.5 (5) 111.7 (5) 111.7 (5) 111.7 (4) 121.8 (5) 119.7 (4) 122.4 (5) 119.7 (4) 121.8 (5) 119.7 (4) 121.7 (5) 121.7 (4) 122.5 (5) 113.7 (4) 112.5 (5) 110.9 (6) 116.0 (6)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2A) \\ O(2E) - O(2B) - O(2B) \\ O(2C) - C(2B) - O(2D) \\ O(2E) - C(2D) - O(2E) \\ C(2B) - C(2D) - O(2E) \\ C(2B) - C(2D) - O(2E) \\ C(2B) - C(2D) - O(2E) \\ O(2E) - C(2E) - O(2E) \\ O(2E) - C(2E) - O(2E) \\ O(2E) - O(2E) \\ O(2E) - O(2E) \\ O(2E) - O(2E) \\ O(2E) - O(2E) \\ O(2E) \\ O(2E)$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 110.2 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (5) \\ 111.6 (3) \\ 110.2 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (5) \\ 111.6 (3) \\ 110.2 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (5) \\ 111.3 (5) \\ 111.3 (5) \\ 111.3 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.3 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.5 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 120.9 (4) \\ 10.$	$ \begin{split} &N(10) - C(11) - C(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &C(14) - C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &N(13) - C(14) - C(144) \\ &C(144) - C(144) - C(144) \\ &C(14) - C(15) - N(16) \\ &C(15) - N(16) - C(17) \\ &C(15) - N(16) - C(17) \\ &N(16) - C(17) - C(174) \\ &N(16) - C(17) - C(18) \\ &C(17) - C(18) - N(19) \\ &C(17) - C(18) - N(19) \\ &O(184) - C(20) - C(204) \\ &N(19) - C(20) - C(21) \\ &C(20) - C(204) - C(206) \\ &C(20) - C(20) - C(206) \\ \\ \\ &C(20) - C(20) - C(20) \\ \\ \\ &C(20) - C(20) - C(20) \\ \\ \\ &C(20) - C(20) - C(20) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	108.6 (4) 108.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 112.0 (4) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (5) 122.4 (5) 115.7 (4) 109.6 (4) 111.7 (5) 122.4 (5) 119.7 (4) 109.6 (4) 111.7 (5) 122.7 (5) 112.1 (4) 111.7 (5) 122.1 (5) 122.5 (5) 109.1 (5) 110.9 (6) 110.9 (6) (5) 109.0 (7)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B - O(2C)) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2D) \\ O(2C) - C(2B) - O(2D) \\ O(2E) - C(2D) - N(2D) \\ C(2E) - C(2D) - O(2E) \\ O(2E) - C(2C) - C(2E) \\ O(2E) - C(2C) - C(2E) \\ O(2E) - C(2C) - C(2E) \\ O(2E) - C(2O) - C(2E) \\ O(2E) - O(3) - N(4) \\ O(3A) - C(3) - N(4) \\ O(3A) - C(5) - O(5A) \\ N(4) - C(5) - C(5A) \\ N(4) - C(5) - C(5A) \\ \end{array}$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 112.6 (4)\\ 112.5 (4)\\ 112.8 (5)\\ 110.7 (4)\\ 112.6 (4)\\ 110.7 (4)\\ 112.6 (4)\\ 112.6 (4)\\ 112.9 (4)\\ 113.1 (5)\\ 123.8 (5)\\ 124.5 (6)\\ 119.6 (4)\\ 123.0 (4)\\ 113.3 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.7 (5)\\ 110.4 (5)\\ 110.$	$\begin{split} N(10) &= C(11) = C(12) \\ C(11) &= C(11) = C(12) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(13) \\ C(12) &= O(13) = C(14) \\ N(13) &= C(14) = C(14) \\ N(13) = C(14) = C(14) \\ N(13) = C(14) = C(14) \\ C(14) = C(15) = O(16) \\ C(15) = O(154) \\ C(14) = C(15) = O(154) \\ C(14) = C(15) = O(16) \\ O(15A) = C(15) = O(16) \\ O(15A) = C(17) = C(18) \\ C(17) = C(18) = O(18) \\ C(17) = C(18) = O(18) \\ C(17) = C(18) = N(19) \\ C(18) = N(19) = C(20) \\ N(19) = C(20) - C(21) \\ C(20) = C(20A) - C(206) \\ N(19) = C(20) - C(21) \\ C(20) = C(20A) - C(206) \\ C(20) = C(20) - C(206) \\ C(20$	108.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (5) 122.4 (5) 115.7 (4) 109.6 (4) 112.7 (5) 121.7 (5) 121.7 (5) 121.7 (5) 121.7 (5) 111.7 (4) 112.5 (5) 109.1 (5) 113.7 (4) 112.5 (5) 110.9 (6) 110.9 (6) 111.0 (6)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ N(2A) - C(2) - C(3) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2D) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2C) - O(2C) \\ C(2B) - C(2C) - O(2C) \\ C(2B) - C(2C) - O(2C) \\ C(2B) - C(2G) - O(2C) \\ C(2B) - C(2G) - O(2C) \\ C(2B) - C(2G) - O(2C) \\ O(2B) - C(2G) - O(2C) \\ N(2D) - C(2K) - C(2M) \\ O(2L) - C(2K) - C(2M) \\ O(2L) - C(2M) - C(2M) \\ C(2M) C(2M) $	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 113.1 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 110.7 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 111.3 (5) \\ 110.7 (4) \\ 122.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 111.3 (4) \\ 110.9 (4) \\ 111.3 (4) \\ 110.9 (4) \\ 111.3 (4) \\$	$ \begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(12) - \mathbb{O}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14) - \mathbb{C}(14B) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14L) \\ &C(14) - \mathbb{C}(15) - \mathbb{N}(16) \\ &O(15A) - \mathbb{C}(15) - \mathbb{N}(16) \\ &C(17) - \mathbb{C}(18) \\ &C(17A) - \mathbb{C}(17A) - \mathbb{O}(17B) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ &C(18) - \mathbb{N}(19) \\ &C(20) - \mathbb{C}(20) \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(21) \\ &C(20A) - \mathbb{C}(20A) - \mathbb{C}(20C) \\ &C(20A) - \mathbb{C}(20A) - \mathbb{C}(20C) \\ &C(20A) - \mathbb{C}(20A) - \mathbb{C}(20C) \\ &C(20A) - \mathbb{C}(20C) - \mathbb{C}(20) \\ \\ \\ \\ &C(20A) - \mathbb{C}(20C) - \mathbb{C}(20) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	113.6 (4) 113.7 (4) 113.7 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 112.0 (4) 112.0 (4) 117.5 (5) 111.9 (5) 112.4 (5) 122.4 (5) 115.7 (4) 121.8 (5) 119.7 (4) 109.6 (4) 111.7 (5) 116.2 (4) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5)
C(1) - C(2) - N(2A) $C(1) - C(2) - C(3)$ $N(2A) - C(2) - C(3)$ $N(2A) - C(2B) - O(2A)$ $N(2A) - C(2B) - O(2A)$ $N(2A) - C(2B) - O(2A)$ $O(2B) - C(2D) - O(2E)$ $O(2B) - C(2G) - O(2E)$ $O(2B) - C(2A) - C(2A)$ $O(2A) - C(2A) - O(2A)$ $O(2A) - C(2A) - N(2E)$ $O(2A) - C(2A) - C(2A)$ $O(2A) - C(2A) - C(2A)$ $O(2A) - C(2A) - C(2A)$ $O(2A) - C(2A) - C(2B)$ $O(2A) - O(2A) - O(2B)$ $O(2A) - O(2B) - O(2B)$ $O(2B) - O(2$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 118.5 (4) \\ 119.4 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 110.3 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 133.0 (4) \\$	$\begin{split} N(10) &= C(11) = C(12) \\ C(11) &= C(11) = C(12) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(13) \\ O(124) = C(12) = N(13) \\ C(12) = N(13) = C(14) \\ N(13) = C(14) = C(13) \\ C(14) = C(14) = C(14) \\ N(13) = C(14) = C(14) \\ C(144) = C(14B) = C(14C) \\ C(144) = C(14B) = C(14C) \\ C(144) = C(14B) = C(14C) \\ C(144) = C(15) = O(15A) \\ C(14) = C(15) = O(15A) \\ C(14) = C(15) = O(16A) \\ C(15) = N(16) = C(17) \\ C(16) = C(17) = C(17) \\ N(16) = C(17) = C(18) \\ C(17) = C(18) = O(18A) \\ C(17) = C(18) = N(19) \\ O(18) = N(19) = C(20) \\ N(19) = C(20) = C(21) \\ C(20A) = C(20A) = C(20A) \\ N(19) = C(20) = C(21) \\ C(20A) = C(20A) = C(20A) \\ C(20B) = C(20A) = C(20B) \\ C(20B) = C(20A) = C(20A) \\ C(20B) = C(20A) \\ C(20B) = C(20A) = C(20A) \\ C(20B) = C(20A) \\ C$	113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 119.5 (5) 122.6 (4) 118.2 (4) 118.4 (4) 114.4 (5) 117.5 (5) 111.9 (5) 111.9 (5) 111.7 (4) 122.4 (5) 119.7 (4) 109.6 (4) 111.7 (5) 111.7 (4) 112.1 (4) 111.7 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 113.7 (4) 112.5 (5) 110.9 (6) 110.9 (6)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - C(2B) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - C(2D) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - N(2D) \\ C(2B) - C(2D) - N(2D) \\ C(2D) - C(2E) - C(2E) \\ C(2D) - C(2E) - C(2E) \\ C(2D) - C(2D) - N(2D) \\ C(2D) - C(2D) - C(2E) \\ C(2D) - C(2G) - O(2L) \\ C(2D) - C(2G) - O(2L) \\ N(2D) - C(2K) - C(2K) \\ C(2K) - C(2M) - C(2K) \\ C(2M) - C(2M) - C(2M) \\ C(2M) \\ C(2M) - C(2M) \\ C(2M) \\ C(2M) - C(2M) \\ C(2M) \\ C(2M) \\ C(2M) - C(2M) \\ C(2M)$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 111.7 (5) \\ 123.6 (5) \\ 110.9 (4) \\ 110.9 (4) \\ 111.3 (5) \\ 111.3 (4) \\ 112.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 112.3 (4) \\ 112.3 (4) \\ 111.3 (4) \\ 111.2 (5) \\$	$\begin{split} N(10) &= C(11) = C(12) \\ C(11) &= C(11) = C(12) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(13) \\ C(12) &= O(13) = C(14) \\ N(13) &= C(14) = C(14) \\ N(13) = C(14) = C(144) \\ N(13) = C(14) = C(144) \\ C(14) = C(14B) = C(144) \\ C(144) = C(14B) = C(144) \\ C(144) = C(14B) = C(144) \\ C(144) = C(15) = N(16) \\ C(15) = N(16) = C(17) \\ C(14) = C(15) = N(16) \\ C(15) = N(16) = C(17) \\ N(16) = C(17) = C(18) \\ C(17) = C(18) = O(174) \\ N(16) = C(17) = C(18) \\ C(17) = C(18) = O(184) \\ C(17) = C(20) - C(204) \\ N(19) = C(20) - C(204) \\ C(20) = C(204) - C(206) \\ C(2$	108.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.7 (4) 118.8 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.7 (5) 111.7 (5) 122.4 (5) 115.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 122.4 (5) 119.7 (4) 122.4 (5) 119.7 (4) 122.4 (5) 119.7 (4) 122.4 (5) 122.4 (5) 119.7 (4) 122.5 (5) 111.7 (5) 121.7 (5) 122.0 (5) 109.1 (5) 109.1 (5) 113.7 (4) 112.5 (5) 113.7 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - O(2D) \\ C(2B) - O(2D) - C(2E) \\ C(2B) - C(2D) - C(2E) \\ C(2B) - C(2D) - N(2D) \\ C(2E) - C(2D) - N(2D) \\ C(2E) - C(2D) - C(2E) \\ C(2E) - C(2E) - C(2C) \\ O(2E) - C(2E) - C(2C) \\ O(2E) - C(2C) - O(2L) \\ O(2E) - C(2C) - C(2E) \\ O(2E) - C(2D) - C(2E) \\ O(2E) \\ O(2E) - C(2E) \\ O(2E) \\ O(2E) - C(2E) \\ O(2E) \\ O(2E)$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 113.1 (5)\\ 123.8 (5)\\ 124.5 (6)\\ 119.6 (4)\\ 122.0 (4)\\ 123.0 (4)\\ 123.0 (4)\\ 110.7 (4)\\ 120.6 (5)\\ 124.5 (6)\\ 119.6 (4)\\ 123.0 (4)\\ 110.7 (4)\\ 110.7 (4)\\ 110.2 (4)\\ 110.7 (4)\\ 110.2 (4)\\ 110.7 (4)\\ 110.2 (4)\\ 110.7 (4)\\ 110.2 (4)\\ 111.3 (5)\\ 117.9 (4)\\ 122.7 (5)\\ 117.9 (4)\\ 122.3 (4)\\ 10.9 (4)\\ 111.3 (4)\\ 112.3 (4)\\ 112.3 (4)\\ 112.3 (5)\\ 110.3 (5)\\ \end{array}$	$\begin{split} &N(10) - C(11) - C(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(12) - N(13) \\ &O(124) - C(14) - C(14) \\ &N(13) - C(14) - C(15) \\ &C(144) - C(144) - C(15) \\ &C(144) - C(144) - C(146) \\ &C(144) - C(146) - C(142) \\ &C(144) - C(145) - O(154) \\ &C(14) - C(15) - N(16) \\ &O(154) - C(15) - N(16) \\ &O(154) - C(15) - N(16) \\ &O(154) - C(17) - O(178) \\ &C(17) - C(18) - N(16) \\ &C(17) - C(18) \\ &C(17) - C(18) - N(19) \\ &O(184) - C(13) - N(19) \\ &O(184) - C(20) - C(204) \\ &N(19) - C(20) - C(204) \\ &N(19) - C(20) - C(204) \\ &N(19) - C(20) - C(204) \\ &C(20) - C(204) - C(206) \\ &C(204) - C(206) \\ \\ &C(204) - C(206) \\ &C(204) - C(206) \\ \\ &C(206) - C(206) \\ &C(206) - C(206) \\ \\ \\ &C(206) - C(206) \\ \\ &C$	113.6 (4) 108.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (5) 122.4 (5) 122.4 (5) 122.4 (5) 115.7 (4) 108.4 (4) 111.7 (5) 112.1 (4) 111.7 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.2 (5) 109.1 (5) 113.7 (4) 122.5 (5) 110.9 (6) 110.9 (6) 110.9 (6) 110.9 (0) 113.8 (9) 122.9 (5) 122.9 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2A) \\ O(2A) - C(2B) - O(2A) \\ O(2B) - C(2D) - C(2B) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2F) - C(2G) \\ O(2F) - C(2G) - O(2F) \\ O(2F) - C(2G) - C(2F) \\ O(2F) \\ O(2F) - C(2F) \\ $	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 110.3 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 120.6 (5) \\ 110.7 (4) \\ 120.6 (5) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 111.3 (5) \\ 111.3 (5) \\ 111.3 (5) \\ 111.3 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 113.3 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 113.3 (4) \\ 113.3 (4) \\ 111.3 (4) \\ 112.3 (4) \\ 111.3 (5) \\ 111.2 (5) \\$	$\begin{split} N(10) &= C(11) = C(12) \\ C(11) &= C(11) = C(12) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(13) \\ C(12) &= O(13) = C(14) \\ N(13) &= C(14) = C(14) \\ N(13) = C(14) = C(14) \\ N(13) = C(14) = C(14) \\ C(14) = C(14B) = C(14d) \\ C(14A) = C(14B) = C(14d) \\ C(14A) = C(14B) = C(14d) \\ C(14A) = C(14B) = C(14d) \\ C(14) = C(15) = O(15A) \\ C(14) = C(15) = O(15A) \\ C(14) = C(15) = O(15A) \\ C(15) = N(16) = C(17) \\ N(16) = C(17) = C(18) \\ C(17) = C(18) = O(17A) \\ N(16) = C(17) = C(18) \\ C(17) = C(18) = O(18A) \\ C(17) = C(18) = O(18A) \\ C(17) = C(18) = N(19) \\ C(18) = N(19) = C(20) \\ N(19) = C(20) - C(21A) \\ N(19) = C(20) - C(21A) \\ N(19) = C(20) - C(21A) \\ C(20) = C(20A) = C(20A) \\ C(20A) = C(20A) = C(20A) \\ C(20A) = C(20A) = C(20A) \\ C(20A) = C(20A) - C(20B) \\ C(20A) = C(20A) - C(20B) \\ C(20A) = C(21) - O(21A) \\ C(21) = O(22) \\ C(21) = O(21) \\ C(2$	113.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.2 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.7 (5) 111.7 (4) 122.4 (5) 115.7 (4) 121.7 (5) 116.2 (4) 112.1 (4) 111.7 (5) 121.7 (5) 121.7 (5) 122.1 (5) 122.1 (5) 122.0 (5) 113.7 (4) 112.5 (5) 113.7 (4) 112.5 (5) 113.7 (4) 122.1 (5) 122.9 (5) 127.8 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2B) \\ O(2C) - C(2B) - O(2D) \\ O(2C) - C(2B) - O(2D) \\ O(2C) - C(2B) - O(2D) \\ O(2D) - C(2E) - O(2C) \\ O(2D) - C(2E) - O(2C) \\ O(2D) - C(2E) - O(2C) \\ O(2D) - O(2E) - O(2C) \\ O(2D) - O(2C) - O(2C) \\ O(2D) - O(2D) - O(2D) \\ O(2D) \\ O(2D) - O(2D) \\ O(2D) - O(2D) \\ O(2D)$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 112.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.2 (4) \\ 112.2 (4) \\ 112.2 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.9 (4) \\ 110.2 (4) \\ 110.7 (4) \\ 110.2 (4) \\ 110.7 (4) \\ 110.2 (4) \\ 110.7 (4) \\ 110.2 (4) \\ 110.7 (4) \\ 110.9 (4) \\ 115.7 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 112.2 (5) \\ 110.3 (5) \\ 111.2 (5) \\ 111.2 (5) \\ 121 (5)$	$\begin{split} N(10) &= C(11) - C(12) \\ C(11) - C(11) - C(12) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - O(13) \\ C(12) - O(13) - C(14) \\ N(13) - C(14) - C(13) \\ C(14) - C(14) - C(14) \\ N(13) - C(14) - C(14) \\ N(13) - C(14) - C(14) \\ N(13) - C(14) - C(14) \\ C(14) - C(144) - C(144) \\ C(14) - C(144) - C(146) \\ C(14) - C(146) - C(142) \\ C(14) - C(146) - C(17) \\ C(14) - C(15) - N(16) \\ C(15) - N(16) - C(17) - C(18) \\ C(17) - C(18) - O(154) \\ C(17) - C(18) - N(19) \\ C(17) - C(20) - C(20) \\ N(19) - C(20) - C(21) \\ C(20) - C(20) - C(20) \\ C(20$	113.6 (4) 108.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 112.5 (5) 122.6 (4) 112.5 (5) 122.6 (4) 112.5 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.7 (4) 108.4 (5) 112.1 (4) 112.1 (4) 111.7 (5) 122.1 (5) 122.2 (5) 10.9 (6) 113.7 (4) 10.9 (6) 113.7 (4) 10.9 (6) 113.7 (4) 10.9 (6) 113.7 (4) 10.9 (6) 113.7 (4) 10.9 (6) 112.7 (5) 110.9 (6) 112.9 (5) 122.9 (5) 122.9 (5) 117.8 (4) 122.9 (5) 122.9
C(1) - C(2) - N(2A) $C(1) - C(2) - C(3)$ $N(2A) - C(2) - C(3)$ $N(2A) - C(2B) - O(2C)$ $N(2A) - C(2B) - O(2A)$ $N(2A) - C(2B) - O(2A)$ $O(2B) - C(2D) - N(2A)$ $C(2B) - C(2D) - N(2A)$ $C(2B) - C(2D) - N(2A)$ $C(2D) - C(2E) - C(2E)$ $C(2D) - C(2C) - O(2H)$ $C(2D) - C(2C) - O(2H)$ $C(2E) - C(2G) - O(2H)$ $C(2E) - C(2E) - C(2E)$ $C(2M) - C(2K) - C(2M)$ $C(2M) - C(2M) - N(2R)$ $C(2M) - C(2O) - C(2P)$ $C(2M) - N(2R) - C(4)$ $C(3) - N(4) - C(5)$ $N(4) - C(5) - C(5A)$ $C(5M) - C(5A) - C(5C)$ $C(5M) - C(5A) - C(5C)$ $C(5M) - C(5A) - C(5C)$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 112.5 (4) \\ 112.5 (5) \\ 110.7 (4) \\ 112.2 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.9 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 123.8 (5) \\ 123.6 (5) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 110.5 (4) \\ 110.5 (4) \\ 110.5 (4) \\ 111.3 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.3 (5) \\ 111.3 (5) \\ 111.3 (5) \\ 111.3 (5) \\ 111.3 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 123.7 (5) \\ 117.9 (4) \\ 110.3 (5) \\ 111.2 (5) \\ 122.1 (5) \\$	$\begin{split} &N(10) - \mathbb{C}(11) - \mathbb{C}(12) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(124) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(11) - \mathbb{C}(12) - \mathbb{O}(13) \\ &C(12) - \mathbb{O}(13) - \mathbb{C}(14) \\ &N(13) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14) - \mathbb{C}(15) \\ &C(14) - \mathbb{C}(14) - \mathbb{C}(14) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14C) \\ &C(14) - \mathbb{C}(14B) - \mathbb{C}(14C) \\ &C(14) - \mathbb{C}(15) - \mathbb{O}(15A) \\ &C(15) - \mathbb{N}(16) \\ &C(15) - \mathbb{N}(16) \\ &C(17) - \mathbb{C}(17) \\ &N(16) - \mathbb{C}(17) - \mathbb{C}(18) \\ &C(17) - \mathbb{C}(18) - \mathbb{O}(18A) \\ &C(17) - \mathbb{C}(18) - \mathbb{N}(19) \\ &C(18) - \mathbb{N}(19) - \mathbb{C}(20) \\ &N(19) - \mathbb{C}(20) - \mathbb{C}(20A) \\ &C(20) - \mathbb{C}(20A) - \mathbb{C}(20B) \\ &C(20) - \mathbb{C}(21) - \mathbb{O}(22) \\ &C(21) - \mathbb{O}(21) - \mathbb{O}(22) \\ &C(21) - \mathbb{O}(22) - \mathbb{C}(21) \\ &C(21) - \mathbb{O}(22) - \mathbb{C}(21) \\ &N(2R) - \mathbb{C}(20) - \mathbb{C}(21) \\ &N(2R) - \mathbb{C}(20) - \mathbb{C}(21) \\ &N(2R) - \mathbb{C}(20) - \mathbb{C}(21) \\ &N(2R) - \mathbb{C}(21) - \mathbb{O}(22) \\ &N(2R) - \mathbb{C}(2N) - \mathbb{C}(2N) \\ &N(2R) - \mathbb{C}(2$	113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 117.1 (4) 123.3 (5) 122.6 (4) 118.2 (4) 118.2 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.9 (5) 111.7 (5) 111.7 (5) 111.7 (4) 121.8 (5) 111.7 (5) 111.7 (5) 122.4 (5) 112.1 (4) 111.7 (5) 121.7 (5) 122.1 (5) 122.0 (5) 122.0 (5) 113.7 (4) 112.5 (5) 110.9 (6) 116.0 (6) (7) 109.0 (7) 113.8 (9) 124.2 (5) 122.9 (5) 117.8 (4) 122.0 (5) 122.9 (5) 117.8 (4) 122.0 (5) 122.9 (5) 117.8 (5) 122.9 (5) 123.8 (
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - C(2B) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ O(2C) - C(2B) - C(2D) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2C) - O(2C) \\ C(2D) - C(2C) - O(2C) \\ C(2D) - C(2C) - O(2C) \\ O(2D) - N(2A) - C(2A) \\ O(2D) - O(2A) - O(2A) \\ O(2D) - O(2A) - O(2A) \\ O(2A) - C(2A) - O(2A) \\ O(3A) - O(3) - N(4) \\ O(3A) - C(5) - O(6) \\ O(5A) - C(5A) - C(5A) \\ O(5A) - C(5A) - C(5A) \\ O(5B) - C(5A) - C(5C) \\ O(5B) - C(5A) - C(5C) \\ O(5A) - C(5A) - C(5C) \\ O(5A) - C(5A) - C(5A) \\ O(5A) - C(5A) - C(5A) \\ O(5A) - C(5A) - C(5A) \\ O(5B) - C(5A) - C(5A) \\ O(5A) - C(5A) \\ O(5A) - C(5A) \\ O(5A) - C(5A) \\ O$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 111.7 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 113.1 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.5 (4) \\ 112.7 (4) \\ 122.7 (5) \\ 117.9 (4) \\ 110.9 (4) \\ 112.3 (4) \\ 112.3 (4) \\ 112.2 (5) \\ 111.2 (5) \\ 111.2 (5) \\ 111.2 (5) \\ 111.2 (5) \\ 112.1 (5) \\$	$\begin{split} &N(10) - C(11) - C(12) \\ &C(11) - C(11) - C(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(13) \\ &C(11) - C(12) - N(13) \\ &C(12) - N(13) - C(14) \\ &N(13) - C(14) - C(14) \\ &C(14) - C(14B) - C(14d) \\ &C(14) - C(15) - N(16) \\ &O(15A) - C(15) - N(16) \\ &O(15A) - C(15) - N(16) \\ &O(15A) - C(17) - C(18) \\ &C(17) - C(18) - O(17d) \\ &N(16) - C(17) - C(18) \\ &C(17) - C(18) - O(17d) \\ &N(16) - C(17) - C(18) \\ &C(17) - C(18) - O(17d) \\ &N(16) - C(17) - C(18) \\ &O(17d) - C(18) - O(17d) \\ &N(16) - C(17d) - O(17d) \\ &N(16d) - C(17d) - O(17d) \\ &N(17d) - C(18d) - N(16d) \\ &O(17d) - C(18d) - N(19d) \\ &O(17d) - C(18d) - O(17d) \\ &N(17d) - C(18d) - N(19d) \\ &O(17d) - C(18d) - O(17d) \\ &N(19d) - C(20d) - C(20d) \\ &C(20d) - C(20d) - C(20d) \\ \\ &C(20d) - C(20d) - C(20d) \\ \\ &C(20d) - C(20d) - C(20d) \\ \\ &C(20d) - C(21) - O(22) \\ \\ &C(21d) - C(2d) - C(2d) \\ \\ &N(2R) - C(4) - C(4) \\ \\ \\ &N(2R) - C(4) - C(4) \\ \\ \\ &N(2R) - C(4) - C(4) \\ \\ \\ \\ &\mathsf$	113.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.2 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) (111.9 (5) 111.7 (5) 122.4 (5) 115.7 (4) 121.8 (5) 119.7 (4) 121.8 (5) 119.7 (4) 122.1 (5) 122.1 (4) 111.7 (5) 121.7 (5) 122.1 (5) 122.0 (5) 109.1 (1) 113.7 (4) 112.5 (5) 113.7 (4) 122.1 (5) 122.0 (5) 109.1 (7) 113.8 (4) 112.5 (5) 113.7 (4) 122.2 (5) 113.8 (4) 122.9 (5) 122.9 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2B) \\ O(2C) - C(2B) - O(2D) \\ C(2B) - C(2D) - C(2E) \\ C(2B) - C(2D) - C(2E) \\ C(2D) - C(2E) - C(2C) \\ O(2D) - C(2E) - C(2C) \\ O(2D) - C(2E) - C(2C) \\ O(2D) - C(2C) - O(2E) \\ O(2D) - C(2C) - C(2E) \\ O(2D) - C(2D) - C(2C) \\ O(2D) - C(2D) - C(2C) \\ O(2D) - C(2D) - C(2E) \\ O(2D) - C(2D) \\ O(2D) - C(2D) \\ O(2D) - C(2D)$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 112.6 (4) \\ 119.4 (5) \\ 119.4 (5) \\ 110.7 (4) \\ 112.4 (5) \\ 110.7 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 112.9 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 133.0 (4) \\ 123.0 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 110.2 (4) \\ 111.3 (5) \\ 111.3 (5) \\ 117.9 (4) \\ 122.7 (5) \\ 117.9 (4) \\ 122.3 (4) \\ 111.2 (5) \\ 122.1 (5) \\$	$\begin{split} &N(10) - C(11) - C(12) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(124) \\ &C(11) - C(12) - O(13) \\ &C(12) - O(13) - C(14) \\ &N(13) - C(14) - C(13) \\ &O(124) - C(12) - N(13) \\ &C(14) - C(14) - C(15) \\ &C(144) - C(144) - C(15) \\ &C(144) - C(144) - C(146) - C(142) \\ &C(144) - C(145) - C(144) \\ &C(144) - C(145) - C(146) - C(146) \\ &C(15) - O(154) \\ &C(14) - C(15) - N(16) \\ &C(15) - N(16) - C(17) - C(18) \\ &C(17) - C(17) - C(18) \\ &C(17) - C(18) - O(154) \\ &C(17) - C(18) - O(154) \\ &C(17) - C(18) - O(17) \\ &N(16) - C(17) - C(18) \\ &C(17) - C(18) - N(19) \\ &C(17) - C(18) - N(19) \\ &C(18) - N(19) - C(20) \\ &N(19) - C(20) - C(204) \\ &C(20) - C(204) - C(206) \\ &C(204) - C(206) \\ &C(206) - C(206) \\ &C(206) - C(206) \\ &C(206) - C(206) \\ &C(206) - C(206) \\ \\ &C(206) - C(206) \\ &C(206) - C(206) \\ &C(206) - C(206) \\ \\ &C(206) - C(206) \\ &C(206) - C(206) \\ \\ &C(206) - C(206) \\ \\ &C(206) - C(206) \\ $	113.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.4 (4) 114.4 (5) 117.1 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.2 (4) 117.5 (5) 111.7 (4) 108.4 (5) 112.1 (4) 111.7 (5) 112.1 (4) 111.7 (5) 122.1 (5) 122.2 (5) 109.1 (5) 113.7 (4) 122.2 (5) 110.9 (6) 110.9 (6) 110.9 (6) 110.9 (6) 112.8 (2) 122.9 (5) 112.8 (5) 122.9 (5) 112.8 (5) 122.9 (5) 117.8 (4) 122.2 (5) 122.2 (5) 115.8 (5) 125.2 (5)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2A) \\ O(2A) - C(2B) - O(2A) \\ O(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2B) - C(2D) - N(2A) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2E) - C(2F) \\ C(2D) - C(2F) - C(2G) \\ O(2F) - C(2G) - O(2F) \\ O(2F) - C(2G) - C(2F) \\ O(2F) - C(2G) - O(2F) \\ O(2F) - C(2G) - O(2F) \\ O(2F) - O(2G) - O(2F) \\ O(2F) - O(2F) \\ O(2F) - O(2G) \\ O(2F) - O(2F)$	$\begin{array}{c} 108.6 (4) \\ 112.0 (4) \\ 112.6 (4) \\ 118.5 (4) \\ 122.8 (5) \\ 117.6 (4) \\ 119.4 (5) \\ 110.7 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 112.6 (4) \\ 113.1 (5) \\ 123.8 (5) \\ 124.5 (6) \\ 119.6 (4) \\ 123.0 (4) \\ 123.0 (4) \\ 123.0 (3) \\ 120.6 (5) \\ 110.7 (4) \\ 120.6 (5) \\ 110.7 (4) \\ 120.6 (5) \\ 110.7 (4) \\ 120.6 (5) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 110.7 (4) \\ 111.3 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.4 (5) \\ 111.3 (4) \\ 120.6 (4) \\ 115.7 (4) \\ 115.7 (4) \\ 115.7 (4) \\ 110.9 (4) \\ 111.3 (4) \\ 112.3 (4) \\ 111.2 (5) \\ 122.1 (5) \\ 122.1 (5) \\ 120.1 (4) \\ 120.1 (4) \end{array}$	$\begin{split} N(10) &= C(11) = C(12) \\ C(11) &= C(11) = C(12) \\ C(11) &= C(12) = O(124) \\ C(11) &= C(12) = O(124) \\ C(11) = C(12) = O(13) \\ C(12) = O(13) = C(14) \\ N(13) = C(14) = C(14) \\ N(13) = C(14) = C(14) \\ N(13) = C(14) = C(14) \\ C(14) = C(14B) = C(14d) \\ C(14) = C(15) = N(16) \\ C(15) = N(16) = C(17) \\ N(16) = C(17) = C(18) \\ C(17) = C(18) = O(18d) \\ C(17) = C(18) = O(17d) \\ C(17) = C(20d) = C(20d) \\ C(20d) = C(20d) = C(20d) \\ C(20d) = C(20d) = C(20d) \\ C(17) = C(20) = C(21d) \\ C(17) = C(20) = C(21d) \\ C(20) = C(20d) = C(20d) \\ C(20) = C(21) = O(22d) \\ C(20) = C(21) = O(22d) \\ C(20) = C(21) = O(22d) \\ $	113.6 (4) 108.6 (4) 113.7 (4) 119.5 (5) 117.1 (4) 123.3 (5) 122.6 (4) 118.2 (4) 118.4 (4) 114.4 (5) 112.0 (4) 117.5 (5) 111.9 (5) 111.7 (5) 111.7 (4) 122.4 (5) 115.7 (4) 121.7 (5) 111.7 (4) 112.1 (4) 111.7 (5) 121.7 (5) 121.7 (5) 122.1 (5) 122.1 (5) 122.0 (5) 113.7 (4) 112.5 (5) 113.7 (4) 112.5 (5) 113.7 (4) 122.1 (5) 122.2 (5) 113.8 (9) 124.2 (5) 122.9 (5) 122.9 (5) 122.9 (5) 122.2 (5) 115.8 (4) 122.2 (5) 115.8 (4)
$\begin{array}{l} C(1) - C(2) - N(2A) \\ C(1) - C(2) - C(3) \\ C(2) - N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2C) \\ N(2A) - C(2B) - O(2B) \\ O(2C) - C(2B) - O(2D) \\ O(2C) - C(2B) - O(2D) \\ O(2C) - C(2B) - O(2C) \\ O(2D) - C(2C) - C(2C) \\ O(2D) - C(2C) - C(2C) \\ O(2D) - C(2C) - C(2C) \\ O(2D) - C(2C) - O(2C) \\ O(2D) - O(2C) - O(2C) \\ O(2D) - O(2D) - O(2D) \\ O(2D) - O(2D)$	$\begin{array}{c} 108.6 (4)\\ 112.0 (4)\\ 112.6 (4)\\ 118.5 (4)\\ 118.5 (4)\\ 119.4 (5)\\ 110.7 (4)\\ 110.7 (4)\\ 112.4 (5)\\ 110.7 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 112.9 (4)\\ 113.1 (5)\\ 123.8 (5)\\ 124.5 (6)\\ 119.6 (4)\\ 123.0 (4)\\ 110.9 (4)\\ 110.2 (4)\\ 110.7 (5)\\ 117.9 (4)\\ 123.7 (5)\\ 117.9 (4)\\ 123.7 (5)\\ 117.9 (4)\\ 123.7 (5)\\ 117.9 (4)\\ 112.3 (4)\\ 112.3 (4)\\ 112.3 (4)\\ 112.2 (5)\\ 122.1 (5)\\ 122.1 (5)\\ 122.1 (5)\\ 122.1 (5)\\ 122.1 (4)\\ 129.0 (4)\\ 121.9 (5)\\ 120.1 (4)\\ 120.2 (4)\\ 120.$	$\begin{split} N(10) &= C(11) - C(12) \\ C(11) - C(11) - C(12) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - O(124) \\ C(11) - C(12) - O(13) \\ C(12) - N(13) - C(14) \\ N(13) - C(14) - C(13) \\ O(124) - C(12) - N(13) \\ C(14) - C(14) - C(15) \\ C(144) - C(144) - C(15) \\ C(144) - C(14B) - C(144) \\ C(14C) - C(14B) - C(144) \\ C(14C) - C(14B) - C(14E) \\ C(14) - C(15) - N(16) \\ C(15) - N(16) - C(17) \\ C(15) - N(16) - C(17) \\ N(16) - C(17) - C(18) \\ C(17) - C(18) - N(19) \\ C(17) - C(20) - C(201) \\ C(20) - C(20) - C(201) \\ C(20) - C(20) - C(21) \\ C(20) - C(20) - C(20) \\ C(20) - C(20) - C(20)$	113.6 (4) 108.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 113.7 (4) 123.3 (5) 122.6 (4) 112.0 (4) 112.0 (4) 112.0 (4) 117.5 (5) 111.9 (5) 111.9 (5) 111.9 (5) 111.7 (4) 108.4 (5) 112.1 (4) 112.1 (4) 111.7 (5) 122.4 (5) 119.7 (4) 109.6 (4) 121.8 (5) 122.4 (5) 119.7 (4) 109.6 (4) 121.7 (5) 116.2 (4) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.1 (5) 122.2 (5) 109.1 (5) 113.7 (4) 109.2 (5) 110.9 (6) 113.8 (9) 122.9 (5) 112.9 (5) 122.9 (5) 115.8 (5) 122.0 (5) 115.8 (5) 122.2 (5) 115.8 (5) 122.2 (5) 115.8 (5) 122.2 (5) 115.8 (5) 122.2 (5) 115.8 (5) 122.2 (5) 115.8 (5) 122.2 (5) 115.8 (5) 122.9 (5) 115.8 (5) 125.8 (5)

Table 2 (cont.)

C(8A)—C(8)—C(9)	110.3 (4)	O(C1) - C(C) - C(D)	111.6 (4)
C(8) - C(8A) - C(8B)	115.1 (4)	$C(C) \rightarrow C(D) \rightarrow C(E)$	112.8 (5)
C(8A) - C(8B) - C(8C)	112.1 (5)	C(D) - C(E) - C(F)	111.9 (5)
$C(8A) \rightarrow C(8B) \rightarrow C(8D)$	108.0 (5)	$C(E) \rightarrow C(F) \rightarrow C(G)$	111.7 (5)
C(8C) - C(8B) - C(8D)	111.0 (5)	$C(F) \rightarrow C(G) \rightarrow C(H)$	114.0 (6)
C(8) - C(9) - O(9A)	120.7 (5)	$C(G) \rightarrow C(H) \rightarrow C(I)$	114.4 (8)
C(8) - C(9) - N(10)	116.6 (4)	C(H) - C(I) - C(J)	113.9 (10)



Fig. 2. Stereoview of WLIP (1).

in the calculations but were not refined. Population factors, 0.9 for O(w1) and 0.1 for O(w2), were assigned to the two water molecules during the refinement. The function minimized in the refinement was $\sum w(F_o^2 - F_c^2)^2$, where weights w were $1/\sigma^2(F_o^2)$. Atomic form factors were from Doyle & Turner (1968) and for H atoms, from Stewart, Davidson & Simpson (1965). In the final refinement cycle, with block-matrix least-squares method, all shifts were < 1.54 σ , R = 0.073, S = 5.08. These values are slightly higher than normal because of the strong thermal motion of atoms [C(H), C(I) and C(J)]which are at the end of the β -hydroxydecanoic acid chain. The final difference Fourier peaks were $< 0.39 \text{ e} \text{ Å}^{-3}$. The CRYM system of computer programs was used (Duchamp, 1984). Final atomic coordinates can be found in Table 1.* All bond distances and angles are within the expected ranges (Table 2).

^{*} Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55144 (47 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR0373]

 Table 3. Close intermolecular contacts between non-H

 atoms (Å)

Symmetry operations listed were performed on the first atom.

C(2N)O(W1)	x - 1, y, z	3.441 (7)
N(2R)O(W1)	x - 1, y, z	2.821 (7)
C(5C)O(W2)	x - 1, y, z	3.443 (34)
O(15A)C(8A)	$\frac{1}{2} - x$, $1 - y$, $z - \frac{1}{2}$	3.275 (7)
O(15A)C(8C)	$\frac{1}{2} - x$, $1 - y$, $z - \frac{1}{2}$	3.473 (7)
N(19)O(9A)	$\frac{1}{2} - x$, $1 - y$, $z - \frac{1}{2}$	2.899 (6)
C(20A)O(9A)	$\frac{1}{2} - x$, $1 - y$, $z - \frac{1}{2}$	3.465 (8)
O(6A)C(2G)	$1-x, y-\frac{1}{2}, -z-\frac{1}{2}$	3.362 (7)
O(6A)O(2H)	$1-x, y-\frac{1}{2}, -z-\frac{1}{2}$	2.608 (6)
O(6A)O(2I)	$1-x, y-\frac{1}{2}, -z-\frac{1}{2}$	3.351 (6)
C(2F)O(18A)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3.427 (7)
N(2J)O(18A)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	2.849 (5)
N(2R)C(1A)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3.473 (8)
O(A1)O(17B)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	2.805 (6)
O(A1)O(18A)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3.497 (5)
C(C)O(11B)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3.422 (7)
O(C1)C(2)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3,432 (6)
O(C1)N(2A)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3.302 (5)
O(C1)C(2B)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3.197 (6)
O(C1)O(2C)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	3.094 (5)
O(C1)O(11B)	$x - \frac{1}{2}, \frac{1}{2} - y, -z$	2.824 (5)
	• •	

Table 4. Hydrogen-bond geometry (Å, °)

D	A		D····A	H… <i>A</i>	<i>D</i> —H… <i>A</i>
N(10)	O(2C)	x, y, z	2.842 (5)	1.94	146
N(4)	O(2L)	x, y, z	2.979 (5)	2.39	116
N(16)	O(3A)	x, y, z	2.917 (5)	1.92	168
N(10)	N(7)	x, y, z	2.823 (6)	2.47	99
N(13)	N(10)	x, y, z	2.735 (6)	2.29	105
O(W1)	O(12A)	x, y, z	2.811 (6)	1.79	168
O(W1)	O(15A)	x, y, z	2.791 (6)	1.94	171
N(19)	N(16)	x, y, z	2.804 (6)	2.50	96
N(2R)	O(W1)	x + 1, y, z	2.821 (7)	1.85	162
N(19)	O(9A)	$\frac{1}{2} - x$, $1 - y$, $z + \frac{1}{2}$	2.899 (6)	2.09	134
N(2J)	O(18A)	$x + \frac{1}{2}, \frac{1}{2} - y, -z$	2.849 (5)	1.86	160

Discussion. The crystal structure of WLIP (Figs. 1 and 2) is significantly different from that deduced for a solution in DMSO- d_6 . In a series of conformers generated by distance geometry and molecular dynamics calculations using distance constraints obtained from two-dimensional NMR experiments in DMSO-d₆ (Mortishire-Smith, Nutkins, Packman, Brodey, Rainey, Johnstone & Williams, 1991), residues Ser6 to Ile9 appear to adopt a type II β -turn conformation. Although several hydrogen-bonding interactions are evident in the crystalline conformation, no β -turn is present between Ser6 and Ile9, and an NOE identified between Ser6 α and Ile9 γ is not satisfied by the crystal structure. Amide exchangerate measurements demonstrate that in DMSO, Ile9NH is solvent inaccessible; in the crystal structure, Ile9NH is intramolecularly hydrogen bonded (Tables 3 and 4).

In the crystal structure (Figs. 1 and 2), the *N*terminal blocking group and residues 1 to 3 adopt a β -turn conformation in which the carbonyl group of the fatty acid is hydrogen bonded to Thr3NH. The stereochemistry of the β -turn residues (OHDec-L-Leu-D-Glu-D-*a*-Thr) prevents an unfavorable 1,3 steric interaction between the i + 1CO and the i + 2side chain. Glu2CO forms a hydrogen bond to Ser6NH, and Ser8NH is hydrogen bonded to

Thr3CO across the peptide macrocycle. The stereochemistry of the β -hydroxy acid is shown to be R.

It is noteworthy that the utilization of the sidechain hydroxyl of threonine to form a macrocyclic lactone, while the amine group of this amino acid is used for side-chain attachment, is a feature found in numerous secondary metabolites [*e.g.* virginiamycin S (Vanderhaeghe & Parmentier, 1960), mikamycin B (also known as ostreogryein B3) (Cox, Eastwood, Snell & Todd, 1970), and didemnin (Rinehart *et al.*, 1982)].

Knowledge of the three-dimensional structures of WLIP and tolaasinl (Mortishire-Smith & Williams, 1991) will aid our investigation of the white-line complex by NMR spectroscopy.

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