Experimental

Crystal data

$C_{15}H_{23}N_3O.C_{15}H_{23}N_3O$
$M_r = 522.73$
Triclinic
$P\overline{1}$
$a = 7.957\ (2)$ Å
$b = 9.400\ (2)$ Å
$c = 10.711\ (3)$ Å
$\alpha = 106.514\ (9)°$
$\beta = 98.163\ (9)°$
$\gamma = 104.922\ (8)°$
$V = 721.9\ (3)$ Å^3
$Z = 1$
$D_x = 1.202$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 3837 reflections
$\theta = 2.5$–$30.5°$
$\mu = 0.077$ mm^{-1}
$T = 102$ K
Prism
Colorless
0.42 × 0.28 × 0.25 mm
Crystal source: local laboratory

Data collection

KappaCCD (with Oxford Cryostream) diffractometer

ω scans with κ offsets

Absorption correction: none

18736 measured reflections

4300 independent reflections

3999 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\rm max} = 30.5°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 13$
$l = -15 \rightarrow 15$
intensity decay: <2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.089$
$S = 1.040$
4300 reflections
366 parameters
H atoms treated by a mixture of independent and constrained refinement

w=$1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.0950P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.28$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.22$ e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.012 (5)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
O1	0.69923 (15)	0.93850 (14)	0.42641 (11)	0.0182 (2)
N1	0.33390 (18)	0.77416 (15)	0.41648 (12)	0.0156 (2)
N2	0.10780 (19)	0.72188 (17)	0.52745 (14)	0.0211 (3)
N3	0.18622 (18)	0.51131 (15)	0.41086 (13)	0.0177 (3)
C2	0.2114 (2)	0.66842 (17)	0.44790 (14)	0.0160 (3)
C4	0.3061 (2)	0.30039 (18)	0.28525 (16)	0.0198 (3)
C5	0.4897 (2)	0.33034 (18)	0.24665 (16)	0.0207 (3)
C6	0.7054 (2)	0.59722 (19)	0.24390 (17)	0.0206 (3)
C7	0.6920 (2)	0.74767 (19)	0.21812 (16)	0.0195 (3)
C8	0.5797 (2)	0.83326 (18)	0.30257 (15)	0.0152 (3)
C9	0.8786 (2)	0.8592 (2)	0.2340 (2)	0.0286 (4)
C3A	0.2895 (2)	0.46229 (17)	0.33282 (14)	0.0160 (3)
C5A	0.5184 (2)	0.48056 (18)	0.20807 (15)	0.0173 (3)
C8A	0.4334 (2)	0.71776 (17)	0.33523 (14)	0.0147 (3)
C8B	0.4087 (2)	0.56072 (17)	0.28692 (14)	0.0152 (3)
C1′	0.4921 (2)	0.92293 (18)	0.22702 (15)	0.0176 (3)
C2′	0.3452 (2)	0.8183 (2)	0.10164 (16)	0.0225 (3)
C3′	0.2475 (2)	0.9069 (2)	0.03653 (18)	0.0245 (3)
C4′	0.1018 (3)	0.8003 (3)	−0.0875 (2)	0.0347 (4)
O2	0.26334 (15)	0.05299 (13)	0.53910 (11)	0.0185 (2)
N4	0.80175 (18)	0.48979 (15)	0.56881 (13)	0.0176 (3)
N5	0.8927 (2)	0.27876 (18)	0.47215 (15)	0.0221 (3)
N6	0.64366 (17)	0.22785 (15)	0.55959 (12)	0.0154 (2)
C10	0.7753 (2)	0.33249 (18)	0.53463 (15)	0.0166 (3)
C11	0.5222 (2)	0.28263 (18)	0.61752 (14)	0.0151 (3)
C12	0.3811 (2)	0.17306 (17)	0.65861 (15)	0.0159 (3)
C13	0.2549 (2)	0.25948 (18)	0.72213 (16)	0.0193 (3)
C14	0.3456 (2)	0.43417 (18)	0.80632 (15)	0.0197 (3)
C15	0.4161 (2)	0.51969 (18)	0.71350 (15)	0.0178 (3)
C16	0.5451 (2)	0.68989 (18)	0.77192 (16)	0.0213 (3)
C17	0.6683 (2)	0.70131 (18)	0.67263 (16)	0.0196 (3)
C18	0.6760 (2)	0.53638 (18)	0.62153 (14)	0.0166 (3)
C19	0.5299 (2)	0.43612 (17)	0.64335 (14)	0.0159 (3)
C20	0.1428 (3)	0.1721 (2)	0.7979 (2)	0.0309 (4)
C21	0.4727 (2)	0.09561 (19)	0.74432 (15)	0.0176 (3)
C22	0.6111 (2)	0.20561 (19)	0.87252 (15)	0.0201 (3)

C23	0.7137 (2)	0.1186 (2)	0.93802 (17)	0.0221 (3)
C24	0.8558 (3)	0.2245 (2)	1.0636 (2)	0.0303 (4)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···N6^{i}	0.87 (2)	2.10 (2)	2.8672 (19)	147 (2)
N2—H21N···O2^{i}	0.86 (2)	2.24 (2)	2.998 (2)	147.5 (19)
N2—H22N···N4^{ii}	0.90 (2)	2.10 (2)	3.001 (2)	177.8 (19)
O2—H2O···N1^{iii}	0.89 (2)	1.97 (2)	2.8142 (18)	157 (2)
N5—H51N···O1^{iii}	0.89 (2)	2.27 (3)	3.033 (2)	144 (2)
N5—H52N···N3^{iv}	0.86 (3)	2.19 (3)	3.047 (2)	176 (2)

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

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
O1	0.69923 (15)	0.93850 (14)	0.42641 (11)	0.0182 (2)
N1	0.33390 (18)	0.77416 (15)	0.41648 (12)	0.0156 (2)
N2	0.10780 (19)	0.72188 (17)	0.52745 (14)	0.0211 (3)
N3	0.18622 (18)	0.51131 (15)	0.41086 (13)	0.0177 (3)
C2	0.2114 (2)	0.66842 (17)	0.44790 (14)	0.0160 (3)
C4	0.3061 (2)	0.30039 (18)	0.28525 (16)	0.0198 (3)
C5	0.4897 (2)	0.33034 (18)	0.24665 (16)	0.0207 (3)
C6	0.7054 (2)	0.59722 (19)	0.24390 (17)	0.0206 (3)
C7	0.6920 (2)	0.74767 (19)	0.21812 (16)	0.0195 (3)
C8	0.5797 (2)	0.83326 (18)	0.30257 (15)	0.0152 (3)
C9	0.8786 (2)	0.8592 (2)	0.2340 (2)	0.0286 (4)
C3A	0.2895 (2)	0.46229 (17)	0.33282 (14)	0.0160 (3)
C5A	0.5184 (2)	0.48056 (18)	0.20807 (15)	0.0173 (3)
C8A	0.4334 (2)	0.71776 (17)	0.33523 (14)	0.0147 (3)
C8B	0.4087 (2)	0.56072 (17)	0.28692 (14)	0.0152 (3)
C1′	0.4921 (2)	0.92293 (18)	0.22702 (15)	0.0176 (3)
C2′	0.3452 (2)	0.8183 (2)	0.10164 (16)	0.0225 (3)
C3′	0.2475 (2)	0.9069 (2)	0.03653 (18)	0.0245 (3)
C4′	0.1018 (3)	0.8003 (3)	−0.0875 (2)	0.0347 (4)
O2	0.26334 (15)	0.05299 (13)	0.53910 (11)	0.0185 (2)
N4	0.80175 (18)	0.48979 (15)	0.56881 (13)	0.0176 (3)
N5	0.8927 (2)	0.27876 (18)	0.47215 (15)	0.0221 (3)
N6	0.64366 (17)	0.22785 (15)	0.55959 (12)	0.0154 (2)
C10	0.7753 (2)	0.33249 (18)	0.53463 (15)	0.0166 (3)
C11	0.5222 (2)	0.28263 (18)	0.61752 (14)	0.0151 (3)
C12	0.3811 (2)	0.17306 (17)	0.65861 (15)	0.0159 (3)
C13	0.2549 (2)	0.25948 (18)	0.72213 (16)	0.0193 (3)
C14	0.3456 (2)	0.43417 (18)	0.80632 (15)	0.0197 (3)
C15	0.4161 (2)	0.51969 (18)	0.71350 (15)	0.0178 (3)
C16	0.5451 (2)	0.68989 (18)	0.77192 (16)	0.0213 (3)
C17	0.6683 (2)	0.70131 (18)	0.67263 (16)	0.0196 (3)
C18	0.6760 (2)	0.53638 (18)	0.62153 (14)	0.0166 (3)
C19	0.5299 (2)	0.43612 (17)	0.64335 (14)	0.0159 (3)
C20	0.1428 (3)	0.1721 (2)	0.7979 (2)	0.0309 (4)
C21	0.4727 (2)	0.09561 (19)	0.74432 (15)	0.0176 (3)
C22	0.6111 (2)	0.20561 (19)	0.87252 (15)	0.0201 (3)

C23	0.7137 (2)	0.1186 (2)	0.93802 (17)	0.0221 (3)
C24	0.8558 (3)	0.2245 (2)	1.0636 (2)	0.0303 (4)

Table 4. *Anisotropic displacement parameters* (Å^2)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0160 (5)	0.0168 (5)	0.0188 (5)	0.0026 (4)	0.0040 (4)	0.0038 (4)
N1	0.0171 (6)	0.0131 (6)	0.0158 (5)	0.0025 (5)	0.0055 (5)	0.0050 (4)
N2	0.0227 (7)	0.0141 (6)	0.0276 (7)	0.0027 (5)	0.0139 (6)	0.0072 (5)
N3	0.0187 (6)	0.0150 (6)	0.0181 (6)	0.0029 (5)	0.0042 (5)	0.0056 (5)
C2	0.0169 (7)	0.0144 (7)	0.0153 (6)	0.0027 (5)	0.0040 (5)	0.0048 (5)
C4	0.0227 (8)	0.0129 (7)	0.0222 (7)	0.0046 (6)	0.0034 (6)	0.0053 (5)
C5	0.0223 (7)	0.0157 (7)	0.0236 (7)	0.0066 (6)	0.0027 (6)	0.0066 (6)
C6	0.0197 (7)	0.0184 (7)	0.0260 (7)	0.0085 (6)	0.0082 (6)	0.0075 (6)
C7	0.0206 (7)	0.0195 (7)	0.0218 (7)	0.0081 (6)	0.0103 (6)	0.0079 (6)
C8	0.0162 (7)	0.0130 (7)	0.0160 (6)	0.0023 (5)	0.0058 (5)	0.0054 (5)
C9	0.0258 (8)	0.0253 (9)	0.0407 (10)	0.0094 (7)	0.0198 (8)	0.0129 (7)
C3A	0.0174 (7)	0.0125 (7)	0.0153 (6)	0.0024 (5)	0.0010 (5)	0.0038 (5)
C5A	0.0210 (7)	0.0147 (7)	0.0171 (6)	0.0077 (6)	0.0054 (5)	0.0043 (5)
C8A	0.0157 (7)	0.0147 (7)	0.0131 (6)	0.0036 (5)	0.0029 (5)	0.0051 (5)
C8B	0.0168 (7)	0.0148 (7)	0.0138 (6)	0.0050 (5)	0.0036 (5)	0.0045 (5)
C1′	0.0210 (7)	0.0151 (7)	0.0172 (6)	0.0046 (6)	0.0055 (5)	0.0067 (5)
C2′	0.0287 (8)	0.0186 (8)	0.0181 (7)	0.0076 (6)	0.0022 (6)	0.0044 (6)
C3′	0.0221 (8)	0.0236 (8)	0.0274 (8)	0.0045 (6)	0.0019 (6)	0.0123 (6)
C4′	0.0311 (10)	0.0376 (11)	0.0305 (9)	0.0050 (8)	−0.0032 (8)	0.0145 (8)
O2	0.0180 (5)	0.0139 (5)	0.0197 (5)	0.0025 (4)	0.0038 (4)	0.0022 (4)
N4	0.0201 (6)	0.0136 (6)	0.0186 (6)	0.0026 (5)	0.0054 (5)	0.0066 (5)
N5	0.0215 (7)	0.0155 (7)	0.0310 (7)	0.0034 (5)	0.0131 (6)	0.0092 (5)
N6	0.0160 (6)	0.0140 (6)	0.0159 (5)	0.0033 (5)	0.0046 (5)	0.0055 (4)
C10	0.0166 (7)	0.0164 (7)	0.0163 (6)	0.0038 (6)	0.0030 (5)	0.0063 (5)
C11	0.0159 (7)	0.0139 (7)	0.0134 (6)	0.0028 (5)	0.0026 (5)	0.0037 (5)
C12	0.0173 (7)	0.0137 (7)	0.0164 (6)	0.0035 (6)	0.0056 (5)	0.0052 (5)
C13	0.0196 (7)	0.0166 (7)	0.0225 (7)	0.0053 (6)	0.0093 (6)	0.0062 (6)
C14	0.0254 (8)	0.0161 (7)	0.0191 (7)	0.0077 (6)	0.0085 (6)	0.0055 (5)
C15	0.0213 (7)	0.0144 (7)	0.0176 (6)	0.0059 (6)	0.0041 (5)	0.0050 (5)
C16	0.0268 (8)	0.0133 (7)	0.0224 (7)	0.0057 (6)	0.0065 (6)	0.0040 (5)
C17	0.0228 (7)	0.0135 (7)	0.0205 (7)	0.0035 (6)	0.0031 (6)	0.0055 (5)
C18	0.0195 (7)	0.0137 (7)	0.0151 (6)	0.0031 (6)	0.0015 (5)	0.0056 (5)
C19	0.0181 (7)	0.0146 (7)	0.0134 (6)	0.0042 (5)	0.0029 (5)	0.0036 (5)
C20	0.0337 (10)	0.0233 (9)	0.0428 (10)	0.0096 (7)	0.0250 (8)	0.0131 (8)
C21	0.0207 (7)	0.0151 (7)	0.0185 (6)	0.0044 (5)	0.0071 (5)	0.0076 (5)
C22	0.0251 (8)	0.0180 (7)	0.0174 (7)	0.0067 (6)	0.0047 (6)	0.0064 (5)

C23	0.0192 (7)	0.0221 (8)	0.0265 (8)	0.0066 (6)	0.0053 (6)	0.0102 (6)
C24	0.0256 (9)	0.0347 (10)	0.0297 (9)	0.0094 (7)	0.0016 (7)	0.0118 (7)

Table 5. *Selected geometric parameters (Å, °)*

O1—C8	1.4333 (18)	C2′—H2′1	0.9900
O1—H1O	0.87 (2)	C2′—H2′2	0.9900
N1—C8A	1.3473 (19)	C3′—C4′	1.524 (3)
N1—C2	1.355 (2)	C3′—H3′1	0.9900
N2—C2	1.352 (2)	C3′—H3′2	0.9900
N2—H21N	0.86 (2)	C4′—H4′1	0.9800
N2—H22N	0.90 (2)	C4′—H4′2	0.9800
N3—C3A	1.326 (2)	C4′—H4′3	0.9800
N3—C2	1.368 (2)	O2—C12	1.4435 (18)
C4—C3A	1.508 (2)	O2—H2O	0.89 (2)
C4—C5	1.553 (2)	N4—C18	1.326 (2)
C4—H4A	0.9900	N4—C10	1.369 (2)
C4—H4B	0.9900	N5—C10	1.343 (2)
C5—C5A	1.552 (2)	N5—H51N	0.89 (2)
C5—H5A	0.9900	N5—H52N	0.86 (3)
C5—H5B	0.9900	N6—C11	1.3521 (19)
C6—C5A	1.524 (2)	N6—C10	1.354 (2)
C6—C7	1.542 (2)	C11—C19	1.373 (2)
C6—H6A	0.9900	C11—C12	1.523 (2)
C6—H6B	0.9900	C12—C21	1.539 (2)
C7—C9	1.536 (2)	C12—C13	1.559 (2)
C7—C8	1.565 (2)	C13—C20	1.528 (2)
C7—H7	1.0000	C13—C14	1.547 (2)
C8—C8A	1.528 (2)	C13—H13	1.0000
C8—C1′	1.543 (2)	C14—C15	1.527 (2)
C9—H9A	0.9800	C14—H14A	0.9900
C9—H9B	0.9800	C14—H14B	0.9900
C9—H9C	0.9800	C15—C19	1.492 (2)
C3A—C8B	1.392 (2)	C15—C16	1.552 (2)
C5A—C8B	1.493 (2)	C15—H15	1.0000
C5A—H5A1	1.0000	C16—C17	1.553 (2)
C8A—C8B	1.369 (2)	C16—H16A	0.9900
C1′—C2′	1.533 (2)	C16—H16B	0.9900
C1′—H1′1	0.9900	C17—C18	1.511 (2)
C1′—H1′2	0.9900	C17—H17A	0.9900
C2′—C3′	1.515 (2)	C17—H17B	0.9900

C18—C19	1.390 (2)	C22—H22A	0.9900
C20—H20A	0.9800	C22—H22B	0.9900
C20—H20B	0.9800	C23—C24	1.518 (3)
C20—H20C	0.9800	C23—H23A	0.9900
C21—C22	1.531 (2)	C23—H23B	0.9900
C21—H21A	0.9900	C24—H24A	0.9800
C21—H21B	0.9900	C24—H24B	0.9800
C22—C23	1.528 (2)	C24—H24C	0.9800
C8—O1—H1O	106.1 (16)	C6—C7—H7	106.5
C8A—N1—C2	116.75 (13)	C8—C7—H7	106.5
C2—N2—H21N	117.1 (14)	O1—C8—C8A	107.86 (12)
C2—N2—H22N	118.4 (13)	O1—C8—C1′	110.68 (13)
H21N—N2—H22N	124 (2)	C8A—C8—C1′	108.86 (12)
C3A—N3—C2	114.64 (13)	O1—C8—C7	107.23 (13)
N2—C2—N1	117.86 (14)	C8A—C8—C7	111.25 (12)
N2—C2—N3	116.00 (14)	C1′—C8—C7	110.91 (12)
N1—C2—N3	126.09 (14)	C7—C9—H9A	109.5
C3A—C4—C5	102.66 (13)	C7—C9—H9B	109.5
C3A—C4—H4A	111.2	H9A—C9—H9B	109.5
C5—C4—H4A	111.2	C7—C9—H9C	109.5
C3A—C4—H4B	111.2	H9A—C9—H9C	109.5
C5—C4—H4B	111.2	H9B—C9—H9C	109.5
H4A—C4—H4B	109.1	N3—C3A—C8B	123.06 (14)
C5A—C5—C4	105.69 (12)	N3—C3A—C4	127.60 (14)
C5A—C5—H5A	110.6	C8B—C3A—C4	109.28 (14)
C4—C5—H5A	110.6	C8B—C5A—C6	107.03 (13)
C5A—C5—H5B	110.6	C8B—C5A—C5	101.45 (13)
C4—C5—H5B	110.6	C6—C5A—C5	119.75 (13)
H5A—C5—H5B	108.7	C8B—C5A—H5A1	109.3
C5A—C6—C7	109.15 (13)	C6—C5A—H5A1	109.3
C5A—C6—H6A	109.9	C5—C5A—H5A1	109.3
C7—C6—H6A	109.9	N1—C8A—C8B	120.73 (14)
C5A—C6—H6B	109.9	N1—C8A—C8	118.64 (13)
C7—C6—H6B	109.9	C8B—C8A—C8	120.58 (13)
H6A—C6—H6B	108.3	C8A—C8B—C3A	118.36 (13)
C9—C7—C6	110.78 (14)	C8A—C8B—C5A	127.61 (14)
C9—C7—C8	111.31 (13)	C3A—C8B—C5A	113.05 (13)
C6—C7—C8	114.70 (13)	C2′—C1′—C8	114.42 (13)
C9—C7—H7	106.5	C2′—C1′—H1′1	108.7

C8—C1′—H1′1	108.7	C21—C12—C13	115.96 (13)
C2′—C1′—H1′2	108.7	C20—C13—C14	111.54 (14)
C8—C1′—H1′2	108.7	C20—C13—C12	112.91 (14)
H1′1—C1′—H1′2	107.6	C14—C13—C12	115.30 (13)
C3′—C2′—C1′	113.85 (14)	C20—C13—H13	105.4
C3′—C2′—H2′1	108.8	C14—C13—H13	105.4
C1′—C2′—H2′1	108.8	C12—C13—H13	105.4
C3′—C2′—H2′2	108.8	C15—C14—C13	107.99 (12)
C1′—C2′—H2′2	108.8	C15—C14—H14A	110.1
H2′1—C2′—H2′2	107.7	C13—C14—H14A	110.1
C2′—C3′—C4′	112.83 (16)	C15—C14—H14B	110.1
C2′—C3′—H3′1	109.0	C13—C14—H14B	110.1
C4′—C3′—H3′1	109.0	H14A—C14—H14B	108.4
C2′—C3′—H3′2	109.0	C19—C15—C14	107.56 (12)
C4′—C3′—H3′2	109.0	C19—C15—C16	101.26 (13)
H3′1—C3′—H3′2	107.8	C14—C15—C16	120.46 (13)
C3′—C4′—H4′1	109.5	C19—C15—H15	109.0
C3′—C4′—H4′2	109.5	C14—C15—H15	109.0
H4′1—C4′—H4′2	109.5	C16—C15—H15	109.0
C3′—C4′—H4′3	109.5	C15—C16—C17	104.74 (12)
H4′1—C4′—H4′3	109.5	C15—C16—H16A	110.8
H4′2—C4′—H4′3	109.5	C17—C16—H16A	110.8
C12—O2—H2O	111.7 (15)	C15—C16—H16B	110.8
C18—N4—C10	114.51 (13)	C17—C16—H16B	110.8
C10—N5—H51N	120.3 (15)	H16A—C16—H16B	108.9
C10—N5—H52N	120.6 (15)	C18—C17—C16	102.27 (13)
H51N—N5—H52N	119 (2)	C18—C17—H17A	111.3
C11—N6—C10	116.91 (13)	C16—C17—H17A	111.3
N5—C10—N6	117.65 (14)	C18—C17—H17B	111.3
N5—C10—N4	116.42 (14)	C16—C17—H17B	111.3
N6—C10—N4	125.93 (14)	H17A—C17—H17B	109.2
N6—C11—C19	120.56 (14)	N4—C18—C19	123.57 (14)
N6—C11—C12	118.97 (13)	N4—C18—C17	127.56 (15)
C19—C11—C12	120.42 (13)	C19—C18—C17	108.82 (14)
O2—C12—C11	108.50 (12)	C11—C19—C18	118.07 (14)
O2—C12—C21	108.80 (12)	C11—C19—C15	128.28 (14)
C11—C12—C21	109.40 (12)	C18—C19—C15	112.88 (13)
O2—C12—C13	103.40 (12)	C13—C20—H20A	109.5
C11—C12—C13	110.41 (12)	C13—C20—H20B	109.5

H20A—C20—H20B	109.5	C21—C22—H22B	109.2
C13—C20—H20C	109.5	H22A—C22—H22B	107.9
H20A—C20—H20C	109.5	C24—C23—C22	113.57 (15)
H20B—C20—H20C	109.5	C24—C23—H23A	108.9
C22—C21—C12	116.51 (13)	C22—C23—H23A	108.9
C22—C21—H21A	108.2	C24—C23—H23B	108.9
C12—C21—H21A	108.2	C22—C23—H23B	108.9
C22—C21—H21B	108.2	H23A—C23—H23B	107.7
C12—C21—H21B	108.2	C23—C24—H24A	109.5
H21A—C21—H21B	107.3	C23—C24—H24B	109.5
C23—C22—C21	111.98 (14)	H24A—C24—H24B	109.5
C23—C22—H22A	109.2	C23—C24—H24C	109.5
C21—C22—H22A	109.2	H24A—C24—H24C	109.5
C23—C22—H22B	109.2	H24B—C24—H24C	109.5
C8A—N1—C2—N2	−178.91 (13)	C7—C8—C8A—N1	174.78 (13)
C8A—N1—C2—N3	3.8 (2)	O1—C8—C8A—C8B	−120.14 (14)
C3A—N3—C2—N2	179.95 (14)	C1′—C8—C8A—C8B	119.72 (14)
C3A—N3—C2—N1	−2.7 (2)	C7—C8—C8A—C8B	−2.80 (19)
C3A—C4—C5—C5A	−27.21 (15)	N1—C8A—C8B—C3A	−5.5 (2)
C5A—C6—C7—C9	−172.04 (13)	C8—C8A—C8B—C3A	172.06 (13)
C5A—C6—C7—C8	60.92 (17)	N1—C8A—C8B—C5A	−173.26 (14)
C9—C7—C8—O1	−38.55 (17)	C8—C8A—C8B—C5A	4.3 (2)
C6—C7—C8—O1	88.22 (16)	N3—C3A—C8B—C8A	6.7 (2)
C9—C7—C8—C8A	−156.27 (14)	C4—C3A—C8B—C8A	−170.61 (13)
C6—C7—C8—C8A	−29.50 (18)	N3—C3A—C8B—C5A	176.25 (14)
C9—C7—C8—C1′	82.40 (17)	C4—C3A—C8B—C5A	−1.10 (17)
C6—C7—C8—C1′	−150.83 (14)	C6—C5A—C8B—C8A	26.0 (2)
C2—N3—C3A—C8B	−2.7 (2)	C5—C5A—C8B—C8A	152.30 (15)
C2—N3—C3A—C4	174.12 (14)	C6—C5A—C8B—C3A	−142.30 (13)
C5—C4—C3A—N3	−159.41 (15)	C5—C5A—C8B—C3A	−16.03 (16)
C5—C4—C3A—C8B	17.78 (16)	O1—C8—C1′—C2′	−172.97 (13)
C7—C6—C5A—C8B	−55.33 (16)	C8A—C8—C1′—C2′	−54.59 (16)
C7—C6—C5A—C5	−169.80 (13)	C7—C8—C1′—C2′	68.14 (17)
C4—C5—C5A—C8B	26.21 (15)	C8—C1′—C2′—C3′	174.06 (14)
C4—C5—C5A—C6	143.60 (14)	C1′—C2′—C3′—C4′	−179.78 (15)
C2—N1—C8A—C8B	0.6 (2)	C11—N6—C10—N5	−177.33 (14)
C2—N1—C8A—C8	−177.02 (13)	C11—N6—C10—N4	3.5 (2)
O1—C8—C8A—N1	57.45 (17)	C18—N4—C10—N5	175.40 (13)
C1′—C8—C8A—N1	−62.70 (16)	C18—N4—C10—N6	−5.5 (2)

C10—N6—C11—C19	2.9 (2)	C10—N4—C18—C19	1.1 (2)
C10—N6—C11—C12	−174.80 (13)	C10—N4—C18—C17	178.25 (14)
N6—C11—C12—O2	−66.97 (17)	C16—C17—C18—N4	−156.79 (15)
C19—C11—C12—O2	115.36 (14)	C16—C17—C18—C19	20.70 (16)
N6—C11—C12—C21	51.59 (17)	N6—C11—C19—C18	−6.7 (2)
C19—C11—C12—C21	−126.07 (15)	C12—C11—C19—C18	170.93 (13)
N6—C11—C12—C13	−179.63 (13)	N6—C11—C19—C15	−175.88 (14)
C19—C11—C12—C13	2.71 (19)	C12—C11—C19—C15	1.7 (2)
O2—C12—C13—C20	79.12 (17)	N4—C18—C19—C11	4.7 (2)
C11—C12—C13—C20	−164.99 (14)	C17—C18—C19—C11	−172.93 (13)
C21—C12—C13—C20	−39.86 (19)	N4—C18—C19—C15	175.48 (13)
O2—C12—C13—C14	−151.05 (13)	C17—C18—C19—C15	−2.13 (17)
C11—C12—C13—C14	−35.16 (17)	C14—C15—C19—C11	25.0 (2)
C21—C12—C13—C14	89.97 (17)	C16—C15—C19—C11	152.28 (15)
C20—C13—C14—C15	−166.61 (14)	C14—C15—C19—C18	−144.60 (13)
C12—C13—C14—C15	62.90 (17)	C16—C15—C19—C18	−17.37 (16)
C13—C14—C15—C19	−53.21 (16)	O2—C12—C21—C22	176.83 (13)
C13—C14—C15—C16	−168.27 (14)	C11—C12—C21—C22	58.46 (17)
C19—C15—C16—C17	29.21 (15)	C13—C12—C21—C22	−67.19 (18)
C14—C15—C16—C17	147.50 (14)	C12—C21—C22—C23	−171.19 (14)
C15—C16—C17—C18	−30.78 (15)	C21—C22—C23—C24	178.47 (14)