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2-(4-Bromophenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole

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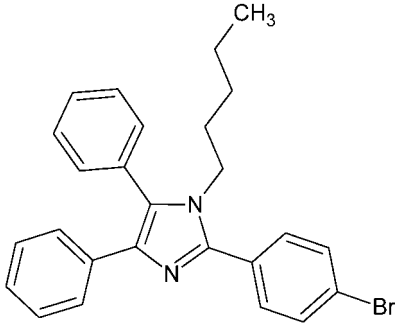
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.007 Å; R factor = 0.066; wR factor = 0.116; data-to-parameter ratio = 16.5.

The title compound, $C_{26}H_{25}BrN_2$, is isomorphous with the chloro derivative [2-(4-chlorophenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole; Mohamed *et al.* (2013). Acta Cryst. E**69**, o846–o847]. The two phenyl rings and the 4-bromophenyl ring are oriented at dihedral angles of 30.1 (2), 64.3 (3) and 42.0 (2)°, respectively, with respect to the imidazole ring. In the crystal, molecules stack in columns along the *b*-axis direction, however, there are no significant intermolecular interactions present.

Related literature

For biological and synthetic applications of imidazole derivatives, see: Maier *et al.* (1989*a*,*b*); Welton (1999); Hermann & Kocher (1997). For related structures, see: Akkurt *et al.* (2013); Mohamed *et al.* (2013); Simpson *et al.* (2013).



Experimental

Crystal data

$C_{26}H_{25}BrN_2$
M_r = 445.39
Monoclinic, $P2_1/n$
a = 10.665 (5) Å
b = 9.619 (5) Å
c = 21.541 (10) Å
β = 91.092 (9)°
V = 2209.4 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.88 mm^{-1}
T = 150 K
0.36 × 0.16 × 0.03 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
T_{min} = 0.600, T_{max} = 0.969
16966 measured reflections
4329 independent reflections
2328 reflections with $I > 2\sigma(I)$
R_{int} = 0.187

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.116
S = 0.88
4329 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −1.05 e Å^{-3}

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2633).

References

Akkurt, M., Mohamed, S. K., Singh, K., Marzouk, A. A. & Abdelhamid, A. A. (2013). *Acta Cryst.* E**69**, o846–o847.
Bruker (2011). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Hermann, W. A. & Kocher, C. (1997). *Angew. Chem. Int. Ed. Engl.* **36**, 2162–2187.
Maier, T., Schmierer, R., Bauer, K., Bieringer, H., Buerstell, H. & Sachse, B. (1989*a*). US Patent 4820335.
Maier, T., Schmierer, R., Bauer, K., Bieringer, H., Buerstell, H. & Sachse, B. (1989*b*). *Chem. Abstr.* **111**, 19494.
Mohamed, S. K., Akkurt, M., Singh, K., Marzouk, A. A. & Abdelhamid, A. A. (2013). *Acta Cryst.* E**69**, o1243.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Simpson, J., Mohamed, S. K., Marzouk, A. A., Talybov, A. H. & Abdelhamid, A. A. (2013). *Acta Cryst.* E**69**, o5–o6.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Welton, T. (1999). *Chem. Rev.* **99**, 2071–2084.

supplementary materials

Acta Cryst. (2013). E**69**, o1417 [doi:10.1107/S1600536813021983]

2-(4-Bromophenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole

Shaaban K. Mohamed, Mehmet Akkurt, Kuldip Singh, Adel A. Marzouk and Mustafa R. Albayati

1. Comment

Many substituted imidazoles exhibit diverse pharmaceutical properties and are known inhibitors of fungicides and herbicides, plant growth regulators and therapeutic agents (Maier *et al.*, 1989*a,b*). Moreover, they are of interest for environmental and green chemistry applications, and have been prepared and used as a large class of ionic liquids and Lewis base catalysts (Welton, 1999; Hermann & Kocher, 1997). As part of our ongoing study of the synthesis (Akkurt *et al.*, 2013; Mohamed *et al.*, 2013; Simpson *et al.*, 2013) and biological applications of tetrasubstituted imidazoles, we herein report on the synthesize and crystal structure of the title compound.

The title compound, Fig. 1, and the chloro derivative, 2-(4-Chlorophenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole, whose crystal structure has been reported by (Mohamed *et al.*, 2013), are isomorphous. In the title compound the phenyl rings (C10–C15 and C16–C21) and the 4-bromophenyl ring (C4–C9) make dihedral angles of 30.1 (2), 64.3 (3) and 42.0 (2)°, respectively, with the imidazole ring (N1/N2/C1–C3). The values of the bond lengths and bond angles fall within the normal range and are comparable with those reported for similar structures (Akkurt *et al.*, 2013; Mohamed *et al.*, 2013; Simpson *et al.*, 2013).

In the crystal, the molecules stack in columns along the b axis direction however, there are no significant intermolecular interactions present (Fig. 2).

2. Experimental

The title compound was synthesized following our previously reported procedure (Mohamed *et al.*, 2013). Colourless plates of the title compound (*M*.p. 396–398 K) were collected with 84% yield. Crystals of sufficient quality for the X-ray diffraction study were obtained by slow evaporation of an ethanol solution of the title compound.

3. Refinement

All H atoms were placed in geometrically idealized positions with C—H = 0.95 - 0.99 Å and refined using a riding model with U_{iso}(H) = 1.5U_{eq}(C-methyl) and = 1.2U_{eq}(C) for other H atoms. The R_{int} value is rather high probably due to the fact that the crystal diffracted weakly beyond 22° in θ.

Computing details

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2011); data reduction: *SAINT* (Bruker, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

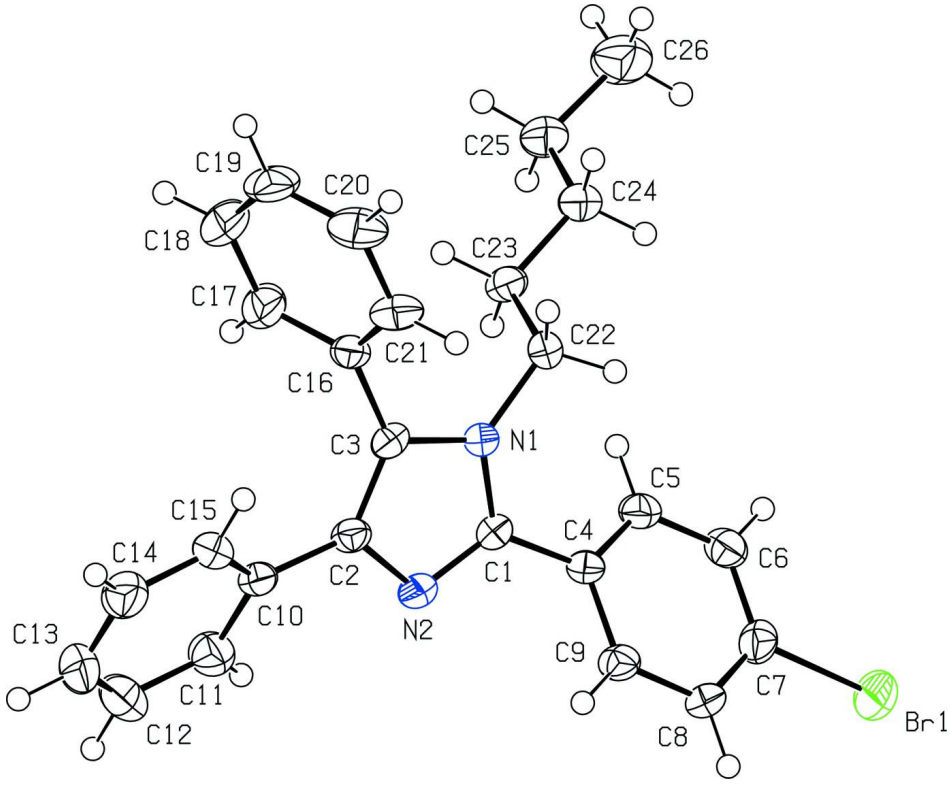

Figure 1

The molecular structure of the title molecule, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

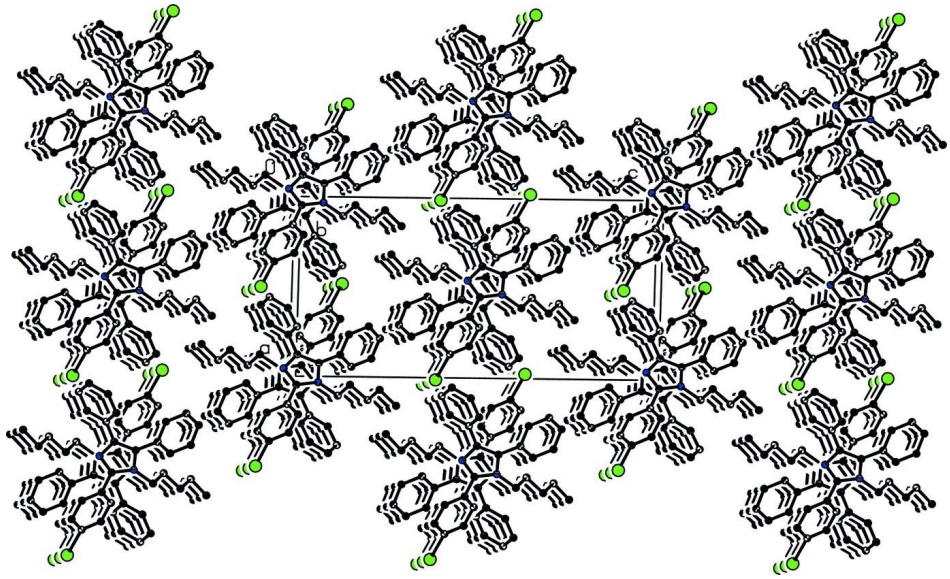

Figure 2

The crystal packing of the title compound, viewed along the *b* axis.

2-(4-Bromophenyl)-1-pentyl-4,5-diphenyl-1*H*-imidazole

Crystal data

$C_{26}H_{25}BrN_2$
$M_r = 445.39$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.665$ (5) Å
$b = 9.619$ (5) Å
$c = 21.541$ (10) Å
$\beta = 91.092$ (9)°
$V = 2209.4$ (19) Å^3
$Z = 4$
$F(000) = 920$
$D_x = 1.339$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 638 reflections
$\theta = 2.3$–$23.5°$
$\mu = 1.88$ mm^{-1}
$T = 150$ K
Plate, colourless
0.36 × 0.16 × 0.03 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and o scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
$T_{min} = 0.600$, $T_{max} = 0.969$
16966 measured reflections
4329 independent reflections
2328 reflections with $I > 2\sigma(I)$
$R_{int} = 0.187$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 11$
$l = -25 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.116$
$S = 0.88$
4329 reflections
263 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -1.05$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.48280 (5)	1.06999 (7)	1.12186 (2)	0.0518 (2)
N1	0.9579 (3)	0.7532 (4)	0.95097 (14)	0.0260 (14)
N2	1.0328 (3)	0.7435 (4)	1.04691 (14)	0.0291 (14)
C1	0.9420 (4)	0.7928 (5)	1.01128 (18)	0.0266 (14)
C2	1.1118 (4)	0.6715 (5)	1.00900 (18)	0.0266 (14)

C3	1.0659 (4)	0.6773 (5)	0.94893 (18)	0.0289 (14)
C4	0.8327 (4)	0.8632 (5)	1.03554 (18)	0.0287 (14)
C5	0.7751 (4)	0.9785 (5)	1.00753 (18)	0.0330 (18)
C6	0.6714 (4)	1.0384 (5)	1.03236 (18)	0.0331 (18)
C7	0.6244 (4)	0.9856 (5)	1.08588 (19)	0.0340 (18)
C8	0.6802 (4)	0.8754 (6)	1.11597 (19)	0.0356 (18)
C9	0.7843 (4)	0.8143 (5)	1.09045 (18)	0.0290 (16)
C10	1.2222 (4)	0.6036 (5)	1.03414 (18)	0.0286 (16)
C11	1.2824 (4)	0.6578 (5)	1.0867 (2)	0.0403 (19)
C12	1.3866 (5)	0.5930 (7)	1.1121 (2)	0.054 (2)
C13	1.4331 (5)	0.4747 (6)	1.0864 (2)	0.053 (2)
C14	1.3738 (4)	0.4185 (6)	1.0344 (2)	0.0462 (19)
C15	1.2697 (4)	0.4841 (5)	1.00872 (19)	0.0344 (18)
C16	1.1136 (4)	0.6206 (5)	0.89021 (18)	0.0287 (16)
C17	1.2266 (4)	0.6687 (6)	0.8681 (2)	0.0426 (19)
C18	1.2736 (5)	0.6162 (6)	0.8134 (2)	0.053 (2)
C19	1.2084 (5)	0.5199 (6)	0.7801 (2)	0.048 (2)
C20	1.0959 (5)	0.4708 (6)	0.80118 (19)	0.047 (2)
C21	1.0490 (5)	0.5224 (5)	0.85652 (18)	0.0366 (16)
C22	0.8836 (4)	0.7999 (5)	0.89621 (18)	0.0304 (16)
C23	0.9433 (4)	0.9208 (5)	0.86564 (18)	0.0313 (14)
C24	0.8586 (4)	0.9869 (5)	0.81709 (19)	0.0360 (18)
C25	0.9148 (4)	1.1120 (6)	0.7870 (2)	0.048 (2)
C26	0.8257 (5)	1.1835 (6)	0.7416 (2)	0.064 (2)
H5	0.80860	1.01570	0.97050	0.0400*
H6	0.63250	1.11590	1.01260	0.0400*
H8	0.64750	0.84160	1.15380	0.0430*
H9	0.82320	0.73770	1.11090	0.0350*
H11	1.25130	0.74020	1.10520	0.0480*
H12	1.42660	0.63130	1.14800	0.0640*
H13	1.50530	0.43110	1.10410	0.0640*
H14	1.40460	0.33530	1.01640	0.0560*
H15	1.23010	0.44580	0.97270	0.0410*
H17	1.27200	0.73790	0.89040	0.0510*
H18	1.35230	0.64800	0.79910	0.0630*
H19	1.24060	0.48620	0.74210	0.0580*
H20	1.05050	0.40230	0.77820	0.0560*
H21	0.97110	0.48900	0.87110	0.0440*
H22A	0.79830	0.82590	0.90930	0.0360*
H22B	0.87570	0.72240	0.86610	0.0360*
H23A	1.02160	0.88990	0.84590	0.0380*
H23B	0.96580	0.99100	0.89750	0.0380*
H24A	0.83830	0.91710	0.78460	0.0430*
H24B	0.77900	1.01430	0.83670	0.0430*
H25A	0.99110	1.08340	0.76480	0.0570*
H25B	0.94060	1.17920	0.81970	0.0570*
H26A	0.79680	1.11660	0.71010	0.0960*
H26B	0.86920	1.26040	0.72130	0.0960*
H26C	0.75340	1.21980	0.76390	0.0960*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0375 (3)	0.0761 (5)	0.0421 (3)	0.0165 (3)	0.0082 (2)	−0.0099 (3)
N1	0.023 (2)	0.035 (3)	0.0199 (19)	0.0012 (18)	0.0009 (16)	0.0006 (17)
N2	0.029 (2)	0.036 (3)	0.0225 (19)	0.0029 (19)	0.0050 (17)	−0.0002 (18)
C1	0.024 (2)	0.032 (3)	0.024 (2)	−0.001 (2)	0.0039 (19)	0.002 (2)
C2	0.030 (2)	0.027 (3)	0.023 (2)	0.002 (2)	0.004 (2)	0.004 (2)
C3	0.027 (2)	0.035 (3)	0.025 (2)	0.001 (2)	0.007 (2)	0.002 (2)
C4	0.027 (2)	0.040 (3)	0.019 (2)	0.000 (2)	0.0001 (19)	−0.002 (2)
C5	0.035 (3)	0.042 (4)	0.022 (2)	0.007 (2)	0.001 (2)	0.000 (2)
C6	0.036 (3)	0.035 (4)	0.028 (2)	0.007 (2)	−0.003 (2)	−0.001 (2)
C7	0.027 (2)	0.044 (4)	0.031 (3)	0.000 (2)	0.002 (2)	−0.014 (2)
C8	0.030 (3)	0.055 (4)	0.022 (2)	0.001 (3)	0.006 (2)	0.001 (2)
C9	0.034 (3)	0.030 (3)	0.023 (2)	0.006 (2)	0.003 (2)	−0.003 (2)
C10	0.028 (2)	0.037 (4)	0.021 (2)	−0.003 (2)	0.0027 (19)	0.000 (2)
C11	0.041 (3)	0.045 (4)	0.035 (3)	0.006 (3)	0.000 (2)	−0.003 (2)
C12	0.046 (3)	0.076 (5)	0.038 (3)	0.012 (3)	−0.011 (2)	−0.001 (3)
C13	0.032 (3)	0.077 (5)	0.051 (3)	0.011 (3)	−0.001 (3)	0.017 (3)
C14	0.042 (3)	0.053 (4)	0.044 (3)	0.012 (3)	0.008 (2)	0.008 (3)
C15	0.032 (3)	0.046 (4)	0.025 (2)	0.004 (2)	−0.002 (2)	0.003 (2)
C16	0.031 (3)	0.034 (3)	0.021 (2)	0.007 (2)	0.0010 (19)	0.003 (2)
C17	0.035 (3)	0.058 (4)	0.035 (3)	0.000 (3)	0.005 (2)	−0.009 (3)
C18	0.044 (3)	0.077 (5)	0.038 (3)	0.006 (3)	0.015 (3)	−0.008 (3)
C19	0.061 (4)	0.061 (5)	0.023 (3)	0.018 (3)	0.011 (3)	−0.002 (3)
C20	0.069 (4)	0.043 (4)	0.028 (3)	0.001 (3)	−0.002 (3)	−0.009 (2)
C21	0.054 (3)	0.031 (3)	0.025 (2)	0.001 (3)	0.006 (2)	0.004 (2)
C22	0.023 (2)	0.042 (4)	0.026 (2)	0.003 (2)	−0.0008 (19)	0.000 (2)
C23	0.032 (2)	0.038 (3)	0.024 (2)	−0.003 (2)	0.0048 (19)	0.001 (2)
C24	0.036 (3)	0.045 (4)	0.027 (2)	0.004 (3)	0.002 (2)	0.004 (2)
C25	0.043 (3)	0.064 (5)	0.037 (3)	0.003 (3)	0.005 (2)	0.020 (3)
C26	0.071 (4)	0.069 (5)	0.052 (3)	0.007 (4)	0.008 (3)	0.023 (3)

Geometric parameters (Å, º)

Br1—C7	1.893 (4)	C23—C24	1.509 (6)
N1—C1	1.368 (5)	C24—C25	1.497 (7)
N1—C3	1.365 (6)	C25—C26	1.516 (7)
N1—C22	1.478 (5)	C5—H5	0.9500
N2—C1	1.313 (5)	C6—H6	0.9500
N2—C2	1.372 (5)	C8—H8	0.9500
C1—C4	1.454 (6)	C9—H9	0.9500
C2—C3	1.376 (6)	C11—H11	0.9500
C2—C10	1.443 (6)	C12—H12	0.9500
C3—C16	1.477 (6)	C13—H13	0.9500
C4—C5	1.399 (6)	C14—H14	0.9500
C4—C9	1.382 (6)	C15—H15	0.9500
C5—C6	1.365 (6)	C17—H17	0.9500
C6—C7	1.364 (6)	C18—H18	0.9500
C7—C8	1.372 (7)	C19—H19	0.9500

C8—C9	1.380 (6)	C20—H20	0.9500
C10—C11	1.392 (6)	C21—H21	0.9500
C10—C15	1.374 (7)	C22—H22A	0.9900
C11—C12	1.378 (7)	C22—H22B	0.9900
C12—C13	1.363 (8)	C23—H23A	0.9900
C13—C14	1.386 (7)	C23—H23B	0.9900
C14—C15	1.383 (6)	C24—H24A	0.9900
C16—C17	1.384 (6)	C24—H24B	0.9900
C16—C21	1.369 (7)	C25—H25A	0.9900
C17—C18	1.385 (7)	C25—H25B	0.9900
C18—C19	1.355 (8)	C26—H26A	0.9800
C19—C20	1.375 (7)	C26—H26B	0.9800
C20—C21	1.393 (6)	C26—H26C	0.9800
C22—C23	1.486 (6)		

C1—N1—C3	107.4 (3)	C4—C9—H9	120.00
C1—N1—C22	126.8 (4)	C8—C9—H9	120.00
C3—N1—C22	125.2 (3)	C10—C11—H11	120.00
C1—N2—C2	106.8 (3)	C12—C11—H11	120.00
N1—C1—N2	110.6 (4)	C11—C12—H12	120.00
N1—C1—C4	125.9 (4)	C13—C12—H12	120.00
N2—C1—C4	123.1 (4)	C12—C13—H13	120.00
N2—C2—C3	109.1 (4)	C14—C13—H13	120.00
N2—C2—C10	120.7 (3)	C13—C14—H14	120.00
C3—C2—C10	130.1 (4)	C15—C14—H14	120.00
N1—C3—C2	106.1 (4)	C10—C15—H15	119.00
N1—C3—C16	122.0 (4)	C14—C15—H15	119.00
C2—C3—C16	131.9 (4)	C16—C17—H17	120.00
C1—C4—C5	124.2 (4)	C18—C17—H17	120.00
C1—C4—C9	117.7 (4)	C17—C18—H18	120.00
C5—C4—C9	118.1 (4)	C19—C18—H18	120.00
C4—C5—C6	121.2 (4)	C18—C19—H19	120.00
C5—C6—C7	119.2 (4)	C20—C19—H19	120.00
Br1—C7—C6	119.7 (3)	C19—C20—H20	120.00
Br1—C7—C8	118.7 (3)	C21—C20—H20	120.00
C6—C7—C8	121.6 (4)	C16—C21—H21	120.00
C7—C8—C9	119.1 (4)	C20—C21—H21	120.00
C4—C9—C8	120.8 (4)	N1—C22—H22A	109.00
C2—C10—C11	119.7 (4)	N1—C22—H22B	109.00
C2—C10—C15	122.2 (4)	C23—C22—H22A	109.00
C11—C10—C15	118.0 (4)	C23—C22—H22B	109.00
C10—C11—C12	120.6 (5)	H22A—C22—H22B	108.00
C11—C12—C13	120.9 (5)	C22—C23—H23A	109.00
C12—C13—C14	119.4 (5)	C22—C23—H23B	109.00
C13—C14—C15	119.7 (5)	C24—C23—H23A	109.00
C10—C15—C14	121.4 (4)	C24—C23—H23B	109.00
C3—C16—C17	119.2 (4)	H23A—C23—H23B	108.00
C3—C16—C21	122.1 (4)	C23—C24—H24A	109.00
C17—C16—C21	118.8 (4)	C23—C24—H24B	109.00

C16—C17—C18	120.2 (5)	C25—C24—H24A	109.00
C17—C18—C19	120.6 (5)	C25—C24—H24B	109.00
C18—C19—C20	120.2 (4)	H24A—C24—H24B	108.00
C19—C20—C21	119.4 (5)	C24—C25—H25A	109.00
C16—C21—C20	120.9 (5)	C24—C25—H25B	109.00
N1—C22—C23	111.3 (3)	C26—C25—H25A	109.00
C22—C23—C24	112.4 (4)	C26—C25—H25B	109.00
C23—C24—C25	113.5 (4)	H25A—C25—H25B	108.00
C24—C25—C26	113.1 (4)	C25—C26—H26A	109.00
C4—C5—H5	119.00	C25—C26—H26B	110.00
C6—C5—H5	119.00	C25—C26—H26C	110.00
C5—C6—H6	120.00	H26A—C26—H26B	109.00
C7—C6—H6	120.00	H26A—C26—H26C	109.00
C7—C8—H8	120.00	H26B—C26—H26C	109.00
C9—C8—H8	120.00		

C3—N1—C1—N2	−1.2 (5)	C1—C4—C5—C6	179.0 (4)
C3—N1—C1—C4	−173.4 (4)	C9—C4—C5—C6	−2.3 (7)
C22—N1—C1—N2	−173.0 (4)	C1—C4—C9—C8	−179.5 (4)
C22—N1—C1—C4	14.9 (7)	C5—C4—C9—C8	1.6 (7)
C1—N1—C3—C2	0.8 (5)	C4—C5—C6—C7	0.8 (7)
C1—N1—C3—C16	−178.5 (4)	C5—C6—C7—Br1	178.7 (3)
C22—N1—C3—C2	172.8 (4)	C5—C6—C7—C8	1.2 (7)
C22—N1—C3—C16	−6.5 (7)	Br1—C7—C8—C9	−179.3 (3)
C1—N1—C22—C23	93.6 (5)	C6—C7—C8—C9	−1.8 (7)
C3—N1—C22—C23	−76.8 (5)	C7—C8—C9—C4	0.3 (7)
C2—N2—C1—N1	1.0 (5)	C2—C10—C11—C12	178.8 (4)
C2—N2—C1—C4	173.5 (4)	C15—C10—C11—C12	0.1 (7)
C1—N2—C2—C3	−0.5 (5)	C2—C10—C15—C14	−178.3 (4)
C1—N2—C2—C10	−179.9 (4)	C11—C10—C15—C14	0.3 (7)
N1—C1—C4—C5	−47.0 (7)	C10—C11—C12—C13	0.1 (8)
N1—C1—C4—C9	134.3 (5)	C11—C12—C13—C14	−0.6 (8)
N2—C1—C4—C5	141.8 (5)	C12—C13—C14—C15	1.0 (7)
N2—C1—C4—C9	−36.9 (7)	C13—C14—C15—C10	−0.9 (7)
N2—C2—C3—N1	−0.2 (5)	C3—C16—C17—C18	179.5 (5)
N2—C2—C3—C16	179.0 (5)	C21—C16—C17—C18	−1.0 (7)
C10—C2—C3—N1	179.1 (5)	C3—C16—C21—C20	179.9 (4)
C10—C2—C3—C16	−1.7 (9)	C17—C16—C21—C20	0.4 (7)
N2—C2—C10—C11	−29.8 (6)	C16—C17—C18—C19	1.6 (8)
N2—C2—C10—C15	148.8 (4)	C17—C18—C19—C20	−1.6 (8)
C3—C2—C10—C11	150.9 (5)	C18—C19—C20—C21	0.9 (8)
C3—C2—C10—C15	−30.5 (8)	C19—C20—C21—C16	−0.3 (8)
N1—C3—C16—C17	115.2 (5)	N1—C22—C23—C24	−169.5 (3)
N1—C3—C16—C21	−64.3 (6)	C22—C23—C24—C25	178.1 (4)
C2—C3—C16—C17	−63.9 (7)	C23—C24—C25—C26	−176.0 (4)
C2—C3—C16—C21	116.6 (6)		