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

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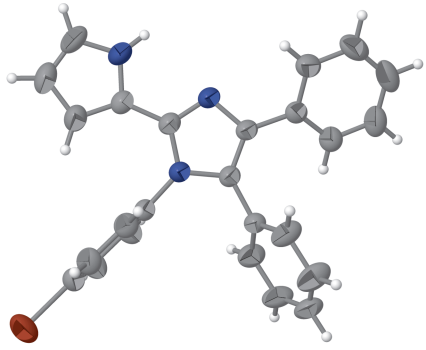
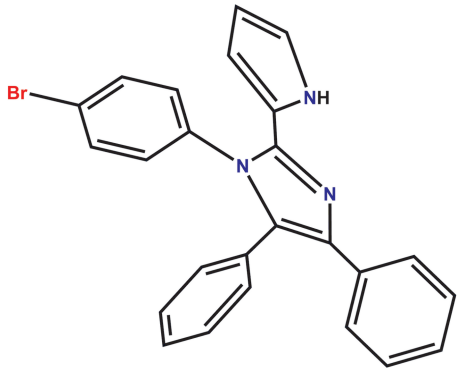
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{25}H_{18}BrN_3$, crystallizes in the triclinic $P\overline{1}$ space group. It is of interest with respect to anticancer activity, antibiotic, antibacterial and antifungal properties. The extended structure features N—H···N, C—H···N, C—H···π, N—H···π, C—H···Br and C—Br···π interactions.

3D view



Chemical scheme



Structure description

Imidazoles are one of the essential building blocks in many natural products and are of importance in the pharmaceutical industry. It is well known that the major constituent of most of the marine sponges contains bromopyrrole-imidazole alkaloids (Forte *et al.*, 2009; Lindel *et al.*, 2017; Zhang *et al.*, 2017). Several metalloenzymes consist of histidine (which contains an imidazole moiety) as one of the amino acids in their protein sequence. In addition, N-substituted imidazoles are vital ingredients in several known pharmacologically active metabolites, namely clotrimazole, ketoconazole, miconazole, oxicanozole (a well-known antibiotic for the treatment of fungal infections), zoledronic acid (used for the treatment of osteoporosis), and nilotinib (an anti-cancer drug) (Yadav *et al.*, 2025). Similarly, several 1,2,4,5-tetra-substituted imidazole-based commercial drugs are available in the form of capravirine (anti-viral drug), losartan (angiotension receptor blocker), olmersatan, and medoximil (anti-hypertensive agent) (Gupta *et al.*, 2004; Narasimhan *et al.*, 2011; Siwach *et al.*, 2021).

Herein, we report the structure of a 1,2,4,5-tetra-substituted imidazole, namely, 1-(4-bromophenyl)-4,5-diphenyl-2-(1*H*-pyrrol-2-yl)-1*H*-imidazole (**1**). To achieve this, many methods of synthesis were demonstrated (Zhang *et al.*, 2016; Hamdi *et al.*, 2024; Parameswari & Jayamoorthy, 2025). Among these, a multicomponent Debus–Radziszewski reaction involving benzil, pyrrole-2-carboxaldehyde, 4-bromoaniline and ammonium acetate (1:1:3:3 ratio) in glacial acetic acid medium under overnight reflux condition afforded the title compound (**1**) as a white solid in very good yield (65–70%).

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N1	0.86	2.52	2.774 (3)	98
C6—H6···N1	0.93	2.61	2.893 (3)	98
C23—H23···N1^{i}	0.93	2.78	3.470 (3)	132
C24—H24···N1^{ii}	0.93	2.98	3.547 (4)	121

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

Compound **1** crystallizes in the triclinic $P\overline{1}$ space group. Its bond parameters are in good agreement with those of previously determined 1,2,4,5-tetra-substituted imidazole derivatives (Gayathri *et al.*, 2010*a*,*b*,*c*,*d*; Xiao *et al.*, 2012; Zhao *et al.*, 2012). Fig. 1 shows the molecular structure of **1** in which the four substituents on the imidazole are depicted as **I** to **IV**. The central imidazole ring is essentially coplanar with the 2-pyrrole ring [dihedral angle = 3.66 (18)]) while it is almost perpendicular to the 4-bromophenyl ring [88.6 (9)°]. The two phenyl rings attached in the 4- and 5-positions of the imidazole ring are not coplanar with it, subtending dihedral angles of 28.7 (9) and 63.3 (9)°, respectively. Intramolecular C—H···N, N—H···N (Table 1) and C—H···π [C2—H2···$\pi_{Ph(II)}$ 3.21Å and 134°] interactions occur.

In the crystal, C—H···N (Table 1), C—H···π [C15—H15···$\pi_{Ph(II)}$ 3.19 Å and 128°; symmetry code: $1-x, 2-y, 1-z$]; C18—H18···$\pi_{pyrrole}$ 3.10 Å and 145°; symmetry code: $1-x, 1-y, -z$; C25—H25···$\pi_{imidazole}$ 2.86 Å and 136°; symmetry code: $1-x, 2-y, 1-z$] and N—H···π [N3—H3A···$\pi_{Ph(III)}$ 3.09 Å and 148°; symmetry code: $1+x, y, z$] interactions are observed. Both intramolecular and intermolecular interactions are shown in (Fig. 2).

It is well established that weak C—H···halogen bonds (Desiraju *et al.*, 2005, 2011; Mazik *et al.*, 2010; Capdevila-Cortada *et al.*, 2015) and weak anion–π interactions (Schottel *et al.*, 2008) play a significant role in crystal engineering and supramolecular chemistry. Herein, the bromine atom participates in various intermolecular interactions *i.e.* C—Br···π interactions (C17—Br···$\pi_{pyrrole}$ 4.26 Å and 122° symmetry code: $1-x, 1-y, -z$) and C—H···Br interactions (C11—H11···Br1 3.64 Å 92°; symmetry code: $x, -1+y, z$; C12—H12···Br1 3.288 Å 133°; symmetry code: $-1+x, y, z$; C21—H21···Br1 3.48 Å and 119°; C22—H22···Br1 3.05 Å 139°; symmetry code: $-x, 1-y, -z$) and eventually leading to the formation of a two-dimensional pillared network type supramolecular architecture (Fig. 3).

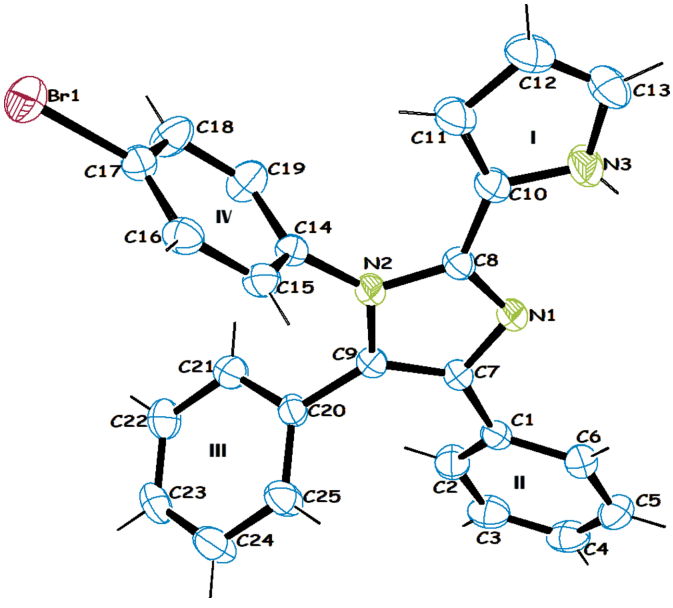

Figure 1
The molecular structure of compound **1** with 50% probability displacement ellipsoids.

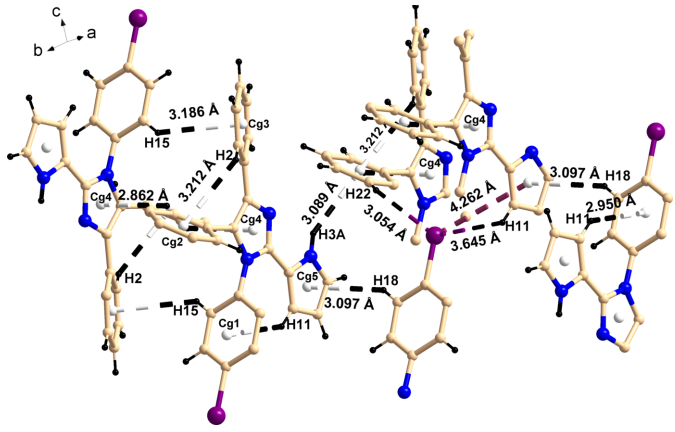

Figure 2
Perspective view of the C—H···π and C—H···Br interactions.

Synthesis and crystallization

A mixture of benzil (1.5324 g 7.28 mmol), 2-pyrrolecarbaldehyde (0.6847 g, 7.2 mmol), 4-bromoaniline (4.9602 g, 28.8 mmol) and ammonium acetate (3.7555 g, 28.8 mmol) was dissolved in 35 ml of glacial acetic acid and the mixture was allowed to reflux overnight. The reaction was monitored by TLC; after completion, the reaction was quenched by pouring the solution in to a crushed ice bath, the obtained white precipitate was filtered and purified by column chromatography using silica gel and hexane and ethylacetate (9:1) as eluents. Yield 65–70%, m.p. 232°C. FT–IR (cm^{-1}) 1010(*s*), 1093(*w*), 1281(*w*), 1489(*w*), 1587(*w*), 3029(*w*), 3204 (*br*).

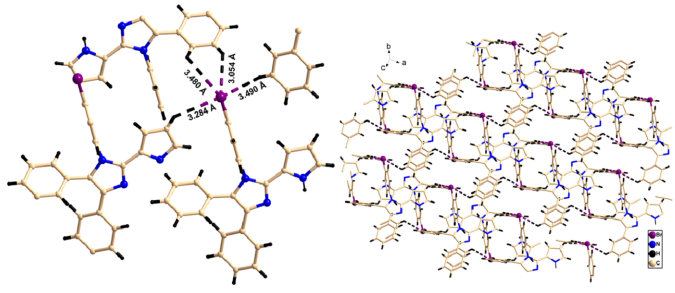

Figure 3
Perspective view of C—H···Br interactions and the supramolecular architecture.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{18}BrN_3$
M_r	440.33
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	300
a, b, c (Å)	9.6044 (9), 9.7662 (7), 12.3705 (11)
α, β, γ (°)	103.837 (3), 92.480 (5), 113.592 (2)
V (Å^3)	1019.82 (15)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.03
Crystal size (mm)	0.29 × 0.20 × 0.17
Data collection	
Diffractometer	Bruker D8 QUEST diffractometer with PHOTON II detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.590, 0.724
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28057, 5046, 3328
R_{int}	0.044
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.111, 1.02
No. of reflections	5046
No. of parameters	262
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.70, −0.67

Computer programs: *APEX4* and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg *et al.*, 2014) and *publCIF* (Westrip, 2010).

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References

Brandenburg, K., Berndt, M. & Putz, H. (2014). *DIAMOND*.Crystal Impact GbR, Bonn, Germany.

Bruker (2012). *APEX4* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Capdevila-Cortada, M. & Novoa, J. J. (2015). *CrystEngComm* **17**, 3354–3365.

Desiraju, G. R. (2005). *Chem. Commun.* pp. 2995.

Desiraju, G. R., Vittal, J. J. & Ramanan, A. (2011). *Crystal Engineering A Textbook*. New Delhi: Cambridge University Press India Pvt Ltd.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Forte, B., Malgesini, B., Piutti, C., Quartieri, F., Scolaro, A. & Papeo, G. (2009). *Marine Drugs* **7**, 705–753.

Gayathri, P., Jayabharathi, J., Saravanan, K., Thiruvalluvar, A. & Butcher, R. J. (2010*b*). *Acta Cryst.* E**66**, o1791.

Gayathri, P., Jayabharathi, J., Srinivasan, N., Thiruvalluvar, A. & Butcher, R. J. (2010*a*). *Acta Cryst.* E**66**, o1703.

Gayathri, P., Thiruvalluvar, A., Saravanan, K., Jayabharathi, J. & Butcher, R. J. (2010*c*). *Acta Cryst.* E**66**, o2219.

Gayathri, P., Thiruvalluvar, A., Srinivasan, N., Jayabharathi, J. & Butcher, R. J. (2010*d*). *Acta Cryst.* E**66**, o2519.

Gupta, P., Hameed, S. & Jain, R. (2004). *Eur. J. Med. Chem.* **39**, 805–814.

Hamdi, A., Daoudi, W., Aaddouz, M., Azzouzi, M., Amhamdi, H., Elyoussfi, A., Aatiaoui, A. E., Verma, D. K., Abboud, M. & Ahari, M. (2024). *Heliyon* **10**, e32153.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Lindel, T. (2017). *Alkaloids* **77**, 117–219.

Mazik, M., Buthe, A. C. & Jones, P. G. (2010). *Tetrahedron* **66**, 385–389.

Narasimhan, B., Sharma, D. & Kumar, P. (2011). *Med. Chem. Res.* **20**, 1119–1140.

Parameswari, M. & Jayamoorthy, K. (2025). *Phosphorus Sulfur Silicon* **200**, 413–430.

Schottel, B. L., Chifotides, H. T. & Dunbar, K. R. (2008). *Chem. Soc. Rev.* **37**, 68–83.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Siwach, A. & Verma, P. K. (2021). *BMC Chem.* **15**, 12.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

Xiao, Y., Yang, L., He, K., Yuan, J. & Mao, P. (2012). *Acta Cryst.* E**68**, o1153.

Yadav, G. & Jain, R. (2025). *Eur. J. Med. Chem.* **290**, 117524–117534.

Zhang, F., Gao, Q., Chen, B., Bai, Y., Sun, W., Lv, D. & Ge, M. (2016). *Phosphorus Sulfur Silicon* **191**, 786–789.

Zhang, H., Dong, M., Chen, J., Wang, H., Tenney, K. & Crews, P. (2017). *Marine Drugs* **15**, 351-380.

Zhao, B., Li, Z., Fan, M., Song, B. & Deng, Q. (2012). *Acta Cryst.* E**68**, o542.

full crystallographic data

IUCrData (2026). **11**, x260107 [https://doi.org/10.1107/S2414314626001070]

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

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Crystal data

$C_{25}H_{18}BrN_3$
M_r = 440.33
Triclinic, $P\overline{1}$
a = 9.6044 (9) Å
b = 9.7662 (7) Å
c = 12.3705 (11) Å
α = 103.837 (3)°
β = 92.480 (5)°
γ = 113.592 (2)°
V = 1019.82 (15) Å^3
Z = 2
$F(000)$ = 448
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9931 reflections
θ = 2.3–23.5°
μ = 2.03 mm^{-1}
T = 300 K
Block, colourless
0.29 × 0.20 × 0.17 mm

Data collection

Bruker D8 QUEST diffractometer with PHOTON II detector
Radiation source: i-mu-s microfocus source
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.590, T_{max} = 0.724
28057 measured reflections
5046 independent reflections
3328 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 28.3°, θ_{min} = 1.7°
h = −12→12
k = −13→13
l = −16→16
4 standard reflections every 19 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 1.02
5046 reflections
262 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.6237P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

Special details

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

Refinement. All the non-hydrogen atoms were refined anisotropically using full-matrix least-square procedures while the hydrogen atoms were included in the idealized position and N—H proton was added from the difference Fourier map. C—H bonds were constrained to 0.95 Å for aromatic C—H (with U_{iso}(H) of 1.2).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.17363 (4)	0.77956 (4)	−0.13312 (3)	0.07507 (15)
N1	0.6881 (2)	0.7667 (2)	0.40296 (17)	0.0435 (5)
N2	0.4941 (2)	0.7513 (2)	0.28907 (16)	0.0424 (5)
N3	0.8849 (3)	0.7915 (3)	0.2437 (2)	0.0631 (7)
H3A	0.919538	0.786406	0.307202	0.076*
C1	0.5738 (3)	0.7303 (3)	0.5743 (2)	0.0424 (5)
C2	0.4476 (3)	0.6416 (3)	0.6162 (2)	0.0542 (7)
H2	0.351403	0.591522	0.571249	0.065*
C3	0.4624 (4)	0.6265 (4)	0.7230 (2)	0.0629 (8)
H3	0.376028	0.567672	0.750074	0.076*
C4	0.6027 (4)	0.6970 (4)	0.7900 (2)	0.0664 (9)
H4	0.612151	0.685934	0.862259	0.080*
C5	0.7299 (4)	0.7845 (4)	0.7499 (2)	0.0689 (9)
H5	0.825907	0.831789	0.794895	0.083*
C6	0.7161 (3)	0.8026 (3)	0.6430 (2)	0.0553 (7)
H6	0.802551	0.863354	0.616948	0.066*
C7	0.5633 (3)	0.7454 (3)	0.45918 (19)	0.0403 (5)
C8	0.6437 (3)	0.7692 (3)	0.3020 (2)	0.0419 (5)
C9	0.4418 (3)	0.7368 (3)	0.39117 (19)	0.0399 (5)
C10	0.7427 (3)	0.7854 (3)	0.2166 (2)	0.0464 (6)
C11	0.7341 (4)	0.7976 (4)	0.1089 (2)	0.0619 (8)
H11	0.650583	0.797226	0.067589	0.074*
C12	0.8737 (4)	0.8109 (4)	0.0719 (3)	0.0693 (9)
H12	0.899548	0.820796	0.001732	0.083*
C13	0.9628 (4)	0.8067 (4)	0.1560 (3)	0.0706 (9)
H13	1.061884	0.813235	0.154215	0.085*
C14	0.4130 (3)	0.7570 (3)	0.19131 (19)	0.0406 (5)
C15	0.4253 (3)	0.8973 (3)	0.1795 (2)	0.0466 (6)
H15	0.481108	0.988158	0.237019	0.056*
C16	0.3550 (3)	0.9038 (3)	0.0824 (2)	0.0501 (6)
H16	0.364313	0.998937	0.073592	0.060*
C17	0.2714 (3)	0.7691 (3)	−0.0007 (2)	0.0478 (6)
C18	0.2563 (4)	0.6277 (3)	0.0102 (2)	0.0623 (8)
H18	0.199101	0.536796	−0.046879	0.075*
C19	0.3278 (4)	0.6230 (3)	0.1077 (2)	0.0596 (7)
H19	0.317994	0.527791	0.116641	0.071*
C20	0.2879 (3)	0.7227 (3)	0.41275 (19)	0.0404 (5)
C21	0.1557 (3)	0.5947 (3)	0.3567 (2)	0.0592 (7)
H21	0.161990	0.516775	0.299562	0.071*
C22	0.0139 (3)	0.5807 (4)	0.3844 (3)	0.0688 (8)
H22	−0.074278	0.493345	0.345820	0.083*
C23	0.0017 (3)	0.6925 (4)	0.4671 (3)	0.0624 (8)
H23	−0.094174	0.681746	0.485665	0.075*
C24	0.1309 (4)	0.8209 (4)	0.5229 (3)	0.0706 (9)
H24	0.123314	0.898620	0.579398	0.085*

C25	0.2730 (3)	0.8356 (3)	0.4957 (3)	0.0594 (7)
H25	0.360480	0.923780	0.534372	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0872 (3)	0.0988 (3)	0.0531 (2)	0.0534 (2)	0.00014 (16)	0.02267 (17)
N1	0.0363 (11)	0.0534 (12)	0.0419 (11)	0.0208 (10)	0.0091 (9)	0.0118 (9)
N2	0.0361 (11)	0.0536 (12)	0.0395 (10)	0.0209 (9)	0.0080 (8)	0.0129 (9)
N3	0.0405 (13)	0.0945 (19)	0.0583 (14)	0.0273 (13)	0.0178 (11)	0.0288 (13)
C1	0.0450 (14)	0.0476 (14)	0.0398 (12)	0.0263 (12)	0.0085 (11)	0.0093 (11)
C2	0.0542 (16)	0.0591 (17)	0.0507 (15)	0.0235 (14)	0.0106 (13)	0.0183 (13)
C3	0.084 (2)	0.0631 (18)	0.0529 (17)	0.0374 (17)	0.0238 (16)	0.0227 (14)
C4	0.105 (3)	0.072 (2)	0.0411 (15)	0.056 (2)	0.0121 (17)	0.0175 (14)
C5	0.076 (2)	0.085 (2)	0.0468 (16)	0.0462 (19)	−0.0089 (15)	0.0020 (15)
C6	0.0500 (16)	0.0701 (18)	0.0473 (15)	0.0307 (14)	0.0055 (12)	0.0099 (13)
C7	0.0353 (13)	0.0457 (14)	0.0398 (12)	0.0184 (11)	0.0071 (10)	0.0092 (10)
C8	0.0380 (13)	0.0442 (13)	0.0435 (13)	0.0176 (11)	0.0101 (11)	0.0114 (11)
C9	0.0372 (13)	0.0433 (13)	0.0388 (12)	0.0174 (11)	0.0077 (10)	0.0100 (10)
C10	0.0437 (14)	0.0490 (15)	0.0480 (14)	0.0199 (12)	0.0135 (11)	0.0147 (11)
C11	0.0630 (18)	0.085 (2)	0.0520 (16)	0.0407 (17)	0.0222 (14)	0.0252 (15)
C12	0.073 (2)	0.082 (2)	0.0587 (18)	0.0331 (18)	0.0336 (17)	0.0251 (16)
C13	0.0494 (18)	0.086 (2)	0.076 (2)	0.0257 (16)	0.0306 (16)	0.0241 (18)
C14	0.0391 (13)	0.0471 (14)	0.0375 (12)	0.0202 (11)	0.0094 (10)	0.0114 (10)
C15	0.0478 (15)	0.0439 (14)	0.0440 (13)	0.0194 (12)	0.0072 (11)	0.0051 (11)
C16	0.0609 (17)	0.0471 (15)	0.0506 (15)	0.0297 (13)	0.0138 (13)	0.0154 (12)
C17	0.0495 (15)	0.0612 (17)	0.0406 (13)	0.0299 (13)	0.0095 (11)	0.0160 (12)
C18	0.078 (2)	0.0446 (16)	0.0490 (16)	0.0191 (14)	−0.0093 (14)	0.0020 (12)
C19	0.075 (2)	0.0434 (15)	0.0551 (16)	0.0234 (14)	−0.0053 (14)	0.0114 (13)
C20	0.0356 (13)	0.0465 (14)	0.0417 (12)	0.0190 (11)	0.0073 (10)	0.0142 (11)
C21	0.0454 (16)	0.0628 (18)	0.0566 (16)	0.0206 (14)	0.0049 (13)	−0.0014 (13)
C22	0.0341 (15)	0.076 (2)	0.078 (2)	0.0147 (14)	0.0019 (14)	0.0055 (17)
C23	0.0400 (16)	0.080 (2)	0.079 (2)	0.0341 (16)	0.0190 (14)	0.0265 (17)
C24	0.0574 (19)	0.0584 (18)	0.094 (2)	0.0293 (16)	0.0272 (17)	0.0063 (17)
C25	0.0427 (15)	0.0496 (16)	0.0750 (19)	0.0157 (13)	0.0168 (14)	0.0037 (14)

Geometric parameters (Å, º)

Br1—C17	1.897 (2)	C11—H11	0.9300
N1—C8	1.312 (3)	C12—C13	1.336 (5)
N1—C7	1.381 (3)	C12—H12	0.9300
N2—C8	1.373 (3)	C13—H13	0.9300
N2—C9	1.397 (3)	C14—C19	1.369 (4)
N2—C14	1.434 (3)	C14—C15	1.371 (3)
N3—C13	1.348 (4)	C15—C16	1.380 (4)
N3—C10	1.366 (3)	C15—H15	0.9300
N3—H3A	0.8600	C16—C17	1.367 (4)
C1—C2	1.385 (4)	C16—H16	0.9300

C1—C6	1.389 (4)	C17—C18	1.370 (4)
C1—C7	1.469 (3)	C18—C19	1.382 (4)
C2—C3	1.372 (4)	C18—H18	0.9300
C2—H2	0.9300	C19—H19	0.9300
C3—C4	1.366 (5)	C20—C25	1.374 (4)
C3—H3	0.9300	C20—C21	1.377 (4)
C4—C5	1.374 (5)	C21—C22	1.380 (4)
C4—H4	0.9300	C21—H21	0.9300
C5—C6	1.383 (4)	C22—C23	1.353 (4)
C5—H5	0.9300	C22—H22	0.9300
C6—H6	0.9300	C23—C24	1.362 (4)
C7—C9	1.370 (3)	C23—H23	0.9300
C8—C10	1.446 (3)	C24—C25	1.379 (4)
C9—C20	1.471 (3)	C24—H24	0.9300
C10—C11	1.368 (4)	C25—H25	0.9300
C11—C12	1.402 (4)		

C8—N1—C7	106.17 (19)	C13—C12—H12	126.2
C8—N2—C9	106.67 (19)	C11—C12—H12	126.2
C8—N2—C14	125.72 (19)	C12—C13—N3	108.6 (3)
C9—N2—C14	127.50 (19)	C12—C13—H13	125.7
C13—N3—C10	109.8 (3)	N3—C13—H13	125.7
C13—N3—H3A	125.1	C19—C14—C15	119.9 (2)
C10—N3—H3A	125.1	C19—C14—N2	120.0 (2)
C2—C1—C6	118.2 (2)	C15—C14—N2	120.1 (2)
C2—C1—C7	122.4 (2)	C14—C15—C16	120.1 (2)
C6—C1—C7	119.3 (2)	C14—C15—H15	120.0
C3—C2—C1	120.9 (3)	C16—C15—H15	120.0
C3—C2—H2	119.6	C17—C16—C15	119.3 (2)
C1—C2—H2	119.6	C17—C16—H16	120.3
C4—C3—C2	120.7 (3)	C15—C16—H16	120.3
C4—C3—H3	119.7	C16—C17—C18	121.4 (2)
C2—C3—H3	119.7	C16—C17—Br1	118.9 (2)
C3—C4—C5	119.4 (3)	C18—C17—Br1	119.7 (2)
C3—C4—H4	120.3	C17—C18—C19	118.7 (2)
C5—C4—H4	120.3	C17—C18—H18	120.7
C4—C5—C6	120.4 (3)	C19—C18—H18	120.7
C4—C5—H5	119.8	C14—C19—C18	120.6 (2)
C6—C5—H5	119.8	C14—C19—H19	119.7
C5—C6—C1	120.3 (3)	C18—C19—H19	119.7
C5—C6—H6	119.9	C25—C20—C21	117.7 (2)
C1—C6—H6	119.9	C25—C20—C9	120.0 (2)
C9—C7—N1	110.3 (2)	C21—C20—C9	122.3 (2)
C9—C7—C1	130.0 (2)	C20—C21—C22	120.7 (3)
N1—C7—C1	119.7 (2)	C20—C21—H21	119.7
N1—C8—N2	111.5 (2)	C22—C21—H21	119.7
N1—C8—C10	122.5 (2)	C23—C22—C21	120.8 (3)
N2—C8—C10	126.0 (2)	C23—C22—H22	119.6

C7—C9—N2	105.3 (2)	C21—C22—H22	119.6
C7—C9—C20	131.4 (2)	C22—C23—C24	119.5 (3)
N2—C9—C20	123.2 (2)	C22—C23—H23	120.2
N3—C10—C11	106.4 (2)	C24—C23—H23	120.2
N3—C10—C8	117.0 (2)	C23—C24—C25	120.0 (3)
C11—C10—C8	136.6 (3)	C23—C24—H24	120.0
C10—C11—C12	107.7 (3)	C25—C24—H24	120.0
C10—C11—H11	126.2	C20—C25—C24	121.3 (3)
C12—C11—H11	126.2	C20—C25—H25	119.3
C13—C12—C11	107.5 (3)	C24—C25—H25	119.3

C6—C1—C2—C3	0.6 (4)	N2—C8—C10—C11	4.6 (5)
C7—C1—C2—C3	178.1 (2)	N3—C10—C11—C12	0.1 (3)
C1—C2—C3—C4	−1.0 (4)	C8—C10—C11—C12	179.9 (3)
C2—C3—C4—C5	0.3 (4)	C10—C11—C12—C13	−0.1 (4)
C3—C4—C5—C6	0.7 (5)	C11—C12—C13—N3	0.0 (4)
C4—C5—C6—C1	−1.1 (4)	C10—N3—C13—C12	0.1 (4)
C2—C1—C6—C5	0.4 (4)	C8—N2—C14—C19	92.0 (3)
C7—C1—C6—C5	−177.2 (2)	C9—N2—C14—C19	−92.4 (3)
C8—N1—C7—C9	−0.7 (3)	C8—N2—C14—C15	−85.6 (3)
C8—N1—C7—C1	177.3 (2)	C9—N2—C14—C15	90.0 (3)
C2—C1—C7—C9	28.5 (4)	C19—C14—C15—C16	−1.6 (4)
C6—C1—C7—C9	−154.0 (3)	N2—C14—C15—C16	176.1 (2)
C2—C1—C7—N1	−149.1 (2)	C14—C15—C16—C17	1.0 (4)
C6—C1—C7—N1	28.4 (3)	C15—C16—C17—C18	−0.2 (4)
C7—N1—C8—N2	0.4 (3)	C15—C16—C17—Br1	179.37 (19)
C7—N1—C8—C10	−178.3 (2)	C16—C17—C18—C19	−0.1 (4)
C9—N2—C8—N1	0.1 (3)	Br1—C17—C18—C19	−179.6 (2)
C14—N2—C8—N1	176.5 (2)	C15—C14—C19—C18	1.3 (4)
C9—N2—C8—C10	178.7 (2)	N2—C14—C19—C18	−176.3 (3)
C14—N2—C8—C10	−4.9 (4)	C17—C18—C19—C14	−0.5 (5)
N1—C7—C9—N2	0.8 (3)	C7—C9—C20—C25	59.9 (4)
C1—C7—C9—N2	−177.0 (2)	N2—C9—C20—C25	−117.1 (3)
N1—C7—C9—C20	−176.5 (2)	C7—C9—C20—C21	−116.3 (3)
C1—C7—C9—C20	5.7 (4)	N2—C9—C20—C21	66.8 (3)
C8—N2—C9—C7	−0.6 (3)	C25—C20—C21—C22	−0.6 (4)
C14—N2—C9—C7	−176.8 (2)	C9—C20—C21—C22	175.6 (3)
C8—N2—C9—C20	177.1 (2)	C20—C21—C22—C23	0.1 (5)
C14—N2—C9—C20	0.8 (4)	C21—C22—C23—C24	0.5 (5)
C13—N3—C10—C11	−0.1 (3)	C22—C23—C24—C25	−0.6 (5)
C13—N3—C10—C8	−179.9 (2)	C21—C20—C25—C24	0.6 (4)
N1—C8—C10—N3	2.7 (4)	C9—C20—C25—C24	−175.7 (3)
N2—C8—C10—N3	−175.7 (2)	C23—C24—C25—C20	0.0 (5)
N1—C8—C10—C11	−177.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1	0.86	2.52	2.774 (3)	98
C6—H6···N1	0.93	2.61	2.893 (3)	98
C23—H23···N1^{i}	0.93	2.78	3.470 (3)	132
C24—H24···N1^{ii}	0.93	2.98	3.547 (4)	121

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