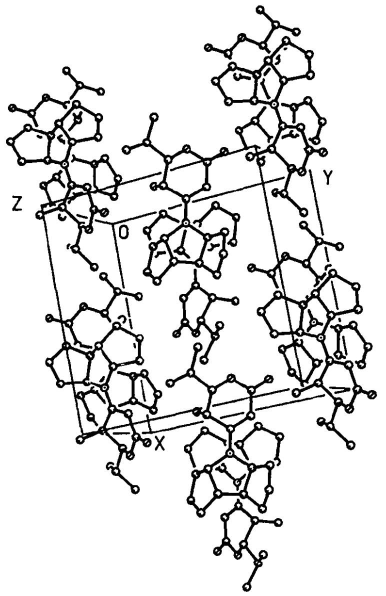

Fig. 2. Molecular packing.

Figures were generated using *SHELXTL-Plus* (Sheldrick, 1987). The positional and equivalent isotropic thermal parameters for the non-H atoms are listed in Table 1, while the bond lengths and angles for the non-H atoms are in Table 2.* The drawing of the molecule with the atomic labeling scheme is shown in Fig. 1, and the packing diagram is in Fig. 2.

Related literature. The tricyclic amine was used for stereochemical control in the formation of the tricyclic aminopyranone where the absolute configuration at the two starred C atoms is controlled by asymmetric induction (Whitesell, Minton & Chen, 1988). Interpretation of these results required knowledge of the absolute stereochemistry at both new chiral centers, determined here by internal correlation with the known configuration of the amine subunit (Lynch, Minton, Whitesell & Davis, 1990). Conformations of similar tricyclic amine compounds are discussed in Chen, Whitesell, Price, Abboud & Davis (1990) and Abboud, Minton, Whitesell & Davis (1990).

Acknowledgement is made to the Donors of the Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research (Grant ACS-PRF AC-20714 to JKW) and to the Robert A. Welch Foundation (Grant F-626 to JKW and F-233 to RED).

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* Lists of structure factors, anisotropic displacement coefficients, H-atom coordinates, bond lengths and angles involving H atoms, torsion angles and a structure determination summary have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52700 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure at 198 K of a Chiral, Tricyclic Aminobiphenyl

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Abstract. (*S*)-(3aα,4aβ,7aβ,7bα)-4-(4-Biphenylyl)-octahydro-1*H*,5*H*-dicyclopenta[*b*,*d*]pyrrole, $C_{22}H_{25}N$, $M_r = 303{\cdot}4$, triclinic, $P1$, $a = 8{\cdot}521$ (2), $b = 8{\cdot}656$ (2), $c = 12{\cdot}002$ (3) Å, $\alpha = 104{\cdot}51$ (2), $\beta = 90{\cdot}18$ (2), $\gamma = 92{\cdot}58$ (2)°, $V = 856{\cdot}1$ (3) Å^3, $Z = 2$ [two independent molecules, (*A*) and (*B*), in the

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asymmetric unit], $D_x = 1{\cdot}177$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}63$ cm^{-1}, $F(000) = 328$, $T = 198$ K, $R = 0{\cdot}0429$ for 2718 reflections [$F_o \geq 6\sigma(F_o)$]. Crystal chirality was assigned to correspond to the known chirality of the parent amine. All five-membered rings in the title compound exhibit similar conformations with slight differences in their puckering. Rings (1), (2) and (3) in each molecule are in envelope conformations [E^4, E^6 and E^7 in (*A*) and $E^{4'}$, $E^{6'}$ and $E^{7'}$ in (*B*)]. A rotational difference is observed in the orientations of the biphenyl groups with respect to the tricyclic amines in the two molecules. The dihedral angle in (*A*) between ring (4) and the plane passing through atoms C(1), C(10) and N is 22·1 (4)° while its counterpart in (*B*) is 12·0 (4)°. Another difference is in the angle between the phenyl rings with a dihedral angle of 35·0 (4)° in (*A*) and 40·9 (5)° in (*B*). The N atom in (*A*) lies at a distance of 0·169 (6) Å from the plane of atoms C(1), C(10) and C(11); in (*B*), N′ lies at a distance of 0·077 (7) Å from the plane of atoms C(1′), C(10′) and C(11′). The independent molecules of this compound pack in a head-to-tail arrangement. A pseudo-inversion center relates the tricyclic amine and the terminal phenyl ring of both molecules, while the inner phenyl rings are nearly perpendicular to each other [dihedral angle 87·7 (5)°], reminiscent of the well known herringbone stacking of aromatics.

Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}(Å^2)
N	−0·0668	0·6982	0·8468	0·040 (1)
C(1)	−0·1899 (5)	0·5707 (6)	0·8212 (4)	0·038 (1)
C(2)	−0·3399 (6)	0·6093 (7)	0·8923 (5)	0·049 (2)
C(3)	−0·4597 (7)	0·6323 (11)	0·8103 (5)	0·102 (3)
C(4)	−0·4196 (6)	0·5579 (9)	0·6960 (5)	0·080 (2)
C(5)	−0·2390 (6)	0·5546 (7)	0·6944 (4)	0·047 (1)
C(6)	−0·1527 (6)	0·6953 (6)	0·6582 (4)	0·044 (1)
C(7)	−0·0729 (6)	0·6444 (7)	0·5403 (4)	0·050 (2)
C(8)	0·0727 (6)	0·5629 (7)	0·5666 (4)	0·050 (2)
C(9)	0·1310 (6)	0·6652 (7)	0·6848 (4)	0·051 (2)
C(10)	−0·0153 (5)	0·7488 (6)	0·7449 (4)	0·037 (1)
C(11)	0·0290 (5)	0·7244 (6)	0·9437 (4)	0·035 (1)
C(12)	0·1632 (5)	0·8281 (6)	0·9575 (4)	0·039 (1)
C(13)	0·2633 (5)	0·8468 (6)	1·0524 (4)	0·039 (1)
C(14)	0·2358 (5)	0·7646 (5)	1·1373 (4)	0·035 (1)
C(15)	0·0985 (5)	0·6679 (6)	1·1257 (4)	0·040 (1)
C(16)	−0·0036 (5)	0·6466 (6)	1·0325 (4)	0·039 (1)
C(17)	0·3512 (5)	0·7735 (5)	1·2316 (4)	0·035 (1)
C(18)	0·5127 (6)	0·7882 (6)	1·2132 (4)	0·040 (1)
C(19)	0·6217 (6)	0·7975 (6)	1·3012 (5)	0·049 (2)
C(20)	0·5722 (7)	0·7909 (6)	1·4099 (5)	0·053 (2)
C(21)	0·4147 (6)	0·7761 (6)	1·4300 (4)	0·054 (2)
C(22)	0·3042 (6)	0·7660 (6)	1·3427 (4)	0·044 (1)
N′	0·5554 (4)	0·2361 (5)	1·0548 (3)	0·041 (1)
C(1′)	0·6764 (5)	0·1239 (6)	1·0601 (4)	0·034 (1)
C(2′)	0·8273 (6)	0·1439 (7)	0·9927 (4)	0·046 (2)
C(3′)	0·9546 (6)	0·2188 (7)	1·0834 (5)	0·054 (2)
C(4′)	0·9078 (5)	0·1574 (7)	1·1871 (5)	0·047 (2)
C(5′)	0·7284 (5)	0·1614 (6)	1·1879 (4)	0·037 (1)
C(6′)	0·6653 (6)	0·3285 (6)	1·2432 (4)	0·038 (1)
C(7′)	0·5955 (6)	0·3442 (7)	1·3618 (4)	0·050 (2)
C(8′)	0·4324 (6)	0·2600 (7)	1·3363 (4)	0·054 (2)
C(9′)	0·3765 (6)	0·3071 (7)	1·2288 (4)	0·048 (1)
C(10′)	0·5258 (5)	0·3460 (6)	1·1659 (4)	0·037 (1)
C(11′)	0·4609 (5)	0·2215 (6)	0·9594 (4)	0·036 (1)
C(12′)	0·3333 (5)	0·3200 (6)	0·9610 (4)	0·039 (1)
C(13′)	0·2330 (6)	0·2969 (6)	0·8671 (4)	0·040 (1)
C(14′)	0·2539 (5)	0·1797 (6)	0·7653 (4)	0·038 (1)
C(15′)	0·3858 (6)	0·0875 (6)	0·7616 (4)	0·039 (1)
C(16′)	0·4862 (6)	0·1066 (6)	0·8559 (4)	0·039 (1)
C(17′)	0·1397 (5)	0·1510 (6)	0·6677 (4)	0·037 (1)
C(18′)	−0·0218 (6)	0·1556 (6)	0·6877 (5)	0·044 (1)
C(19′)	−0·1294 (6)	0·1262 (6)	0·5973 (5)	0·048 (2)
C(20′)	−0·0781 (6)	0·0926 (6)	0·4848 (5)	0·048 (2)
C(21′)	0·0803 (6)	0·0862 (6)	0·4635 (4)	0·050 (2)
C(22′)	0·1886 (6)	0·1158 (6)	0·5536 (4)	0·042 (1)

Experimental. The tricyclic aminobiphenyl (see scheme below for the ring labelling) was prepared by nucleophilic aromatic substitution of 4-fluorobiphenyl with the tricyclic amine and potassium hydride. Crystallization of the racemic mixture from ethanol afforded material as a conglomerate with m.p. 373–374 K. The data crystal had dimensions 0·31 × 0·33 × 0·42 mm. A Nicolet *R3m/V* diffractometer equipped with a graphite monochromator and a Nicolet LT-2 low-temperature delivery system (198 K) was used to collect the data. The lattice parameters were obtained from the least-squares refinement of 50 reflections with $17{\cdot}85 < 2\theta < 22{\cdot}63°$. The data were collected using the ω-scan technique with a 2θ range from 3·0–55·0° and 1·0° ω scan at 3–6° min^{-1} (two hemispheres: $h = -11 \rightarrow 11$, $k = -11 \rightarrow 11$, $l = -15 \rightarrow 15$). Of the 7858 reflections measured, 3930 were unique, with $R_{\text{int}} = 0{\cdot}0162$ from averaging reflections of the two hemispheres (ignoring the minor anomalous-dispersion differences, with no atom heavier than N, and using Mo $K\alpha$ radiation). Four reflections ($0\bar{2}\bar{1}$, $\bar{1}\bar{2}0$, 021, 120) were remeasured every 96 reflections to monitor instrument and crystal stability (maximum correction on *I* was < 1·01%). The data were also corrected for Lp effects and for absorption (numerical corrections based on measurement of indexed crystal faces, $\mu = 0{\cdot}63$ cm^{-1}). Reflections having $F_o < 6\sigma(F_o)$ were considered unobserved (1212 reflections). Minimum and maximum transmission were 0·9735 and 0·9784, respectively. Data reduction and decay correction were performed using the Nicolet XRD *SHELXTL-Plus* software package (Sheldrick, 1987). The struc-

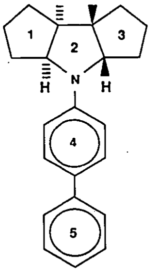

Table 2. *Bond lengths* (Å) *and angles* (°) *of the non*-H *atoms*

N—C(1)	1·462 (4)	N—C(10)	1·460 (5)
N—C(11)	1·384 (4)	C(1)—C(2)	1·541 (7)
C(1)—C(5)	1·548 (7)	C(2)—C(3)	1·469 (9)
C(3)—C(4)	1·412 (8)	C(4)—C(5)	1·541 (7)
C(5)—C(6)	1·549 (8)	C(6)—C(7)	1·542 (7)
C(6)—C(10)	1·540 (6)	C(7)—C(8)	1·524 (8)
C(8)—C(9)	1·539 (7)	C(9)—C(10)	1·557 (7)
C(11)—C(12)	1·404 (6)	C(11)—C(16)	1·419 (7)
C(12)—C(13)	1·392 (7)	C(13)—C(14)	1·396 (7)
C(14)—C(15)	1·394 (6)	C(14)—C(17)	1·482 (6)
C(15)—C(16)	1·385 (7)	C(17)—C(18)	1·400 (7)
C(17)—C(22)	1·409 (7)	C(18)—C(19)	1·389 (7)
C(19)—C(20)	1·387 (8)	C(20)—C(21)	1·370 (8)
C(21)—C(22)	1·390 (7)	N′—C(1′)	1·459 (6)
N′—C(10′)	1·461 (5)	N′—C(11′)	1·375 (6)
C(1′)—C(2′)	1·548 (7)	C(1′)—C(5′)	1·545 (7)
C(2′)—C(3′)	1·536 (7)	C(3′)—C(4′)	1·518 (9)
C(4′)—C(5′)	1·531 (6)	C(5′)—C(6′)	1·554 (7)
C(6′)—C(7′)	1·522 (7)	C(6′)—C(10′)	1·541 (7)
C(7′)—C(8′)	1·533 (7)	C(8′)—C(9′)	1·528 (8)
C(9′)—C(10′)	1·549 (7)	C(11′)—C(12′)	1·409 (7)
C(11′)—C(16′)	1·408 (6)	C(12′)—C(13′)	1·380 (7)
C(13′)—C(14′)	1·396 (6)	C(14′)—C(15′)	1·402 (7)
C(14′)—C(17′)	1·485 (6)	C(15′)—C(16′)	1·388 (7)
C(17′)—C(18′)	1·399 (7)	C(17′)—C(22′)	1·396 (7)
C(18′)—C(19′)	1·384 (7)	C(19′)—C(20′)	1·384 (7)
C(20′)—C(21′)	1·375 (7)	C(21′)—C(22′)	1·387 (7)
C(1)—N—C(10)	113·0 (3)	C(1)—N—C(11)	121·8 (3)
C(10)—N—C(11)	121·0 (3)	N—C(1)—C(2)	114·3 (3)
N—C(1)—C(5)	105·2 (4)	C(2)—C(1)—C(5)	106·1 (4)
C(1)—C(2)—C(3)	105·3 (4)	C(2)—C(3)—C(4)	111·1 (5)
C(3)—C(4)—C(5)	106·3 (4)	C(1)—C(5)—C(4)	104·7 (4)
C(1)—C(5)—C(6)	106·1 (4)	C(4)—C(5)—C(6)	115·5 (5)
C(5)—C(6)—C(7)	113·2 (4)	C(5)—C(6)—C(10)	105·2 (4)
C(7)—C(6)—C(10)	104·4 (4)	C(6)—C(7)—C(8)	103·4 (4)
C(7)—C(8)—C(9)	104·3 (4)	C(8)—C(9)—C(10)	106·2 (4)
N—C(10)—C(6)	104·3 (3)	N—C(10)—C(9)	115·1 (4)
C(6)—C(10)—C(9)	105·9 (4)	N—C(11)—C(12)	121·3 (4)
N—C(11)—C(16)	121·4 (4)	C(12)—C(11)—C(16)	117·3 (4)
C(11)—C(12)—C(13)	120·7 (5)	C(12)—C(13)—C(14)	122·2 (4)
C(13)—C(14)—C(15)	116·7 (4)	C(13)—C(14)—C(17)	121·5 (4)
C(15)—C(14)—C(17)	121·7 (5)	C(14)—C(15)—C(16)	122·6 (5)
C(11)—C(16)—C(15)	120·3 (4)	C(14)—C(17)—C(18)	120·9 (4)
C(14)—C(17)—C(22)	121·9 (4)	C(18)—C(17)—C(22)	117·1 (4)
C(17)—C(18)—C(19)	121·4 (5)	C(18)—C(19)—C(20)	120·3 (5)
C(19)—C(20)—C(21)	119·5 (5)	C(20)—C(21)—C(22)	120·9 (5)
C(17)—C(22)—C(21)	120·8 (5)	C(1′)—N′—C(10′)	113·5 (4)
C(1′)—N′—C(11′)	122·7 (4)	C(10′)—N′—C(11′)	123·0 (4)
N′—C(1′)—C(2′)	115·1 (4)	N′—C(1′)—C(5′)	105·6 (3)
C(2′)—C(1′)—C(5′)	105·6 (4)	C(1′)—C(2′)—C(3′)	106·2 (4)
C(2′)—C(3′)—C(4′)	103·8 (4)	C(3′)—C(4′)—C(5′)	104·0 (4)
C(1′)—C(5′)—C(4′)	105·6 (4)	C(1′)—C(5′)—C(6′)	105·0 (4)
C(4′)—C(5′)—C(6′)	114·1 (4)	C(5′)—C(6′)—C(7′)	114·2 (5)
C(5′)—C(6′)—C(10′)	105·3 (3)	C(7′)—C(6′)—C(10′)	104·8 (4)
C(6′)—C(7′)—C(8′)	103·8 (4)	C(7′)—C(8′)—C(9′)	103·8 (5)
C(8′)—C(9′)—C(10′)	106·7 (4)	N′—C(10′)—C(6′)	104·6 (4)
N′—C(10′)—C(9′)	116·1 (4)	C(6′)—C(10′)—C(9′)	105·7 (4)
N′—C(11′)—C(12′)	121·5 (4)	N′—C(11′)—C(16′)	121·5 (4)
C(12′)—C(11′)—C(16′)	116·9 (4)	C(11′)—C(12′)—C(13′)	120·8 (4)
C(12′)—C(13′)—C(14′)	122·7 (5)	C(13′)—C(14′)—C(15′)	116·4 (4)
C(13′)—C(14′)—C(17′)	121·8 (4)	C(15′)—C(14′)—C(17′)	121·8 (4)
C(14′)—C(15′)—C(16′)	121·8 (4)	C(11′)—C(16′)—C(15′)	121·2 (4)
C(14′)—C(17′)—C(18′)	120·6 (4)	C(14′)—C(17′)—C(22′)	121·7 (4)
C(18′)—C(17′)—C(22′)	117·7 (4)	C(17′)—C(18′)—C(19′)	121·1 (5)
C(18′)—C(19′)—C(20′)	120·1 (5)	C(19′)—C(20′)—C(21′)	119·6 (5)
C(20′)—C(21′)—C(22′)	120·5 (5)	C(17′)—C(22′)—C(21′)	120·9 (5)

ture was solved by direct methods (Sheldrick, 1987) and refined by full-matrix least squares (Sheldrick, 1976). In all, 596 parameters were refined. The non-H atoms were refined with anisotropic thermal parameters. The H-atom positions were obtained from a ΔF map. The H atoms were refined with isotropic thermal parameters except for those bonded to C(3) and C(4) which were calculated in idealized positions and their isotropic thermal parameters fixed. The function $\sum w(|F_o| - |F_c|)^2$ was minimized, where $w = 1/[\sigma(F_o)]^2$ and $\sigma(F_o) = \{0{\cdot}5kI^{-1/2}\,[(\sigma I)^2 + (0{\cdot}02I)^2]^{1/2}\}$. The intensity, I, is given by $(I_{\text{peak}} - I_{\text{background}}) \times$ (scan rate); the factor 0·02 serves to downweight intense reflections and to account for instrument instability and k is the correction due to Lp effects and decay. $\sigma(I)$ was estimated from counting statistics as $\sigma(I) = [(I_{\text{peak}} + I_{\text{background}})^{1/2} \times \text{(scan rate)}]$. The final $R = 0{\cdot}0429$ for 2718 reflections, with $wR = 0{\cdot}0455$ ($R_{\text{all}} = 0{\cdot}0709$, $wR_{\text{all}} = 0{\cdot}0545$) and goodness-of-fit = 1·50. The mini-

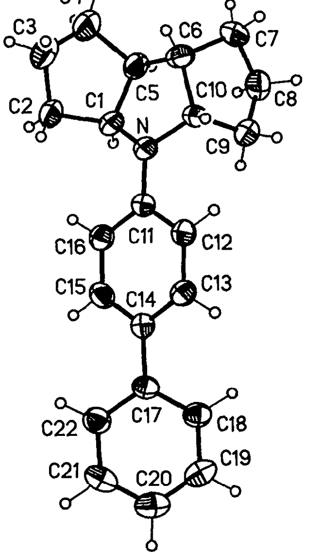

Fig. 1. Molecular structure of (*A*), with 50% probability ellipsoids, showing the atom-numbering scheme.

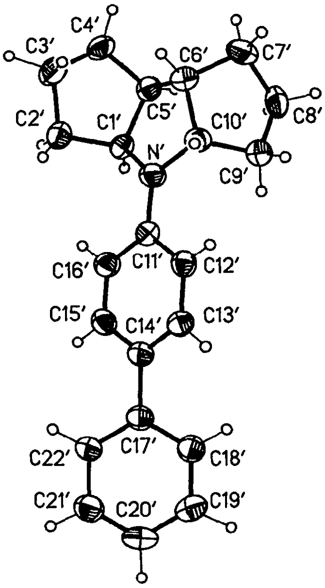

Fig. 2. Molecular structure of (*B*), with 50% probability ellipsoids, showing the atom-numbering scheme.

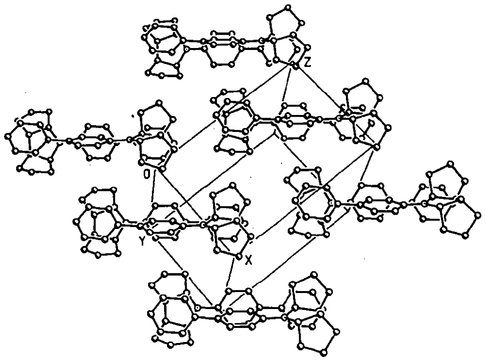

Fig. 3. Molecular packing.

mum and maximum peaks in the final ΔF map were -0.23 and 0.17 e Å^{-3}, respectively, and the maximum $|\Delta/\sigma|$ was 0·024. The scattering factors for the non-H atoms were taken from Cromer & Mann (1968), with the anomalous-dispersion corrections taken from the work of Cromer & Liberman (1970). The scattering factors for the H atoms were obtained from Stewart, Davidson & Simpson (1965). Values used to calculate the linear absorption coefficient are from *International Tables for X-ray Crystallography* (1974). Figures generated using *SHELXTL-Plus* (Sheldrick, 1987). Positional and equivalent isotropic thermal parameters for the non-H atoms are listed in Table 1, while the bond lengths and angles for the non-H atoms are listed in Table 2.* The drawings of molecules (*A*) and (*B*) with the atom-labeling schemes are shown in Figs. 1 and 2, respectively, and the packing diagram is in Fig. 3.

Related literature. The aminobiphenyl substituted with the chiral tricyclic amine (Whitesell, Minton & Chen, 1988) was prepared as a chiral analog of biphenyl as a possible candidate for non-linear optical, second harmonic generation (Chemla & Zyss, 1987). Single-crystal X-ray analysis was undertaken to investigate the influence of the C_2 symmetric amine subunit on crystal packing.

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* Tables of anisotropic thermal parameters, H-atom positional parameters, bond lengths and angles involving H atoms, torsion angles and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52708 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of the Complex of Imidazole and Picric Acid*

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Abstract. $C_6H_2N_3O_7^-.C_3H_5N_2^+$, $M_r = 297.2$, orthorhombic, *Pbca*, $a = 8.944\,(2)$, $b = 13.496\,(5)$, $c = 20.195\,(7)$ Å, $V = 2438\,(1)$ Å^3, $Z = 8$, $D_x = 1.61$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0.133$ mm^{-1}, $F(000) = 1216$, $T = 293$ K, $R = 0.061$ for 1369 observed reflections. The imidazole ring is protonated and makes a dihedral angle of 112·6 (1)° with the six-membered ring of the picric acid. The imidazole ring dimensions are in good agreement

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