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Structures of the Antileprosy Phenazine Derivatives B673 and B741: 3-(*p*-Chloroanilino)-10-(*p*-chlorophenyl)-2-cyclohexylimino-2,10-dihydrophenazine, $C_{30}H_{26}Cl_2N_4$, and 3-(*p*-Chloroanilino)-10-(*p*-chlorophenyl)-2,10-dihydro-2-(4-methylcyclohexylimino)phenazine, $C_{31}H_{28}Cl_2N_4$

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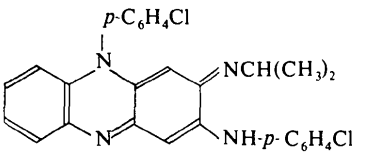
Abstract. B673: $M_r = 513{\cdot}47$, triclinic, $P\bar{1}$, $a = 10{\cdot}992\ (3)$, $b = 12{\cdot}191\ (7)$, $c = 10{\cdot}458\ (6)$ Å, $\alpha = 112{\cdot}13\ (5)$, $\beta = 91{\cdot}57\ (3)$, $\gamma = 88{\cdot}58\ (3)°$, $U = 1298\ (2)$ Å^3, $Z = 2$, $D_m = 1{\cdot}29\ (2)$, $D_x = 1{\cdot}31$ Mg m^{-3}, Mo $K\alpha_1$, $\lambda = 0{\cdot}70926$ Å, $\mu = 0{\cdot}28$ mm^{-1}, $F(000) = 536$, $T = 295$ K, $R = 0{\cdot}068$ for 1861 reflections. B741: $M_r = 527{\cdot}49$, triclinic, $P\bar{1}$, $a = 12{\cdot}161\ (14)$, $b = 12{\cdot}692\ (4)$, $c = 10{\cdot}448\ (7)$ Å, $\alpha = 111{\cdot}60\ (4)$, $\beta = 113{\cdot}52\ (6)$, $\gamma = 91{\cdot}92\ (5)°$, $U = 1344\ (4)$ Å^3, $Z = 2$, $D_m = 1{\cdot}29\ (2)$, $D_x = 1{\cdot}30$ Mg m^{-3}, Mo $K\alpha_1$, $\lambda = 0{\cdot}70926$ Å, $\mu = 0{\cdot}27$ mm^{-1}, $F(000) = 552$, $T = 295$ K, $R = 0{\cdot}042$ for 1784 reflections. The two compounds have substantially similar structures, except that in B673 the imino nitrogen atom N(2) is equatorial to the cyclohexyl group while in B741 it is axial to the 4-methylcyclohexyl group. Consequently, approach to the presumed active sites at N(2) and N(3) is unhindered in B673 but hindered in B741.

Introduction. The substituted iminodihydrophenazine clofazimine (I) and its analogs are of considerable current significance because of their use and/or potential as antileprosy drugs. Indeed, clofazimine has been in use for more than twenty years (Browne & Hogerzeil, 1962) and is still regarded by many workers as the best drug available (Jacobson, 1981). Regrettably, as has been the case for the sulfone dapsone, 4,4′-diaminodiphenyl sulfone, for many years (Pearson, 1981; Guinto, Cellona, Fajardo & de la Cruz, 1981), bacterial resistance to clofazimine has recently emerged (Warndorff-van Diepin, 1982). Consequently, the need for the development of suitable clofazimine analogs is both great and immediate.



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The design of active analogs, however, is hampered by a lack of understanding of the mode of action of clofazimine at the molecular level. Consequently, we have initiated a program of structural investigations of active and inactive clofazimine analogs in the hope of establishing structure–activity relationships for this class of molecules. We here report the structures of two closely related analogs, both of which differ from (I) only in the alkyl substituent at the imino nitrogen atom. In B673, this substituent is cyclohexyl, while in B741 it is 4-methylcyclohexyl. The cyclohexyl compound (B673) is more active than clofazimine *in vitro* and is active *via* the oral route against tuberculosis; the 4-methylcyclohexyl compound (B741) is less active *in vitro* but shows the same activity as B673 against tuberculosis (Conalty, 1982). Neither drug has been tested against *M. leprae* in the mouse foot pad.

Experimental. Compounds donated by Dr M. L. Conalty, Dublin, Ireland. Crystals grown from acetone solutions, D_m by flotation. Data collected on Enraf–Nonius CAD-4 diffractometer, structures solved using *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), other programs from *SDP* package (Enraf–Nonius, 1979). Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Weighting scheme as defined by Corfield, Doedens & Ibers (1967) with $p = 0{\cdot}01$; data for B741 corrected for linear decomposition; other parameters in Table 1.

Discussion. Final atomic coordinates for B673 and B741, with their standard deviations as estimated from the inverse matrix, are listed in Tables 2 and 3, respectively.* Views of single molecules of B673 and B741 are shown in Figs. 1 and 2, respectively. The bond lengths and angles in B673 and B741 are compared in Tables 4 and 5, respectively.

As is apparent in the figures, the principal difference between the two structures is in the orientation of the cyclohexyl ring at N(2). In B673, the cyclohexyl group has the nitrogen atom in the equatorial position as expected, and this causes the cyclohexyl group to be arrayed on the same side of the molecule as the *p*-chlorophenyl group at N(10). Consequently, as is readily seen in Fig. 1, the bulky cyclohexyl group is far removed from N(3) and H(3), and approach to the potential hydrogen-bonding sites at N(2) and N(3)–H(3) is unhindered. In B741, however, the *cis* configuration of the 4-methylcyclohexylimino group

* Lists of observed and calculated structure amplitudes, unrefined hydrogen-atom coordinates, bond lengths and angles in the phenyl rings, and anisotropic thermal parameters for both compounds have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39219 (36 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Experimental parameters for* B673 *and* B741

	B673	B741
Crystal shape and size (mm)	Rectangular plate 1·0 × 0·4 × 0·35	Rectangular plate 0·6 × 0·5 × 0·12
Number and range of reflections used to calculate cell constants	23 reflections $10 < \theta < 16°$	25 reflections $8 < \theta < 16°$
Max. $(\sin\theta/\lambda)$ (Å^{-1})	0·574	0·594
Range of *hkl*	$-12 < h < 12$ $-13 < k < 13$ $0 < l < 11$	$0 < h < 14$ $-15 < k < 15$ $-12 < l < 12$
Standard reflections (variation)	−5 2 −3 (4%) −4 −2 0 (5%) −9 1 0 (7%)	3 −4 4 (7%) 1 4 4 (7%) 6 5 −7 (6%)
Number of unique reflections	4061	4727
Number of unobserved reflections [$I < 3{\cdot}0\sigma(I)$]	1868	1785
Location and refinement of hydrogen atoms	Calculated positions; only H(3) refined	Calculated positions; only H(3) refined
Parameters refined (LS refinement based on *F*)	329	338
R	0·068	0·042
wR	0·063	0·031
S	3·3	1·7
Final Δ/σ	0·11	0·4
Max. height in final difference map (e Å^{-3})	0·2	0·1

Table 2. *Atomic positional and thermal parameters for* B673

$$U_{eq} = (6\pi^2)^{-1}\sum\beta_{ij}\mathbf{a}_i\mathbf{a}_j$$

	x	*y*	*z*	U_{eq}(Å^2)
Cl(18)	1·5116 (2)	0·1691 (2)	−0·3780 (2)	0·112 (1)
Cl(24)	0·7788 (2)	0·4039 (2)	0·9454 (2)	0·105 (1)
N(2)	1·2723 (4)	0·3281 (4)	0·3281 (4)	0·060 (1)
N(3)	1·0775 (4)	0·3436 (4)	0·4644 (4)	0·060 (1)
N(5)	0·8555 (4)	0·1330 (4)	0·0470 (5)	0·059 (1)
N(10)	1·0613 (4)	0·1286 (4)	−0·1088 (4)	0·052 (1)
C(1)	1·1721 (5)	0·2306 (5)	0·1022 (5)	0·054 (2)
C(2)	1·1791 (5)	0·2828 (5)	0·2515 (5)	0·055 (2)
C(3)	1·0634 (5)	0·2846 (5)	0·3242 (5)	0·050 (2)
C(4)	0·9609 (5)	0·2356 (5)	0·2544 (5)	0·053 (2)
C(6)	0·7463 (6)	0·0291 (6)	−0·1611 (6)	0·071 (2)
C(7)	0·7396 (6)	−0·0261 (6)	−0·3012 (6)	0·076 (2)
C(8)	0·8414 (6)	−0·0298 (5)	−0·3791 (6)	0·071 (2)
C(9)	0·9486 (5)	0·0214 (5)	−0·3188 (6)	0·060 (2)
C(11)	0·9544 (5)	0·0769 (5)	−0·1760 (6)	0·053 (2)
C(12)	0·8540 (5)	0·0806 (5)	−0·0963 (6)	0·054 (2)
C(13)	0·9573 (5)	0·1807 (5)	0·1074 (5)	0·048 (2)
C(14)	1·0686 (5)	0·1819 (5)	0·0351 (5)	0·050 (2)
C(15)	1·1677 (5)	0·1357 (5)	−0·1818 (5)	0·048 (2)
C(16)	1·2547 (6)	0·0460 (5)	−0·2124 (6)	0·064 (2)
C(17)	1·3602 (6)	0·0572 (6)	−0·2735 (6)	0·071 (2)
C(18)	1·3765 (5)	0·1499 (5)	−0·3053 (6)	0·062 (2)
C(19)	1·2906 (6)	0·2406 (5)	−0·2765 (6)	0·068 (2)
C(20)	1·1828 (5)	0·2277 (5)	−0·2150 (6)	0·060 (2)
C(21)	0·9989 (5)	0·3558 (5)	0·5730 (5)	0·042 (2)
C(22)	0·9125 (5)	0·2745 (5)	0·5664 (6)	0·058 (2)
C(23)	0·8433 (5)	0·2890 (5)	0·6821 (6)	0·066 (2)
C(24)	0·8634 (5)	0·3885 (5)	0·8011 (5)	0·62 (2)
C(25)	0·9484 (6)	0·4673 (5)	0·8085 (6)	0·064 (2)
C(26)	1·0173 (5)	0·4547 (5)	0·6946 (5)	0·057 (2)
C(27)	1·3893 (5)	0·3208 (6)	0·2600 (6)	0·075 (2)
C(28)	1·4091 (6)	0·4265 (7)	0·2352 (7)	0·109 (2)
C(29)	1·5343 (7)	0·4267 (8)	0·1724 (8)	0·133 (3)
C(30)	1·6335 (6)	0·4121 (8)	0·2635 (7)	0·127 (3)
C(31)	1·6158 (6)	0·3108 (8)	0·2984 (8)	0·138 (3)
C(32)	1·4890 (7)	0·3114 (7)	0·3590 (7)	0·111 (3)
H(3)	1·151 (3)	0·374 (3)	0·484 (4)	0·04 (1)

Table 3. *Atomic positional and thermal parameters for* B741

$$U_{eq} = (6\pi^2)^{-1}\sum\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}(Å^2)
Cl(18)	0·4548 (1)	0·48849 (8)	0·2333 (1)	0·102 (1)
Cl(24)	0·0506 (1)	−0·23636 (9)	0·9642 (1)	0·102 (1)
N(2)	0·2032 (3)	0·2433 (2)	0·6617 (3)	0·062 (1)
N(3)	0·1576 (3)	0·0571 (2)	0·6863 (3)	0·068 (1)
N(5)	0·3275 (2)	−0·1418 (2)	0·3462 (3)	0·056 (1)
N(10)	0·3781 (2)	0·0589 (2)	0·3107 (2)	0·050 (1)
C(1)	0·2923 (3)	0·1584 (3)	0·4828 (3)	0·052 (1)
C(2)	0·2363 (3)	0·1588 (3)	0·5810 (3)	0·053 (1)
C(3)	0·2137 (3)	0·0469 (3)	0·5931 (3)	0·053 (1)
C(4)	0·2436 (3)	−0·0474 (3)	0·5132 (3)	0·056 (1)
C(6)	0·4152 (3)	−0·2414 (3)	0·1789 (3)	0·065 (1)
C(7)	0·4746 (3)	−0·2437 (3)	0·0910 (4)	0·071 (1)
C(8)	0·5032 (3)	−0·1446 (3)	0·0763 (3)	0·064 (1)
C(9)	0·4725 (3)	−0·0436 (3)	0·1472 (3)	0·056 (1)
C(11)	0·4128 (3)	−0·0402 (3)	0·2372 (3)	0·049 (1)
C(12)	0·3837 (3)	−0·1403 (3)	0·2549 (3)	0·050 (1)
C(13)	0·3003 (3)	−0·0473 (3)	0·4179 (3)	0·049 (1)
C(14)	0·3243 (3)	0·0625 (2)	0·4061 (3)	0·046 (1)
C(15)	0·3994 (3)	0·1628 (2)	0·2905 (3)	0·048 (1)
C(16)	0·5060 (3)	0·2446 (3)	0·3912 (3)	0·059 (1)
C(17)	0·5229 (3)	0·3458 (3)	0·3727 (4)	0·068 (1)
C(18)	0·4334 (3)	0·3604 (3)	0·2539 (3)	0·062 (1)
C(19)	0·3279 (3)	0·2785 (3)	0·1516 (3)	0·060 (1)
C(20)	0·3115 (3)	0·1780 (3)	0·1699 (3)	0·055 (1)
C(21)	0·1320 (3)	−0·0208 (3)	0·7426 (3)	0·054 (1)
C(22)	0·2069 (3)	−0·0949 (3)	0·7788 (3)	0·058 (1)
C(23)	0·1824 (3)	−0·1619 (3)	0·8473 (3)	0·063 (1)
C(24)	0·0817 (3)	−0·1546 (3)	0·8758 (3)	0·060 (1)
C(25)	0·0062 (3)	−0·0823 (3)	0·8389 (4)	0·070 (1)
C(26)	0·0307 (3)	−0·0152 (3)	0·7724 (3)	0·062 (1)
C(27)	0·2199 (3)	0·3571 (3)	0·6610 (4)	0·070 (1)
C(28)	0·2381 (4)	0·4485 (3)	0·8137 (4)	0·080 (1)
C(29)	0·1245 (4)	0·4416 (3)	0·8399 (4)	0·085 (1)
C(30)	0·0120 (4)	0·4466 (3)	0·7129 (4)	0·097 (1)
C(31)	−0·0052 (4)	0·3590 (3)	0·5611 (4)	0·100 (2)
C(32)	0·1079 (4)	0·3643 (3)	0·5333 (4)	0·090 (2)
C(33)	−0·1025 (4)	0·4373 (4)	0·7375 (6)	0·150 (2)
H(3)	0·127 (3)	0·115 (2)	0·700 (3)	0·09 (3)

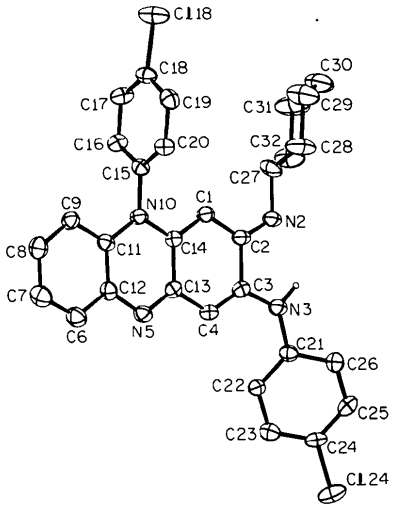

Fig. 1. View of a single molecule of B673 [3-(*p*-chloroanilino)-10-(*p*-chlorophenyl)-2-cyclohexylimino-2,10-dihydrophenazine]. Atom H(3) is shown as a sphere of arbitary size, other hydrogen atoms are omitted. Thermal ellipsoids are drawn at the 25% probability level.

leads to axial–equatorial geometry, the observed conformer having the methyl group equatorial and the imino nitrogen atom axial. This conformer is expected to be lower in energy than the one with axial methyl and equatorial nitrogen (Eliel & Masilamani, 1971) and is, therefore, probably the predominant isomer in solution also. Consequently, as is seen in Fig. 2, the bulky 4-methylcyclohexyl group is on the same side of the molecule as N(3)—H, and approach to N(2) and N(3)—H by a potential hydrogen-bonding moiety (*e.g.* guanosine) is severely restricted in this conformer. The observed difference in activity between B673 and B741 may well be explained by this conformational difference. Presumably, if an isomer of B741 with the *trans*-4-methylcyclohexylimino group were synthesized, its structure would be similar to that of B673 with equatorial–equatorial conformation; this (unknown) isomer would probably be as active as B673 and may prove to be a valuable drug.

The phenazine moieties of both compounds are remarkably planar for dihydrophenazine derivatives. In B673 the central (nitrogen-containing) ring is planar, and in the entire fourteen-atom dihydrophenazine skeleton no atom deviates from the least-squares plane by more than 0·031 (5) Å. In B741 the deviation from planarity is more marked but is still much smaller than in clofazimine itself (Broom, Eggleston & Hodgson, 1984). As expected, the *p*-chlorophenyl ring at N(10) is approximately perpendicular to the phenazine plane in both structures, the dihedral angle C(14)—N(10)—C(15)—C(16) being 91·0 (5) and 87·2 (4)° in B673 and B741, respectively.

The aromatic rings at N(3) are more nearly coplanar with the phenazine rings, the interplanar angles being 31·8 (4) and 38·4 (3)° in B673 and B741, respectively. These values are similar to those of 29·0 to

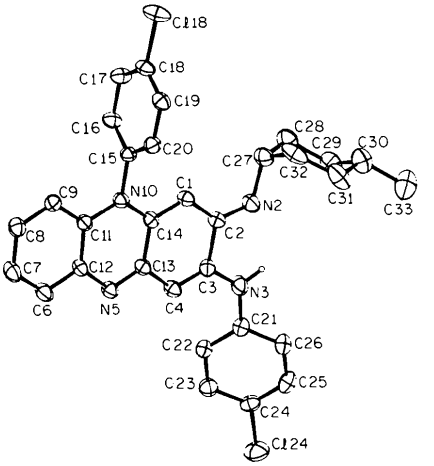

Fig. 2. View of a single molecule of B741 [3-(*p*-chloroanilino)-10-(*p*-chlorophenyl)-2,10-dihydro-2-(4-methylcyclohexylimino)-phenazine], drawn as in Fig. 1.

Table 4. *Bond distances* (Å)

	B673	B741		B673	B741
C(1)–C(2)	1·448 (5)	1·439 (4)	N(10)–C(11)	1·389 (4)	1·390 (3)
C(1)–C(14)	1·347 (4)	1·356 (4)	N(10)–C(14)	1·397 (4)	1·383 (3)
C(2)–C(3)	1·494 (4)	1·497 (4)	N(10)–C(15)	1·436 (4)	1·441 (3)
C(2)–N(2)	1·283 (4)	1·287 (3)	C(11)–C(12)	1·390 (4)	1·402 (4)
C(3)–C(4)	1·349 (4)	1·341 (4)	C(13)–C(14)	1·459 (4)	1·473 (4)
C(3)–N(3)	1·375 (4)	1·369 (4)	C(21)–N(3)	1·407 (4)	1·405 (4)
C(4)–C(13)	1·426 (5)	1·419 (4)	C(27)–N(2)	1·472 (4)	1·455 (4)
N(5)–C(12)	1·390 (4)	1·383 (4)	C(27)–C(28)	1·430 (6)	1·509 (4)
N(5)–C(13)	1·307 (4)	1·294 (3)	C(27)–C(32)	1·519 (6)	1·514 (4)
C(6)–C(12)	1·387 (5)	1·397 (4)	C(28)–C(29)	1·542 (6)	1·518 (5)
C(6)–C(7)	1·364 (5)	1·371 (4)	C(29)–C(30)	1·479 (7)	1·502 (5)
C(7)–C(8)	1·391 (5)	1·372 (4)	C(30)–C(31)	1·433 (7)	1·489 (5)
C(8)–C(9)	1·370 (5)	1·373 (4)	C(31)–C(32)	1·545 (6)	1·519 (5)
C(9)–C(11)	1·389 (5)	1·390 (4)	C(30)–C(33)		1·521 (5)

Table 5. *Bond angles* (°)

	B673	B741
C(2)–C(1)–C(14)	121·3 (4)	122·2 (3)
C(1)–C(2)–C(3)	115·8 (4)	116·4 (3)
N(2)–C(2)–C(1)	127·7 (4)	128·6 (3)
N(2)–C(2)–C(3)	116·5 (4)	114·9 (3)
C(2)–C(3)–C(4)	121·7 (4)	120·2 (3)
N(3)–C(3)–C(2)	111·2 (4)	111·2 (3)
N(3)–C(3)–C(4)	127·2 (4)	128·6 (4)
C(3)–C(4)–C(13)	121·5 (4)	123·3 (4)
C(13)–N(5)–C(12)	117·2 (3)	118·7 (3)
C(12)–C(6)–C(7)	120·4 (4)	121·5 (3)
C(6)–C(7)–C(8)	119·5 (4)	119·4 (5)
C(7)–C(8)–C(9)	121·7 (4)	121·1 (3)
C(8)–C(9)–C(11)	118·2 (4)	120·0 (3)
C(11)–N(10)–C(14)	121·1 (3)	122·0 (3)
C(11)–N(10)–C(15)	122·6 (3)	120·2 (3)
C(14)–N(10)–C(15)	116·3 (3)	117·8 (3)
N(10)–C(11)–C(9)	120·8 (4)	122·8 (3)
N(10)–C(11)–C(12)	118·3 (4)	117·4 (3)
C(9)–C(11)–C(12)	121·0 (4)	119·8 (4)
C(11)–C(12)–C(6)	119·3 (4)	118·2 (3)
C(11)–C(12)–N(5)	123·3 (4)	122·6 (3)
N(5)–C(12)–C(6)	117·4 (4)	119·2 (3)
N(5)–C(13)–C(4)	118·1 (4)	119·3 (3)
N(5)–C(13)–C(14)	124·6 (4)	123·6 (3)
C(4)–C(13)–C(14)	117·3 (4)	117·2 (3)
C(13)–C(14)–C(1)	122·4 (4)	120·7 (3)
C(13)–C(14)–N(10)	115·7 (4)	115·6 (3)
C(1)–C(14)–N(10)	122·0 (4)	123·7 (3)
C(3)–N(3)–C(21)	130·8 (4)	130·3 (4)
C(2)–N(2)–C(27)	117·8 (3)	120·8 (3)
N(2)–C(27)–C(28)	110·6 (4)	109·0 (3)
N(2)–C(27)–C(32)	107·3 (4)	109·7 (3)
C(28)–C(27)–C(32)	107·6 (4)	109·7 (3)
C(27)–C(28)–C(29)	112·7 (4)	112·5 (3)
C(28)–C(29)–C(30)	110·7 (5)	112·9 (4)
C(29)–C(30)–C(31)	111·8 (5)	110·6 (4)
C(30)–C(31)–C(32)	112·5 (5)	113·9 (4)
C(31)–C(32)–C(27)	110·5 (4)	112·1 (3)
C(29)–C(30)–C(33)		113·0 (4)
C(31)–C(30)–C(33)		112·4 (5)

35·9° reported for the related molecules clofazimine and B1912 (Eggleston, Marsh & Hodgson, 1984), the value of 38·4 (3)° in B741 lying slightly outside this range. These values are probably small enough to allow significant π interaction between the phenazine and *p*-chlorophenyl moieties. Necessarily, these relatively small interplanar angles lead to potentially severe H(4)–H(22) interactions, the distances being 2·01 (5) and 2·18 (4) Å in B673 and B741, respectively. The H···H contacts are relieved in part by the relatively large values of the C(3)–N(3)–C(21) angles [130·8 (4) and 130·3 (4)°] and C(4)–C(3)–N(3) angles [127·2 (4) and 128·6 (4)°]. It is noteworthy, also, that in all of the molecules of this type which have been examined the C(3)–N(3) bond is shorter than the N(3)–C(21) bond. In the present molecules these values are 1·375 (4) and 1·407 (4) Å in B673 and 1·369 (4) and 1·405 (4) Å in B741.

There is probably a weak intramolecular N(3)–H(3)···N(2) hydrogen bond in both compounds. The N(3)···N(2) and H(3)···N(2) distances and N(3)–H(3)···N(2) angle are 2·568 (5), 2·04 (3) Å and 117 (2)° (B673) and 2·536 (4), 2·08 (3) Å and 114 (3)° (B741). The existence of such a planar five-membered intramolecular hydrogen bond has been postulated in a variety of other molecules, including the dipeptides α-L-leucyl-L-glutamic acid (Eggleston & Hodgson, 1983) and L-prolyl-L-glutamic acid (Eggleston & Hodgson, 1982); the geometries of all of these postulated interactions are comparable.

The cyclohexyl groups in both structures are in the classical chair conformation. In both compounds the four basal atoms C(28), C(29), C(31), C(32) are coplanar, with no atom deviating from the least-squares plane by more than 1σ. In B673 C(27) sits 0·689 (6) Å above this plane and C(30) is 0·605 (8) Å below it, while in B741 the corresponding distances are 0·650 (4) and 0·614 (5) Å. These values are comparable to those of 0·65 to 0·71 Å in B1912 (Eggleston, Marsh & Hodgson, 1984).

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