N(3)–C(12) and C(12)–C(13) bonds is approximately 'perpendicular' with torsion angles N(2)–N(3)–C(12)–C(13) = 83·0 (4), C(9)–N(3)–C(12)–C(13) = −89·4 (5), N(3)–C(12)–C(13)–C(14) = −99·7 (4) and N(3)–C(12)–C(13)–C(18) = 79·5 (5)°. The C(11) methyl H atoms are staggered relative to the S(10)–C(5) bond.

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N-Cyclohexylbicyclo[3.2.1]octane-3-spiro-3′-succinimide

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Abstract. $C_{17}H_{25}NO_2$, M_r = 275·39, orthorhombic, *Pbca*, a = 24·520 (7), b = 11·795 (2), c = 10·577 (2) Å, V = 3059 (1) Å^3, Z = 8, D_x = 1·196 g cm^{-3}, μ = 0·7226 cm^{-1}, λ = 0·7107 Å. The structure was solved by direct methods and refined to an R value of 0·078 for 1528 observed reflections. The bicyclic system adopts an envelope–boat conformation.

Introduction. The compound was prepared and crystallized by P. Ballesteros and E. De la Cuesta of the Facultad de Farmacia de la Universidad Complutense de Madrid, Spain. The crystal used for data collection was a parallelepiped of dimensions 0·20 × 0·30 × 0·35 mm. Cell parameters and intensities were obtained on a four-circle automatic Nonius CAD-4 diffractometer with the θ–2θ scan method and graphite-monochromatized Mo $K\alpha$ radiation. 3611 reflections were collected up to 2θ = 60°. The intensities were corrected for Lorentz and polarization effects, but not for absorption.

The crystal structure was solved with *MULTAN* 80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). The complete non-H skeleton was found and the refinement of these atoms with isotropic temperature factors by the least-squares full-matrix methods gave $R = \sum ||F_o| - |F_c|| / \sum |F_o| = 0·130$. H atoms were located from a difference map. The final refinement (R = 0·078) was based on 1528 observed reflections having $I > 2\sigma(I)$ and included isotropic and anisotropic thermal parameters for the H and non-H atoms respectively. The weights were calculated (Martínez-Ripoll & Cano, 1975) as $W = K/\sigma^2$, $\sigma = a + b|F_o|$ and K = 0·575 (a = 6·111, b = −5·380 when $|F_o|$ = 0·30–0·84; a = 1·526, b = 0·149 when $|F_o|$ = 0·85–5·89; a = 4·284, b = 0·264 when $|F_o|$ > 5·89). No trends in sin θ/λ were observed.

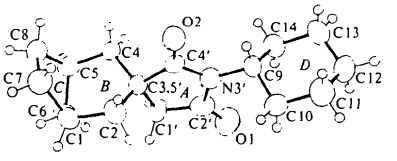

Fig. 1. Perspective view and labelling of the molecule with H atoms.

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Scattering factors were obtained from *International Tables for X-ray Crystallography* (1974). Computations were carried out with programs of the XRAY 70 system (Stewart, Kundell & Baldwin, 1970) and *PLALIN* (Nardelli, 1980).

Discussion. Atomic coordinates are given in Table 1.* Fig. 1 shows the molecule with the labelling of the atoms. Table 2 shows the bond lengths and angles; torsion angles are given in Table 3.

The molecule contains a cyclohexane ring and a five-membered ring joined by a common C—C—C bridge, and a succinimide group substituted at the spiranic C(3,5′) which has a cyclohexane ring substituted at the N atom. The cyclohexane ring of the

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36824 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates and isotropic thermal parameters (for non-*H *atoms* $\times 10^3$, *for* H $\times 10^2$)

$U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j$.

$U = \exp[-8\pi^2 U(\sin\theta/\lambda)^2]$.

	x	*y*	*z*	U_{eq}/U (Å^2)
C(1)	0·3615 (2)	0·0313 (5)	0·4776 (5)	46 (2)
C(2)	0·3053 (2)	0·0227 (5)	0·5424 (5)	43 (2)
C(3,5′)	0·2676 (2)	0·1257 (4)	0·5157 (4)	40 (2)
C(4)	0·2995 (3)	0·2383 (5)	0·5245 (7)	53 (2)
C(5)	0·3587 (2)	0·2304 (5)	0·4781 (6)	49 (2)
C(6)	0·3637 (2)	0·1309 (5)	0·3852 (5)	47 (2)
C(7)	0·4056 (2)	0·0655 (6)	0·5734 (7)	53 (2)
C(8)	0·3985 (3)	0·1955 (6)	0·5863 (7)	59 (2)
C(9)	0·1193 (2)	0·1347 (5)	0·6238 (4)	45 (2)
C(10)	0·0897 (2)	0·2432 (5)	0·5894 (6)	53 (2)
C(11)	0·0361 (3)	0·2513 (7)	0·6623 (7)	66 (3)
C(12)	0·0011 (3)	0·1480 (6)	0·6437 (7)	66 (3)
C(13)	0·0314 (3)	0·0409 (7)	0·6807 (8)	66 (3)
C(14)	0·0844 (3)	0·0303 (5)	0·6051 (7)	55 (2)
C(1′)	0·2356 (2)	0·1140 (7)	0·3901 (5)	54 (2)
C(2′)	0·1763 (2)	0·1157 (5)	0·4228 (5)	54 (2)
N(3′)	0·1717 (2)	0·1250 (4)	0·5544 (4)	46 (1)
C(4′)	0·2222 (2)	0·1284 (5)	0·6134 (4)	41 (2)
O(1)	0·1382 (2)	0·1107 (5)	0·3512 (4)	80 (2)
O(2)	0·2275 (2)	0·1329 (4)	0·7267 (3)	59 (1)
H(11)	0·371 (2)	0·038 (6)	0·434 (6)	1 (2)
H(21)	0·314 (3)	0·024 (6)	0·638 (7)	3 (2)
H(22)	0·286 (3)	−0·047 (6)	0·521 (6)	2 (2)
H(41)	0·298 (2)	0·263 (6)	0·612 (7)	2 (2)
H(42)	0·281 (3)	0·294 (6)	0·481 (7)	3 (2)
H(51)	0·372 (3)	0·304 (6)	0·452 (6)	4 (2)
H(61)	0·335 (3)	0·130 (6)	0·316 (6)	4 (2)
H(62)	0·400 (3)	0·139 (5)	0·348 (6)	−2 (2)
H(71)	0·442 (3)	0·059 (5)	0·545 (6)	1 (2)
H(72)	0·395 (3)	0·032 (6)	0·653 (7)	3 (2)
H(81)	0·380 (3)	0·220 (5)	0·671 (7)	7 (2)
H(82)	0·435 (3)	0·230 (6)	0·577 (6)	4 (2)
H(91)	0·132 (2)	0·139 (5)	0·711 (6)	3 (2)
H(101)	0·080 (2)	0·245 (5)	0·498 (6)	3 (2)
H(102)	0·117 (2)	0·308 (5)	0·607 (6)	3 (2)
H(111)	0·019 (3)	0·318 (6)	0·641 (7)	3 (2)
H(112)	0·048 (3)	0·268 (6)	0·753 (7)	5 (2)
H(121)	−0·011 (3)	0·147 (6)	0·553 (7)	3 (2)
H(122)	−0·034 (3)	0·147 (5)	0·691 (6)	5 (2)
H(131)	0·011 (3)	−0·024 (6)	0·667 (6)	6 (2)
H(132)	0·041 (3)	0·047 (6)	0·772 (7)	2 (2)
H(141)	0·106 (3)	−0·035 (6)	0·626 (6)	−2 (2)
H(142)	0·075 (3)	0·018 (5)	0·511 (7)	5 (2)
H(1′1)	0·244 (3)	0·043 (6)	0·345 (6)	3 (2)
H(2′1)	0·243 (3)	0·173 (6)	0·339 (7)	6 (2)

Table 2. *Bond distances* (Å) *and angles* (°)

C(1)–C(2)	1·543 (8)	C(1)–H(11)	0·97 (7)
C(1)–C(6)	1·530 (8)	C(2)–H(21)	1·04 (7)
C(1)–C(7)	1·536 (9)	C(2)–H(22)	0·98 (7)
C(2)–C(3,5′)	1·552 (8)	C(4)–H(41)	0·97 (7)
C(3,5′)–C(4)	1·544 (8)	C(4)–H(42)	0·93 (7)
C(3,5′)–C(1′)	1·548 (7)	C(5)–H(51)	0·96 (7)
C(3,5′)–C(4′)	1·519 (7)	C(6)–H(61)	1·01 (7)
C(4)–C(5)	1·537 (9)	C(6)–H(62)	0·97 (7)
C(5)–C(6)	1·536 (8)	C(7)–H(71)	0·96 (7)
C(5)–C(8)	1·558 (9)	C(7)–H(72)	0·96 (7)
C(7)–C(8)	1·549 (9)	C(8)–H(81)	1·05 (7)
C(9)–C(10)	1·516 (8)	C(8)–H(82)	0·99 (6)
C(9)–C(14)	1·512 (8)	C(9)–H(91)	0·97 (6)
C(9)–N(3′)	1·483 (6)	C(10)–H(101)	1·00 (6)
C(10)–C(11)	1·527 (9)	C(10)–H(102)	1·02 (6)
C(11)–C(12)	1·503 (10)	C(11)–H(111)	0·92 (7)
C(12)–C(13)	1·517 (11)	C(11)–H(112)	1·03 (7)
C(13)–C(14)	1·532 (10)	C(12)–H(121)	1·00 (7)
C(1′)–C(2′)	1·493 (9)	C(12)–H(122)	1·00 (7)
C(2′)–N(3′)	1·401 (7)	C(13)–H(131)	0·93 (7)
C(2′)–O(1)	1·205 (7)	C(13)–H(132)	1·00 (7)
N(3′)–C(4′)	1·388 (7)	C(14)–H(141)	0·96 (7)
C(4′)–O(2)	1·208 (6)	C(14)–H(142)	1·03 (7)
		C(1′)–H(1′1)	0·98 (7)
		C(1′)–H(2′1)	0·90 (7)

C(6)–C(1)–C(7)	101·3 (5)	C(10)–C(9)–N(3′)	111·2 (4)
C(2)–C(1)–C(7)	110·7 (5)	C(10)–C(9)–C(14)	112·7 (5)
C(2)–C(1)–C(6)	111·4 (5)	C(9)–C(10)–C(11)	110·1 (5)
C(1)–C(2)–C(3,5′)	113·6 (5)	C(10)–C(11)–C(12)	112·0 (6)
C(2)–C(3,5′)–C(4′)	109·2 (4)	C(11)–C(12)–C(13)	111·3 (6)
C(2)–C(3,5′)–C(1′)	112·9 (4)	C(12)–C(13)–C(14)	110·4 (6)
C(2)–C(3,5′)–C(4)	111·1 (5)	C(9)–C(14)–C(13)	110·3 (5)
C(1′)–C(3,5′)–C(4′)	102·4 (4)	C(3,5′)–C(1′)–C(2′)	107·1 (5)
C(4)–C(3,5′)–C(4′)	108·2 (4)	C(1′)–C(2′)–O(1)	127·5 (6)
C(4)–C(3,5′)–C(1′)	112·6 (5)	C(1′)–C(2′)–N(3′)	108·1 (5)
C(3,5′)–C(4)–C(5)	114·1 (5)	N(3′)–C(2′)–O(1)	124·4 (6)
C(4)–C(5)–C(8)	111·9 (5)	C(9)–N(3′)–C(2′)	124·6 (4)
C(4)–C(5)–C(6)	109·0 (5)	C(2′)–N(3′)–C(4′)	112·1 (4)
C(6)–C(5)–C(8)	102·6 (5)	C(9)–N(3′)–C(4′)	123·2 (4)
C(1)–C(6)–C(5)	100·1 (5)	C(3,5′)–C(4′)–N(3′)	110·3 (4)
C(1)–C(7)–C(8)	103·8 (5)	N(3′)–C(4′)–O(2)	123·0 (5)
C(5)–C(8)–C(7)	105·5 (5)	C(3,5′)–C(4′)–O(2)	126·7 (5)
C(14)–C(9)–N(3′)	111·3 (5)		

Table 3. *Torsion angles* (°)

C(1)–C(2)–C(3,5′)–C(4)	−42·9 (6)	C(1′)–C(3,5′)–C(4′)–N(3′)	−2·7 (5)
C(2)–C(3,5′)–C(4)–C(5)	34·8 (7)	C(3,5′)–C(4′)–N(3′)–C(2′)	2·2 (6)
C(3,5′)–C(4)–C(5)–C(6)	24·1 (7)	C(4′)–N(3′)–C(2′)–C(1′)	−0·7 (6)
C(4)–C(5)–C(6)–C(1)	−74·6 (6)	N(3′)–C(2′)–C(1′)–C(3,5′)	−1·1 (6)
C(5)–C(6)–C(1)–C(2)	66·3 (6)	C(2′)–C(1′)–C(3,5′)–C(4′)	2·3 (6)
C(6)–C(1)–(2)–C(3,5′)	−8·9 (7)		
		C(9)–C(14)–C(13)–C(12)	56·2 (7)
C(1)–C(7)–C(8)–C(5)	−10·8 (7)	C(14)–C(13)–C(12)–C(11)	−56·9 (8)
C(7)–C(8)–C(5)–C(6)	−20·6 (6)	C(13)–C(12)–C(11)–C(10)	56·4 (8)
C(8)–C(5)–C(6)–C(1)	44·2 (6)	C(12)–C(11)–C(10)–C(9)	−54·2 (7)
C(5)–C(6)–C(1)–C(7)	−51·5 (5)	C(11)–C(10)–C(9)–C(14)	55·5 (6)
C(6)–C(1)–C(7)–C(8)	38·4 (6)	C(10)–C(9)–C(14)–C(13)	−56·0 (7)

Table 4. *Least-squares planes and deviations* (Å) *of atoms from those planes, and some dihedral angles* (°)

Deviations of atoms used in calculating the least-squares planes are denoted by asterisks.

	A	*B*	*C*	*D*	*E*
C(1)	−1·106 (6)	*0·038 (5)	*−0·027 (5)	–	–
C(2)	−1·237 (6)	*−0·035 (5)	–	–	–
C(3,5′)	*0·010 (5)	0·533 (4)	–	–	–
C(4)	1·315 (6)	*0·071 (7)	–	–	–
C(5)	1·236 (6)	*−0·053 (6)	*0·033 (6)	–	–
C(6)	0·136 (6)	0·855 (5)	0·749 (5)	–	–
C(7)	−0·796 (7)	−1·340 (7)	*0·061 (6)	–	–
C(8)	0·726 (7)	−1·470 (7)	*−0·085 (7)	–	–
C(9)	0·088 (6)	–	–	0·646 (4)	*0·000 (4)
C(10)	1·402 (6)	–	–	*−0·006 (6)	0·655 (6)
C(11)	1·461 (8)	–	–	*0·009 (7)	*−0·001 (7)
C(12)	0·273 (7)	–	–	0·663 (7)	*0·001 (7)
C(13)	−1·027 (8)	–	–	*−0·011 (8)	−0·679 (9)
C(14)	−1·113 (6)	–	–	*0·008 (7)	*−0·001 (7)
C(1′)	*−0·018 (8)	2·069 (5)	–	–	–
C(2′)	*−0·001 (6)	–	–	–	–
N(3′)	*0·008 (5)	–	–	–	–
C(4′)	*−0·017 (6)	0·028 (4)	–	–	–
O(1)	0·011 (6)	–	–	–	–
O(2)	−0·055 (5)	–	–	–	–

Plane *A*: $-0{\cdot}0155\,(25)X + 0{\cdot}9972\,(2)Y - 0{\cdot}0737\,(33)Z = 0{\cdot}965\,(22)$
B: $-0{\cdot}3985\,(36)X - 0{\cdot}0486\,(23)Y - 0{\cdot}9159\,(16)Z = -8{\cdot}215\,(21)$
C: $0{\cdot}7162\,(29)X + 0{\cdot}0480\,(27)Y - 0{\cdot}6963\,(29)Z = 2{\cdot}875\,(43)$
D: $-0{\cdot}5156\,(41)X - 0{\cdot}0355\,(28)Y - 0{\cdot}8561\,(24)Z = -6{\cdot}567\,(11)$
E: $-0{\cdot}0603\,(31)X + 0{\cdot}1996\,(41)Y - 0{\cdot}9780\,(8)Z = -6{\cdot}313\,(15)$

Dihedral angles $A \wedge B$ 88·6 (2), $B \wedge C$ 69·5 (3), $A \wedge D$ 88·0 (3).

bicyclic system adopts a highly distorted boat conformation; this deformation is shown by the values of the asymmetry parameters (Duax & Norton, 1975): $\Delta C_s^{3,5'} = 1{\cdot}0\,(5)$ and $\Delta C_s^{1-2} = 32{\cdot}7\,(6)°$ and by the deviations of C(3,5′) and C(6) from the least-squares plane through C(1), C(2), C(4), C(5) (Table 4).

The boat conformation of the fused cyclohexane ring is assumed in order to avoid the interaction between O(2) and the C(7)–C(8) bond which would occur if the cyclohexane ring adopted the chair conformation, the most common in this series of compounds. This boat is a little flattened in the C(1), C(2), C(3,5′), C(4), C(5) part; consequently the non-bonded distance C(6)···C(3,5′) is 2·732 (7) Å, slightly larger than the corresponding distance in an ideal boat (2·56 Å) (Webb & Becker, 1967).

The five-membered ring adopts a distorted 6,1-half-chair conformation [$\Delta = 11{\cdot}24\,(2)$ and $\varphi = 51{\cdot}3\,(5)°$, Altona, Geise & Romers, 1968]. The deviations of C(6) and C(1) from the least-squares plane through C(1), C(5), C(7) and C(8) are given in Table 4.

The decrease of the C(1)–C(6)–C(5) bond angle to 100·1 (5)° is related to the half-chair conformation adopted by this ring, instead of the envelope conformation found in other compounds of this series (Florencio, Smith-Verdier & García-Blanco, 1979, and references therein).

The cyclohexane ring substituted at N(3′) has a highly symmetrical chair conformation, all asymmetry parameters being below 2: $\Delta C_s^{10} = 0{\cdot}3\,(5)$, $\Delta C_2^{9-10} = 1{\cdot}3\,(7)$ and $\Delta C_2^{11-12} = 2{\cdot}0\,(8)°$. Mirror symmetry is dominant [C_s plane through C(10) and C(13)] with near equal displacements of C(10) and C(13) on opposite sides from the least-squares plane through C(9), C(11), C(12), C(14).

The succinimide ring is planar and the symmetry of the whole molecule approximates to *m* with a mirror plane through the succinimide ring. As can be seen in Fig. 1 and Table 4, the two cyclohexane rings are nearly perpendicular to the succinimide plane.

The distances for intermolecular contacts correspond to normal van der Waals interactions.

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Structure of (6*S*,13b*R*)-1,2,3,5,6,13b-Hexahydro-6-isopropyl-8*H*-pyrrolo[1′,2′:1,2]pyrazino[3,4-*b*]quinazoline-5,8-dione

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Abstract. $C_{17}H_{19}N_3O_2$, monoclinic, $P2_1$, $a = 5{\cdot}382$ (1), $b = 17{\cdot}534$ (4), $c = 8{\cdot}198$ (1) Å, $\beta = 100{\cdot}46$ (1)°, $Z = 2$, $d_m = 1{\cdot}323$, $d_c = 1{\cdot}299$ Mg m^{-3}, $F(000) = 316$, μ(Cu $K\alpha$) = 0·618 mm^{-1}. $R = 0{\cdot}052$ for 1284 significant reflections. The proline-containing *cis*-peptide unit which forms part of a six-membered ring deviates from perfect planarity. The torsion angle about the peptide bond is 3·0 (5)° and the peptide bond length is 1·313 (5) Å. The conformation of the proline ring is C_s—C$^{\beta}$-*endo*. The crystal structure is stabilized by C—H···O interactions.

Introduction. The proline ring plays an important role in the bend regions of protein chains. The title compound (Fig. 1) with a dipeptide-like fragment with prolyl and valyl residues affords a possibility of studying the conformations of these two side chains. NMR studies had indicated (Rajappa & Advani, 1973) an axial conformation of the valyl side chain.

In the present compound, there are no proton donors of type O—H or N—H. The only possible proton donor is the C—H group. C—H···O and C—H···N interactions have been previously observed in crystal structures (Sutor, 1962; Leiserowitz, 1976). Evidence for significant C—H···O interactions has been obtained from an X-ray powder diffraction study of the neutral–ionic phase transition in tetrathiafulvalene–chloranil (Batail, La Placa, Mayerle & Torrence, 1981). It is of interest to look for similar interactions in the present situation.

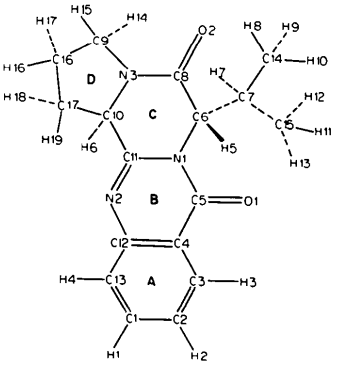

Fig. 1. The atomic numbering.

The title compound, a tetracyclic quinazolone, was derived from *cyclo*(-L-Val-L-Pro-), but during its synthesis, the proline centre epimerized, so that the product has the *S* configuration at the valine and the *R*

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