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The Crystal and Molecular Structure of 3β-Acetoxy-17α-hydroxy-16β-bromo-5α-pregnan-11,20-dione*

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The crystal structure of 3β-acetoxy-17α-hydroxy-16β-bromo-5α-pregnan-11,20-dione has been determined by three-dimensional X-ray analysis and refined to a final R value of 0·090. Unit cell constants are $a=11{\cdot}521$, $b=19{\cdot}587$, $c=10{\cdot}390$ Å, space group $P2_12_12_1$. Standard deviations for bond lengths and angles are in the ranges of 0·02–0·03 Å and 1–2° respectively. Neighboring molecules are hydrogen bonded *via* the 11-ketone and 17-hydroxyl groups. Molecular geometry and packing of the molecules are discussed.

Introduction

Many hypotheses may be formulated in an attempt to explain the molecular stacking arrangements of steroids in the crystalline state, such as the presence or absence of heavy atoms, angular methyl groups, side chains, *etc.* (Norton, 1965; Norton & Ohrt, 1966). The present paper presents the first in a series of structure determinations undertaken to augment the information presently available in this area. Three steroids of the 5α-pregnane series have been selected. Two, 3β,17α-dihydroxy-21-bromo-5α-pregnan-11,20-dione and 3β,17α-dihydroxy-16β-bromo-5α-pregnan-11,20-dione, are isomers, the difference being in the position of attachment of the heavy atom; the third varies in that it has an acetate side chain attached to carbon 3, namely, 3β-acetoxy-17α-hydroxy-16β-bromo-5α-pregnan-11,20-dione (Fig. 1), the structure of which is herein presented.

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Experimental

Crystals of the steroid were grown from methanol and from 95% ethanol solutions by slow evaporation at room temperature. These solvents provided two different crystal modifications: monoclinic from methanol and orthorhombic from ethanol. Crystal data for the two modifications are:

$C_{23}H_{33}O_5Br$, $M=469{\cdot}43$ λ (Cu $K\alpha$) = 1·5418 Å

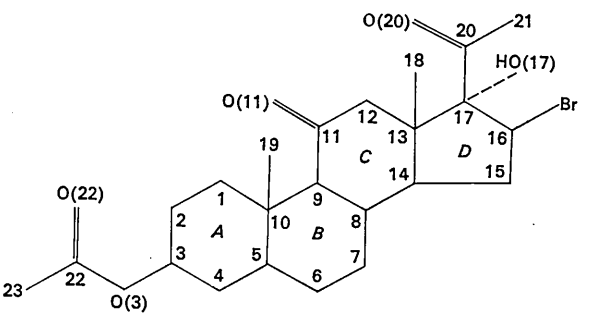


Fig. 1. 3β-Acetoxy-17α-hydroxy-16β-bromo-5α-pregnan-11,20-dione. Schematic drawing showing the numbering scheme used in the discussion.

Monoclinic modification

Solvent methanol, $a=7{\cdot}142\pm0{\cdot}001$, $b=26{\cdot}208\pm0{\cdot}008$, $c=7{\cdot}088\pm0{\cdot}001$ Å, $\beta=113{\cdot}56\pm0{\cdot}02°$, $V_0=1216{\cdot}18$ Å^3, $D_m=1{\cdot}292\pm0{\cdot}005$ g.cm^{-3}, $Z=2$, $D_c=1{\cdot}274$ g.cm^{-3}. Space group $P2_1$ (C_2^2; no.4). Thin plates.

Orthorhombic modification

Solvent ethanol, $a=11{\cdot}521\pm0{\cdot}003$, $b=19{\cdot}587\pm0{\cdot}001$, $c=10{\cdot}390\pm0{\cdot}001$ Å, $V_0=2344{\cdot}63$ Å^3, $D_m=1{\cdot}314\pm0{\cdot}005$ g.cm^{-3}, $Z=4$, $D_c=1{\cdot}321$ g.cm^{-3}. Space group $P2_12_12_1$ (D_2^4; no.19). Prismatic blocks.

Owing to the more regular nature of the orthorhombic crystals, these were used for the intensity measurements, for which a crystal of dimensions $0{\cdot}3\times0{\cdot}1\times0{\cdot}05$ mm was selected. Intensity measurements were made with a General Electric single-crystal orienter by the stationary-counter–stationary-crystal method using balanced nickel and cobalt filters (ten seconds count with each filter). A total of 2396 reflections were measured with the use of Cu $K\alpha$ radiation. Approximate absorption corrections were applied and the intensities were corrected for Lorentz and polarization effects.

A three-dimensional Patterson synthesis was computed from $|F^2|$ values modified to represent point atoms with thermal motion, and the bromine atom was located from the Harker sections. The positions of the other twenty-eight carbon and oxygen atoms in the asymmetric unit were determined by routine application of the heavy atom method. No attempt was made to locate the hydrogen atoms.

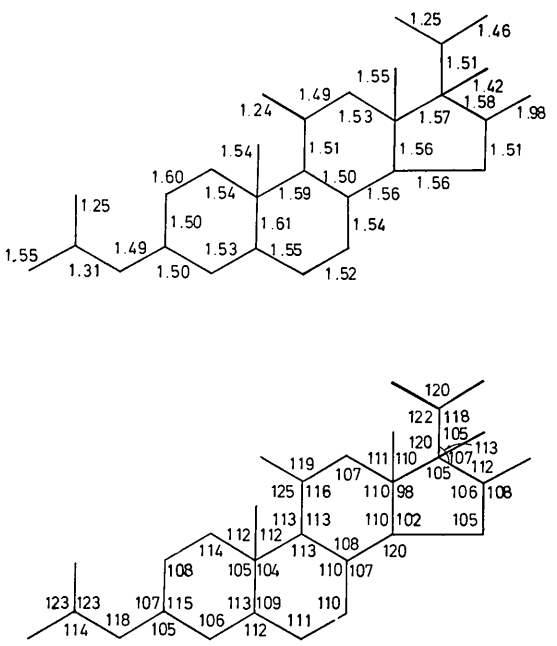


Fig. 2. Interatomic distances and angles. Standard deviations are in the ranges of 0·02 and 0·03 Å and 1–2° respectively.

The positional and thermal parameters of all atoms and the anisotropic thermal parameters of the bromine atom were refined by block-diagonal least squares in which the bromine atom and C(16), to which the bromine atom is bonded, were included in a single enlarged (13×13) matrix block to take account of interaction between these two atoms. The refinement converged with an R index (defined as $\Sigma\,||F_o|-|F_c||/|F_o|$) of 0·090 omitting 'unobserved' reflections. During the refinement, the atomic scattering factors used were those given in *International Tables for X-ray Crystallography* (1962) and the bromine scattering factors were corrected for the real part of the anomalous dispersion correction only. The quantity minimized was $\Sigma\, w(|F_o|-|F_c|)^2$ where $w^{1/2}=1$ if $|F_o|\leq20$ and $w^{1/2}=20/|F_o|$ if $|F_o|>20$. The refined parameters are listed in Table 1.

Table 1. *Positional and vibrational parameters of the atoms*

The standard deviations in the last two digits of each number are given in parenthesis.

	x/a	y/b	z/c	B(iso)
Br	0·5236 (2)	0·3261 (1)	1·0087 (3)	6·32 (–)*
O(3)	0·4402 (11)	0·9264 (6)	1·0303 (12)	4·72 (27)
O(11)	0·3520 (12)	0·6323 (7)	0·7226 (13)	5·25 (30)
O(17)	0·2183 (10)	0·4350 (6)	1·0094 (14)	4·61 (25)
O(20)	0·3159 (13)	0·3731 (7)	0·7383 (14)	5·32 (30)
O(22)	0·2556 (17)	0·9607 (10)	1·0128 (21)	9·64 (49)
C(1)	0·3472 (18)	0·7581 (9)	0·8765 (18)	4·54 (42)
C(2)	0·3780 (17)	0·8375 (9)	0·8851 (18)	4·25 (40)
C(3)	0·4013 (16)	0·8538 (9)	1·0241 (19)	4·58 (39)
C(4)	0·4979 (17)	0·8133 (9)	1·0839 (19)	4·34 (41)
C(5)	0·4584 (15)	0·7388 (8)	1·0799 (17)	3·52 (34)
C(6)	0·5438 (21)	0·6909 (11)	1·1512 (23)	5·93 (52)
C(7)	0·4965 (17)	0·6184 (9)	1·1600 (20)	4·57 (41)
C(8)	0·4733 (15)	0·5900 (8)	1·0245 (17)	3·66 (32)
C(9)	0·3912 (14)	0·6361 (7)	0·9530 (15)	2·74 (31)
C(10)	0·4403 (16)	0·7111 (8)	0·9351 (17)	3·58 (36)
C(11)	0·3455 (17)	0·6052 (9)	0·8297 (19)	4·17 (39)
C(12)	0·2908 (15)	0·5363 (8)	0·8408 (16)	3·16 (33)
C(13)	0·3795 (16)	0·4896 (9)	0·9065 (17)	3·73 (37)
C(14)	0·4121 (14)	0·5196 (7)	1·0410 (14)	2·92 (32)
C(15)	0·4770 (19)	0·4586 (10)	1·1057 (18)	5·00 (43)
C(16)	0·4107 (19)	0·3959 (10)	1·0657 (20)	4·83 (42)
C(17)	0·3278 (15)	0·4198 (7)	0·9529 (15)	2·88 (33)
C(18)	0·4862 (18)	0·4774 (9)	0·8193 (18)	4·57 (39)
C(19)	0·5532 (18)	0·7122 (10)	0·8563 (19)	4·54 (42)
C(20)	0·3033 (18)	0·3639 (9)	0·8568 (19)	4·44 (41)
C(21)	0·2516 (20)	0·3004 (11)	0·9034 (23)	5·70 (51)
C(22)	0·3608 (19)	0·9738 (10)	1·0249 (21)	5·76 (47)
C(23)	0·4112 (20)	1·0474 (11)	1·0196 (23)	5·89 (47)

* Equivalent B(iso). The anisotropic thermal parameters for the bromine atom in the form $\exp[-\Sigma(h_ih_jb_{ij}\times10^{-5})]$ are:

b_{11}	b_{22}	b_{33}	b_{12}	b_{31}	b_{23}
1176 (19)	369 (6)	1635 (28)	262 (10)	−44 (28)	38 (15)

Discussion

The least-squares planes through important regions of the steroid nucleus, distances of atoms from these planes and interplanar angles are given in Table 2 and the interatomic distances and angles are summarized in Fig. 2. The least-squares planes through rings *A*, *B*, *C*, and *D* are almost parallel [Table 2(*c*)] and the r.m.s.

Table 2(*a*). *Least-squares planes through the atoms**

Plane	Atoms	*l*	*m*	*n*	*p*
*A*1	C(2), C(3), C(4)	0·6558	0·7021	−0·2774	11·823
*A*2	C(1), C(2), C(4), C(5)	0·8093	−0·1920	−0·5551	−4·700
*A*3*B*1	C(1), C(5), C(6), C(10)	0·7406	0·5942	−0·3138	8·956
*B*2	C(6), C(7), C(9), C(10)	0·7944	−0·3529	−0·4943	−5·698
*B*3*C*1	C(7), C(8), C(9), C(11)	0·7724	0·4709	−0·4263	5·051
*C*2	C(8), C(11), C(12), C(14)	0·7167	−0·4106	−0·5637	−6·855
*C*3*D*1	C(12), C(13), C(14), C(15)	0·8164	0·4067	−0·4100	3·512
*D*2	C(13), C(15), C(16), C(17)	0·7205	−0·3944	−0·5703	−6·067
*D*3	C(14), C(15), C(16), C(17)	−0·7020	0·0681	0·7090	4·977
A	C(1), C(2), C(3), C(4), C(5), C(10)	0·8487	0·1265	−0·5135	0·825
B	C(5), C(6), C(7), C(8), C(9), C(10)	0·8775	−0·0293	−0·4787	−0·884
C	C(8), C(9), C(11), C(12), C(13), C(14)	0·8055	−0·1069	−0·5829	−3·281
D	C(13), C(14), C(15), C(16), C(17)	0·8061	−0·1925	−0·5596	−3·891
C(1)–C(17)		0·8275	−0·0550	−0·5587	−2·486

* The planes are in the form $lx+my+nz=p$, where x, y, z and p are in Å and x, y and z are referred to the crystal axes with x||**a**, y||**b** and z||**c**.

Table 2(*b*). *Distances from the least-squares planes*

	A	*B*	*C*	*D*	*A*2	*A*3*B*1	*B*2	*B*3*C*1	*C*2	*C*3*D*1	*D*2	*D*3	C(1)–C(17)
C(1)	−0·23				0·03	−0·03							−0·11
C(2)	0·22				−0·03								0·05
C(3)	−0·25				−0·68								−0·55
C(4)	0·27				0·03								0·07
C(5)	−0·27	−0·28			−0·03	0·03	−0·76						−0·21
C(6)		0·26				−0·03	−0·01						0·24
C(7)		−0·22					0·01	−0·07					−0·18
C(8)		0·23	0·23				0·69	−0·06	0·02				0·42
C(9)		−0·27	−0·19				−0·01	0·08	−0·61				−0·00
C(10)	0·25	0·28			0·74	0·03	0·01						0·49
C(11)			0·19					−0·08	−0·02				0·31
C(12)			−0·24						0·02	−0·09			−0·20
C(13)			0·29	0·30					0·74	0·10	0·06	−0·72	0·32
C(14)			−0·29	−0·29					−0·02	0·07	0·69	0·05	−0·19
C(15)				0·16						−0·08	−0·07	−0·08	0·12
C(16)				0·02							0·10	0·08	−0·21
C(17)				−0·19							−0·10	−0·05	−0·37

deviation of atoms C(1)–C(17) from the least-squares plane through the steroid nucleus is 0·28 Å. The length of the steroid nucleus [C(3)–C(16)] is 8·98 Å. Rings *A*, *B*, *C*, and *D* are *trans*-fused and rings *A*, *B*, and *C* are chair shaped. Ring *D* has a distorted half-chair configuration with torsional angles C(14)–C(15)–C(16)–C(17) and C(15)–C(16)–C(17)–C(13) of +13° and +17° respectively.

Table 2(*c*). *Interplanar angles*

Plane 1	Plane 2	Angle
*A*1	*A*2	123°
*A*3*B*1	*A*2	131
*A*3*B*1	*B*2	122
*B*3*C*1	*B*2	131
*B*3*C*1	*C*2	127
*C*3*D*1	*C*2	130
*C*3*D*1	*D*2	131
*C*3*D*1	*D*3	33
A	*B*	171
B	*C*	171
C	*D*	175
C(1)–C(17)	(100)	146
C(1)–C(17)	(010)	87
C(1)–C(17)	(001)	56

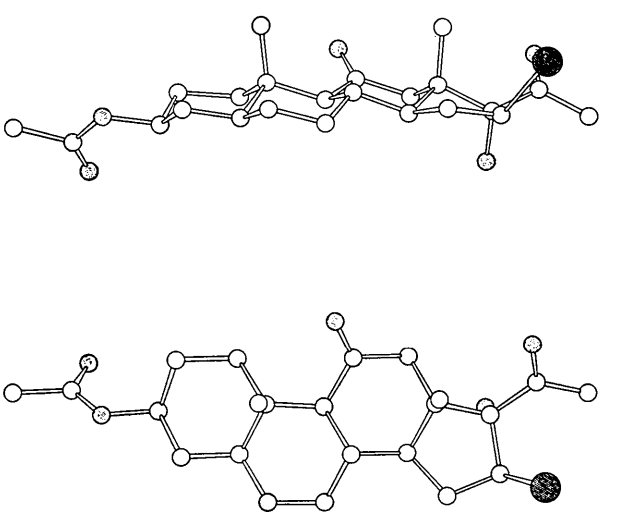


Fig. 3. Perspective views of the molecule. Large shaded circles: Br; small shaded circles: O; open circles: C. The plane of the acetate side chain lies at 55° to that of the *A* ring and that of the acetyl group at 40° to that of the *D* ring.

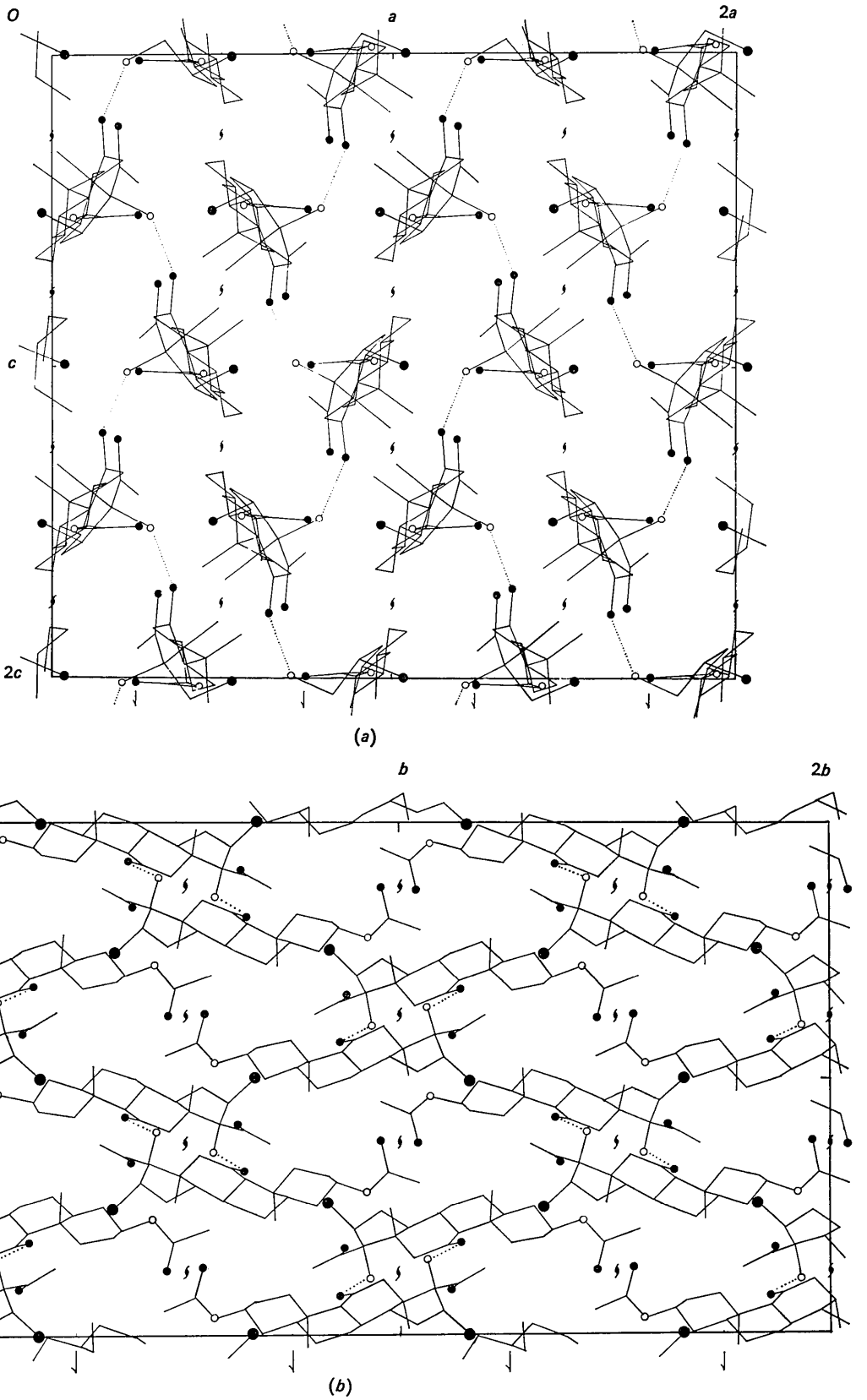
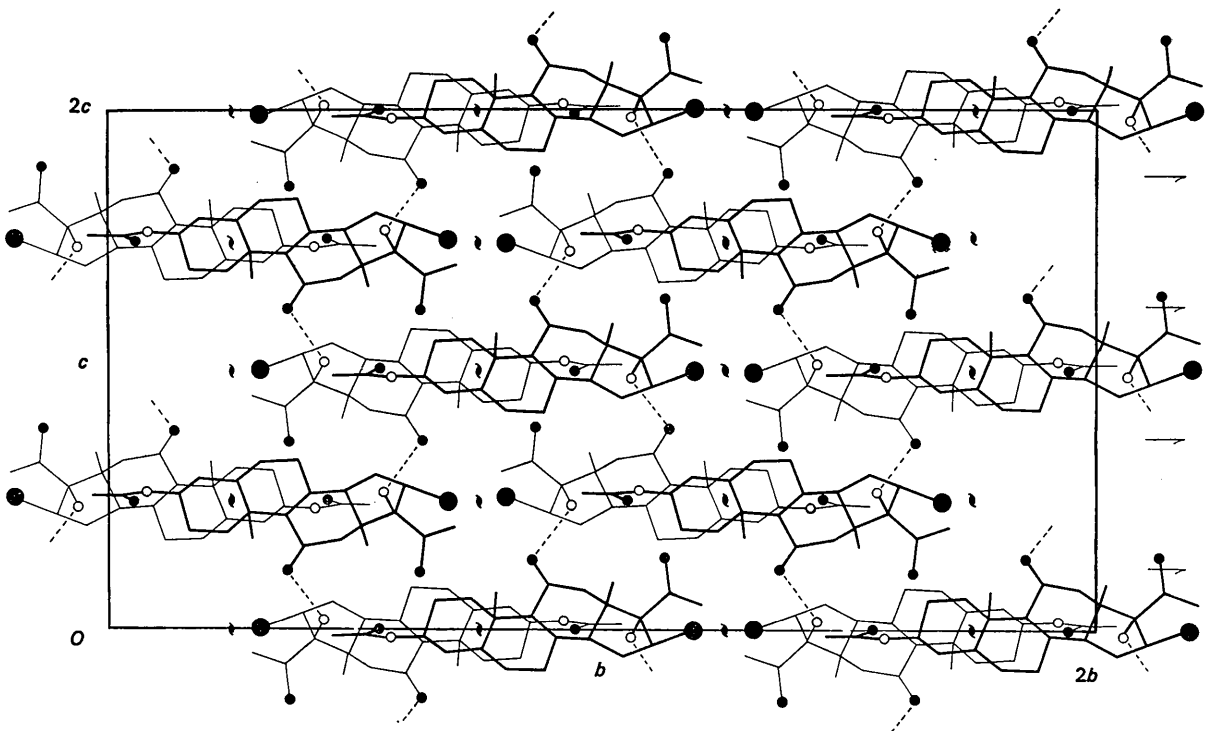


Fig. 4. Projections of four unit cells onto the planes (*a*) (010), (*b*) (001). The hydrogen bonding between the 17α-hydroxyl and the 11-keto oxygen is shown by dotted lines.



(c)

Fig.4 *(cont.)* *(c)* Projection of four unit cells onto the plane (100).

Table 3. *Intermolecular distances less than* 4·0 Å

The equivalent positions are:

1	x	y	z
2	$\frac{1}{2}-x$	$\bar{y}$	$\frac{1}{2}+z$
3	$\bar{x}$	$\frac{1}{2}-y$	$\frac{1}{2}-z$

O(20)–C(14) (2/01$\bar{1}$) means O(20) at equivalent position 1 to [C(14) at equivalent position 2, translated one unit cell in the y direction and one unit cell in the $\bar{z}$ direction].

	Position	Distance		Position	Distance
O(11)–O(17)	2/01$\bar{1}$	2·70 Å	C(12)–C(15)	2/01$\bar{1}$	3·94 Å
O(11)–C(16)	2/01$\bar{1}$	3·48	C(12)–C(16)	2/01$\bar{1}$	3·92
O(11)–C(17)	2/01$\bar{1}$	3·63	C(18)–O(3)	3/1$\bar{1}$1	3·86
O(11)–C(21)	2/01$\bar{1}$	3·76	O(20)–C(2)	3/1$\bar{1}$1	3·82
C(11)–O(17)	2/01$\bar{1}$	3·50	O(20)–C(19)	3/1$\bar{1}$1	3·63
C(12)–O(17)	2/01$\bar{1}$	3·49	C(18)–C(2)	3/1$\bar{1}$1	3·80
O(20)–C(7)	2/01$\bar{1}$	3·70	C(18)–C(22)	3/1$\bar{1}$1	3·99
O(20)–C(9)	2/0$\bar{1}$1	3·81	C(18)–C(23)	3/1$\bar{1}$1	3·96
O(20)–C(14)	2/01$\bar{1}$	3·94	C(21)–C(19)	3/1$\bar{1}$1	3·92

The acetate side chain [C(3), O(3), C(22), O(22), and C(23)] is planar but this plane lies at 55° to the plane of the *A* ring, instead of being perpendicular to it as might be expected (Mathieson, 1965), (see Fig. 3). This effect is due to the steric hindrance between the acetate group of one molecule and the C(18) methyl group of adjacent molecules, which approach each other to within 3·8 Å. The acetyl side chain is planar, lying at 40° to the plane of the *D* ring and C(13) lies in this plane.

Table 4. *Comparison between the values of $|F_o|$ and $|F_c|$ calculated for the refined atomic parameters*

$|F_o|$ and $|F_c|$ are given on ten times the absolute scale.

H	K	L	FOBS	FCAL
0	0	2	2322	2849
0	0	4	856	968
0	0	6	525	656
0	0	8	285	303
0	0	12	76	55
0	1	1	276	102
0	1	2	400	461
0	1	3	1115	1059
0	1	4	93	86
0	1	5	626	666
0	1	6	75	57
0	1	7	262	233
0	1	8	158	158
0	1	9	262	251
0	1	10	138	103
0	1	11	91	91
0	2	0	80	103
0	2	1	98	40
0	2	2	157	164
0	2	3	415	356
0	2	4	372	359
0	2	5	498	497
0	2	6	139	141
0	2	7	267	309
0	2	8	164	147
0	2	10	97	56
0	2	11	91	39
0	2	12	76	34
0	3	1	311	197
0	3	2	254	255
0	3	3	325	377
0	3	4	430	322
0	3	5	488	485
0	3	6	141	175
0	3	7	211	184
0	3	8	93	60
0	3	9	98	36
0	3	10	97	78
0	3	12	75	50
0	4	0	440	643
0	4	1	253	222
0	4	2	178	192
0	4	4	736	701
0	4	5	481	426
0	4	6	204	171
0	4	7	232	217
0	4	8	133	106
0	4	9	98	50
0	4	10	97	71
0	5	1	597	729
0	5	2	406	359
0	5	3	427	484
0	5	4	95	31
0	5	5	357	405
0	5	6	80	58
0	5	7	177	234
0	5	8	246	220
0	5	9	99	68
0	5	10	96	91
0	5	12	70	22
0	6	0	879	878
0	6	1	171	161
0	6	2	404	458
0	6	3	60	56
0	6	4	329	359
0	6	5	154	148
0	6	6	262	270
0	6	7	120	55
0	6	8	213	220
0	6	9	99	109
0	6	10	95	126
0	6	11	85	41
0	6	12	68	35
0	7	1	766	832
0	7	2	172	147
0	7	3	470	483
0	7	4	70	51
0	7	5	438	453
0	7	6	179	157
0	7	7	304	293
0	7	9	197	201
0	7	10	94	31
0	7	11	117	134
0	7	12	65	44
0	8	0	424	447
0	8	1	115	64
0	8	2	1207	1232
0	8	3	119	75
0	8	4	428	493
0	8	5	222	202
0	8	6	88	430
0	8	7	93	87
0	8	8	206	201
0	8	9	98	102
0	8	10	92	133
0	8	11	137	61
0	8	12	61	36
0	9	1	587	558
0	9	2	132	157
0	9	3	642	635
0	9	5	177	182
0	9	6	127	102
0	9	7	135	94
0	9	11	77	32
0	10	0	204	161
0	10	1	113	78
0	10	2	174	152
0	10	3	101	39
0	10	4	203	217
0	10	5	115	105
0	10	6	131	101
0	10	7	97	37
0	10	8	186	157
0	10	10	88	33
0	10	11	72	33
0	11	1	340	399
0	11	3	297	320
0	11	4	120	97
0	11	5	390	401
0	11	6	94	112

H	K	L	FOBS	FCAL
0	11	7	191	207
0	11	8	274	296
0	11	9	93	66
0	11	10	83	71
0	11	11	68	30
0	12	0	105	107
0	12	1	79	27
0	12	2	633	673
0	12	3	85	42
0	12	4	308	305
0	12	5	93	80
0	12	6	164	148
0	12	7	99	96
0	12	8	97	100
0	12	9	91	53
0	12	10	105	115
0	12	11	62	44
0	13	1	316	314
0	13	2	66	35
0	13	3	362	364
0	13	5	191	212
0	13	6	98	67
0	13	7	98	56
0	13	10	74	28
0	14	0	404	327
0	14	1	117	73
0	14	2	229	206
0	14	3	175	182
0	14	4	127	77
0	14	5	97	88
0	14	6	192	202
0	14	8	92	77
0	14	9	82	49
0	14	10	68	78
0	15	1	341	315
0	15	2	234	227
0	15	3	453	443
0	15	4	329	371
0	15	5	208	205
0	15	7	94	111
0	15	9	76	64
0	15	10	59	39
0	16	0	135	97
0	16	1	95	63
0	16	3	97	57
0	16	4	99	72
0	16	6	96	43
0	16	7	91	50
0	16	8	82	54
0	17	1	138	97
0	17	2	160	210
0	17	3	192	209
0	17	4	98	44
0	17	6	92	53
0	17	8	75	75
0	18	0	99	66
0	18	1	99	159
0	18	2	99	57
0	18	3	97	74
0	18	4	96	47
0	18	5	93	66
0	18	6	88	60
0	18	8	68	61
0	19	1	239	225
0	19	3	168	185
0	19	4	92	48
0	19	5	88	144
0	19	7	71	84
0	20	0	209	205
0	20	2	92	126
0	20	4	164	183
0	20	6	72	89
0	20	7	62	24
0	21	1	89	73
0	21	3	84	44
0	21	5	72	60
0	22	0	82	31
0	22	1	81	40
0	22	2	79	35
0	22	3	76	66
0	22	4	69	50
0	23	2	69	42
0	23	3	65	57
0	23	4	58	47
0	24	0	81	44
0	24	1	60	25
1	0	1	238	267
1	0	2	760	771
1	0	3	827	817
1	0	4	140	124
1	0	5	438	515
1	0	6	386	434
1	0	7	283	329
1	0	9	147	158
1	0	10	138	112
1	0	11	91	105
1	0	12	76	24
1	1	0	943	979
1	1	1	1030	1073
1	1	2	521	495
1	1	3	250	148
1	1	4	201	218
1	1	5	164	150
1	1	6	157	134
1	1	7	153	116
1	1	8	139	110
1	1	9	98	96
1	1	10	97	108
1	1	11	91	30
1	2	0	827	970
1	2	1	700	687
1	2	2	1162	1234
1	2	3	233	234
1	2	4	618	700
1	2	5	157	116
1	2	6	169	166
1	2	7	86	28
1	2	8	202	242
1	2	9	163	152
1	2	10	163	186

H	K	L	FOBS	FCAL
1	2	11	90	48
1	2	12	75	44
1	3	0	303	322
1	3	1	1046	1156
1	3	2	254	284
1	3	3	1017	1024
1	3	4	291	252
1	3	5	660	721
1	3	6	197	237
1	3	7	458	480
1	3	8	168	209
1	3	9	98	96
1	3	10	147	128
1	3	11	90	34
1	3	12	74	22
1	4	0	635	673
1	4	1	331	452
1	4	2	1006	993
1	4	3	874	900
1	4	4	793	827
1	4	5	333	354
1	4	6	458	460
1	4	7	173	126
1	4	8	320	349
1	4	9	95	34
1	4	10	174	160
1	4	12	72	54
1	5	0	635	701
1	5	1	772	790
1	5	3	392	405
1	5	4	505	506
1	5	5	412	449
1	5	6	277	355
1	5	7	200	200
1	5	8	152	134
1	5	9	133	139
1	5	10	96	59
1	5	11	87	38
1	5	12	70	43
1	6	0	226	296
1	6	1	339	355
1	6	2	158	155
1	6	3	262	265
1	6	4	156	167
1	6	5	102	54
1	6	6	143	132
1	6	7	130	122
1	6	8	96	45
1	6	9	141	123
1	6	10	151	95
1	6	11	85	40
1	6	12	68	21
1	7	0	121	105
1	7	1	160	164
1	7	2	561	530
1	7	3	326	308
1	7	4	131	148
1	7	5	135	163
1	7	6	85	107
1	7	7	92	90
1	7	8	97	69
1	7	10	93	111
1	7	11	82	43
1	7	12	65	38
1	8	0	1087	997
1	8	1	384	348
1	8	2	388	418
1	8	3	142	96
1	8	4	74	105
1	8	5	149	133
1	8	6	281	288
1	8	7	94	32
1	8	8	175	178
1	8	9	97	93
1	8	10	92	105
1	8	11	79	73
1	8	12	60	69
1	9	0	620	530
1	9	1	146	56
1	9	2	117	99
1	9	3	457	459
1	9	4	128	149
1	9	5	340	366
1	9	6	142	95
1	9	7	195	212
1	9	9	160	180
1	9	10	90	47
1	9	11	76	34
1	10	0	927	960
1	10	1	120	90
1	10	2	736	779
1	10	3	109	79
1	10	4	455	452
1	10	5	88	37
1	10	6	250	249
1	10	7	97	44
1	10	8	95	85
1	10	9	95	93
1	10	11	71	30
1	11	0	132	125
1	11	1	464	511
1	11	2	297	257
1	11	3	520	511
1	11	4	121	111
1	11	5	487	478
1	11	7	232	247
1	11	8	98	47
1	11	9	93	127
1	11	10	83	53
1	11	11	67	58
1	12	0	281	316
1	12	1	113	155
1	12	2	205	261
1	12	3	85	36
1	12	4	140	164
1	12	5	217	268
1	12	6	97	54
1	12	7	99	186
1	12	8	96	53
1	12	9	91	69

H	K	L	FOBS	FCAL
1	12	10	78	101
1	13	0	84	96
1	13	1	160	141
1	13	2	208	200
1	13	3	139	108
1	13	4	145	138
1	13	5	187	199
1	13	6	98	35
1	13	7	146	149
1	13	10	73	47
1	14	0	241	305
1	14	1	152	164
1	14	2	148	96
1	14	3	225	232
1	14	4	162	174
1	14	5	146	150
1	14	6	99	147
1	14	7	96	39
1	14	8	92	49
1	15	0	258	289
1	15	1	281	330
1	15	2	147	117
1	15	3	279	280
1	15	4	160	154
1	15	5	99	217
1	15	6	131	138
1	15	7	94	87
1	15	8	88	113
1	15	9	76	66
1	15	10	59	77
1	16	0	235	266
1	16	1	150	156
1	16	2	263	267
1	16	3	97	47
1	16	4	174	188
1	16	5	146	125
1	16	6	95	74
1	16	7	91	43
1	16	8	82	81
1	16	9	68	38
1	17	0	98	46
1	17	1	196	190
1	17	2	218	249
1	17	3	224	209
1	17	4	98	105
1	17	5	137	131
1	17	6	92	46
1	17	7	85	87
1	17	8	75	33
1	17	9	60	60
1	18	0	208	212
1	18	1	99	47
1	18	2	174	162
1	18	3	97	50
1	18	4	128	122
1	18	5	92	29
1	18	6	116	100
1	18	7	79	47
1	18	8	67	56
1	19	0	97	86
1	19	1	97	75
1	19	2	96	32
1	19	3	95	76
1	19	4	92	42
1	19	5	88	60
1	19	6	81	28
1	19	7	70	37
1	20	2	92	34
1	20	3	91	33
1	20	4	87	45
1	20	7	60	27
1	21	1	89	66
1	21	3	84	27
1	21	4	79	28
1	21	5	71	56
1	22	0	81	81
1	22	1	81	31
1	22	2	79	90
1	22	4	69	90
1	22	5	61	27
1	23	1	94	110
1	23	2	68	50
1	23	3	65	100
1	24	0	60	23
1	24	1	59	40
2	0	0	1702	1783
2	0	1	1659	1791
2	0	2	1200	1394
2	0	3	313	281
2	0	4	394	359
2	0	5	299	347
2	0	6	400	357
2	0	7	137	80
2	0	8	93	44
2	0	9	209	205
2	0	10	97	90
2	0	11	90	53
2	0	12	74	42
2	1	0	1022	1036
2	1	1	615	712
2	1	2	836	805
2	1	3	845	809
2	1	4	302	288
2	1	5	593	676
2	1	6	142	124
2	1	7	274	338
2	1	8	158	149
2	1	9	223	216
2	1	10	97	64
2	1	11	90	62
2	2	0	886	1037
2	2	1	753	771
2	2	2	732	832
2	2	3	492	507
2	2	4	424	475
2	2	5	465	484
2	2	6	275	344
2	2	7	137	108
2	2	8	188	143
2	2	9	98	59

H	K	L	FOBS	FCAL
2	2	10	97	81
2	2	11	89	27
2	2	12	73	80
2	3	0	83	90
2	3	1	177	258
2	3	2	130	134
2	3	3	658	630
2	3	4	293	256
2	3	5	503	479
2	3	6	315	309
2	3	7	243	243
2	3	8	185	158
2	3	9	97	79
2	3	10	96	38
2	3	11	88	48
2	3	12	71	53
2	4	0	89	45
2	4	1	454	414
2	4	2	653	694
2	4	3	340	337
2	4	4	292	311
2	4	5	136	155
2	4	6	290	332
2	4	7	205	209
2	4	8	130	98
2	4	9	158	168
2	4	10	96	38
2	4	11	87	41
2	5	0	317	262
2	5	1	521	593
2	5	2	257	263
2	5	3	984	992
2	5	4	242	243
2	5	5	420	384
2	5	6	83	85
2	5	7	167	110
2	5	9	149	151
2	5	10	95	111
2	5	11	85	36
2	5	12	68	42
2	6	0	834	859
2	6	1	272	262
2	6	2	632	651
2	6	3	311	308
2	6	4	512	565
2	6	5	174	194
2	6	6	394	409
2	6	7	124	107
2	6	8	154	186
2	6	9	99	66
2	6	10	94	94
2	6	12	66	30
2	7	0	177	207
2	7	1	1120	1106
2	7	2	396	372
2	7	3	623	649
2	7	4	272	300
2	7	5	490	587
2	7	6	87	53
2	7	7	341	351
2	7	8	140	128
2	7	9	98	97
2	7	10	92	34
2	7	11	81	68
2	8	0	758	652
2	8	1	498	433
2	8	2	311	321
2	8	3	95	56
2	8	4	377	339
2	8	5	112	81
2	8	6	191	162
2	8	7	163	126
2	8	8	182	202
2	8	9	97	51
2	8	10	91	48
2	8	11	78	65
2	9	0	418	353
2	9	1	473	317
2	9	2	179	136
2	9	3	205	215
2	9	5	147	125
2	9	7	166	156
2	9	8	99	60
2	9	9	96	91
2	9	10	89	90
2	10	0	328	299
2	10	1	138	107
2	10	3	184	187
2	10	4	112	121
2	10	5	153	133
2	10	6	162	158
2	10	7	233	231
2	10	8	99	62
2	10	10	85	51
2	10	11	69	35
2	11	0	340	323
2	11	1	147	160
2	11	2	165	152
2	11	3	131	103
2	11	4	117	78
2	11	5	219	161
2	11	6	171	164
2	11	7	99	92
2	11	8	168	170
2	11	9	92	69
2	11	10	81	112
2	12	0	517	509
2	12	1	140	141
2	12	2	388	388
2	12	3	249	222
2	12	4	432	431
2	12	5	206	191
2	12	6	186	195
2	12	7	156	140
2	12	8	137	129
2	12	9	89	80
2	12	10	77	62
2	12	11	58	30
2	13	0	178	167
2	13	1	568	547

H	K	L	FOBS	FCAL
2	13	2	162	150
2	13	3	280	248
2	13	4	126	75
2	13	5	285	310
2	13	6	182	163
2	13	7	181	208
2	13	8	93	135
2	13	9	85	48
2	14	0	405	408
2	14	1	155	130
2	14	2	351	355
2	14	3	215	221
2	14	4	248	258
2	14	5	98	48
2	14	6	99	100
2	14	7	96	60
2	14	8	91	95
2	14	9	80	49
2	14	10	65	78
2	15	0	93	63
2	15	1	383	373
2	15	2	187	155
2	15	3	351	325
2	15	4	187	186
2	15	5	209	205
2	15	6	97	128
2	15	7	93	106
2	15	8	86	55
2	15	9	74	41
2	16	1	130	82
2	16	2	97	54
2	16	3	98	43
2	16	4	99	80
2	16	5	97	67
2	16	6	95	43
2	17	1	261	245
2	17	2	99	60
2	17	3	99	102
2	17	4	97	70
2	17	5	95	30
2	17	6	92	37
2	17	7	84	36
2	17	8	72	26
2	18	0	182	130
2	18	1	147	169
2	18	2	139	123
2	18	3	153	159
2	18	4	95	56
2	18	5	92	81
2	18	6	86	48
2	18	7	77	55
2	18	8	65	42
2	19	0	96	35
2	19	1	137	134
2	19	2	95	79
2	19	3	94	134
2	19	4	91	65
2	19	5	87	78
2	19	6	79	44
2	19	7	68	21
2	20	0	160	138
2	20	1	92	33
2	20	2	130	121
2	20	4	85	77
2	20	6	70	88
2	20	7	58	22
2	21	1	87	106
2	21	2	85	42
2	21	3	82	71
2	21	5	69	65
2	22	0	80	43
2	22	2	77	95
2	22	3	72	40
2	22	4	68	58
2	22	5	58	54
2	23	0	69	34
2	23	1	69	36
2	23	3	62	42
3	0	1	1305	1397
3	0	2	371	315
3	0	3	445	562
3	0	4	117	158
3	0	5	252	225
3	0	6	81	95
3	0	7	89	34
3	0	8	95	94
3	0	9	164	162
3	0	10	96	34
3	1	0	418	323
3	1	1	751	711
3	1	2	468	408
3	1	3	325	365
3	1	4	254	249
3	1	5	72	455
3	1	6	395	387
3	1	7	212	220
3	1	8	256	220
3	1	9	235	211
3	1	10	96	94
3	1	11	87	65
3	1	12	73	36
3	2	0	527	483
3	2	1	458	477
3	2	2	658	633
3	2	3	577	576
3	2	4	570	584
3	2	5	252	267
3	2	6	329	346
3	2	7	142	140
3	2	8	216	191
3	2	10	160	165
3	2	11	87	43
3	2	12	69	53
3	3	0	872	894
3	3	1	762	831
3	3	2	400	402
3	3	3	471	476
3	3	4	325	258
3	3	5	417	465
3	3	6	164	180

H	K	L	FOBS	FCAL
3	3	7	242	270
3	3	8	263	249
3	3	9	178	179
3	3	10	95	88
3	3	11	85	48
3	4	0	429	426
3	4	1	682	704
3	4	2	875	908
3	4	3	311	295
3	4	4	676	768
3	4	5	158	179
3	4	6	165	166
3	4	7	233	242
3	4	8	142	124
3	4	9	99	137
3	4	10	94	76
3	4	11	84	36
3	5	0	254	243
3	5	1	56	846
3	5	2	130	71
3	5	3	348	370
3	5	4	215	168
3	5	5	295	297
3	5	6	165	151
3	5	7	250	238
3	5	8	97	103
3	5	10	93	36
3	5	11	83	37
3	6	0	473	465
3	6	1	404	354
3	6	2	307	299
3	6	3	538	530
3	6	4	218	228
3	6	5	144	108
3	6	6	162	163
3	6	7	186	157
3	6	8	97	116
3	6	9	98	73
3	6	10	92	32
3	6	11	80	30
3	6	12	62	50
3	7	0	306	248
3	7	1	142	102
3	7	2	227	202
3	7	3	121	55
3	7	4	197	216
3	7	5	213	219
3	7	6	135	109
3	7	7	164	145
3	7	8	98	99
3	7	9	97	48
3	7	10	91	81
3	7	11	78	25
3	7	12	57	53
3	8	0	710	690
3	8	1	434	404
3	8	2	337	344
3	8	3	434	457
3	8	4	231	207
3	8	5	249	264
3	8	6	163	146
3	8	7	206	202
3	8	8	95	34
3	8	9	96	29
3	8	11	75	73
3	9	0	762	789
3	9	1	412	488
3	9	2	583	605
3	9	3	466	501
3	9	4	269	294
3	9	5	243	252
3	9	6	174	125
3	9	7	208	210
3	9	8	99	57
3	9	9	95	147
3	9	10	86	46
3	9	11	70	79
3	10	0	687	647
3	10	1	145	149
3	10	2	605	583
3	10	3	81	83
3	10	4	385	378
3	10	5	195	185
3	10	6	224	191
3	10	7	133	157
3	10	8	193	203
3	10	9	93	108
3	10	10	83	83
3	10	11	67	63
3	11	0	132	102
3	11	1	243	227
3	11	2	141	149
3	11	3	386	382
3	11	4	160	170
3	11	5	336	348
3	11	6	97	111
3	11	7	264	277
3	11	8	96	113
3	11	9	91	34
3	11	10	78	37
3	12	0	331	311
3	12	1	135	111
3	12	2	189	179
3	12	3	320	307
3	12	4	171	96
3	12	5	194	156
3	12	6	188	163
3	12	7	98	101
3	12	9	87	46
3	12	10	73	39
3	13	0	139	120
3	13	1	164	124
3	13	2	248	247
3	13	3	133	128
3	13	4	182	199
3	13	5	175	183
3	13	6	95	115
3	13	7	97	62
3	13	8	92	51
3	13	10	68	32

H	K	L	FOBS	FCAL
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3	14	1	125	88
3	14	2	126	130
3	14	3	144	128
3	14	4	139	106
3	14	5	170	135
3	14	6	156	127
3	14	8	89	39
3	14	10	60	57
3	15	1	307	321
3	15	2	166	144
3	15	3	233	238
3	15	4	99	60
3	15	5	99	43
3	15	6	96	53
3	15	7	92	81
3	15	9	70	73
3	16	0	276	283
3	16	1	187	168
3	16	2	282	257
3	16	3	141	119
3	16	4	156	143
3	16	5	139	141
3	16	6	148	126
3	16	7	87	80
3	16	8	77	77
3	16	9	63	64
3	17	0	99	78
3	17	1	227	218
3	17	2	149	121
3	17	3	188	159
3	17	4	138	145
3	17	5	127	130
3	17	6	90	42
3	17	7	81	85
3	17	8	•69	22
3	18	0	132	111
3	18	1	98	65
3	18	2	192	209
3	18	3	96	34
3	18	4	174	190
3	18	5	90	38
3	18	6	83	87
3	18	7	74	38
3	18	8	60	38
3	19	0	95	28
3	19	1	95	43
3	19	2	94	39
3	19	3	92	72
3	19	4	89	62
3	19	5	84	98
3	19	6	76	35
3	19	7	65	30
3	20	2	90	31
3	20	3	87	39
3	20	4	82	45
3	20	5	76	99
3	20	6	67	36
3	21	0	85	82
3	21	1	84	57
3	21	2	83	71
3	21	4	74	39
3	21	5	67	49
3	22	0	77	56
3	22	1	76	58
3	22	2	74	60
3	22	3	69	68
3	22	4	64	36
3	23	0	67	28
3	23	1	66	46
3	23	3	57	61
4	0	0	819	799
4	0	1	78	142
4	0	2	551	682
4	0	3	450	412
4	0	4	315	318
4	0	5	109	90
4	0	6	460	489
4	0	7	375	416
4	0	8	161	183
4	0	10	94	128
4	0	12	66	127
4	1	0	419	621
4	1	1	865	878
4	1	2	645	701
4	1	3	557	560
4	1	4	566	585
4	1	5	264	286
4	1	6	129	79
4	1	7	292	298
4	1	8	163	126
4	1	9	150	154
4	1	10	94	60
4	1	11	83	55
4	1	12	66	52
4	2	0	328	447
4	2	1	591	610
4	2	2	600	591
4	2	3	323	302
4	2	4	356	319
4	2	5	265	246
4	2	6	85	66
4	2	7	255	267
4	2	9	99	114
4	2	10	93	35
4	2	11	83	53
4	2	12	65	48
4	3	0	103	71
4	3	1	294	248
4	3	2	171	154
4	3	3	343	351
4	3	4	125	114
4	3	5	118	133
4	3	6	256	266
4	3	7	192	176
4	3	8	348	331
4	3	9	98	60
4	3	10	93	92
4	3	11	82	33
4	3	12	64	85

Table 4 (*cont.*)

H	K	L	FOBS	FCAL
4	4	0	243	179
4	4	1	175	177
4	4	2	280	292
4	4	3	176	151
4	4	4	205	211
4	4	5	80	28
4	4	6	180	146
4	4	7	147	68
4	4	8	97	118
4	4	9	98	41
4	4	10	92	63
4	4	11	80	51
4	4	12	62	22
4	5	0	696	709
4	5	1	677	670
4	5	2	346	349
4	5	3	576	574
4	5	4	211	210
4	5	5	243	238
4	5	6	274	314
4	5	7	162	159
4	5	8	223	246
4	5	10	92	58
4	5	11	79	30
4	5	12	59	35
4	6	0	319	344
4	6	1	689	703
4	6	2	216	265
4	6	3	543	540
4	6	4	194	209
4	6	5	275	303
4	6	6	265	246
4	6	7	199	218
4	6	8	99	106
4	6	9	97	123
4	6	10	90	36
4	6	11	76	70
4	7	1	658	702
4	7	2	325	296
4	7	3	492	493
4	7	4	267	262
4	7	5	87	329
4	7	6	147	102
4	7	7	148	154
4	7	8	99	41
4	7	9	96	110
4	7	10	88	58
4	7	11	74	40
4	8	0	946	1024
4	8	1	206	206
4	8	2	588	628
4	8	3	265	262
4	8	4	400	425
4	8	5	147	93
4	8	6	203	211
4	8	7	97	68
4	8	8	99	156
4	8	10	85	75
4	8	11	70	21
4	9	0	135	67
4	9	1	155	177
4	9	2	172	173
4	9	3	124	100
4	9	4	143	139
4	9	5	185	187
4	9	6	152	143
4	9	7	98	111
4	9	8	97	61
4	9	9	92	122
4	9	10	82	77
4	9	11	66	72
4	10	0	131	142
4	10	1	180	197
4	10	2	82	116
4	10	3	115	100
4	10	4	90	28
4	10	5	134	124
4	10	6	97	66
4	10	7	99	126
4	10	8	96	83
4	10	9	91	32
4	11	0	372	374
4	11	1	329	311
4	11	2	236	217
4	11	3	164	125
4	11	4	165	132
4	11	5	137	116
4	11	6	156	166
4	11	7	149	139
4	11	8	95	53
4	11	9	88	73
4	11	10	74	41
4	12	0	117	121
4	12	1	188	218
4	12	2	284	272
4	12	3	250	262
4	12	4	419	426
4	12	5	214	197
4	12	6	141	156
4	12	7	97	35
4	12	8	92	108
4	12	9	83	55
4	12	10	68	50
4	13	0	151	159
4	13	1	227	229
4	13	2	252	274
4	13	3	128	105
4	13	4	263	244
4	13	5	241	246
4	13	6	170	155
4	13	7	152	138
4	13	8	90	88
4	13	9	78	65
4	13	10	63	57
4	14	0	373	391
4	14	1	272	235
4	14	2	279	277
4	14	3	207	176
4	14	4	216	191
4	14	5	189	178
4	14	6	97	94
4	14	7	92	79
4	14	8	85	49
4	14	9	72	32
4	15	0	146	158
4	15	1	146	107
4	15	2	140	144
4	15	3	182	190
4	15	5	97	64
4	15	6	94	34
4	15	7	89	82
4	15	8	79	48
4	15	9	66	79
4	16	0	98	119
4	16	1	99	74
4	16	2	157	171
4	16	3	99	41
4	16	4	97	77
4	16	5	95	79
4	16	6	91	92
4	16	7	83	35
4	16	8	72	61
4	17	0	99	80
4	17	1	99	31
4	17	2	98	66
4	17	3	97	87
4	17	4	95	61
4	17	5	92	79
4	17	6	66	31
4	17	7	77	45
4	17	8	65	46
4	18	0	97	61
4	18	1	96	89
4	18	2	96	106
4	18	3	94	133
4	18	4	138	151
4	18	5	87	118
4	18	6	79	50
4	18	7	69	28
4	19	0	93	125
4	19	1	126	117
4	19	2	92	58
4	19	3	128	132
4	19	4	86	88
4	19	5	132	148
4	19	6	71	46
4	19	7	59	58
4	20	0	140	125
4	20	1	88	74
4	20	2	87	90
4	20	3	83	91
4	20	4	78	61
4	20	5	71	67
4	20	6	102	88
4	21	0	81	80
4	21	1	81	59
4	21	2	79	55
4	21	3	75	89
4	21	4	69	41
4	21	5	61	26
4	22	0	72	55
4	22	1	71	22
4	22	2	69	68
4	22	4	57	49
4	23	0	61	37
4	23	1	60	27
5	0	1	158	130
5	0	2	366	345
5	0	3	361	282
5	0	4	264	262
5	0	6	89	78
5	0	7	134	135
5	0	8	98	80
5	0	9	97	85
5	0	11	78	35
5	0	12	58	27
5	1	0	467	470
5	1	1	421	480
5	1	2	350	328
5	1	3	238	225
5	1	4	263	311
5	1	5	229	235
5	1	6	150	127
5	1	7	252	248
5	1	8	98	48
5	1	9	97	44
5	1	10	92	68
5	1	11	78	63
5	1	12	58	39
5	2	0	420	438
5	2	1	337	361
5	2	2	204	220
5	2	3	368	413
5	2	4	345	395
5	2	5	83	251
5	2	6	213	183
5	2	7	221	227
5	2	8	98	78
5	2	9	97	118
5	3	0	648	683
5	3	1	540	561
5	3	2	137	142
5	3	3	535	502
5	3	4	423	433
5	3	5	308	277
5	3	6	329	354
5	3	7	345	320
5	3	8	193	172
5	3	9	97	136
5	3	11	77	25
5	4	0	638	672
5	4	1	562	540
5	4	2	566	541
5	4	3	490	489
5	4	4	351	365
5	4	5	315	302
5	4	6	275	248
5	4	7	256	222
5	4	8	157	164
5	4	9	96	119
5	4	10	89	67
5	4	11	75	68
5	5	0	108	101
5	5	1	225	222
5	5	2	295	329
5	5	3	75	253
5	5	4	145	109
5	5	5	315	288
5	5	6	256	294
5	5	7	160	136
5	5	8	147	150
5	5	9	96	89
5	5	10	88	70
5	5	11	73	47
5	6	0	220	261
5	6	1	106	70
5	6	2	476	484
5	6	3	310	278
5	6	4	154	150
5	6	5	163	152
5	6	6	213	199
5	6	7	97	69
5	6	8	138	144
5	6	9	94	78
5	6	10	86	80
5	7	0	277	279
5	7	1	194	171
5	7	2	236	205
5	7	3	153	126
5	7	4	209	220
5	7	5	160	119
5	7	6	175	142
5	7	7	98	124
5	7	8	144	152
5	7	9	93	40
5	7	10	83	75
5	7	11	68	47
5	8	0	381	368
5	8	1	308	333
5	8	2	292	302
5	8	3	128	100
5	8	4	222	219
5	8	5	196	208
5	8	6	140	155
5	8	7	180	177
5	8	9	92	70
5	8	10	81	62
5	8	11	64	26
5	9	0	356	339
5	9	1	382	449
5	9	2	508	538
5	9	3	299	278
5	9	4	361	338
5	9	5	94	94
5	9	6	133	123
5	9	7	99	46
5	9	8	96	37
5	9	9	90	63
5	9	10	77	24
5	9	11	59	29
5	10	0	115	139
5	10	1	168	174
5	10	2	257	287
5	10	3	182	178
5	10	4	141	140
5	10	5	160	159
5	10	6	150	155
5	10	7	98	136
5	10	8	94	78
5	10	9	87	53
5	10	10	72	51
5	11	0	227	224
5	11	1	240	198
5	11	2	220	247
5	11	3	355	389
5	11	4	95	43
5	11	5	252	277
5	11	6	95	82
5	11	7	97	76
5	11	9	83	47
5	11	10	68	38
5	12	0	243	222
5	12	1	152	115
5	12	2	302	303
5	12	3	249	245
5	12	4	278	246
5	12	5	95	103
5	12	6	133	125
5	12	7	95	67
5	12	8	89	82
5	12	9	78	45
5	12	10	62	69
5	13	0	94	44
5	13	1	128	72
5	13	2	137	146
5	13	3	96	87
5	13	4	98	106
5	13	5	99	93
5	13	6	97	54
5	13	7	92	114
5	13	8	85	94
5	14	0	153	92
5	14	1	301	341
5	14	3	163	169
5	14	4	99	32
5	14	5	97	40
5	14	6	94	98
5	14	7	90	65
5	14	8	80	92
5	14	9	67	57
5	15	1	194	210
5	15	2	163	162
5	15	3	99	96
5	15	4	148	143
5	15	5	95	82
5	15	6	92	121
5	15	7	84	41
5	15	8	74	35
5	15	9	58	48
5	16	0	99	39
5	16	1	182	167
5	16	2	177	159
5	16	3	97	129
5	16	4	165	160
5	16	5	92	66
5	16	6	87	69
5	16	7	78	112
5	16	8	100	98
5	17	0	97	126
5	17	1	97	81
5	17	2	96	113
5	17	3	129	115
5	17	4	92	115
5	17	5	88	72
5	17	6	81	56
5	17	7	71	38
5	18	0	158	190
5	18	1	94	92
5	18	2	93	106
5	18	3	92	30
5	18	4	88	145
5	18	5	82	43
5	18	6	74	84
5	18	7	63	24
5	19	1	90	80
5	19	3	85	34
5	19	4	81	93
5	19	5	74	56
5	19	6	65	70
5	20	0	84	102
5	20	1	84	33
5	20	2	82	59
5	20	3	78	56
5	20	4	72	33
5	21	0	76	81
5	21	1	75	23
5	21	2	73	72
5	21	3	68	31
5	21	4	63	53
5	22	0	94	69
5	22	1	66	72
5	22	2	63	64
6	0	0	382	457
6	0	1	550	567
6	0	2	276	280
6	0	3	428	462
6	0	4	123	87
6	0	5	250	270
6	0	6	199	157
6	0	7	254	259
6	0	8	99	107
6	0	9	95	147
6	0	10	87	45
6	0	11	71	27
6	1	0	193	181
6	1	1	354	340
6	1	2	685	660
6	1	3	443	427
6	1	4	415	432
6	1	5	283	306
6	1	6	157	136
6	1	7	97	130
6	1	9	95	65
6	1	10	138	118
6	1	11	71	40
6	2	0	304	326
6	2	1	206	238
6	2	2	390	417
6	2	3	137	93
6	2	4	340	325
6	2	5	201	208
6	2	6	171	165
6	2	7	267	244
6	2	8	187	197
6	2	9	94	72
6	2	10	86	40
6	2	11	70	42
6	3	1	104	90
6	3	2	229	213
6	3	3	212	203
6	3	4	84	48
6	3	5	156	129
6	3	6	305	284
6	3	7	171	126
6	3	8	165	135
6	3	10	85	67
6	3	11	69	61
6	4	0	340	340
6	4	1	229	238
6	4	2	115	113
6	4	3	269	222
6	4	4	85	151
6	4	5	170	170
6	4	6	94	45
6	4	7	98	64
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6	4	9	93	30
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6	5	1	158	183
6	5	2	167	198
6	5	3	205	214
6	5	4	189	175
6	5	5	171	152
6	5	6	173	139
6	5	7	171	163
6	5	8	97	69
6	5	9	92	100
6	5	10	82	71
6	6	0	230	216
6	6	1	576	661
6	6	2	302	292
6	6	3	483	506
6	6	4	268	256
6	6	5	190	204
6	6	6	137	106
6	6	7	99	84
6	6	8	97	112
6	6	9	92	89
6	6	10	80	80
6	6	11	63	30
6	7	0	361	330
6	7	1	466	451
6	7	2	227	207
6	7	3	182	155
6	7	4	257	297
6	7	5	269	279
6	7	6	205	212
6	7	7	99	165
6	7	8	96	98
6	8	0	83	33
6	8	1	206	189
6	8	2	398	457
6	8	3	214	215
6	8	4	208	188
6	8	5	267	250
6	8	6	98	138
6	8	7	137	153
6	8	8	95	59
6	8	9	88	92
6	8	10	74	29
6	9	0	311	335
6	9	1	140	132
6	9	2	226	204
6	9	3	223	212
6	9	4	252	260
6	9	5	134	87
6	9	6	99	103
6	9	7	135	118
6	9	8	93	90
6	9	9	84	55
6	10	0	90	113
6	10	1	90	153
6	10	2	193	167
6	10	3	298	287
6	10	4	155	188
6	10	5	98	142
6	10	6	158	173
6	10	7	96	39
6	10	9	80	38
6	10	10	66	20
6	11	0	321	331
6	11	1	141	87
6	11	2	280	272
6	11	3	95	74
6	11	4	283	271
6	11	5	99	95
6	11	6	142	174
6	11	8	88	69
6	11	10	59	28
6	12	0	177	166
6	12	1	247	265
6	12	2	308	304
6	12	3	182	174
6	12	4	98	93
6	12	5	99	116
6	12	6	96	63
6	12	7	92	113
6	12	9	71	89
6	13	0	309	312
6	13	1	97	102
6	13	2	176	167
6	13	3	141	169
6	13	4	99	143
6	13	5	97	141
6	13	6	94	64
6	13	7	89	71
6	13	8	79	64
6	13	9	65	44
6	14	0	250	311
6	14	1	149	108
6	14	2	211	206
6	14	3	99	143
6	14	4	97	81
6	14	5	95	103
6	14	6	144	146
6	14	7	84	44
6	14	8	72	54
6	15	0	99	60
6	15	1	99	44
6	15	2	98	78
6	15	3	97	116
6	15	4	95	44
6	15	5	92	68
6	15	6	87	85
6	15	7	78	71
6	16	0	140	163
6	16	1	97	38
6	16	2	96	57
6	16	3	95	43
6	16	4	92	71
6	16	5	89	46
6	16	6	81	46
6	16	7	71	76
6	17	0	95	118
6	17	1	94	100
6	17	2	93	47
6	17	3	92	70
6	17	4	88	95
6	17	5	82	102
6	17	6	74	66
6	17	7	64	24
6	18	1	144	158
6	18	3	87	66
6	18	5	75	94
6	18	6	67	28
6	19	0	129	142
6	19	1	85	71
6	19	2	119	144
6	19	3	79	72
6	19	4	74	88
6	19	5	67	79
6	20	0	118	126
6	20	1	77	66
6	20	2	75	67
6	20	3	71	91
6	20	4	65	105
6	21	1	113	113
6	21	3	60	74
7	0	1	79	48
7	0	2	81	27
7	0	3	127	66
7	0	5	92	73
7	0	6	96	140
7	0	8	195	200
7	0	9	91	39
7	0	11	62	39
7	1	0	78	35
7	1	1	274	260
7	1	2	223	241
7	1	3	252	227
7	1	4	89	68
7	1	5	246	233
7	1	6	96	44
7	1	7	99	115
7	1	8	97	65
7	1	9	91	78
7	1	10	79	65
7	1	11	62	58
7	2	0	79	98
7	2	1	362	378
7	2	2	339	349
7	2	3	376	340
7	2	4	143	60
7	2	5	274	266
7	2	6	97	65
7	2	7	141	144
7	2	8	96	62
7	2	9	91	128
7	2	10	79	63
7	2	11	61	82
7	3	0	423	387
7	3	1	115	112
7	3	2	412	435
7	3	3	283	275
7	3	4	270	247
7	3	5	298	274
7	3	6	275	255
7	3	7	158	162
7	3	8	96	72
7	3	9	90	76
7	3	10	78	39
7	4	0	276	257
7	4	1	390	455
7	4	2	258	236
7	4	3	369	382
7	4	4	91	87
7	4	5	179	157
7	4	6	139	76
7	4	7	99	51
7	4	8	96	39
7	4	9	89	78
7	4	10	76	44
7	5	0	426	453
7	5	1	84	151
7	5	2	182	164
7	5	3	160	135
7	5	4	146	142
7	5	5	95	78
7	5	6	164	127
7	5	7	98	40
7	5	8	135	133
7	5	9	88	105
7	6	0	692	797
7	6	1	121	45
7	6	2	196	151
7	6	3	135	151
7	6	4	93	64
7	6	5	96	53
7	6	6	191	172
7	6	7	98	47
7	6	8	133	103
7	6	10	71	46
7	7	0	88	76
7	7	1	158	182
7	7	2	359	310
7	7	3	243	228
7	7	4	170	156
7	7	5	212	191
7	7	6	99	75
7	7	7	97	71
7	7	8	92	76
7	7	9	83	54
7	7	10	68	58
7	8	0	208	235
7	8	1	229	223
7	8	2	128	101
7	8	3	197	222
7	8	4	96	74
7	8	5	168	176
7	8	6	99	138
7	8	7	96	145
7	8	9	80	79
7	9	0	231	229
7	9	1	237	260
7	9	2	227	179
7	9	3	295	297
7	9	4	304	316
7	9	5	168	125
7	9	6	137	172
7	9	7	94	66
7	9	8	88	70
7	9	9	77	65
7	9	10	60	26
7	10	0	212	140
7	10	1	250	259
7	10	2	95	64
7	10	3	178	195
7	10	4	137	133
7	10	5	167	182
7	10	6	97	56
7	10	7	92	152
7	10	8	85	81
7	10	9	72	63
7	11	0	321	332
7	11	1	194	211
7	11	2	237	236
7	11	3	185	193
7	11	4	166	108
7	11	5	135	163
7	11	6	95	48
7	11	7	90	92
7	11	8	81	86
7	12	0	206	216
7	12	1	171	162
7	12	2	151	142
7	12	3	158	139
7	12	4	98	127
7	12	5	96	78
7	12	6	93	74
7	12	7	87	30
7	12	8	76	36
7	13	1	99	33
7	13	2	99	48
7	13	3	98	44
7	13	4	97	46
7	13	5	94	58
7	13	6	90	45
7	13	7	82	53
7	13	8	70	34
7	14	0	99	47
7	14	1	98	188
7	14	2	98	101
7	14	3	97	101
7	14	4	95	58
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7	14	6	85	37
7	14	7	76	65
7	14	8	64	36
7	15	0	97	50
7	15	1	155	53
7	15	2	96	81
7	15	3	94	48
7	15	4	146	157
7	15	5	88	54
7	15	6	80	71
7	15	7	69	30
7	16	0	151	58
7	16	1	186	225
7	16	2	93	56
7	16	3	91	128
7	16	4	88	68
7	16	5	117	112
7	16	6	73	74
7	16	7	62	42
7	17	0	137	145
7	17	1	122	137
7	17	2	134	147
7	17	3	86	73
7	17	4	81	113
7	17	5	75	80
7	17	6	66	88
7	18	0	85	98
7	18	2	131	135
7	18	4	74	94
7	18	5	67	27
7	19	1	78	63
7	19	2	75	23
7	19	3	71	86
7	19	4	66	29
7	20	0	69	31
7	20	1	68	78
7	20	2	67	24
7	20	3	62	23
7	21	0	59	75
7	21	1	58	31
8	0	0	143	182
8	0	1	283	335
8	0	2	178	174
8	0	3	271	270
8	0	5	267	240
8	0	6	99	38
8	0	7	97	106
8	0	8	93	46
8	0	10	70	115
8	1	0	343	393
8	1	1	146	142
8	1	2	271	245
8	1	3	146	102
8	1	4	185	183
8	1	5	163	119
8	1	6	99	87
8	1	7	97	48
8	1	8	93	104
8	1	9	84	34
8	1	10	69	70
8	2	1	208	206
8	2	2	137	136
8	2	3	186	188
8	2	4	199	175
8	2	5	243	240
8	2	6	141	169
8	2	7	97	115
8	2	8	92	65
8	2	9	83	69
8	2	10	69	40
8	3	0	140	114
8	3	1	215	225
8	3	2	214	180
8	3	3	132	64
8	3	6	99	29
8	3	7	97	45
8	3	8	92	38
8	3	9	82	44
8	3	10	68	20
8	4	0	89	35
8	4	1	212	213
8	4	2	91	34
8	4	3	141	98
8	4	4	153	105
8	4	6	99	65
8	4	7	96	68
8	4	8	92	48
8	4	9	81	67
8	4	10	67	62
8	5	0	339	313
8	5	1	91	138
8	5	2	213	172
8	5	3	164	134
8	5	4	233	179
8	5	5	98	127
8	5	6	172	170
8	5	7	96	79
8	5	8	90	62
8	5	9	79	76
8	5	10	64	26
8	6	0	337	363
8	6	1	530	601
8	6	2	290	251
8	6	3	346	329
8	6	4	169	180
8	6	5	263	228
8	6	6	98	124
8	6	7	143	147
8	6	9	77	48
8	6	10	61	62
8	7	0	93	31
8	7	1	149	171
8	7	2	297	278
8	7	4	307	332
8	7	5	99	87
8	7	6	138	166
8	7	7	93	79
8	7	8	87	108
8	7	9	74	36
8	8	0	94	77
8	8	1	134	105
8	8	2	136	76
8	8	3	97	67
8	8	4	99	150
8	8	5	99	94
8	8	7	92	119
8	8	8	83	82
8	8	9	70	54
8	9	0	143	100
8	9	1	209	204
8	9	2	137	133
8	9	3	176	155
8	9	4	99	109
8	9	5	97	90
8	9	6	95	75
8	9	7	133	121
8	9	8	80	28
8	9	9	67	24
8	10	0	97	84
8	10	1	97	68
8	10	2	98	61
8	10	3	99	90
8	10	4	98	109
8	10	5	143	155
8	10	6	93	70
8	10	7	87	56
8	10	8	76	54
8	10	9	62	41
8	11	0	99	150
8	11	1	99	138
8	11	2	99	118
8	11	3	175	169
8	11	4	97	76
8	11	5	95	32
8	11	6	91	121
8	11	7	83	66
8	11	8	71	58
8	12	0	99	42
8	12	1	99	78
8	12	2	98	79
8	12	3	135	152
8	12	4	95	59
8	12	5	92	80
8	12	6	87	28
8	12	7	78	58
8	12	8	67	39
8	13	0	274	274
8	13	1	97	52
8	13	2	231	267
8	13	3	95	48
8	13	4	93	142
8	13	5	90	55
8	13	6	82	101
8	13	7	72	36
8	13	8	59	64
8	14	0	192	195
8	14	1	131	137
8	14	2	130	139
8	14	3	162	170
8	14	4	90	74
8	14	5	85	107
8	14	6	77	62
8	14	7	67	68
8	15	0	135	153
8	15	1	93	60
8	15	2	92	106
8	15	3	90	118
8	15	4	85	63
8	15	5	79	90
8	15	6	70	42
8	15	7	58	75
8	16	0	90	108
8	16	2	88	102
8	16	3	84	31
8	16	4	79	48
8	16	6	63	28
8	17	0	84	107
8	17	1	83	57
8	17	2	117	126
8	17	3	78	47
8	17	4	72	101
8	17	5	65	44
8	18	1	115	96
8	18	2	74	33
8	18	3	69	103
8	18	4	64	40
8	19	0	92	81
8	19	1	68	43
8	19	2	66	66
8	19	3	60	56
9	0	1	93	76
9	0	2	94	58
9	0	4	98	72

Table 4 (*cont.*)

H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL
9	0	5	99	46	9	15	0	126	120	10	12	2	89	41	11	15	1	60	47
9	0	6	97	52	9	15	1	86	95	10	12	5	85	101	12	0	0	92	2h
9	0	8	87	28	9	15	2	115	117	10	12	5	74	99	12	0	3	89	83
9	1	0	212	171	9	15	3	91	40	10	12	6	65	45	12	0	4	H4	3h
9	1	1	93	91	9	15	4	76	86	10	13	0	87	104	12	0	6	78	44
9	1	2	204	174	9	15	5	88	34	10	13	2	125	145	12	0	8	69	25
9	1	3	146	141	9	15	6	97	43	10	13	3	81	33	12	1	0	92	51
9	1	4	149	131	9	16	0	81	37	10	13	4	76	83	12	1	1	92	33
9	1	5	95	95	9	16	1	86	131	10	13	6	58	48	12	1	2	91	134
9	1	6	97	88	9	16	2	78	71	10	14	0	82	56	12	1	4	84	78
9	1	7	93	62	9	16	3	74	101	10	14	1	81	58	12	1	5	78	40
9	1	8	80	29	9	16	4	64	47	10	14	2	75	51	12	1	6	68	72
9	1	9	74	24	9	16	5	60	71	10	14	3	75	83	12	2	1	92	116
9	2	1	263	282	9	17	0	74	87	10	14	4	69	22	12	2	2	91	34
9	2	2	95	65	9	17	1	73	56	10	14	5	62	54	12	2	3	88	60
9	2	3	288	272	9	17	2	70	83	10	15	0	76	82	12	2	5	77	31
9	2	4	98	116	9	17	3	67	31	10	15	1	75	67	12	3	0	92	84
9	2	5	166	164	9	17	4	60	89	10	15	2	72	51	12	3	2	90	65
9	2	6	97	96	9	18	1	65	51	10	15	3	66	92	12	3	3	87	52
9	2	7	134	127	9	18	2	62	39	10	15	4	63	48	12	3	4	82	52
9	2	8	85	30	10	0	0	97	40	10	16	0	68	76	12	3	5	76	44
9	3	0	295	269	10	0	1	220	225	10	16	1	68	49	12	3	6	67	29
9	3	1	94	92	10	0	2	98	53	10	16	2	66	79	12	4	1	91	57
9	3	2	188	204	10	0	4	264	319	10	16	4	60	28	12	4	2	89	51
9	3	3	148	140	10	0	4	98	41	10	17	0	60	38	12	4	3	86	49
9	3	4	98	148	10	0	5	205	205	10	17	1	59	27	12	4	4	81	56
9	3	5	99	118	10	0	6	92	43	11	0	1	98	63	12	4	6	66	4C
9	3	6	97	100	10	0	7	86	42	11	0	2	97	43	12	5	0	103	107
9	3	7	92	90	10	1	0	256	325	11	0	3	96	68	12	5	1	89	71
9	3	8	84	9H	10	1	1	98	80	11	0	8	60	40	12	5	2	105	175
9	3	9	72	2h	10	1	2	245	225	11	1	0	98	57	12	5	4	79	65
9	4	0	331	384	10	1	3	93	34	11	1	1	98	88	12	5	5	72	48
9	4	1	274	275	10	1	4	172	185	11	1	2	97	44	12	5	6	63	60
9	4	2	234	240	10	1	6	92	90	11	1	3	96	42	12	6	0	88	53
9	4	3	262	235	10	1	7	86	40	11	1	4	93	61	12	6	1	88	8C
9	4	4	141	9C	10	1	H	75	68	11	1	5	90	35	12	6	3	H2	124
9	4	5	165	185	10	1	9	60	21	11	1	6	83	40	12	6	4	77	59
9	4	6	98	64	10	2	0	141	142	11	1	7	74	23	12	6	5	69	73
9	4	7	92	113	10	2	1	98	142	11	1	8	60	23	12	6	6	59	89
9	4	8	83	27	10	2	2	99	54	11	2	0	98	110	12	7	0	85	10H
9	4	9	70	57	10	2	3	99	102	11	2	1	140	173	12	7	1	85	46
9	5	0	248	222	10	2	4	98	119	11	2	2	97	67	12	7	2	83	76
9	5	1	145	117	10	2	5	96	81	11	2	3	145	182	12	7	3	79	121
9	5	2	214	202	10	2	6	92	36	11	2	5	90	116	12	7	4	74	78
9	5	3	149	106	10	2	7	85	49	11	2	6	82	35	12	7	5	67	58
9	5	4	186	183	10	2	9	59	35	11	2	7	72	21	12	8	1	124	107
9	5	5	98	95	10	3	0	98	110	11	2	H	55	20	12	8	2	80	47
9	5	6	194	176	10	3	1	98	H4	11	3	0	250	289	12	8	3	109	85
9	5	7	91	49	10	3	2	97	58	11	3	1	97	85	12	8	4	70	32
9	5	8	82	58	10	3	3	99	48	11	3	2	147	151	12	H	5	63	61
9	5	9	6H	25	10	3	4	97	102	11	3	3	95	102	12	9	0	79	64
9	6	0	154	175	10	3	5	95	37	11	3	4	92	84	12	9	1	79	73
9	6	1	169	193	10	3	6	92	57	11	3	5	86	63	12	9	2	77	58
9	6	2	97	96	10	3	7	84	29	11	3	6	82	66	12	9	3	72	55
9	6	3	98	64	10	3	9	59	23	11	3	H	5H	49	12	9	4	67	4C
9	6	4	97	109	10	4	0	98	89	11	4	0	97	63	12	9	5	5H	38
9	6	5	97	93	10	4	1	99	107	11	4	1	97	106	12	10	0	75	112
9	6	6	94	83	10	4	2	98	H5	11	4	2	9H	30	12	10	1	75	46
9	6	7	89	45	10	4	3	9H	67	11	4	3	94	84	12	10	2	72	61
9	6	8	79	4C	10	4	4	97	1C2	11	4	4	92	98	12	10	4	62	40
9	6	9	66	48	10	4	5	95	6C	11	4	5	8H	77	12	11	0	70	51
9	7	0	97	13C	10	4	6	91	53	11	4	7	7C	49	12	11	1	69	28
9	7	1	97	127	10	4	7	83	35	11	5	0	96	115	12	11	2	68	4C
9	7	2	98	120	10	5	0	165	179	11	5	1	9H	76	12	11	3	63	32
9	7	3	149	94	10	5	1	206	215	11	5	2	175	184	12	12	0	66	45
9	7	4	140	124	10	5	2	99	96	11	5	3	93	46	12	12	1	65	65
9	7	5	97	4C	10	5	3	98	109	11	5	4	145	132	12	12	2	62	5H
9	7	6	93	6H	10	5	4	97	H4	11	5	5	8H	60	12	13	0	58	7H
9	7	7	87	81	10	5	5	9H	4C	11	5	6	78	41	13	0	2	78	2H
9	7	8	77	67	10	5	6	9C	29	11	5	7	6H	47	13	0	3	74	43
9	7	9	63	6H	10	5	7	81	72	11	6	0	95	35	13	0	5	60	20
9	8	1	98	44	10	5	H	69	43	11	6	2	94	128	13	1	0	81	37
9	8	3	148	153	10	6	0	140	162	11	6	3	92	75	13	1	1	80	62
9	8	5	95	1CC	10	6	1	99	143	11	6	4	9C	70	13	1	3	74	4H
9	8	7	79	65	10	6	2	99	73	11	6	5	8H	8C	13	1	4	69	37
9	8	8	73	27	10	6	3	171	173	11	6	6	7E	49	13	2	0	80	A1
9	8	9	5d	65	10	6	4	96	38	11	6	7	6E	79	13	2	1	80	75
9	9	0	17H	22C	10	6	5	188	169	11	7	1	94	79	13	2	2	77	44
9	9	1	93	71	10	6	7	78	95	11	7	2	93	40	13	2	3	74	73
9	9	2	156	161	10	6	H	6H	24	11	7	3	91	115	13	2	5	59	65
9	9	4	97	114	10	7	0	99	105	11	7	4	8H	40	13	3	0	79	74
9	9	5	94	53	10	7	1	98	36	11	7	5	81	91	13	3	1	79	4H
9	9	6	9C	126	10	7	2	191	174	11	7	6	73	60	13	3	2	76	9H
9	9	7	81	32	10	7	3	97	128	11	7	7	62	35	13	3	3	72	4C
9	9	8	69	6A	10	7	4	95	130	11	8	0	148	153	13	3	4	67	89
9	10	1	274	316	10	7	5	139	140	11	8	2	92	142	13	3	5	58	30
9	10	2	98	85	10	7	6	129	144	11	8	3	89	55	13	4	1	77	51
9	10	3	222	234	10	7	7	76	80	11	8	4	84	46	13	4	3	70	33
9	10	5	209	195	10	7	H	64	88	11	8	5	78	8C	13	4	4	65	42
9	10	6	86	35	10	8	1	208	224	11	9	0	91	109	13	5	0	76	91
9	10	7	77	85	10	8	3	154	172	11	9	1	91	35	13	5	2	72	102
9	10	8	65	43	10	8	4	93	46	11	9	2	89	107	13	5	3	68	48
9	11	0	97	132	10	8	5	90	120	11	9	3	86	27	13	5	4	63	73
9	11	1	97	6C	10	8	7	73	47	11	9	4	81	66	13	6	0	74	6H
9	11	2	199	19A	10	8	H	59	35	11	9	5	75	41	13	6	1	72	4C
9	11	3	134	134	10	9	0	97	69	11	9	6	6E	17	13	6	2	7C	51
9	11	4	93	129	10	9	1	96	117	11	10	1	8E	14H	13	6	4	67	104
9	11	5	89	66	10	9	2	96	132	11	10	2	8E	91	13	6	4	59	29
9	11	6	82	38	10	9	3	94	101	11	10	3	82	142	13	7	1	69	35
9	11	7	72	45	10	9	4	92	60	11	10	5	7C	81	13	7	2	68	93
9	11	8	59	22	10	9	5	87	132	11	10	6	6C	42	13	7	3	63	3H
9	12	0	218	231	10	9	A	79	37	11	11	0	103	171	13	H	C	68	85
9	12	1	96	52	10	9	7	69	57	11	11	1	84	51	14	0	1	67	53
9	12	2	156	162	10	10	1	95	81	11	11	2	82	98	13	8	2	64	69
9	12	3	93	47	10	10	2	96	62	11	11	3	78	59	13	8	3	5H	71
9	12	4	91	82	10	10	3	92	47	11	11	4	72	26	13	9	0	115	84
9	12	5	85	43	10	10	4	89	71	11	11	5	66	24	13	9	1	62	41
9	12	6	78	55	10	10	5	83	47	11	12	1	75	44	13	9	2	58	55
9	12	7	68	49	10	10	6	75	35	11	12	3	73	76	14	0	0	64	33
9	13	1	93	131	10	10	7	65	37	11	12	4	68	39	14	0	1	63	21
9	13	3	91	6H	10	11	0	167	175	11	12	5	59	43	14	0	2	59	6H
9	13	4	87	35	10	11	1	93	44	11	13	1	74	47	14	1	0	64	55
9	13	5	80	42	10	11	2	151	152	11	13	2	71	29	14	1	1	61	23
9	13	7	6C	44	10	11	3	9C	42	11	13	3	6E	66	14	2	C	63	35
9	14	1	91	93	10	11	4	69	53	11	13	4	61	22	14	2	1	62	6H
9	14	2	8H	6H	10	11	5	79	47	11	14	0	6E	8E	14	4	C	59	54
9	14	3	89	91	10	11	6	70	56	11	14	1	6E	39					
9	14	4	81	51	10	11	7	5E	5C	11	14	2	6E	17					
9	14	5	75	42	10	12	C	91	78	11	14	3	6C	61					
9	14	6	66	35	10	12	1	9C	132	11	15	0	62	65					

The plane through atoms C(13)C(16)C(17) is perpendicular to plane C(17)C(20)O(17) (88°) and the angles which O(17) makes with C(17) are as expected. The angles which C(17) makes with C(20) are increased, however, to about 116° (± two standard deviations), this distortion being due to the hydrogen bonding between the keto oxygen atom O(11) and the hydroxyl group attached to C(17). This bonding brings the acetyl side chain [C(17), C(20), C(21), and O(20)] into close proximity with the *B* and *C* rings of the adjacent hydrogen bonded molecule, causing a distortion of the *D* ring in the vicinity of C(17).

The steroid molecules are hydrogen bonded *via* the 11-ketone and 17-hydroxyl groups, the OH···O distance being 2·70 Å. The 'bonded' molecules are α–α (bottom-to-bottom) oriented and are stacked in sheets which occur in pairs in which the molecules are packed top-to-top. This arrangement may be regarded as closest packing in which the 'bimolecular' sheets each have six similar sheets in contact with them (Fig. 4).

Apart from the hydrogen bonding, there are only seventeen intermolecular distances less than 4·0 Å (Table 3). Of the eleven internuclear contacts, four involve the oxygen atom of the acetyl group and the remaining seven are between atoms brought together by the hydrogen bonding. Six contacts involve the methyl groups, four of which are between the C(18) methyl group and C(3) acetate group, and two are between the C(19) methyl and C(17) acetyl groups.

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