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The Crystal Structure of 5,6-Epoxy-4-hydroxy-2-methoxy-4,6-di-*t*-butylcyclohex-2-enone

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The crystal structure of 5,6-epoxy-4-hydroxy-2-methoxy-4,6-di-*t*-butylcyclohex-2-enone, $C_{15}H_{24}O_4$, has been determined by single-crystal X-ray diffraction techniques. The unit cell is triclinic, space group $P\bar{1}$, with dimensions $a=12.833$, $b=11.695$, $c=10.861$ Å, $\alpha=104.49$, $\beta=94.62$, $\gamma=96.83°$. There are four molecules in the unit cell. Data were collected on an computer-controlled Philips PW 1100 diffractometer. The structure was determined by direct methods and refined by full-matrix least-squares; the final value of the conventional R index is 0.062.

The title compound may be prepared by autooxidation of 4,6-di-*t*-butylguaiacol in alkaline solution. The two molecules in the asymmetric unit are joined together by two hydrogen bonds, one from the hydroxyl oxygen of each molecule to the epoxide oxygen of the other. With the atoms of one molecule designated by primer, the distances $O'(15)\cdots H(O14)$ and $O(15)\cdots H(O'14)$ are 1.83 and 1.97 Å, respectively, and the angles $O(15)\cdots H(O'14)-O'(14)$ and $O'(15)\cdots H(O14)-O(14)$ are 171 and 167°, respectively. Since the hydroxyl group and the epoxide ring are found to be *cis* to each other,

Table 1. Starting phases obtained from the convergence map. The correct phases are those without parentheses.

h			ϕ_h	$\|E_h\|$
0	3	1	0	3.58
7	−4	6	0	3.55
5	8	−7	0	3.02
3	7	−7	0,(π)	3.65
3	−12	5	0,(π)	3.22
4	7	−8	0,(π)	3.04
6	−9	5	0,(π)	2.73
9	−8	−4	(0),π	2.46

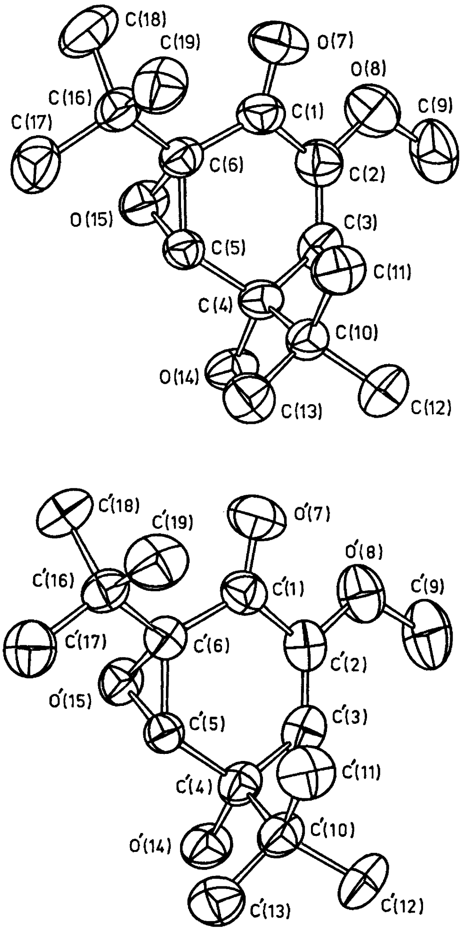

Fig. 1. Perspective views of the two separate molecules in the asymmetric unit.

Table 2. Positional and anisotropic thermal parameters of the non-hydrogen atoms. The β-values refer to the temperature factor expression $\exp[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})]$. Estimated standard deviations are given in parentheses. Values are $\times 10^4$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	2482 (3)	8337 (3)	2389 (3)	79 (3)	91 (3)	75 (3)	35 (5)	−5 (5)	42 (5)
C(2)	3262 (3)	8875 (3)	1678 (3)	59 (3)	96 (3)	97 (4)	13 (4)	−10 (5)	30 (5)
C(3)	2967 (3)	9224 (3)	639 (3)	60 (2)	91 (3)	90 (4)	−7 (4)	19 (4)	35 (5)
C(4)	1841 (3)	9153 (3)	114 (3)	61 (2)	62 (3)	78 (3)	12 (4)	10 (4)	43 (4)
C(5)	1098 (3)	9071 (3)	1123 (3)	62 (2)	63 (3)	75 (3)	26 (4)	11 (4)	34 (4)
C(6)	1379 (3)	8648 (3)	2267 (3)	73 (3)	62 (3)	75 (3)	25 (4)	22 (4)	38 (4)
O(7)	2735 (2)	7677 (3)	3033 (3)	106 (3)	168 (4)	148 (4)	90 (5)	15 (4)	178 (6)
O(8)	4268 (2)	8880 (3)	2190 (3)	65 (2)	162 (3)	137 (3)	24 (4)	−24 (4)	74 (5)
C(9)	5090 (3)	9322 (4)	1543 (5)	58 (3)	162 (5)	172 (6)	46 (6)	6 (6)	27 (8)
C(10)	1526 (3)	8106 (3)	−1128 (3)	66 (2)	69 (3)	75 (3)	22 (4)	18 (4)	33 (4)
C(11)	1594 (4)	6910 (3)	−823 (4)	120 (4)	70 (3)	107 (4)	34 (5)	20 (6)	25 (5)
C(12)	2278 (3)	8252 (4)	−2121 (4)	95 (3)	115 (4)	91 (4)	19 (5)	48 (5)	27 (6)
C(13)	405 (3)	8105 (3)	−1696 (4)	83 (3)	97 (4)	103 (4)	21 (5)	−19 (5)	10 (6)
O(14)	1708 (2)	10228 (2)	−260 (2)	103 (2)	65 (2)	81 (2)	6 (3)	10 (3)	47 (3)
O(15)	1416 (2)	9909 (2)	2347 (2)	96 (2)	64 (2)	85 (2)	23 (3)	28 (3)	29 (3)
C(16)	539 (3)	8133 (3)	2994 (3)	86 (3)	87 (3)	91 (4)	33 (5)	53 (5)	66 (5)
C(17)	−577 (3)	8566 (4)	2768 (4)	94 (3)	126 (4)	153 (5)	43 (6)	105 (6)	106 (7)
C(18)	917 (4)	8540 (5)	4424 (4)	145 (5)	171 (6)	89 (4)	50 (8)	91 (7)	87 (8)
C(19)	373 (4)	6774 (4)	2537 (4)	114 (4)	92 (4)	163 (5)	13 (6)	93 (7)	106 (7)
C′(1)	4257 (3)	13041 (3)	2299 (3)	60 (3)	81 (3)	99 (4)	20 (4)	17 (5)	45 (5)
C′(2)	4288 (3)	12516 (3)	3423 (3)	62 (2)	65 (3)	97 (4)	12 (4)	−16 (5)	39 (5)
C′(3)	3547 (3)	12596 (3)	4205 (3)	81 (3)	73 (3)	85 (3)	6 (4)	−8 (5)	66 (5)
C′(4)	2555 (3)	13133 (3)	4048 (3)	61 (2)	70 (3)	75 (3)	−9 (4)	15 (4)	42 (5)
C′(5)	2382 (3)	13348 (3)	2734 (3)	55 (2)	67 (3)	73 (3)	5 (4)	8 (4)	32 (4)
C′(6)	3204 (2)	13356 (3)	1858 (3)	56 (2)	58 (3)	77 (3)	4 (4)	10 (4)	35 (4)
O′(7)	5033 (2)	13157 (3)	1761 (3)	71 (2)	218 (4)	168 (4)	82 (5)	73 (4)	188 (7)
O′(8)	5181 (2)	12023 (2)	3519 (3)	79 (2)	97 (3)	147 (3)	55 (3)	−20 (4)	74 (4)
C′(9)	5357 (4)	11555 (4)	4584 (5)	107 (4)	141 (5)	182 (6)	83 (7)	−52 (7)	143 (9)
C′(10)	2538 (3)	14322 (3)	5098 (3)	78 (3)	79 (3)	76 (3)	−4 (4)	18 (4)	24 (5)
C′(11)	3339 (3)	15316 (3)	4893 (4)	96 (3)	77 (3)	134 (5)	−21 (5)	31 (6)	−1 (6)
C′(12)	2814 (4)	14123 (4)	6428 (4)	121 (4)	132 (4)	75 (4)	13 (6)	10 (6)	24 (6)
C′ (13)	1432 (3)	14703 (4)	5036 (4)	94 (3)	103 (4)	114 (4)	32 (3)	44 (6)	20 (6)
O′(14)	1676 (2)	12304 (2)	4182 (2)	81 (2)	85 (2)	97 (3)	−35 (5)	37 (3)	44 (4)
O′(15)	2393 (2)	12328 (2)	1672 (2)	72 (2)	67 (2)	82 (2)	−22 (3)	6 (3)	29 (3)
C′(16)	3155 (3)	14021 (3)	797 (3)	74 (3)	83 (3)	93 (3)	23 (4)	32 (3)	80 (5)
C′(17)	2042 (3)	14298 (4)	528 (4)	103 (4)	131 (4)	128 (5)	69 (6)	24 (6)	147 (7)
C′(18)	3456 (3)	13237 (4)	−424 (4)	107 (4)	128 (4)	85 (4)	35 (6)	41 (5)	75 (6)
C′(19)	3906 (4)	15199 (4)	1227 (4)	111 (4)	95 (4)	151 (5)	−13 (6)	50 (7)	102 (7)

these hydrogen bonds are probably responsible for the boat conformation of the cyclohexene ring.

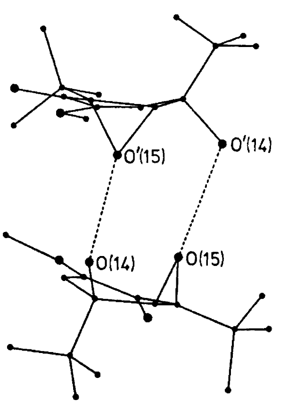

Fig. 2. The hydrogen-bonding system in the dimer molecule.

As part of a series of investigations on oxidation products of phenols, the crystal structure of the autooxidation product of 4,6-di-*t*-butylguaiacol in alkaline solution has been determined.

Butylated hydroxyanisoles (BHA) are used extensively as antioxidants in food.[1,2] The aim of this investigations was to establish the

Table 3. Positional parameters (× 10^3) of the hydrogen atoms.

	x	y	z		x	y	z
H(C3)	353	954	18	H(C′3)	356	1228	493
H(C5)	34	906	81	H(C′5)	175	1382	259
H1(C9)	499	1027	158	H1(C′9)	480	1096	463
H2(C9)	507	882	66	H2(C′9)	532	1210	548
H3(C9)	571	921	197	H3(C′9)	598	1126	465
H1(C11)	137	628	−156	H1(C′11)	306	1553	406
H2(C11)	240	693	−53	H2(C′11)	338	1596	561
H3(C11)	111	679	−23	H3(C′11)	397	1501	488
H1(C12)	208	759	−291	H1(C′12)	275	1482	707
H2(C12)	229	893	−234	H2(C′12)	359	1401	659
H3(C12)	303	813	−190	H3(C′12)	230	1348	660
H1(C13)	31	868	−186	H1(C′13)	88	1402	508
H2(C13)	27	761	−249	H2(C′13)	120	1488	413
H3(C13)	15	800	−115	H3(C′13)	141	1543	575
H(O14)	189	1093	46	H(O′14)	163	1155	346
H1(C17)	−85	833	189	H1(C′17)	184	1489	128
H2(C17)	−103	834	323	H2(C′17)	159	1365	39
H3(C17)	−142	932	304	H3(C′17)	203	1468	−24
H1(C18)	160	811	467	H1(C′18)	418	1312	−37
H2(C18)	49	834	485	H2(C′18)	341	1350	−117
H3(C18)	104	947	487	H3(C′18)	299	1246	−76
H1(C19)	22	655	175	H1(C′19)	386	1564	61
H2(C19)	102	644	264	H2(C′19)	370	1574	201
H3(C19)	14	639	280	H3(C′19)	451	1517	147

structure and stereochemistry of the epoxide formed upon oxidation of 4,6-di-*t*-butylguaiacol to gain information concerning the mechanism of formation of the epoxide.[1–3]

EXPERIMENTAL

Intensities were measured with monochromated Cu*K*α radiation by a computer-controlled Philips PW 1100 diffractometer. Unit-cell dimensions were determined by measurement of the angular positions of 25 accurately centered reflexions found by the "Peak Hunting Program". The unit cell and orientation parameters were obtained from these angular coordinates by the method of least squares. Crystal data are: space group $P\bar{1}$, $a = 12.833(2)$, $b = 11.695(2)$, $c = 10.861$ (2) Å, $\alpha = 104.49$ (2), $\beta = 94.62$ (2), $\gamma = 96.83$ (2)°, $V = 1299$ Å^3, $Z = 4$, $D_c = 1.371$ g cm^{-3}.

The $\theta - 2\theta$ scan technique was employed to

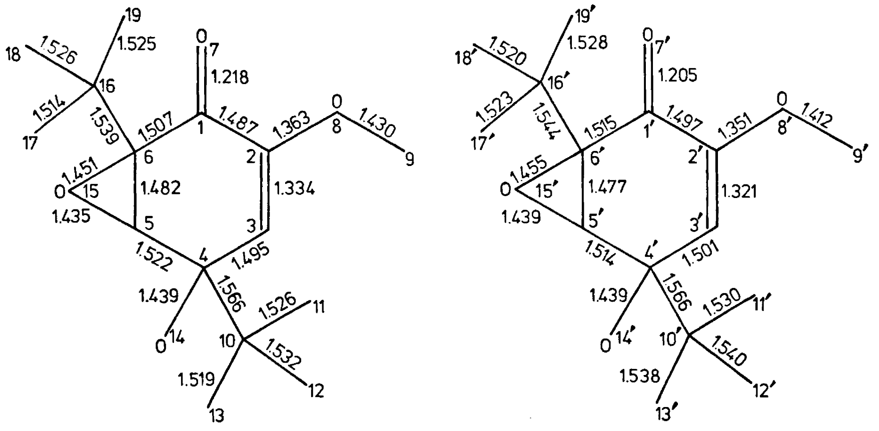
19
1.525
18
1.526
16
1.514
17
1.539
O
7
1.218
1.507
1
1.487
1.363
O
8
1.430
9
6
2
1.451
O
15
1.482
1.334
1.435
5
3
1.522
4
1.495
1.439
1.566
1.526
11
O
14
10
1.532
1.519
12
13
19′
1.528
18′
1.520
16′
1.523
17′
1.544
O
7′
1.205
1.515
1′
1.497
1.351
O
8′
1.412
9′
6′
2′
1.455
O
15′
1.477
1.321
1.439
5′
3′
1.514
4′
1.501
1.439
1.566
1.530
11′
O
14′
10′
1.540
1.538
12′
13′

Fig. 3. The interatomic bond distances.

Table 4. Observed and calculated structure amplitudes. The columns use the running index *k*, $10|F_o|$, and $10|F_c|$, respectively.

H=	0	L=-11
1	59	57
3	47	42
4	61	65
5	97	103
9	29	28
H=	0	L=-10
1	70	72
4	33	32
6	29	32
7	101	109
H=	0	L=-9
1	37	49
2	102	106
3	141	145
4	69	56
6	57	47
7	30	24
8	37	33
9	70	79
11	52	46
H=	0	L=-8
2	149	145
7	40	46
8	70	61
10	67	90
12	24	25
H=	0	L=-7
1	92	92
2	176	123
4	61	73
5	119	113
6	43	43
7	161	166
8	60	53
9	48	50
10	60	54
11	51	50
H=	0	L=-6
1	53	64
2	30	28
3	280	267
5	127	113
6	104	98
7	128	119
8	92	96
10	72	71
11	38	38
12	51	46
13	45	42
H=	0	L=-5
1	67	57
2	488	458
3	410	409
5	28	3
6	28	32
7	59	61
8	79	71
10	55	55
11	36	35
H=	0	L=-4
1	312	295
2	343	317
3	521	490
4	302	274
5	168	158
6	136	125
7	160	143
8	106	100
9	49	36
10	79	73
11	61	50
12	40	38
H=	0	L=-3
1	579	577
2	27	16
3	117	123
4	224	196
5	223	194
6	130	130
7	89	79
8	84	82
10	95	85
H=	0	L=-2
1	406	393
2	281	284
3	190	171
4	195	173
5	306	283
6	207	167
7	138	127
8	50	44
9	149	148
H=	0	L=-1
1	774	781
2	397	358
3	325	298
4	286	273
5	156	146
6	282	199
8	142	134
9	64	60
10	140	138
H=	0	L= 0
1	308	292
2	626	632
3	396	397
5	52	46
6	174	169
8	86	86
9	170	181
10	53	59
11	29	30
12	90	94
13	36	35
H=	0	L= 1
0	282	303
1	176	173
2	965	978
3	1314	1357
4	246	201
5	237	224
6	139	124
7	148	138
9	76	79
10	77	76
11	46	51
12	36	44
H=	0	L= 2
0	266	279
1	516	497
2	1020	1073
3	96	93
4	513	474
5	103	97
6	328	306
7	116	112
8	139	139
H=	0	L= 3
0	473	483
1	404	407
6	93	90
7	33	30
8	93	81
9	52	51
H=	0	L= 4
0	330	337
1	583	559
2	318	290
3	198	179
6	305	288
7	179	178
8	41	41
10	35	36
H=	0	L= 5
0	116	109
1	523	489
2	118	114
3	91	79
4	38	33
6	94	89
7	106	109
8	38	40
9	72	77
H=	0	L= 6
1	156	143
2	105	113
4	144	140
6	37	41
7	92	96
8	31	33
9	37	36
H=	0	L= 7
0	82	82
1	107	94
2	145	139
4	97	95
7	41	44
8	31	31
9	28	21
H=	0	L= 8
1	37	42
2	196	198
4	37	43
6	53	48
7	46	49
H=	0	L= 9
1	229	224
2	64	69
5	36	34
H=	0	L= 10
4	38	39
5	58	58
H=	0	L= 11
0	36	38
1	36	36
2	31	35
H=	0	L= 12
0	56	51
1	51	47
H=	1	L=-12
0	41	42
1	96	90
2	28	26
3	44	44
5	108	100
H=	1	L=-11
-3	58	56
-2	27	28
-1	36	37
0	74	76
2	42	51
3	37	33
5	71	76
6	63	63
7	32	30
9	29	26
H=	1	L=-10
-5	24	17
-4	47	42
-3	31	36
0	60	62
1	39	49
2	64	64
3	105	104
5	27	31
8	55	54
9	51	57
H=	1	L=-9
-6	44	38
-3	45	57
-2	82	79
0	76	78
1	209	210
2	52	49
3	47	40
4	125	119
5	139	140
6	53	52
7	61	62
8	40	36
9	37	38
H=	1	L=-8
-6	65	67
-5	38	35
-3	90	90
-2	134	139
-1	142	149
0	147	144
1	53	45
2	109	104
5	37	30
6	50	57
7	92	96
8	93	94
9	86	89
11	39	32
12	37	34
H=	1	L=-7
-9	54	56
-7	33	26
-6	44	46
-3	264	275
-2	71	56
-1	98	97
0	78	77
1	59	67
2	362	362
4	118	111
5	120	109
6	200	204
7	240	252
8	47	36
9	72	61
H=	1	L=-6
-10	42	35
-7	87	96
-5	55	59
-4	88	107
-3	70	74
-2	42	29
-1	33	26
0	250	235
1	36	34
2	226	228
4	113	112
5	110	104
6	185	185
7	76	70
8	58	52
9	144	141
H=	1	L=-5
-8	40	39
-7	90	96
-5	176	180
-4	81	77
-3	185	173
-2	242	221
-1	195	177
0	51	45
1	231	223
2	129	131
3	135	122
4	109	105
5	197	178
6	106	94
7	63	46
8	33	35
9	118	109
10	36	40
11	35	43
12	74	72
H=	1	L=-4
-11	70	73
-9	95	103
-8	69	70
-5	200	223
-4	173	130
-3	43	46
-2	384	367
-1	203	207
1	181	185
2	209	198
3	248	227
4	108	97
5	79	76
6	218	191
7	81	66
8	51	55
9	55	49
11	29	22
12	45	42
H=	1	L=-3
-12	48	51
-11	33	31
-10	43	46
-8	101	108
-7	115	122
-6	222	234
-5	339	343
-4	123	142
-3	255	237
-2	549	579
-1	165	153
0	103	115
1	54	68
2	47	44
3	562	552
4	28	34
5	214	194
6	198	180
8	158	159
9	127	124
10	35	35
11	71	61
12	64	59
H=	1	L=-2
-12	31	31
-10	117	126
-9	107	109
-8	156	155
-7	81	85
-6	292	287
-5	88	79
-4	283	254
-3	82	85
-2	331	343
-1	308	323
2	970	1031
3	48	31
4	150	140
5	338	302
6	390	360
8	114	112
9	28	32
10	65	79
11	34	40
12	32	25
H=	1	L=-1
-12	56	53
-10	68	77
-9	222	240
-8	225	233
-7	123	127
-6	41	29
-5	186	182
-4	198	202
-3	222	229
-2	651	667
-1	466	471
0	924	1085
1	149	198
2	84	53
3	287	253
4	195	182
5	272	259
6	170	164
7	192	191
8	30	27
10	101	90
12	58	54
H=	1	L= 0
-13	28	28
-11	32	34
-10	184	181
-9	86	90
-6	287	297
-5	512	504
-3	369	375
-2	975	1212
-1	416	437
0	49	47
1	293	291
2	1205	1317
3	114	74
4	167	156
5	29	40
6	66	82
7	95	92
8	37	28
9	31	48
10	138	145
11	87	97
12	27	35
H=	1	L= 1
-13	49	50
-12	41	42
-11	114	127
-10	61	67
-9	39	31
-8	106	111
-6	150	143
-5	367	378
-4	288	300
-3	35	17
-2	29	2
-1	620	684
0	783	881
1	696	745
2	120	93
3	334	333
4	192	184
5	143	132
6	124	104
7	68	68
8	130	123
9	192	200
10	38	38
11	31	38
12	34	36
H=	1	L= 2
-11	42	48
-9	67	55
-8	57	27
-7	32	12
-6	110	100
-4	240	225
-3	185	181
-2	26	13
-1	787	848
0	62	71
1	631	636
2	834	907
3	234	221
4	726	689
5	180	158
6	26	20
7	95	92
8	187	175
11	32	34
12	65	69
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6	336	310
7	47	90
8	85	87
9	30	27
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-1	83	95
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2	294	285
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5	93	95
6	208	217
7	60	59
8	87	85
9	87	88
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3	351	322
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5	95	106
6	67	67
8	159	170
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2	104	108
3	133	146
4	81	80
5	70	71
8	32	41
9	34	34
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3	81	82
4	110	107
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2	141	143
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6	42	37
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1	144	139
2	62	67
3	63	68
4	30	31
6	28	30
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1	34	35
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0	74	71
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1	42	39
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H=	2	L=-11
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-2	29	23
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4	28	34
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8	66	71
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1	59	57
2	59	59
4	62	65
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-1	233	235
0	137	133
1	115	110
2	53	51
3	172	171
4	118	122
5	57	52
6	112	108
8	40	35
9	53	59
11	36	33
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2	38	32
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4	141	139
5	42	42
6	82	78
7	219	215
8	41	34
9	31	32
11	33	29
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3	70	59
4	113	118
7	158	153
8	232	235
9	223	215
10	49	49
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-2	137	118
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1	86	85
2	82	72
3	37	32
4	138	120
5	56	48
6	259	256
8	128	120
9	112	113
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1	405	394
2	35	31
3	63	73
4	90	69
5	85	76
6	73	68
7	100	93
9	201	205
10	114	115
11	55	65
12	39	43
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1	158	173
2	31	33
3	244	230
4	134	134
5	97	78
6	134	129
7	87	67
8	184	181
9	77	67
10	104	96
11	49	48
12	80	78
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0	253	265
1	80	81
2	395	411
3	281	279
4	115	113
5	33	19
6	317	283
7	113	115
8	141	132
9	111	103
10	129	129
11	46	45
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-8	156	150
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-4	286	270
-3	69	87
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-1	349	363
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2	48	29
3	125	123
4	424	448
5	327	301
6	238	214
7	78	65
8	191	194
9	118	112
10	158	158
12	43	45
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-9	148	151
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-6	50	46
-5	64	74
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-2	356	356
-1	382	388
0	438	453
1	91	87
2	125	131
3	26	30
4	61	46
5	115	99
6	24	20
7	76	69
8	35	34
10	66	57
11	36	46
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-9	49	49
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-6	171	157
-5	107	97
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-2	22	9
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1	871	989
2	314	329
3	406	406
4	152	148
5	431	385
6	169	171
8	74	65
9	220	224
10	31	30
12	29	30
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-6	38	22
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-4	65	79
-3	164	167
-1	854	956
0	71	27
1	153	124
2	291	291
3	69	63
4	130	163
5	429	415
6	78	88
7	81	80
8	230	236
9	78	80
12	79	79
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-2	384	407
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0	89	31
1	218	222
2	111	92
3	242	286
4	240	226
5	228	200
6	235	214
7	268	247
9	76	83
11	70	82
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-5	97	82
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-1	139	144
0	137	156
1	128	139
2	189	189
6	60	70
8	34	23
10	49	52
11	33	40
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-12	27	21
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-5	393	380
-3	34	15
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1	106	101
2	200	187
3	117	113
4	63	63
5	149	144
6	125	124
7	110	99
8	120	122
9	42	46
10	29	25
H=	2	L= 5
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1	106	83
2	99	96
3	64	62
4	46	37
5	104	109
6	164	167
7	42	39
8	67	73
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2	119	110
4	97	63
6	64	64
7	77	78
8	64	72
9	37	44
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-7	142	137
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1	79	80
2	267	251
4	115	107
5	70	68
7	35	30

Table 4. Continued.

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-3	69	73
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2	53	47
5	30	24
7	28	29
H=	2 L=	9
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-8	77	69
-7	41	42
-5	43	52
-4	42	46
-3	59	60
-2	64	60
0	32	24
1	65	69
2	62	65
4	79	82
6	53	58
H=	2 L=	10
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-9	33	29
-7	35	40
-5	44	39
-4	52	62
-3	39	40
-2	33	46
0	90	90
2	62	70
3	27	31
H=	2 L=	11
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-4	90	86
-3	77	75
0	27	28
1	32	29
2	28	27
H=	2 L=	12
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-6	74	70
-5	51	46
-3	40	37
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H=	3 L=	-12
3	41	37
5	46	47
6	26	26
7	31	29
H=	3 L=	-11
-3	51	47
-2	33	35
0	64	67
1	81	79
2	42	51
3	66	71
4	33	37
5	74	77
8	27	21
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1	58	66
3	42	40
4	139	144
5	29	25
6	50	51
7	42	42
8	84	90
10	31	25
H=	3 L=	-9
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0	93	90
1	221	217
2	228	236
3	209	201
4	124	124
6	73	76
9	68	71
10	25	27
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6	67	61
7	53	56
8	32	27
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0	81	91
1	33	24
2	45	48
3	219	214
6	249	248
7	318	313
8	60	71
9	53	55
10	71	81
11	34	34
12	40	43
H=	3 L=	-6
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1	112	108
2	24	27
3	104	104
4	185	180
5	104	101
6	159	151
7	137	142
8	147	143
9	161	166
10	29	34
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1	47	58
2	77	74
3	107	103
4	35	54
5	26	29
6	127	129
7	117	122
9	173	166
10	96	98
11	81	87
12	34	40
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-9	92	95
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2	524	496
4	226	223
5	68	51
7	304	283
8	73	65
9	106	110
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2	379	378
3	26	33
4	138	133
5	182	173
7	58	51
8	204	197
9	139	153
10	145	146
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1	186	188
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3	158	158
4	423	463
5	99	98
6	277	239
7	58	62
8	150	145
10	63	60
12	42	47
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3	120	114
4	67	71
5	91	91
7	126	134
8	82	77
9	171	177
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2	183	217
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4	344	320
5	208	179
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7	40	39
8	85	99
9	85	80
10	61	64
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3	471	456
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5	293	300
6	34	31
7	214	219
8	118	127
9	54	51
10	69	72
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-3	209	221
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1	88	68
2	186	167
4	79	80
5	116	90
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8	162	172
9	64	63
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5	140	132
6	35	20
7	192	185
8	54	57
9	66	69
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2	219	202
3	69	66
5	97	98
8	68	69
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1	199	181
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3	27	30
5	98	98
8	91	98
9	26	25
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-9	158	167
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-1	27	31
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3	104	102
4	84	85
5	47	46
6	75	73
7	34	36
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1	127	134
2	28	38
3	102	94
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2	99	100
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1	97	96
3	54	54
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3	34	28
H=	3 L=	11
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H=	4 L=	-12
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1	36	40
5	24	20
6	62	56
H=	4 L=	-11
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3	26	18
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8	44	41
H=	4 L=	-10
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-4	29	24
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1	39	48
3	72	75
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6	53	57
7	88	93
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3	149	151
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7	45	46
8	40	39
9	46	50
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3	33	33
4	132	135
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6	58	59
7	207	212
9	27	22
10	39	36
H=	4 L=	-7
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1	287	285
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4	83	71
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9	57	41
10	62	62
11	28	22
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H=	4 L=	-6
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-1	79	83
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2	89	90
5	155	150
8	197	185
9	86	86
11	32	38
12	31	31
H=	4 L=	-5
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1	249	221
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3	252	258
4	133	109
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7	211	203
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8	30	31
9	225	222
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2	404	420
3	161	144
4	99	82
5	387	367
7	59	57
8	211	218
9	55	59
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6	75	70
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7	96	105
8	66	69
9	87	99
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3	119	113
4	225	214
5	123	134
7	112	120
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2	46	50
3	225	223
4	147	155
5	29	19
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7	82	80
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2	112	109
3	49	52
5	70	75
6	134	132
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1	45	43
2	57	60
3	106	95
4	28	30
5	82	84
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2	76	74
4	30	34
6	25	25
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2	78	84
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H=	5 L=	-11
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2	27	30
4	30	24
8	41	40
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3	106	116
4	112	117
6	64	72
7	28	32
H=	5 L=	-9
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-2	33	39
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3	110	111
5	114	110
6	34	34
7	69	76
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1	102	101
3	87	82
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6	144	142
7	68	72
8	57	59
9	57	57
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-1	35	39
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1	27	20
2	75	79
3	49	42
5	273	285
6	111	122
7	116	121
8	188	192
9	67	66
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-3	28	27
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1	44	59
2	95	88
3	52	45
5	203	204
6	146	140
7	237	232
8	138	149
9	86	88
11	57	55
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3	26	23
4	164	166
5	124	130
6	49	49
7	79	71
8	168	159
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-6	52	40
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-2	37	38
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2	216	189
3	49	61
4	99	106
5	40	35
7	61	55
8	138	128
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-8	69	64
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0	147	140
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2	445	418
3	357	347
4	130	112
5	48	64
6	187	181
7	66	62
8	81	80
10	58	57

Table 4. Continued.

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-1	77	89
0	105	114
2	186	172
3	43	41
4	404	371
5	207	183
6	32	1
7	101	96
8	57	46
9	100	98
10	36	25
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-8	185	191
-6	95	96
-5	69	59
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-2	108	105
-1	239	267
0	193	210
1	249	247
2	238	226
3	145	142
4	184	166
6	54	39
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-8	32	31
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0	206	215
1	51	49
2	142	146
3	184	174
4	47	44
5	74	79
6	153	137
7	49	35
8	46	52
10	49	59
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2	56	44
4	123	137
6	35	35
7	224	221
8	77	78
10	41	37
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-5	34	33
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2	109	82
4	28	37
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7	40	25
8	57	54
9	155	170
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4	145	140
5	39	43
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-3	132	130
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2	250	245
4	208	207
5	61	61
6	45	40
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1	38	34
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3	53	53
4	43	48
6	35	30
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2	44	52
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4	65	68
7	54	55
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5	62	62
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2	126	124
3	117	105
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7	192	188
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4	33	29
5	207	209
8	80	80
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2	285	273
3	55	37
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3	185	175
4	295	285
5	91	88
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4	35	40
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7	41	11
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3	114	118
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7	105	93
9	44	55
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4	96	99
5	108	97
6	43	46
7	152	147
8	30	37
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0	182	188
1	60	57
2	158	175
3	124	103
4	49	37
6	108	102
7	98	99
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2	124	119
3	69	77
4	195	197
5	47	29
6	71	80
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3	79	81
4	107	113
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7	97	94
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2	129	131
3	38	40
4	88	80
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4	78	76
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5	62	55
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H=	7	L= -9
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2	50	59
4	44	45
5	67	64
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7	31	42
10	70	65
H=	7	L= -7
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-6	28	28
-5	42	48
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1	97	103
5	107	109
6	37	37
7	61	73
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H=	7	L= -6
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4	171	179
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7	131	139
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3	73	80
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6	106	108
7	94	93
9	28	27
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4	68	55
6	100	97
7	34	37
9	30	33
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5	68	56
6	160	168
9	47	40
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9	74	82
10	66	70
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7	111	123
8	64	59
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6	99	93
7	101	100
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3	92	91
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3	46	47
4	67	67
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6	39	45
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3	30	45
4	77	73
6	30	33
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3	135	123
4	62	64
5	43	50
6	28	28
8	43	53
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4	79	66
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4	70	60
5	100	108
7	38	45
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8	34	30
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6	75	66
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Table 4. Continued.

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2	234	239
3	28	23
4	43	39
5	52	53
6	34	34
9	43	43
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2	56	49
3	97	96
4	72	75
8	49	47
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1	60	67
2	29	36
5	37	37
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1	87	82
3	76	75
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H= 9 L= -9		
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5	39	37
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4	67	68
H= 9 L= -7		
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2	64	71
5	91	91
9	26	27
H= 9 L= -6		
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-7	35	33
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0	33	36
3	79	66
4	96	109
6	42	51
8	57	50
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2	67	77
5	38	39
6	90	103
7	90	100
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3	58	53
6	93	89
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3	165	165
5	64	63
7	80	83
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6	73	81
8	28	14
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4	39	42
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7	87	98
8	90	83
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3	58	57
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1	95	97
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3	46	49
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3	150	157
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6	42	50
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4	129	140
6	121	134
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8	35	32
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3	139	136
5	108	106
6	45	42
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1	153	150
2	231	232
3	123	113
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2	120	118
3	86	63
4	61	57
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6	60	59
7	33	37
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3	128	124
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5	51	58
6	94	108
7	50	55
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3	71	68
4	67	68
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4	32	29
5	103	95
6	73	73
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2	29	29
3	69	74
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3	44	43
5	48	48
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H= 10 L= 6		
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3	62	64
4	26	20
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2	64	63
5	82	87
6	53	57
7	30	34
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5	35	46
8	59	51
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0	187	184
1	124	126
2	246	238
3	91	86
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1	104	110
3	52	51
4	92	94
5	49	52
6	59	56
H= 11 L= 1		
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4	51	56
5	28	26
6	45	43
H= 11 L= 2		
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2	32	30
4	61	54
6	57	47
H= 11 L= 3		
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3	49	47
4	42	37
H= 11 L= 4		
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4	30	28
5	36	41
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3	28	22
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H= 11 L= 7		
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0	42	41
H= 12 L= -8		
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0	25	13
2	63	56
3	24	24
H= 12 L= -7		
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2	55	55
4	28	18
H= 12 L= -6		
-5	41	38
-4	30	24
-2	39	38
0	26	13
2	27	18
4	39	46
6	25	32
H= 12 L= -5		
-6	26	27
-5	44	45
-4	41	42
-2	67	62
-1	36	45
0	57	49
4	26	25
5	50	56
H= 12 L= -4		
-4	49	41
-3	43	49
-2	43	39
2	96	102
H= 12 L= -3		
-6	30	36
-5	29	26
-4	42	45
-2	60	67
-1	60	53
0	31	35
1	37	47
2	30	31
6	35	30
H= 12 L= -2		
-8	39	39
-6	32	28
-5	36	28
-3	38	36
-2	59	52
-1	54	44
0	40	43
2	70	66
4	26	15
5	37	34
H= 12 L= -1		
-5	38	46
-4	49	54
-3	38	40
-1	45	45
1	160	162
2	94	103
3	46	45
4	37	35
H= 12 L= 0		
-8	37	33
-7	40	46
-5	51	54
-4	37	53
-2	53	56
0	128	128
1	37	39
2	60	64
3	92	98
4	60	58
5	25	25
H= 12 L= 1		
-7	86	86
-6	46	53
-2	39	49
-1	41	28
0	29	33
2	95	99
3	91	92
4	34	39
5	35	29
H= 12 L= 2		
-9	30	31
-8	29	27
-5	47	42
-4	109	112
-2	63	68
0	32	20
4	35	31
5	45	39
H= 12 L= 3		
-9	57	51
-6	36	35
-5	57	68
-2	39	35
-1	31	24
0	74	83
1	40	49
3	27	22
H= 12 L= 4		
-5	42	36
-4	54	50
-3	74	71
-2	114	120
-1	34	41
3	37	32
H= 12 L= 5		
-7	54	50
-4	46	49
-1	46	41
0	57	53
1	37	37
H= 12 L= 6		
-6	45	38
-5	35	29
0	25	23
H= 13 L= -7		
0	35	27
1	37	30
H= 13 L= -6		
0	55	59
1	41	40
2	27	21
3	24	26
H= 13 L= -5		
-5	47	44
-3	35	34
0	41	38
2	44	44
3	30	26
H= 13 L= -4		
-4	28	30
-3	42	36
-2	75	73
0	51	51
1	29	28
5	27	18
H= 13 L= -3		
-5	33	28
-3	37	26
-2	29	24
4	25	31
H= 13 L= -2		
-3	49	44
-2	64	62
0	38	27
1	39	39
3	34	37
H= 13 L= -1		
-8	49	45
-5	37	36
-3	36	30
-2	54	50
-1	70	74
H= 13 L= 0		
-6	91	85
-5	64	66
-4	40	27
0	46	41
1	33	35
2	33	28
H= 13 L= 1		
-6	26	29
-5	50	49
-4	49	51
-3	29	25
-2	39	34
-1	35	32
1	27	25
4	49	44
H= 13 L= 2		
-1	34	27
H= 13 L= 3		
-7	23	16
-5	44	46
-3	28	34
-2	26	29
1	31	25
H= 13 L= 4		
-2	45	49
-1	29	34
0	38	34
H= 13 L= 5		
-5	26	18
-2	31	19
-1	27	28
H= 14 L= -5		
-2	43	44
H= 14 L= -4		
2	45	44
H= 14 L= -3		
-5	27	22
-3	63	57
-2	28	29
H= 14 L= -2		
-1	58	60
0	37	39
H= 14 L= -1		
-6	36	29
-3	50	48
-1	30	26
H= 14 L= 0		
-4	28	14
-1	38	35
3	23	20
H= 14 L= 1		
0	25	21
H= 14 L= 2		
-1	42	42
0	27	32
H= 14 L= 3		
-5	37	27
H= 15 L= -2		
-1	31	25
H= 15 L= -1		
-1	43	40
H= 15 L= 0		
-2	62	56
-1	37	32

measure 5274 reflexions out to $\theta = 65°$ at a scan speed of 0.026 degrees per second. Backgrounds were estimated by stationary counting at $\pm 0.75°$ 2θ from the peak maxima. Three monitor reflexions were measured every 90 min. Lorentz and polarization corrections were applied to the data but no correction for absorption was made. The 3546 reflexions for which $\sigma(I)/I \leq 0.25$, where I is the net intensity and $\sigma(I)$ its estimated standard deviation, based on counter statistics, were used in refinement of the structure.

STRUCTURE DETERMINATION AND REFINEMENTS

The absolute scale and overall temperature factor for calculation of normalized structure factor magnitudes, $|E|$, were estimated by Wilson's method.[4] The structure was solved by a modified version of the MULTAN direct phase determination procedure[5] from the 358 reflexions with $|E|$ values ≥ 1.85. The three origin specifying reflexions and five reflexions used as variables in the starting set of phases are given in Table 1. An E map computed with the signs of the most reliable set showed all the non-hydrogen atoms.

The positional parameters and isotropic temperature factors of all the 38 non-hydrogen atoms were subjected to four cycles of full-matrix least-squares refinement ($R = 0.164$) by a modified version of the program LALS.[6] A Hughes'[7] weighting scheme was used in the refinement. One cycle of refinement of the non-hydrogen atoms with anisotropic temperature factors reduced R to 0.095. A difference Fourier synthesis computed at this point revealed the positions of all the hydrogen atoms. Additional cycles of least-squares calculations with hydrogen atoms included with fixed positional and thermal ($B = 3.5$ Å^2) parameters reduced R to 0.062 for 3546 reflexions. Freeman's[8] scattering factors for oxygen and carbon and that of Stewart, Davidson and Simpson[9] for hydrogen, were used throughout the analysis.

The final positional and thermal parameters of the non-hydrogen atoms, together with their standard deviations, are listed in Table 2 and those of the hydrogen atoms in Table 3. A list of the observed and calculated structure amplitudes is given in Table 4.

RESULTS AND DISCUSSION

The autooxidation product of 4,6-di-*t*-butylguaiacol in alkaline solution was established to be 5,6-epoxy-4-hydroxy-2-methoxy-4,6-di-*t*-butylcyclohex-2-enone with the hydroxyl group and epoxide ring *cis* to each other. The molecular structure is shown in Fig. 1; the two molecules are identically numbered, with the numbers of one distinguished by primes.

Table 5. Bond distances (Å) between non-hydrogen atoms, with estimated standard deviations in parentheses.

C(1)–C(2)	1.487 (4)	C′(1)–C′(2)	1.497 (4)
C(1)–C(6)	1.507 (4)	C′(1)–C′(6)	1.515 (4)
C(1)–O(7)	1.218 (4)	C′(1)–O′(7)	1.205 (4)
C(2)–C(3)	1.334 (4)	C′(2)–C′(3)	1.321 (4)
C(2)–O(8)	1.363 (4)	C′(2)–O′(8)	1.351 (4)
C(3)–C(4)	1.495 (4)	C′(3)–C′(4)	1.501 (4)
C(4)–C(5)	1.522 (4)	C′(4)–C′(5)	1.514 (4)
C(4)–C(10)	1.566 (4)	C′(4)–C′(10)	1.566 (4)
C(4)–O(14)	1.439 (3)	C′(4)–O′(14)	1.439 (4)
C(5)–C(6)	1.482 (4)	C′(5)–C′(6)	1.477 (4)
C(5)–O(15)	1.435 (3)	C′(5)–O′(15)	1.439 (3)
C(6)–O(15)	1.451 (3)	C′(6)–O′(15)	1.455 (3)
C(6)–C(16)	1.539 (4)	C′(6)–C′(16)	1.544 (4)
O(8)–C(9)	1.430 (5)	O′(8)–C′(9)	1.412 (5)
C(10)–C(11)	1.526 (4)	C′(10)–C′(11)	1.530 (5)
C(10)–C(12)	1.532 (5)	C′(10)–C′(12)	1.540 (5)
C(10)–C(13)	1.519 (5)	C′(10)–C′(13)	1.538 (5)
C(16)–C(17)	1.514 (5)	C′(16)–C′(17)	1.523 (5)
C(16)–C(18)	1.526 (5)	C′(16)–C′(18)	1.520 (5)
C(16)–C(19)	1.525 (5)	C′(16)–C′(19)	1.528 (5)

Table 6. Interatomic angles (°), with estimated standard deviations in parentheses.

C(2)–C(1)–C(6)	116.8 (3)	C′(2)–C′(1)–C′(6)	116.7 (3)
C(2)–C(1)–O(7)	120.9 (3)	C′(2)–C′(1)–O′(7)	120.4 (3)
C(6)–C(1)–O(7)	122.3 (3)	C′(6)–C′(1)–O′(7)	122.9 (3)
C(1)–C(2)–C(3)	122.0 (3)	C′(1)–C′(2)–C′(3)	122.5 (3)
C(1)–C(2)–O(8)	110.7 (3)	C′(1)–C′(2)–O′(8)	110.0 (3)
C(3)–C(2)–O(8)	127.1 (3)	C′(3)–C′(2)–O′(8)	127.4 (3)
C(2)–C(3)–C(4)	123.8 (3)	C′(2)–C′(3)–C′(4)	125.6 (3)
C(3)–C(4)–C(5)	111.3 (3)	C′(3)–C′(4)–C′(5)	111.2 (3)
C(3)–C(4)–C(10)	111.6 (3)	C′(3)–C′(4)–C′(10)	113.0 (3)
C(3)–C(4)–O(14)	109.1 (3)	C′(3)–C′(4)–O′(14)	108.2 (3)
C(5)–C(4)–C(10)	111.8 (3)	C′(5)–C′(4)–C′(10)	109.6 (3)
C(5)–C(4)–O(14)	106.8 (3)	C′(5)–C′(4)–O′(14)	108.0 (3)
C(10)–C(4)–O(14)	105.9 (2)	C′(10)–C′(4)–O′(14)	106.6 (3)
C(4)–C(5)–C(6)	123.4 (3)	C′(4)–C′(5)–C′(6)	124.4 (3)
C(4)–C(5)–O(15)	114.9 (3)	C′(4)–C′(5)–O′(15)	115.6 (3)
C(6)–C(5)–O(15)	59.6 (2)	C′(6)–C′(5)–O′(15)	59.8 (2)
C(1)–C(6)–C(5)	114.8 (3)	C′(1)–C′(6)–C′(5)	116.1 (3)
C(1)–C(6)–O(15)	110.2 (3)	C′(1)–C′(6)–O′(15)	109.2 (2)
C(1)–C(6)–C(16)	119.3 (3)	C′(1)–C′(6)–C′(16)	118.7 (3)
C(5)–C(6)–O(15)	58.5 (2)	C′(5)–C′(6)–O′(15)	58.8 (2)
C(5)–C(6)–C(16)	122.4 (3)	C′(5)–C′(6)–C′(16)	122.4 (3)
O(15)–C(6)–C(16)	115.2 (3)	O′(15)–C′(6)–C′(16)	115.2 (3)
C(2)–O(8)–C(9)	115.8 (3)	C′(2)–O′(8)–C′(9)	116.7 (3)
C(4)–C(10)–C(11)	110.2 (3)	C′(4)–C′(10)–C′(11)	110.1 (3)
C(4)–C(10)–C(12)	109.6 (3)	C′(4)–C′(10)–C′(12)	109.1 (3)
C(4)–C(10)–C(13)	110.7 (3)	C′(4)–C′(10)–C′(13)	110.4 (3)
C(11)–C(10)–C(12)	109.1 (3)	C′(11)–C′(10)–C′(12)	109.7 (3)
C(11)–C(10)–C(13)	108.7 (3)	C′(11)–C′(10)–C′(13)	108.8 (3)
C(12)–C(10)–C(13)	108.7 (3)	C′(12)–C′(10)–C′(13)	108.7 (3)
C(5)–O(15)–C(6)	61.8 (2)	C′(5)–O′(15)–C′(6)	61.4 (2)
C(6)–C(16)–C(17)	112.5 (3)	C′(6)–C′(16)–C′(17)	110.7 (3)
C(6)–C(16)–C(18)	108.8 (3)	C′(6)–C′(16)–C′(18)	109.2 (3)
C(6)–C(16)–C(19)	109.5 (3)	C′(6)–C′(16)–C′(19)	109.6 (3)
C(17)–C(16)–C(18)	108.3 (3)	C′(17)–C′(16)–C′(18)	108.5 (3)
C(17)–C(16)–C(19)	107.5 (3)	C′(17)–C′(16)–C′(19)	108.3 (3)
C(18)–C(16)–C(19)	110.2 (3)	C′(18)–C′(16)–C′(19)	110.5 (3)

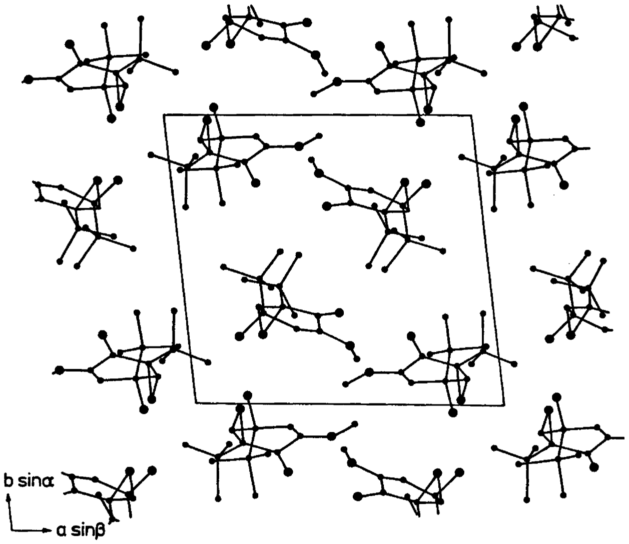

Fig. 4. Projection of the crystal structure along the *c* direction. •, carbon; ●, oxygen.

Table 7. Intermolecular distances shorter than 3. 8 Å.

Superscript	Coordinates	Superscript	Coordinates
none	$x;\ y;\ z$	iii	$1-x;\ 2-y;\ -z$
i	$x;\ -1+y;\ z$	iv	$1-x;\ 2-y;\ 1-z$
ii	$-x;\ 2-y;\ -z$	v	$1-x;\ 3-y;\ 1-z$

C(13)–O(15$^{\mathrm{ii}}$)	3.632 (4)	C(11)–C′(17$^{\mathrm{i}}$)	3.788 (5)
O(14)–C(17$^{\mathrm{ii}}$)	3.645 (5)	C(12)–O′(8$^{\mathrm{iii}}$)	3.720 (4)
C(3)–O′(15)	3.703 (4)	C(13)–C′(5$^{\mathrm{ii}}$)	3.728 (4)
C(4)–O′(15)	3.632 (3)	C(13)–O′(14$^{\mathrm{ii}}$)	3.541 (4)
O(7)–C′(9$^{\mathrm{iv}}$)	3.285 (5)	C(13)–O′(15$^{\mathrm{ii}}$)	3.569 (4)
O(7)–C′(19$^{\mathrm{i}}$)	3.629 (5)	O(14)–O′(15)	2.797 (3)
O(8)–O′(8)	3.608 (4)	O(15)–O′(14)	2.967 (3)
O(8)–C′(9)	3.579 (5)	O(15)–O′(15)	3.233 (3)
O(8)–C′(9$^{\mathrm{iv}}$)	3.666 (5)	C′(2)–C′(11$^{\mathrm{v}}$)	3.740 (5)
C(9)–O′(8)	3.328 (5)	O′(8)–C′(11$^{\mathrm{v}}$)	3.413 (4)
C(9)–C′(9)	3.624 (6)	C′(9)–C′(11$^{\mathrm{v}}$)	3.724 (6)
C(9)–C′(18$^{\mathrm{iii}}$)	3.713 (6)		

Table 8. Least-squares planes and deviations (Å). The planes are described in terms of normalized equations in the orthogonal coordinate system (m, n, p) having $p \parallel c$, n in the bc plane and m in the a,b,c-octant.

Plane A $0.1693m+0.9350n+0.3154p= 9.1427$
Plane B $0.3487m+0.9027n+0.2522p= 9.1738$
Plane C $-0.0403m+0.9264n+0.3745p= 8.1605$
Plane A′ $0.3964m+0.8868n+0.2375p=13.9480$
Plane B′ $0.3145m+0.9375n+0.1489p=14.5499$
Plane C′ $0.4577m+0.8169n+0.3263p=13.4030$

Plane A		Plane B		Plane C	
Atom	Deviation	Atom	Deviation	Atom	Deviation
C(1)^a	−0.267	C(1)	0.004	C(1)	0.004
C(2)	0.009	C(2)^a	0.513	C(2)	0.009
C(3)	−0.009	C(3)^a	0.487	C(3)	−0.009
C(4)^a	−0.258	C(4)	−0.005	C(4)	0.004
C(5)	0.008	C(5)	0.009	C(5)^a	0.531
C(6)	−0.008	C(6)	−0.009	C(6)^a	0.525

Plane A′		Plane B′		Plane C′	
Atom	Deviation	Atom	Deviation	Atom	Deviation
C′(1)^a	0.169	C′(1)	−0.009	C′(1)	0.007
C′(2)	−0.022	C′(2)^a	−0.355	C′(2)	−0.017
C′(3)	0.022	C′(3)^a	−0.303	C′(3)	0.017
C′(4)^a	0.172	C′(4)	0.010	C′(4)	−0.008
C′(5)	−0.020	C′(5)	−0.020	C′(5)^a	−0.367
C′(6)	0.019	C′(6)	0.019	C′(6)^a	−0.328

[a] These atoms were omitted from the calculations of the least-squares planes.

The crystallographic asymmetric unit contains two molecules joined together by two hydrogen-bonds (Fig. 2). The hydroxyl oxygen O(14) in one molecule is hydrogen-bonded to the epoxide oxygen O′(15) of the other. The distances O′(15)···H(O14) and O(15)···H(O′14) are 1.83 and 1.97 Å, respectively, and the angles O′(15)···H(O14)–O(14) and O(15)···H(O′14)–O′(14) are 171 and 167°, respectively.

Fig. 3 indicates the numbering system used in all tables and shows the bond lengths within the two molecules. Bond distances and angles for the structure are listed in Tables 5 and 6. No correction for thermal vibrations have been made. The estimated standard deviations, based solely on least-squares parameters, are about 0.004 Å for the bonds and 0.3° for the angles. No distance between bonded non-hydrogen atoms in one molecule of the asymmetric unit differs by more than 0.019 Å from the corresponding distance in the other molecule.

The mean $C(sp^3)-C(sp^3)$ bond distance, excluding C(5) – C(6), is 1.532 Å. The longer bonds are between the highly substituted carbon atoms C(4),C(10) and C(6),C(16). The shortness of the C(5) – C(6) bond length reflects the strain caused by the epoxide ring. The $C(sp^2)-C(sp^3)$ bonds have an average length of 1.504 Å in good agreement with usually observed values. The $C(sp^2)-C(sp^2)$ single bond is slightly shorter, 1.492 Å. The $C(sp^3)-O$ bonds and the $C(sp^2)-O$ bond have mean lengths of 1.430 and 1.357 Å, respectively.

The molecular packing is shown in Fig. 4. Intermolecular contacts less than 3.8 Å are listed in Table 7. The hydrogen-bonded dimers are held in position in the unit cell by van der Waals forces. Some of the van der Waals distances are shorter than normal, for example the $O(7)-C'(9^{iv})$ distance of 3.285 Å.

The best least-square planes through the ring are given for each of the dimer molecules in Table 8. In the non-primed molecule, the sets of atoms C(1), C(2), C(3), C(4); C(1), C(4), C(5), C(6); and C(2), C(3), C(5), C(6) are each coplanar within ±0.009 Å. In the primed molecule the deviations from the best planes for the same sets of atoms are ±0.017, ±0.020, and ±0.022 Å, respectively. All hydrogen atoms lie in chemically reasonable positions with apparent bond distances ranging from 0.76 to 1.12 Å, mean value 0.96 Å.

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