of the protons on C′(6) straddle the $O(5^{I})$–$C(5^{I})$ bond. The other proton is located then between the methylene protons of $C(5^{I})$ and directed towards $C(6^{IV})$. A similar meshing of the C(6) protons with the O′(5)–C′(5) bond and the methylene protons of C′(5) is necessary to account for the short distances of 3·39 Å and 3·75 Å between $C(6^{IV})$ and O′(5) and C′(5). If this arrangement of the methyl protons is basically correct, then the approach distance between C′(6) and $C(6^{I})$, and C′(6) and $C(6^{II})$, should be approximately 4·4 Å and 3·7 Å, if the proton van der Waals radius is taken as 1·2 Å. The observed distances are 4·11 Å and 3·62 Å respectively.

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Crystal and Molecular Structure of L-α-Glycerylphosphorylcholin

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The crystal structure of L-α-glycerylphosphorylcholin – the basic unit of the lecithins – has been determined and refined to an R value of 0·062 by anisotropic least-squares treatment.

Introduction

Our X-ray studies of lipids in the solid state have been undertaken to contribute to the knowledge of the structure of important biological systems with partly ordered lipid molecules such as cell membranes and the myelin sheath of nerves. Phosphatides with zwitterion structure (lecithins, cephalins, sphingomyelins) are important components in such systems. In order to obtain accurate structural information on the polar regions in the lecithins, we have performed a single-crystal analysis of the basic unit, glycerylphosphorylcholin (GPC).

Experimental

Optically active L-α-GPC ($C_8H_{20}O_6NP$) was synthesized according to Baer & Kates (1948). The compound was purified by four recrystallizations of its $CdCl_2$ complex. GPC was recovered by dissolving the complex in water and passing the solution through an ion exchanger (Tattrie & McArthur, 1958) and finally dried in vacuum over phosphorus pentoxide.

Crystals of GPC were obtained from ethanol (99·5%). They grow in long prisms and are often twinned. As GPC is very hygroscopic the crystals had to be handled in a water-free atmosphere and mounted in glass capillaries for the X-ray work.

The crystals are monoclinic ($P2_1$) with the following cell dimensions (Cu $K\alpha$ radiation): $a = 10·10$, $b = 7·71$, $c = 16·62$ Å, $\beta = 102·7°$.

A reasonable value for the calculated density of the crystals, 1·320 g.cm^{-3}, is obtained if there are four molecules per cell. The Patterson series also conforms with two molecules per asymmetric unit.

Table 1. *Fractional atomic coordinates with standard deviations* × 10^5 (within brackets) *for the heavier atoms of the structure*

	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$
P(1)	0·75618	(14)	0·50164	(45)	0·07638	(10)
N(1)	1·17855	(47)	0·46781	(95)	0·12375	(27)
O(1)	0·36688	(34)	0·91207	(84)	0·14787	(22)
O(2)	0·71364	(35)	1·02920	(85)	0·12976	(23)
O(3)	0·68363	(38)	0·68369	(80)	0·05967	(25)
O(4)	0·88628	(37)	0·53917	(84)	0·15116	(21)
O(5)	0·67329	(42)	0·37357	(92)	0·11188	(30)
O(6)	0·80509	(38)	0·45962	(77)	−0·00003	(24)
C(1)	0·49754	(54)	0·99843	(122)	0·16559	(35)
C(2)	0·58712	(50)	0·93828	(109)	0·10709	(32)
C(3)	0·61784	(54)	0·74153	(127)	0·11985	(35)
C(4)	0·98227	(58)	0·66480	(118)	0·13862	(36)
C(5)	1·12703	(53)	0·60826	(106)	0·17234	(30)
C(6)	1·11141	(62)	0·29848	(108)	0·12782	(36)
C(7)	1·16462	(64)	0·52642	(136)	0·03370	(31)
C(8)	1·32862	(54)	0·44543	(134)	0·16279	(45)
P(1′)	0·78699	(14)	0·77195	(35)	0·60243	(8)
N(1′)	1·20830	(45)	0·84521	(100)	0·63007	(28)
O(1′)	0·39722	(39)	0·36879	(83)	0·60716	(23)
O(2′)	0·74924	(37)	0·23669	(73)	0·62904	(23)
O(3′)	0·71735	(37)	0·58362	(63)	0·59421	(19)
O(4′)	0·92882	(36)	0·73692	(74)	0·66865	(21)
O(5′)	0·71143	(38)	0·89129	(71)	0·64452	(23)
O(6′)	0·81460	(35)	0·80981	(68)	0·52009	(21)
C(1′)	0·51099	(35)	0·30496	(103)	0·57736	(33)
C(2′)	0·63732	(52)	0·32404	(87)	0·64726	(30)
C(3′)	0·68024	(50)	0·50816	(105)	0·66657	(28)
C(4′)	1·02850	(56)	0·62383	(103)	0·64619	(38)
C(5′)	1·17216	(53)	0·69586	(105)	0·67766	(34)
C(6′)	1·12992	(65)	1·00917	(121)	0·63900	(40)
C(7′)	1·18714	(83)	0·80890	(144)	0·54095	(40)
C(8′)	1·35720	(67)	0·88858	(164)	0·66630	(55)

Table 2. *U_{ij}'s together with standard deviations* (x10^4) *within brackets*

Allowance was made for anisotropic vibration with

$$\exp -2\pi^2(h^2a^{*2} . U_{11}+k^2b^{*2} . U_{22}+l^2c^{*2} . U_{33}+2kl . b^*c^* . U_{23}+2lhc^*a^* . U_{31}+2hka^*b^* . U_{12})$$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P(1)	0·0445 (7)	0·0352 (20)	0·0606 (8)	0·0003 (10)	0·0093 (6)	−0·0026 (10)
N(1)	0·0588 (24)	0·0381 (66)	0·0489 (23)	0·0073 (29)	0·0133 (18)	0·0079 (30)
O(1)	0·0527 (18)	0·0858 (49)	0·0571 (20)	0·0050 (25)	0·0217 (13)	0·0042 (24)
O(2)	0·0566 (19)	0·0299 (43)	0·0790 (20)	−0·0017 (25)	0·0231 (15)	−0·0025 (22)
O(3)	0·0545 (21)	0·0385 (45)	0·0709 (23)	0·0010 (24)	0·0178 (17)	0·0091 (21)
O(4)	0·0535 (19)	0·0504 (44)	0·0494 (18)	−0·0012 (24)	0·0089 (15)	−0·0003 (24)
O(5)	0·0653 (23)	0·0396 (56)	0·1084 (30)	0·0075 (32)	0·0245 (20)	0·0051 (30)
O(6)	0·0653 (21)	0·0435 (50)	0·0646 (21)	−0·0125 (23)	0·0064 (16)	0·0023 (24)
C(1)	0·0584 (29)	0·0641 (71)	0·0719 (31)	0·0015 (40)	0·0234 (22)	0·0174 (37)
C(2)	0·0533 (25)	0·0326 (64)	0·0590 (28)	0·0051 (35)	0·0198 (19)	−0·0060 (31)
C(3)	0·0682 (28)	0·0436 (69)	0·0809 (31)	0·0013 (38)	0·0373 (21)	−0·0073 (36)
C(4)	0·0637 (32)	0·0239 (70)	0·0672 (31)	−0·0137 (37)	0·0174 (24)	−0·0023 (36)
C(5)	0·0593 (30)	0·0302 (67)	0·0430 (25)	−0·0114 (30)	0·0063 (21)	0·0019 (33)
C(6)	0·0828 (34)	0·0187 (66)	0·0652 (31)	0·0005 (36)	0·0245 (24)	0·0011 (36)
C(7)	0·1217 (39)	0·0594 (69)	0·0417 (25)	0·0015 (35)	0·0319 (23)	0·0070 (45)
C(8)	0·0525 (28)	0·0772 (91)	0·0982 (45)	0·0172 (52)	0·0234 (27)	0·0137 (37)
P(1′)	0·0482 (6)	0·0314 (16)	0·0451 (6)	0·0009 (8)	0·0128 (4)	−0·0023 (9)
N(1′)	0·0610 (25)	0·0605 (62)	0·0567 (24)	0·0165 (29)	0·0185 (19)	−0·0034 (30)
O(1′)	0·0620 (22)	0·1248 (49)	0·0582 (20)	−0·0288 (26)	0·0145 (15)	−0·0020 (28)
O(2′)	0·0730 (20)	0·0310 (45)	0·0787 (21)	0·0061 (25)	0·0334 (16)	0·0047 (26)
O(3′)	0·0659 (21)	0·0357 (40)	0·0429 (16)	−0·0022 (19)	0·0162 (14)	−0·0122 (21)
O(4′)	0·0599 (19)	0·0513 (42)	0·0510 (17)	−0·0005 (22)	0·0127 (14)	−0·0086 (24)
O(5′)	0·0813 (23)	0·0182 (44)	0·0795 (21)	−0·0024 (24)	0·0320 (16)	−0·0020 (24)
O(6′)	0·0545 (19)	0·0674 (45)	0·0587 (19)	0·0086 (23)	0·0114 (15)	−0·0058 (22)
C(1′)	0·0664 (28)	0·0511 (64)	0·0599 (28)	−0·0117 (33)	0·0187 (21)	−0·0192 (32)
C(2)′	0·0613 (29)	0·0310 (56)	0·0497 (24)	−0·0006 (27)	0·0123 (21)	−0·0036 (28)
C(3′)	0·0579 (26)	0·0481 (61)	0·0388 (22)	0·0058 (31)	0·0160 (18)	−0·0000 (34)
C(4′)	0·0630 (30)	0·0408 (65)	0·0891 (35)	0·0215 (37)	0·0131 (27)	0·0028 (36)
C(5′)	0·0607 (28)	0·0528 (64)	0·0564 (30)	0·0264 (32)	0·0040 (24)	−0·0026 (31)
C(6′)	0·0934 (40)	0·0538 (70)	0·0836 (35)	0·0105 (43)	0·0364 (29)	−0·0027 (46)
C(7′)	0·1461 (55)	0·0648 (95)	0·0642 (32)	0·0098 (45)	0·0392 (33)	0·0126 (56)
C(8′)	0·0556 (35)	0·1569 (104)	0·1489 (56)	0·0621 (69)	0·0189 (36)	−0·0116 (51)

Multiple film Weissenberg photographs were recorded for the 0–4 layers about the *b* axis and the 0 and 2 layers about the *c* axis. The intensities were measured visually and corrected for the Lorentz and polarization factors but not for absorption.

Structure determination

A three-dimensional Patterson series was calculated with coefficients sharpened to correspond to those from point atoms at rest (Abrahamsson & Maslen, 1963). The positions of the two phosphorus atoms were easily derived from the series. They have different *y* coordinates, and no false symmetry is introduced in the electron density series based on the phases of the two atoms. The series in fact showed most of the other atoms in the structure but only the highest peaks were used for the following stage. After four rounds of Fourier refinement all atoms except hydrogen atoms had been located and the *R* value was 0·20.

The structure was further refined by anisotropic least-squares treatment using the full matrix. The progress of the refinement was checked at some stages by calculating difference syntheses. In the first of these, 13 of the hydrogen atoms showed up distinctly and were included in the following structure factor calculations. Each hydrogen atom was assigned an isotropic temperature factor calculated from the anisotropic vibration parameters of the hydrogen-carrying heavier atom. The second difference series calculated at $R=0{\cdot}09$ gave equally clearly the positions of the remaining hydrogen atoms except H(71′), H(73′) and H(81′) which, however, were included in the structure factor calculations with their expected coordinates as they belonged to CH_3 groups of which the other hydrogen atoms had been located from the difference maps. After six more least-squares cycles with all atoms of the molecule included the shifts were small (one-third of the standard deviations) and the refinement was stopped. The hydrogen parameters, however, had not been refined. As 289 parameters were varied simultaneously only the right hand sides of the normal equations matrix were calculated in some of the last cycles in order to reduce the computing time and the inverse matrix of an earlier stage was used for forming the shifts.

The final *R* value for the 1597 observed reflexions is 0·062. The scattering curves given in *International Tables for X-ray Crystallography* (1962), p. 202, were used. The calculations were performed on the Datasaab D21 computer with the program system developed by Abrahamsson, Aleby, Larsson, Nilsson, Selin & Westerdahl (1965). The weight used for each observation in the least-squares refinement was (Mills & Rollett, 1960)

$$w=\frac{1}{1+[(|F_o|-10|F_{\min}|)/4|F_{\min}|]^2}\,.$$

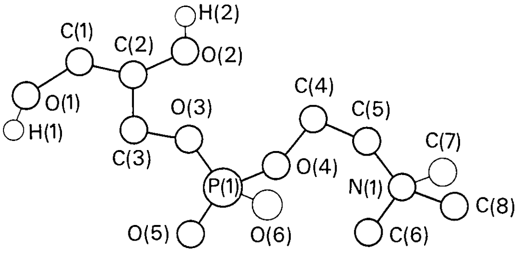

Fig. 1. Numbering of the atoms of the GPC molecule. The two molecules of the asymmetric unit have identical numbering but are differentiated by a prime.

Discussion

The atomic parameters used in the final calculation of structure factors are given with standard deviations in Tables 1–3. Observed and calculated structure factors are listed in Table 4. The numbering of atoms in the molecule is illustrated in Fig. 1. Primed symbols refer to the second molecule of the asymmetric unit.

The two molecules of the asymmetric unit are shown in Fig. 2. Their conformation and orientation in the unit cell is such that one is roughly related to the other by a *c*-glide plane at $y=0{\cdot}13$. As the molecule is optically active this relationship is, of course, not valid at

Table 3. *Parameters for the hydrogen atoms*

	x	y	z	B
H(1)	0·3300	0·8600	0·1000	4·84 Å^2
H(2)	0·7200	1·1550	0·1200	4·07
H(11)	0·4812	0·8620	0·1586	5·02
H(12)	0·5491	0·9694	0·2288	5·02
H(21)	0·5331	0·9603	0·0430	3·89
H(31)	0·6827	0·7191	0·1807	4·81
H(32)	0·5233	0·6684	0·1149	4·81
H(41)	0·9640	0·7839	0·1698	3·72
H(42)	0·9680	0·6884	0·0729	3·72
H(51)	1·1345	0·5587	0·2349	3·12
H(52)	1·1926	0·7200	0·1742	3·12
H(61)	1·1297	0·2558	0·1920	3·34
H(62)	1·0027	0·3120	0·1034	3·34
H(63)	1·1530	0·2038	0·0916	3·34
H(71)	1·0575	0·5516	0·0065	5·21
H(72)	1·2229	0·6438	0·0323	5·21
H(73)	1·2013	0·4240	−0·0007	5·21
H(81)	1·3817	0·5680	0·1593	5·88
H(82)	1·3413	0·4081	0·2273	5·88
H(83)	1·3718	0·3455	0·1299	5·88
H(1′)	0·3200	0·4400	0·5700	5·47
H(2′)	0·7500	0·1100	0·6300	4·73
H(11′)	0·4958	0·1682	0·5607	4·44
H(12′)	0·5241	0·3787	0·5239	4·44
H(21′)	0·6153	0·2659	0·7027	3·29
H(31′)	0·5966	0·5806	0·6820	3·73
H(32′)	0·7671	0·5104	0·7187	3·73
H(41′)	1·0081	0·6103	0·5796	5·58
H(42′)	1·0215	0·4958	0·6740	5·58
H(51′)	1·2447	0·5907	0·6749	4·31
H(52′)	1·1829	0·7358	0·7414	4·31
H(61′)	1·0211	0·9854	0·6172	5·85
H(62′)	1·1498	1·0479	0·7038	5·85
H(63′)	1·1608	1·1133	0·6027	5·85
H(71′)	1·2519	0·6999	0·5317	6·85
H(72′)	1·0821	0·7770	0·5160	6·85
H(73′)	1·2159	0·9231	0·5097	6·85
H(81′)	1·3701	0·9219	0·7311	8·39
H(82′)	1·4202	0·7766	0·6600	8·39
H(83′)	1·3876	0·9983	0·6329	8·39

Table 4. *Observed and calculated structure factors* (x100) *with phase angles* (*as fractions of one revolution*)

H	K	L	FOBS	FCALC	FI
0	0	2	3753	3499	1.0000
0	0	3	2081	2019	1.0000
0	0	4	20719	19439	0.5000
0	0	6	4388	4205	1.0000
0	0	7	289	157	1.0000
0	0	8	3983	3972	1.0000
0	0	9	798	814	0.5000
0	0	10	778	753	0.5000
0	0	11	1237	1233	0.5000
0	0	12	945	1002	1.0000
0	0	13	887	904	1.0000
0	0	15	1462	1483	0.0000
0	0	16	370	492	0.5000
0	0	17	498	316	0.0000
1	0	1	1819	1923	0.5000
1	0	2	6766	6823	1.0000
1	0	3	2616	2880	1.0000
1	0	4	7499	6864	1.0000
1	0	5	2761	2897	1.0000
1	0	6	701	575	1.0000
1	0	7	822	717	0.5000
1	0	8	2106	2181	0.5000
1	0	9	825	922	0.5000
1	0	10	1215	1247	0.5000
1	0	11	1085	1157	0.5000
1	0	13	1105	1154	0.5000
1	0	14	808	949	0.0000
1	0	16	364	377	1.0000
1	0	17	538	637	0.0000
1	0	-1	964	995	1.0000
1	0	-2	7549	6561	0.5000
1	0	-3	329	248	0.9999
1	0	-4	3287	3446	0.5000
1	0	-5	3798	3718	0.5000
1	0	-6	6315	6095	1.0000
1	0	-8	3808	3635	1.0000
1	0	-9	1808	1765	1.0000
1	0	-11	1225	1180	1.0000
1	0	-12	456	383	0.5000
1	0	-13	1962	2131	1.0000
1	0	-14	1051	1116	0.5000
1	0	-15	745	704	1.0000
1	0	-17	1070	1154	0.5000
1	0	-19	416	432	0.5000
2	0	0	12728	12575	0.5000
2	0	1	440	311	0.5000
2	0	2	9210	8825	0.5000
2	0	3	7461	7094	0.5000
2	0	4	1803	1827	1.0000
2	0	5	2953	2983	0.5000
2	0	6	2116	2239	1.0000
2	0	7	4082	4221	1.0000
2	0	8	1492	1420	0.5000
2	0	9	2033	2191	1.0000
2	0	10	1889	1987	0.5000
2	0	11	2229	2360	0.5000
2	0	13	1684	1859	0.5000
2	0	14	755	991	0.0000
2	0	-1	1020	976	1.0000
2	0	-2	191	133	0.5001
2	0	-3	290	242	0.5001
2	0	-4	5231	5005	1.0000
2	0	-5	2824	2584	1.0000
2	0	-6	1061	1002	1.0000
2	0	-8	2300	2215	0.5000
2	0	-9	481	411	1.0000
2	0	-14	1125	1193	0.5000
2	0	-15	2614	2741	0.5000
2	0	-16	375	164	0.5000
2	0	-17	442	509	0.5000
2	0	-18	499	589	1.0000
2	0	-19	1105	1123	1.0000
3	0	1	3197	3354	1.0000
3	0	2	9415	9138	0.5000
3	0	3	2882	2882	1.0000
3	0	4	6804	6655	0.5000
3	0	5	3620	3829	0.5000
3	0	6	1579	1553	1.0000
3	0	7	3548	3697	0.5000
3	0	8	1597	1594	1.0000
3	0	9	1393	1467	1.0000
3	0	10	1040	1138	0.5000
3	0	11	1445	1451	0.0000
3	0	12	426	447	0.5000
3	0	-1	440	436	1.0000
3	0	-2	2903	3207	1.0000
3	0	-3	999	986	0.5000
3	0	-4	2357	2092	0.5000
3	0	-5	901	906	0.5000
3	0	-6	2990	2869	0.5000
3	0	-7	2135	2131	1.0000
3	0	-8	2616	2405	0.5000
3	0	-9	256	226	1.0000
3	0	-10	1661	1625	0.5000
3	0	-11	2891	3049	0.5000
3	0	-12	595	383	1.0000
3	0	-13	1764	1785	0.5000
3	0	-14	1267	1320	1.0000
3	0	-15	462	573	1.0000
3	0	-17	1000	1001	1.0000
4	0	0	412	489	1.0000
4	0	1	2710	2615	0.5000
4	0	2	6368	6560	1.0000
4	0	3	3733	3653	1.0000
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10	1	-6	799	729	0.9548
10	1	-7	792	747	0.5456
10	1	-8	428	400	0.1275
10	1	-9	1306	1211	0.1394
10	1	-10	409	390	0.5090
10	1	-11	821	745	0.0823
10	1	-12	376	312	0.6132
10	1	-13	538	472	0.6456
10	1	-16	235	196	0.0702
10	1	1	696	645	0.3046
10	1	2	662	628	0.1501
10	1	3	741	621	0.3433
10	1	4	638	516	0.0746
10	1	6	421	153	0.6762
11	1	0	652	526	0.5884
11	1	-1	314	288	0.6450
11	1	-2	504	474	0.7171
11	1	-3	455	409	0.7367
11	1	-4	790	710	0.0446
11	1	-5	454	334	0.2138
11	1	-6	390	410	0.1510
11	1	-7	769	727	0.1745
11	1	-8	751	701	0.4921
11	1	-10	451	407	0.4391
11	1	-11	330	238	0.0542
11	1	-12	249	262	0.0708
11	1	-13	224	147	0.3338
11	1	-14	268	236	0.6369
11	1	4	307	237	0.1072
11	1	5	552	475	0.3664
11	1	6	541	537	0.1556
12	1	0	230	245	0.9581
12	1	-1	241	155	0.5167
12	1	-2	557	542	0.1150
12	1	-3	359	292	0.2592
12	1	-4	314	264	0.2676
12	1	-5	701	603	0.2361
12	1	-6	473	472	0.4734
12	1	-7	427	372	0.0941
12	1	-8	445	345	0.4454
12	1	-9	225	256	0.7606
12	1	-10	147	169	0.9934
12	1	-11	341	333	0.5929
12	1	1	151	164	0.7933
12	1	2	574	542	0.6207
0	1	2	9702	8726	0.9014
0	1	3	3552	3352	0.7175
1	1	0	4263	3764	0.3163
1	1	1	5169	5352	0.6393
1	1	-1	6716	6767	0.1463
1	1	-2	7771	8311	0.3913
1	1	-3	9083	9169	0.1461
2	1	1	4900	4649	0.1039
2	1	-1	4208	4392	0.6735
0	2	2	2073	1812	0.7159
0	2	3	1636	1763	0.4614
0	2	4	2226	2038	0.2273
0	2	5	804	812	0.4142
0	2	6	1533	1433	0.9731
0	2	7	1661	1616	0.3966
0	2	8	3177	3023	0.7331
0	2	9	1253	1165	0.6106
0	2	10	1158	1200	0.5914
0	2	11	1392	1335	0.6705
0	2	12	1319	1313	0.0664
0	2	13	547	413	0.9757
0	2	14	1302	1224	0.7707
0	2	15	471	469	0.4678
0	2	16	223	81	0.4967
1	2	1	3032	3108	0.0408
1	2	2	564	535	0.0789
1	2	3	4980	4752	0.7689
1	2	4	3085	2653	0.6107
1	2	5	1146	1147	0.8367
1	2	6	461	311	0.3350
1	2	7	2904	2722	0.4053
1	2	9	1566	1548	0.3507
1	2	10	1643	1943	0.5530
1	2	11	1095	1042	0.6551
1	2	12	1492	1478	0.5201
1	2	13	577	640	0.7624
1	2	14	792	627	0.9056
1	2	15	294	251	0.1134
1	2	16	657	717	0.9591
1	2	17	448	296	0.0320
1	2	-1	1800	1724	0.4283
1	2	-3	2206	2261	0.4551
1	2	-5	3316	3068	0.1111
1	2	-6	3535	3263	0.3772
1	2	-7	3665	3038	0.9483
1	2	-8	1396	1332	0.1103
1	2	-9	1514	1506	0.6073
1	2	-10	1951	1636	0.9297
1	2	-11	910	911	0.1706
1	2	-12	1318	1316	0.1773
1	2	-13	649	711	0.3567
1	2	-14	658	677	0.1277
1	2	-15	1479	1423	0.5887
1	2	-16	563	554	0.5445
1	2	-17	436	342	0.7277
1	2	-18	794	657	0.5003
2	2	0	3541	3354	0.3442
2	2	1	2096	2056	0.5040
2	2	2	2136	1927	0.6722
2	2	3	2217	1992	0.1501
2	2	4	1015	966	0.0774
2	2	5	595	621	0.6770
2	2	6	1065	1074	0.1707
2	2	7	2378	2425	0.7233
2	2	8	1429	1574	0.1257
2	2	9	1777	1793	0.5107
2	2	10	191	200	0.3044
2	2	11	1363	1997	0.3354
2	2	12	2067	2056	0.5527
2	2	13	897	956	0.1434
2	2	14	1296	1312	0.5163
2	2	17	325	221	0.5496
2	2	18	326	266	0.9576
2	2	19	253	232	0.0142
2	2	-2	1437	1306	0.3164
2	2	-3	2930	2331	0.5875
2	2	-4	2215	1911	0.6315
2	2	-5	6109	5635	0.9643
2	2	-6	4624	4159	0.2929
2	2	-7	1901	1944	0.3535
2	2	-8	2423	2169	0.2119
2	2	-9	3285	3075	0.4108
2	2	-10	2206	2171	0.6382
2	2	-11	963	1035	0.9532
2	2	-12	277	270	0.1454
2	2	-13	614	534	0.7711
2	2	-14	1363	1361	0.3700
2	2	-15	819	874	0.4623
2	2	-16	602	634	0.5640
2	2	-17	465	416	0.0610
2	2	-18	510	377	0.9606
2	2	-20	725	634	0.0515
3	2	0	484	432	0.0266
3	2	2	3483	3601	0.3236
3	2	3	2836	2657	0.4821
3	2	4	1036	1112	0.3723
3	2	5	1041	988	0.4692
3	2	6	2436	2285	0.6148
3	2	7	1693	1696	0.0003
3	2	8	743	816	0.3472
3	2	9	571	652	0.1007
3	2	10	2260	2261	0.0445
3	2	11	1207	1255	0.5816
3	2	12	1034	1073	0.9596
3	2	13	452	454	0.7046
3	2	14	963	862	0.4461
3	2	15	889	808	0.1886
3	2	16	666	719	0.4515
3	2	17	615	510	0.3692
3	2	-2	3101	2936	0.1969
3	2	-3	1825	1912	0.0111
3	2	-4	2668	2709	0.3111
3	2	-5	1933	1931	0.9964
3	2	-6	1063	1051	0.7436
3	2	-7	1913	1757	0.4880
3	2	-8	351	326	0.7934
3	2	-9	1675	1575	0.6151
3	2	-10	756	763	0.4371
3	2	-11	422	405	0.5126
3	2	-12	768	747	0.6070
3	2	-13	624	494	0.1604
3	2	-14	516	444	0.4731
3	2	-15	660	696	0.0466
3	2	-16	292	366	0.1606
3	2	-18	526	592	0.0026
3	2	-19	387	240	0.2760
3	2	-20	237	167	0.6413

Table 4 (*cont.*)

H	K	L	FOBS	FCALC	FI
4	2	0	2109	2105	0.2960
4	2	1	2616	2725	0.0722
4	2	2	1566	1558	0.0471
4	2	3	1390	1415	0.4607
4	2	4	2032	2006	0.9025
4	2	5	3662	3656	0.5564
4	2	6	2006	2172	0.4364
4	2	7	482	644	0.3518
4	2	8	1639	1726	0.4165
4	2	9	1767	1824	0.1023
4	2	10	1059	1129	0.9239
4	2	11	845	677	0.8312
4	2	12	1095	1002	0.0074
4	2	13	872	845	0.6666
4	2	14	827	797	0.1052
4	2	15	277	301	0.2617
4	2	16	365	281	0.8946
4	2	17	339	362	0.0269
4	2	-1	2760	2783	0.9499
4	2	-2	843	739	0.6617
4	2	-3	1627	1546	0.6833
4	2	-4	3156	3004	0.7391
4	2	-5	1416	1462	0.4830
4	2	-6	2262	2025	0.8344
4	2	-7	2026	1985	0.4680
4	2	-8	1479	1416	0.3166
4	2	-9	1074	1079	0.6638
4	2	-10	1569	1544	0.4109
4	2	-11	549	455	0.9841
4	2	-12	881	927	0.6986
4	2	-13	1558	1512	0.1346
4	2	-14	516	474	0.8213
4	2	-15	1114	1039	0.0722
4	2	-16	330	441	0.9996
4	2	-19	365	288	0.4922
4	2	-20	462	409	0.4491
5	2	0	3179	3184	0.6359
5	2	1	4521	4491	0.0094
5	2	2	2096	2105	0.8996
5	2	3	3036	3102	0.9999
5	2	4	3159	3272	0.0240
5	2	5	1098	1096	0.6414
5	2	6	381	306	0.2163
5	2	7	509	477	0.5743
5	2	8	1023	1005	0.5950
5	2	9	725	691	0.1653
5	2	10	583	572	0.6737
5	2	12	353	458	0.4357
5	2	13	273	277	0.7086
5	2	14	614	564	0.0956
5	2	15	401	381	0.6377
5	2	16	769	755	0.0098
5	2	-1	609	616	0.2231
5	2	-2	941	995	0.7399
5	2	-3	1298	1340	0.4528
5	2	-4	622	666	0.0651
5	2	-5	1741	1675	0.6357
5	2	-6	1264	1257	0.4496
5	2	-8	713	646	0.5275
5	2	-9	3009	2782	0.0968
5	2	-10	844	859	0.7493
5	2	-11	1055	971	0.0055
5	2	-12	901	881	0.8835
5	2	-13	1404	1382	0.6307
5	2	-14	897	860	0.0678
5	2	-15	208	301	0.6626
5	2	-18	658	536	0.6408
6	2	0	507	556	0.6951
6	2	1	837	889	0.4661
6	2	2	3267	3403	0.4958
6	2	3	1379	1357	0.0636
6	2	4	797	763	0.7427
6	2	5	1888	2042	0.0102
6	2	6	2633	2834	0.9741
6	2	7	434	629	0.9180
6	2	8	744	820	0.0256
6	2	9	701	673	0.5890
6	2	10	534	570	0.5020
6	2	12	744	669	0.5499
6	2	13	555	466	0.1311
6	2	14	698	644	0.5678
6	2	15	189	169	0.2887
6	2	-1	773	778	0.4851
6	2	-2	1333	1370	0.9416
6	2	-3	845	940	0.1825
6	2	-4	1415	1427	0.3798
6	2	-5	307	319	0.1506
6	2	-7	1018	1019	0.9390
6	2	-8	1457	1531	0.8897
6	2	-9	2159	2081	0.9943
6	2	-10	594	507	0.9662
6	2	-11	445	408	0.6096
6	2	-13	2073	2048	0.5480
6	2	-14	449	351	0.4742
6	2	-15	454	357	0.5731
6	2	-17	617	550	0.0249
7	2	0	2417	2560	0.1415
7	2	1	3010	3170	0.4890
7	2	2	1095	1122	0.5495
7	2	3	761	726	0.4434
7	2	4	2295	2597	0.5499
7	2	5	1028	1000	0.0835
7	2	6	669	760	0.3609
7	2	7	472	456	0.2669
7	2	8	780	790	0.0363
7	2	9	256	334	0.7756
7	2	10	580	569	0.9279
7	2	13	243	242	0.2426
7	2	14	461	415	0.5183
7	2	-1	860	866	0.7329
7	2	-2	1456	1468	0.0796
7	2	-3	2230	2354	0.9532
7	2	-4	1017	1013	0.7142
7	2	-5	751	661	0.1915
7	2	-6	421	397	0.6377
7	2	-7	565	509	0.2009
7	2	-8	575	549	0.0706
7	2	-9	413	395	0.7505
7	2	-10	363	406	0.1306
7	2	-11	1743	1721	0.5427
7	2	-12	618	777	0.3740
7	2	-13	910	863	0.4695
7	2	-14	575	524	0.3931
7	2	-15	672	629	0.0697
7	2	-17	402	318	0.0296
7	2	-18	316	267	0.8847
7	2	-19	315	311	0.6158
8	2	0	975	982	0.0561
8	2	1	513	511	0.4450
8	2	2	942	1034	0.0156
8	2	3	1251	1264	0.6175
8	2	4	598	571	0.2614
8	2	5	579	549	0.5648
8	2	6	666	755	0.4602
8	2	7	477	484	0.3527
8	2	8	1222	1095	0.5329
8	2	9	445	379	0.4136
8	2	10	236	202	0.3237
8	2	12	870	738	0.0409
8	2	-1	292	876	0.0198
8	2	-2	633	641	0.4542
8	2	-3	813	881	0.9451
8	2	-4	772	802	0.7421
8	2	-5	668	609	0.3456
8	2	-6	587	525	0.1884
8	2	-7	1529	1559	0.5344
8	2	-8	1613	1706	0.3157
8	2	-9	1652	1812	0.5526
8	2	-11	785	799	0.2039
8	2	-12	714	720	0.7934
8	2	-13	1766	1629	0.0664
8	2	-14	331	268	0.6403
8	2	-15	359	368	0.8872
8	2	-17	566	516	0.5691
8	2	-18	279	263	0.0749
9	2	1	441	419	0.1067
9	2	3	529	477	0.0090
9	2	4	1171	1128	0.0189
9	2	5	340	348	0.6244
9	2	6	841	717	0.0173
9	2	7	355	313	0.6332
9	2	8	681	765	0.5146
9	2	10	532	530	0.5192
9	2	-1	211	210	0.6700
9	2	-2	423	414	0.5003
9	2	-3	702	642	0.6422
9	2	-4	501	546	0.4037
9	2	-5	1225	1104	0.4453
9	2	-6	401	407	0.2597
9	2	-7	[illegible]	719	0.4273
9	2	-9	881	947	0.9275
9	2	-10	706	666	0.7943
9	2	-11	1176	1167	0.0205
9	2	-12	272	274	0.9415
9	2	-13	665	562	0.0642
9	2	-15	461	406	0.5662
9	2	-17	[illegible]	[illegible]	0.4901
10	2	0	462	466	0.5745
10	2	1	315	282	0.1080
10	2	2	632	529	0.6504
10	2	3	474	431	0.9517
10	2	6	686	765	0.0650
10	2	8	476	442	0.0232
10	2	-1	466	459	0.3475
10	2	-2	640	627	0.4837
10	2	-3	742	758	[illegible]
10	2	-4	342	306	0.0481
10	2	-5	573	520	[illegible]
10	2	-6	1365	[illegible]	[illegible]
10	2	-7	1321	1280	0.1266
10	2	-8	784	670	0.7552
10	2	-9	429	734	0.0501
10	2	-11	592	272	0.5936
10	2	-12	376	452	0.2171
10	2	-13	296	371	0.5073
10	2	-14	346	246	0.2745
11	2	0	169	112	0.5906
11	2	4	612	566	0.5316
11	2	-1	364	249	0.6959
11	2	-2	558	474	0.9764
11	2	-3	176	270	0.6569
11	2	-4	779	697	0.9360
11	2	-5	835	767	0.0738
11	2	-6	410	383	0.6257
11	2	-7	775	625	0.0726
11	2	-8	490	502	0.4321
11	2	-9	461	411	0.5674
11	2	-10	311	299	0.3073
11	2	-11	771	717	0.5155
12	2	0	397	426	0.0010
12	2	-1	423	366	0.6486
12	2	-3	408	297	0.1388
12	2	-4	325	306	0.4732
12	2	-5	455	373	0.2014
12	2	-6	557	504	0.4035
12	2	-7	508	450	0.5450
12	2	-8	125	154	0.3163
12	2	-9	719	675	0.5916
12	2	-10	360	383	0.9127
0	2	1	7989	7979	0.0426
1	2	0	5594	5757	0.2966
1	2	-2	4996	4903	0.8536
1	2	-4	5414	4614	0.7743
2	2	-1	7928	8096	0.5247
3	2	1	5526	5474	0.5455
3	2	-1	5420	5452	0.5331
0	3	1	1061	1058	0.2740
0	3	2	1474	1314	0.1352
0	3	3	1059	1006	0.3521
0	3	4	2356	2456	0.6356
0	3	5	1166	1159	0.8763
0	3	6	1589	1596	0.6901
0	3	7	1095	1133	0.9762
0	3	8	1451	1501	0.0163
0	3	9	1545	1605	0.3123
0	3	10	375	297	0.4145
0	3	11	1268	1371	0.2216
0	3	12	1516	1553	0.5347
0	3	13	1279	1350	0.0101
0	3	14	479	561	0.7937
0	3	15	630	699	0.7176
0	3	16	773	767	[illegible]
0	3	17	819	812	0.5717
1	3	2	960	1035	0.6735
1	3	3	1693	2060	0.2925
1	3	4	1767	1638	0.8171
1	3	5	1622	1686	0.3575
1	3	7	2484	2550	0.6719
1	3	8	632	630	[illegible]
1	3	9	960	966	0.7019
1	3	10	1337	1314	0.0830
1	3	11	1201	1201	0.3827
1	3	12	1331	1372	0.2685
1	3	13	1174	1223	0.1671
1	3	14	719	672	0.4567
1	3	15	889	679	0.1646
1	3	18	364	364	0.0843
1	3	-1	765	633	0.6200
1	3	-2	2237	2330	0.1304
1	3	-3	2463	2269	0.3735
1	3	-4	2613	2461	0.2275
1	3	-5	660	626	0.9070
1	3	-6	1058	1070	0.1061
1	3	-7	430	353	0.7677
1	3	-8	1212	1167	0.6004
1	3	-9	723	760	0.7583
1	3	-10	1541	1461	[illegible]
1	3	-11	554	514	0.5563
1	3	-12	2109	2204	0.2160
1	3	-13	1390	1460	0.2656
1	3	-14	525	332	0.3145
1	3	-15	699	[illegible]	0.1244
1	3	-16	287	303	0.7066
1	3	-17	606	492	0.7665
1	3	-18	336	247	0.0075
1	3	-19	361	463	0.5466
2	3	1	867	769	0.3158
2	3	3	3519	3446	0.9135
2	3	4	1242	1274	0.0167
2	3	5	373	383	[illegible]
2	3	6	367	400	0.4359
2	3	7	869	823	0.4407
2	3	8	946	917	0.4917
2	3	9	1326	1221	0.7920
2	3	10	1359	1407	0.9406
2	3	11	797	735	0.7104
2	3	12	1199	1240	0.0485
2	3	13	642	589	0.4965
2	3	14	913	979	0.3457
2	3	15	261	323	0.1637
2	3	16	477	513	0.4253
2	3	17	680	710	0.1553
2	3	-3	1751	1735	[illegible]
2	3	-4	2961	3016	0.6685
2	3	-6	1922	1889	0.2577
2	3	-7	1160	1132	0.5230
2	3	-8	1035	1019	0.0783
2	3	-9	1906	1842	0.3935
2	3	-10	828	841	0.0052
2	3	-11	1218	1248	0.1543
2	3	-12	543	649	0.2367
2	3	-13	423	336	0.0512
2	3	-14	622	647	0.4997
3	3	0	1619	1605	0.8554
3	3	1	3602	3618	0.4663
3	3	2	1208	1063	0.3172
3	3	3	1302	1200	0.5472
3	3	4	1663	1643	0.3129
3	3	5	690	638	0.1930
3	3	6	920	831	0.0545
3	3	7	1275	1310	0.3151
3	3	8	1058	1059	0.3630
3	3	9	639	574	0.9263
3	3	10	911	1058	0.3650
3	3	11	852	609	0.7468
3	3	12	982	1039	0.8277
3	3	13	1054	1066	0.6093
3	3	14	699	693	0.8493
3	3	15	473	478	0.7259
3	3	16	409	375	0.1857
3	3	17	331	304	0.0796
3	3	-1	3267	3010	0.9066
3	3	-2	4378	4450	0.6611
3	3	-3	4212	4060	0.8677
3	3	-4	3906	3757	0.7059
3	3	-5	1614	1680	0.3810
3	3	-6	2852	3005	0.1156
3	3	-7	2334	2220	0.3297
3	3	-8	1363	1266	0.2619
3	3	-9	714	620	0.9666
3	3	-10	3094	3148	0.6671
3	3	-11	1051	1034	0.0236
3	3	-12	1262	1376	0.7018
3	3	-13	300	331	0.1264
3	3	-15	424	587	0.6063
4	3	0	1803	1885	0.7355
4	3	1	625	602	0.3791
4	3	2	2760	2784	0.6866
4	3	3	1343	1326	0.5226
4	3	4	1694	1570	0.7717
4	3	5	2239	2259	0.6743
4	3	6	476	523	0.2032
4	3	7	514	525	0.5173
4	3	8	1306	1417	0.3452
4	3	9	1902	2005	0.1967
4	3	10	505	511	0.5804
4	3	11	899	926	0.1703
4	3	12	692	649	0.6399
4	3	13	664	564	0.6751
4	3	15	677	618	0.6567
4	3	16	539	482	0.9694
4	3	-1	4489	4374	0.9105
4	3	-2	1246	1209	0.4462
4	3	-3	752	781	0.1209
4	3	-4	1743	1713	0.3895
4	3	-5	5807	5697	0.4114
4	3	-6	689	675	0.8956
4	3	-7	362	343	0.9465
4	3	-8	1496	1430	0.7294
4	3	-9	2971	3009	0.9305
4	3	-10	1461	1454	0.6345
4	3	-11	750	740	0.5610
4	3	-12	555	604	0.6578
4	3	-13	917	914	0.5754
4	3	-15	514	490	0.8353
5	3	0	1611	1646	0.3173
5	3	1	704	700	0.1463
5	3	2	1788	1707	0.5164
5	3	3	2272	2400	0.0247
5	3	4	2060	2081	0.7046
5	3	5	458	374	0.0327
5	3	6	1586	1677	0.8245
5	3	7	1700	1732	0.6340
5	3	8	576	610	0.9648
5	3	9	479	502	0.6064
5	3	11	862	810	0.1888
5	3	12	529	549	0.5074
5	3	13	645	629	0.0769
5	3	14	502	554	0.3582
5	3	15	404	361	0.1503
5	3	-1	2661	2645	0.3569
5	3	-2	2741	2732	0.1662
5	3	-3	1958	1944	0.4197
5	3	-4	1665	1630	0.1027
5	3	-5	1253	1177	0.6881
5	3	-6	1710	1721	0.6868
5	3	-7	2089	2099	0.8438
5	3	-8	1881	1935	0.5866
5	3	-9	1160	1110	0.6820
5	3	-10	574	618	0.1726
5	3	-11	1069	1072	0.4667
5	3	-12	1205	1285	0.0501
5	3	-13	676	643	0.4946
5	3	-15	412	405	0.9006
5	3	-16	276	343	0.5275
5	3	-17	440	480	0.0879
6	3	0	2244	2282	0.0108
6	3	1	2112	2181	0.4384
6	3	2	2344	2379	0.2602
6	3	3	1083	1140	0.1952
6	3	4	1563	1566	0.3624
6	3	5	1585	1665	0.0851
6	3	6	791	796	0.7864
6	3	7	524	523	0.0730
6	3	8	813	850	0.8731
6	3	9	685	667	0.7096
6	3	11	705	689	0.6757
6	3	12	361	340	0.8477
6	3	-1	597	606	0.5627
6	3	-2	966	1070	0.9791
6	3	-3	2026	2076	0.9064
6	3	-4	1177	1260	0.4833
6	3	-5	1036	981	[illegible]
6	3	-6	1492	1427	0.7962
6	3	-7	196	216	0.7563
6	3	-8	804	809	0.0912
6	3	-9	921	889	0.4904
6	3	-10	2505	2713	0.1927
6	3	-11	905	913	0.4479
6	3	-12	1301	1284	0.1716
6	3	-13	639	671	0.0440
6	3	-14	588	610	[illegible]
6	3	-15	445	460	0.0546
6	3	-16	789	725	0.6233
7	3	0	1606	1702	0.7776
7	3	1	1678	1729	[illegible]
7	3	2	1591	1691	0.0244
7	3	3	749	771	0.3235
7	3	4	1394	1469	0.2243
7	3	5	507	538	0.1037
7	3	6	629	672	0.3610
7	3	9	561	537	0.2613
7	3	10	373	304	0.2324
7	3	11	241	333	0.7313
7	3	12	476	466	0.0506
7	3	13	462	490	0.7122
7	3	-1	1638	1675	0.7917
7	3	-2	1776	1742	[illegible]
7	3	-3	1619	1693	0.0497
7	3	-4	1148	1296	0.3272
7	3	-5	536	507	0.2821
7	3	-6	2126	2172	0.2173
7	3	-7	1358	1413	0.4663
7	3	-8	1413	1437	0.0703
7	3	-9	990	1071	0.3031
7	3	-10	332	377	0.9194
7	3	-11	851	770	0.1358
7	3	-12	921	1016	0.4793
7	3	-13	565	523	[illegible]
7	3	-14	356	408	0.5447
7	3	-15	375	316	0.7693
7	3	-16	575	471	0.9259
7	3	-17	606	472	0.5771
7	3	-18	341	319	0.0655
8	3	0	1170	1225	0.5296
8	3	1	1328	1424	0.6457
8	3	2	875	984	[illegible]
8	3	3	690	782	0.5369
8	3	4	965	701	0.6443
8	3	5	725	774	0.5996
8	3	7	341	270	0.7525
8	3	8	300	385	0.2154
8	3	9	423	403	0.1241
8	3	10	595	570	0.4256
8	3	11	441	441	0.2204
8	3	-1	572	605	0.5289
8	3	-2	1503	1556	0.5327
8	3	-3	1900	2007	0.3024
8	3	-4	1647	1719	0.0913
8	3	-5	1061	1140	0.2787
8	3	-6	1171	1261	0.1279
8	3	-7	773	871	0.6956
8	3	-8	1209	1311	0.6267
8	3	-10	1225	1326	0.5554
8	3	-11	899	916	0.0248
8	3	-12	327	273	0.6657
8	3	-13	337	321	0.7844
8	3	-14	367	381	0.0355
8	3	-15	718	719	0.4945
8	3	-16	438	406	0.0938
8	3	-17	402	349	0.3169
9	3	0	423	446	0.2871
9	3	1	1152	1218	0.1603
9	3	2	717	690	0.6029
9	3	4	684	595	0.5567
9	3	5	600	604	0.6484
9	3	6	509	526	0.8556
9	3	7	712	671	0.6561
9	3	8	467	392	0.8948
9	3	-1	623	608	0.2565
9	3	-2	830	904	0.2732
9	3	-3	1243	1277	0.5549
9	3	-4	719	771	0.6372
9	3	-5	601	551	0.7058
9	3	-6	1038	1063	0.7634
9	3	-7	960	1069	0.9636
9	3	-8	950	939	0.5991
9	3	-9	290	328	0.6817
9	3	-10	766	750	0.6654
9	3	-13	349	257	0.3779
9	3	-14	622	623	0.1721
9	3	-15	404	302	0.3611
9	3	-16	316	192	0.4019
10	3	0	414	423	0.1642
10	3	1	499	522	0.3306
10	3	2	347	311	0.3390
10	3	3	839	778	0.1466
10	3	4	316	350	0.4819
10	3	5	219	312	0.0572
10	3	-1	923	879	0.6166
10	3	-2	719	738	0.8814
10	3	-3	487	530	0.7835
10	3	-4	1056	980	0.7386
10	3	-5	686	691	0.0093
10	3	-6	833	895	0.5348
10	3	-7	274	216	0.9611
10	3	-8	380	412	0.3137
10	3	-9	261	271	0.4244
10	3	-10	795	733	0.0755
10	3	-11	447	390	0.4359
10	3	-12	373	345	0.1638
10	3	-13	352	283	0.5358
10	3	-14	332	248	0.4642
11	3	0	418	393	0.9640
11	3	1	428	396	0.7165
11	3	2	331	305	0.9415
11	3	3	226	209	0.5047
11	3	-1	206	217	0.8856
11	3	-2	197	229	0.6164
11	3	-3	238	205	0.9243
11	3	-4	414	438	0.4630
11	3	-5	238	242	0.1188
11	3	-6	536	482	0.8318
11	3	-7	489	517	0.3699
11	3	-8	669	617	0.1226
11	3	-9	477	441	0.5058
11	3	-10	401	368	0.0491
11	3	-11	318	328	0.9383
1	3	0	2379	2323	0.1469
1	3	1	5419	5709	0.9203
2	3	0	4540	4200	0.1830
2	3	2	5094	4985	0.8050
2	3	-1	5380	5141	0.4178
2	3	-2	4947	4706	0.7517
0	4	1	4426	4396	0.8159
0	4	2	1265	1253	0.0988
0	4	3	1175	1195	0.8425
0	4	4	1233	1177	0.6392
0	4	5	1755	1678	0.3140
0	4	6	1122	1140	0.6592
0	4	8	581	592	0.3257
0	4	9	1203	1197	0.7062
0	4	10	927	842	0.0682
0	4	11	716	722	0.5663
0	4	12	579	535	0.9286
0	4	13	791	718	0.4877
0	4	14	181	379	0.6551
0	4	15	945	887	0.0119
0	4	16	615	548	0.7734
0	4	17	339	287	0.4487
0	4	18	358	317	0.8059
1	4	0	1971	2012	[illegible]
1	4	1	1220	1154	0.9714
1	4	2	4094	4150	0.0705
1	4	3	2787	2762	0.8058
1	4	4	924	848	0.7571
1	4	5	2143	2146	0.7567
1	4	6	1413	1411	0.6046
1	4	7	812	738	0.0009
1	4	8	467	446	0.5389
1	4	9	497	441	0.3605
1	4	10	604	738	0.6053
1	4	11	1844	1909	[illegible]
1	4	12	368	395	[illegible]
1	4	13	581	815	[illegible]
1	4	14	774	584	0.1604
1	4	15	465	554	0.9763
1	4	16	871	861	0.5806
1	4	17	299	449	0.0838
1	4	-1	1237	1256	0.2807
1	4	-2	2821	3084	0.5672
1	4	-3	1760	1606	0.9307
1	4	-4	1354	1258	0.4850
1	4	-5	1871	1796	0.3836
1	4	-6	1420	1387	0.1475
1	4	-7	961	1009	0.5109
1	4	-8	1460	1463	0.0653
1	4	-9	2140	2146	0.7958
1	4	-10	1336	1315	0.0163
1	4	-11	1240	1243	0.0793
1	4	-12	699	933	0.7253
1	4	-13	1625	1565	0.1618
1	4	-14	1409	1295	0.6708
1	4	-15	529	430	0.5931
1	4	-16	266	228	0.8096
1	4	-17	1083	888	0.5456
1	4	-18	440	322	0.2799
2	4	0	2604	2768	0.5498
2	4	1	2315	2221	0.3535
2	4	2	1235	1155	0.5641
2	4	3	2045	1938	0.3639
2	4	4	2068	2011	0.1825
2	4	5	462	464	0.1314
2	4	6	1550	1582	0.0795
2	4	7	1070	1085	0.9580
2	4	8	1079	1164	0.7005
2	4	9	385	320	0.1519
2	4	10	1326	1399	[illegible]
2	4	11	367	363	0.4288
2	4	12	583	615	0.2814
2	4	13	724	691	0.6004
2	4	14	424	514	0.1697
2	4	15	769	742	0.5573
2	4	16	358	292	0.3605
2	4	-1	1522	1434	0.2958
2	4	-2	1681	1606	0.4915
2	4	-3	510	394	0.0820
2	4	-4	1241	1178	0.0127
2	4	-5	427	503	0.5797
2	4	-6	1797	1725	0.0611
2	4	-7	341	296	0.3650
2	4	-9	1688	1675	0.0728
2	4	-10	716	628	0.7979
2	4	-11	1222	1276	0.1536
2	4	-12	257	261	0.6026
2	4	-13	1106	1196	0.4690
2	4	-14	962	966	0.3688
2	4	-15	971	896	0.5877
2	4	-16	781	731	0.2318
2	4	-17	324	357	0.0977
2	4	-18	320	236	0.9629
2	4	-19	557	553	0.1400
3	4	0	4243	4172	0.5853
3	4	1	332	376	0.3565
3	4	2	2266	2207	0.6272
3	4	3	1787	1793	0.3596
3	4	4	436	373	0.6176
3	4	5	1720	1697	0.4679
3	4	6	856	888	0.1523
3	4	7	841	778	0.4569
3	4	8	1199	1281	0.2129
3	4	9	1371	1401	0.0894
3	4	10	259	405	0.3484
3	4	11	1166	1165	0.0301
3	4	12	660	618	0.7774
3	4	13	282	256	0.3132
3	4	15	571	561	0.4343
3	4	16	437	449	0.2818
3	4	17	325	361	0.5705
3	4	-1	675	769	0.2724
3	4	-2	357	402	0.2125
3	4	-3	1820	1630	0.2447
3	4	-4	3890	4100	0.0500
3	4	-5	914	826	0.8222
3	4	-6	514	608	0.7697
3	4	-7	326	376	0.8557
3	4	-8	2664	2620	0.5498
3	4	-9	2119	2141	0.2865
3	4	-10	1173	1194	0.2835
3	4	-11	1036	997	0.3732
3	4	-12	1318	1385	0.2532
3	4	-13	1031	1011	0.7143
3	4	-14	256	286	0.4269
3	4	-15	499	395	0.8791
3	4	-16	861	754	0.9726
3	4	-17	602	541	0.1699
3	4	-18	391	390	0.0672
4	4	0	1794	1760	0.0219
4	4	1	1183	1141	0.9843
4	4	2	284	196	0.3997
4	4	3	959	974	0.9662
4	4	4	2347	2238	0.5433
4	4	6	1569	1502	0.6940
4	4	7	1672	1703	0.4531
4	4	8	766	756	0.9494
4	4	9	758	837	0.5232
4	4	10	737	858	0.1732
4	4	11	689	894	0.9702
4	4	13	898	875	0.1115
4	4	14	149	263	0.6741
4	4	15	363	345	0.1127
4	4	-1	1257	1214	0.8115
4	4	-2	1887	1802	0.0664
4	4	-3	1437	1520	0.4887
4	4	-4	749	654	0.9999
4	4	-5	990	1045	0.1668
4	4	-6	2821	2855	0.5649
4	4	-7	933	936	0.0731
4	4	-8	2508	2442	0.5293
4	4	-9	1770	1825	0.5291
4	4	-10	1385	1394	0.1041
4	4	-11	1200	1122	0.6569
4	4	-12	1342	1385	0.0577
4	4	-13	1359	1350	0.9069
4	4	-14	486	471	0.7224
4	4	-15	388	316	0.9877
4	4	-18	519	397	0.2838
5	4	0	793	750	0.8630
5	4	1	1585	1534	0.7292
5	4	2	2671	2705	0.9885
5	4	3	1078	1087	0.0780
5	4	4	1883	1971	0.1430
5	4	5	1706	1716	0.0561
5	4	6	1341	1329	0.4917
5	4	7	684	713	0.7601
5	4	8	1072	1025	0.6769
5	4	9	1096	1120	0.6107
5	4	10	719	762	0.9591
5	4	11	244	315	0.4822
5	4	14	344	350	0.6054
5	4	15	251	307	0.9272
5	4	-1	1621	1775	0.7838
5	4	-2	1505	1454	0.3658
5	4	-3	1588	1471	0.3044
5	4	-4	1417	1359	0.5473
5	4	-5	1165	1156	0.4486
5	4	-6	1578	1468	0.6076
5	4	-7	3049	2929	0.7594
5	4	-8	1138	1155	0.0465
5	4	-9	1646	1686	0.8087
5	4	-10	1423	1404	0.9877
5	4	-11	636	717	0.1989
5	4	-12	639	668	0.7481
5	4	-13	548	500	0.2773
5	4	-14	435	445	0.6821
5	4	-16	296	318	0.5143
5	4	-17	330	334	0.8883
5	4	-18	181	202	0.3375
6	4	0	1583	1570	0.5689
6	4	1	2156	2358	0.5875
6	4	2	1226	1197	0.0687
6	4	3	1087	1056	0.5115
6	4	4	1505	1552	0.0514
6	4	5	1612	1679	0.0582
6	4	7	1141	1168	0.9586
6	4	8	363	404	0.4969
6	4	10	167	269	0.0650
6	4	11	531	444	0.4873
6	4	13	584	594	0.6002
6	4	14	217	207	0.5080
6	4	-1	977	1008	0.8872
6	4	-2	2139	2082	0.4952
6	4	-3	898	904	0.0968
6	4	-4	707	811	0.1234
6	4	-5	683	756	0.7087
6	4	-6	1969	2103	0.9686
6	4	-7	749	854	0.6858
6	4	-8	901	800	0.9869

Table 4 (*cont.*)

H	K	L	FOBS	FCALC	FI
6	4	-9	756	830	0.1843
6	4	-11	760	763	0.2621
6	4	-12	505	542	0.5603
6	4	-14	765	713	0.5618
6	4	-15	406	301	0.6195
6	4	-16	358	218	0.6762
6	4	-17	181	248	0.5693
6	4	-18	498	457	0.9829
7	4	0	1086	1135	0.5443
7	4	1	729	818	0.3551
7	4	2	1330	1330	0.4961
7	4	3	1321	1361	0.5539
7	4	5	608	642	0.5885
7	4	6	443	465	0.0882
7	4	8	435	458	0.9464
7	4	9	575	525	0.0041
7	4	10	207	228	0.5210
7	4	11	596	545	0.0427
7	4	12	505	531	0.3586
7	4	-1	1727	1773	0.0827
7	4	-2	1269	1343	0.9408
7	4	-3	879	881	0.9515
7	4	-4	1620	1664	0.0846
7	4	-5	991	1046	0.4665
7	4	-6	789	916	0.2376
7	4	-7	1216	1248	0.2480
7	4	-8	260	257	0.5440
7	4	-9	541	570	0.0761
7	4	-10	757	783	0.5722
7	4	-11	653	695	0.6427
7	4	-12	890	813	0.5725
7	4	-13	170	242	0.4505
7	4	-14	295	325	0.0551
7	4	-15	390	366	0.3191
7	4	-16	525	525	0.0601
8	4	0	689	709	0.1729
8	4	1	1214	1281	0.0660
8	4	2	536	550	0.6520
8	4	3	428	535	0.1640
8	4	4	470	502	0.5668
8	4	5	549	668	0.4663
8	4	6	576	605	0.4174
8	4	7	823	785	0.5341
8	4	9	397	352	0.4355
8	4	11	454	466	0.0460
8	4	-1	563	577	0.2402
8	4	-2	1146	1229	0.0446
8	4	-3	690	730	0.4662
8	4	-4	350	347	0.6847
8	4	-6	1009	1032	0.5261
8	4	-7	385	436	0.3437
8	4	-8	408	383	0.6206
8	4	-9	360	338	0.3858
8	4	-10	487	414	0.5763
8	4	-11	343	352	0.9559
8	4	-12	208	374	0.2617
8	4	-14	1016	973	0.0752
8	4	-15	182	139	0.3985
8	4	-16	265	198	0.0396
9	4	0	304	332	0.1161
9	4	2	657	565	0.9637
9	4	3	1058	1005	0.0515
9	4	4	317	316	0.7983
9	4	5	601	545	0.0634
9	4	6	381	301	0.4269
9	4	7	266	247	0.4932
9	4	9	441	503	0.5126
9	4	-1	1121	1065	0.5164
9	4	-2	436	473	0.6701
9	4	-3	253	164	0.5814
9	4	-4	865	855	0.6139
9	4	-5	641	564	0.4072
9	4	-6	684	632	0.4645
9	4	-8	217	231	0.2245
9	4	-10	687	670	0.0697
9	4	-12	806	746	0.0517
9	4	-15	367	328	0.0344
10	4	0	206	260	0.3070
10	4	1	667	625	0.6512
10	4	2	429	389	0.7999
10	4	3	542	503	0.6242
10	4	4	316	276	0.7992
10	4	5	436	442	0.0466
10	4	6	176	228	0.0052
10	4	-1	222	231	0.7957
10	4	-2	707	616	0.4120
10	4	-4	304	265	0.6333
10	4	-6	426	372	0.9620
10	4	-7	376	268	0.9591
10	4	-8	529	484	0.0631
10	4	-9	434	360	0.3012
10	4	-10	532	360	0.0672
10	4	-11	161	236	0.6569
11	4	-3	221	235	0.0756
11	4	-4	349	276	0.[illegible]600
11	4	-5	383	267	0.[illegible]415
11	4	-6	452	346	0.9936
11	4	-7	471	461	0.7109
11	4	-8	340	281	0.0407
11	4	-9	265	325	0.6145
11	4	-10	263	259	0.5266

the asymmetric glycerol carbon atom. The differences in conformation are illustrated in Fig. 3 showing projections down the C(2)–C(3) and C(2′)–C(3′) bonds. The indicated dihedral angles $\varphi_{O(2)O(3)}$ and $\varphi_{O(2)C(1)}$ for one molecule are 71° and 179° respectively. The corresponding angles for the other GPC molecule of the asymmetric unit are 61° and 63°. In the first case a *gauche-trans* conformation has thus been adopted and a *gauche-gauche* conformation in the latter case. These arrangements also make possible an effective hydrogen bond system similar for both independent molecules.

As observed in 2-aminoethanol phosphate (Kraut, 1961) a *gauche* conformation is adopted about the bond between the two ethyl carbon atoms of the nitrogen

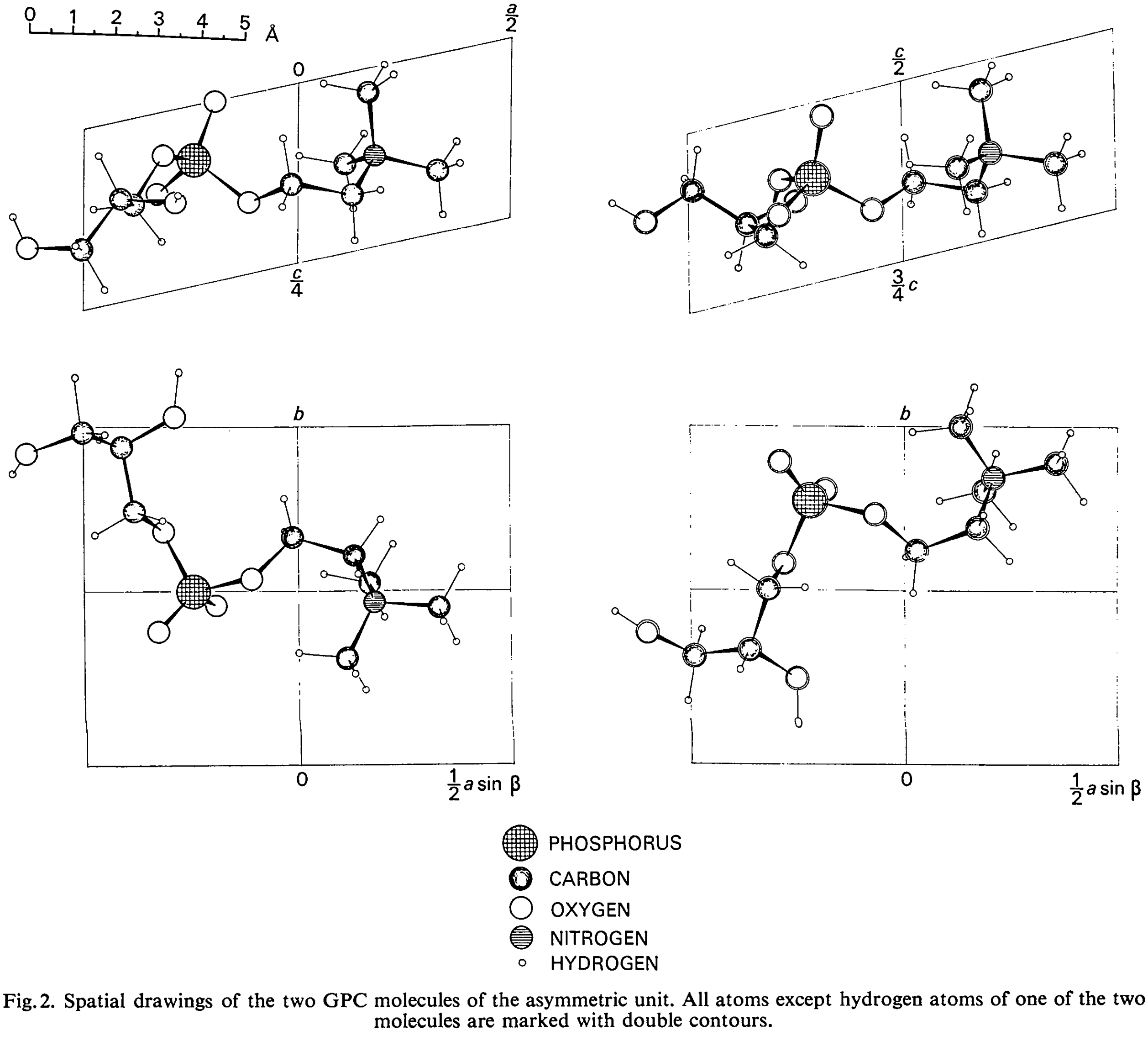

Fig. 2. Spatial drawings of the two GPC molecules of the asymmetric unit. All atoms except hydrogen atoms of one of the two molecules are marked with double contours.

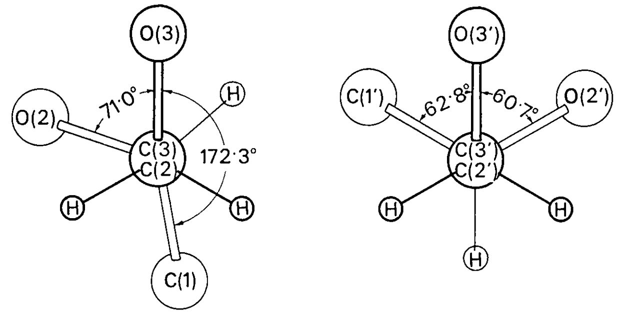

Fig. 3. Conformation of the independent GPC molecules as seen along the C(3)–C(2) and C(3')–C(2') bonds. C(2) and C(2') represent the asymmetric carbon atoms of the molecules.

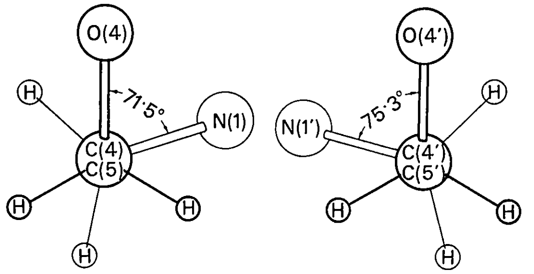

Fig. 4. Conformation of the two GPC molecules of the asymmetric unit as seen along the C(4)–C(5) and C(4')–C(5') bonds.

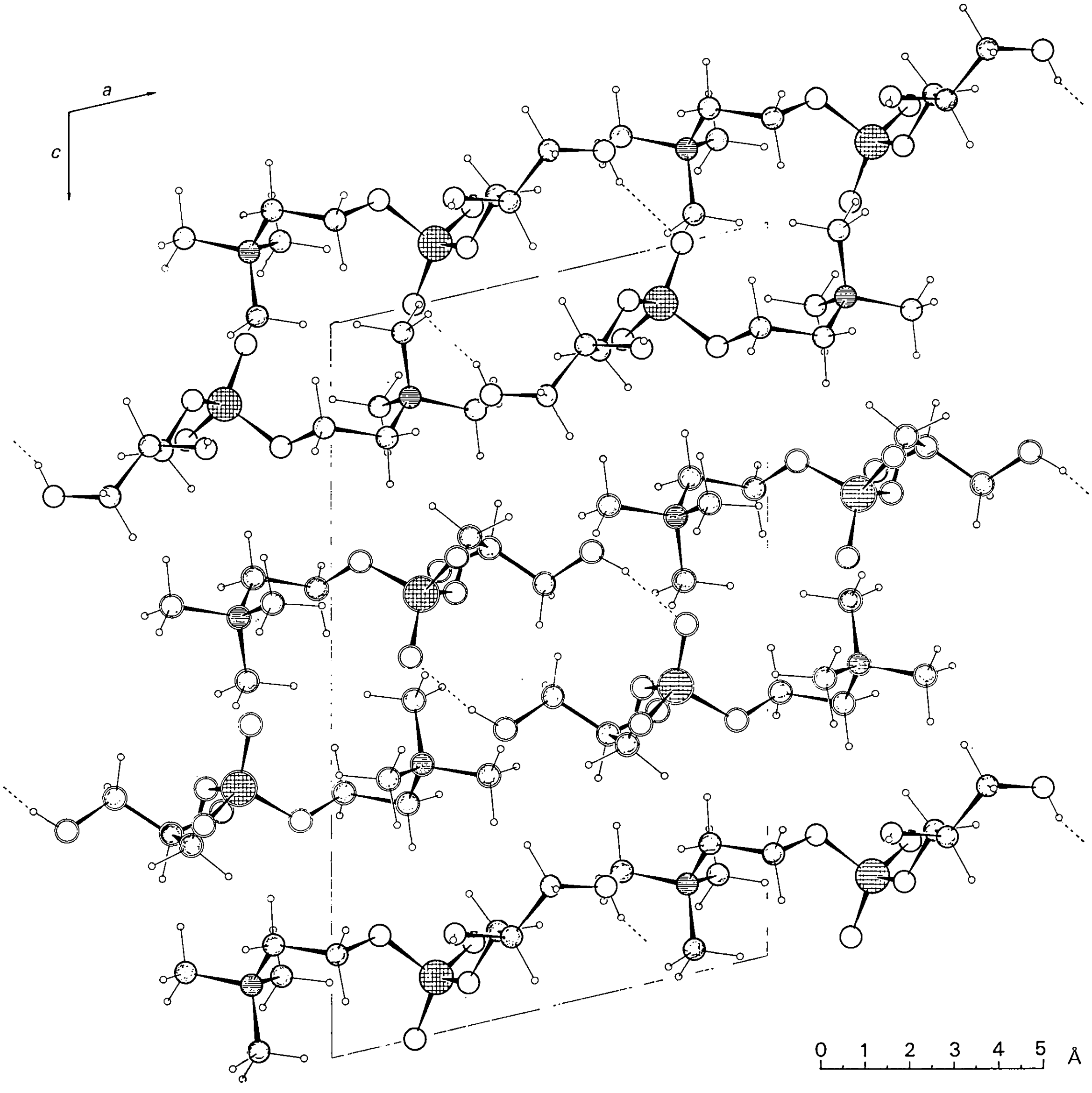

Fig. 5. Illustration of the molecular packing of GPC as seen along the *b* axis. Dashed lines indicate hydrogen bonds. For key to atoms see Fig. 2.

base. The dihedral angles $\varphi_{O(4)N(1)}$ and $\varphi_{O(4')N(1')}$ as seen along the C(4)–C(5) and C(4')–C(5') bonds (Fig. 4) are 72° and 75° respectively.

Bond distances and angles for the two independent molecules of the asymmetric unit are given in Tables 5 and 6. Standard deviations in distances and angles are also listed. They were calculated according to Ahmed & Cruickshank (1953) and Darlow (1960). The maximum deviations from the mean values of identical bonds of the two molecules of the asymmetric unit are, except in a few cases, smaller than 3σ. The standard deviations are, however, slightly underestimated as they have been calculated from the diagonal elements of the inverse least-squares matrix.

The distances in the phosphate group agree well with the recent analyses of adenosine-5'-phosphate (Kraut & Jensen, 1963) and di-*p*-chlorophenyl hydrogen phosphate (DPDPHP) (Calleri & Speakman, 1964). In their paper, Calleri & Speakman surveyed the P–O distances in sixteen earlier accurate structure determinations and calculated that the mean value of the sum of the four P–O distances of the phosphate group was $6{\cdot}177 \pm 0{\cdot}030$ Å. This sum should also be almost constant according to Cruickshank (1961). The value for adenosine 5'-phosphate is 6·185 Å, for DPCPHP 6·151 Å, and for the two GPC molecules 6·196 Å and 6·184 Å.

It is often stated in the literature that each molecule of GPC is associated with a molecule of water. This is obviously not the case in this structure. The zwitterion character of the molecule is evident from the two equivalent short distances between the phosphorus atom and the unsubstituted oxygen atoms [O(5) and O(6)]. The corresponding O–P–O angle is larger in GPC (mean value 121·6°) than adenosine 5'-phosphate (118°). The charge distribution is also different

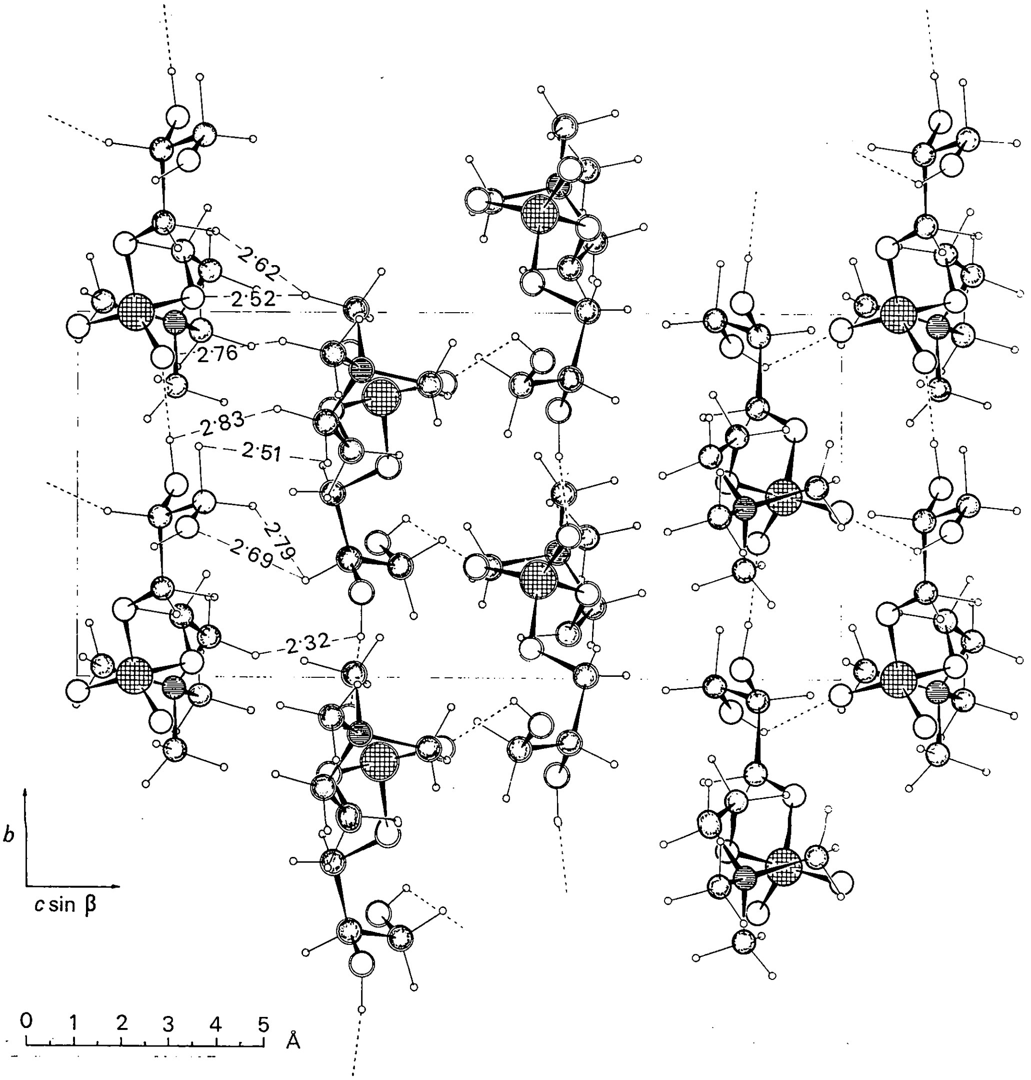

Fig. 6. Molecular packing of GPC as seen along the *a* axis. The hydrogen bonds forming the double layers are indicated as well as some of the shorter contacts between these layers. For key to atoms see Fig. 2.

Table 5. *Bond distances with standard deviations for the two independent molecules of the asymmetric unit*

	Molecule 1		Molecule 1′	
Bond	Length	σ	Length	σ
P(1)–O(3)	1·580 Å	0·0065 Å	1·606 Å	0·0053 Å
–O(4)	1·624	0·0037	1·626	0·0035
–O(5)	1·497	0·0065	1·467	0·0052
–O(6)	1·496	0·0047	1·484	0·0041
N(1)–C(5)	1·510	0·0095	1·487	0·0100
–C(6)	1·480	0·0105	1·516	0·0111
–C(7)	1·540	0·0076	1·476	0·0083
–C(8)	1·522	0·0069	1·529	0·0082
O(1)–C(1)	1·449	0·0077	1·435	0·0077
O(2)–C(2)	1·433	0·0073	1·405	0·0073
O(3)–C(3)	1·390	0·0082	1·457	0·0068
O(4)–C(4)	1·418	0·0093	1·442	0·0083
C(1)–C(2)	1·538	0·0089	1·532	0·0067
C(2)–C(3)	1·553	0·0127	1·498	0·0102
C(4)–C(5)	1·510	0·0080	1·534	0·0080

Table 6. *Bond angles with standard deviations in degrees for the two independent molecules of the asymmetric unit*

	Molecule 1		Molecule 1′	
Angle	θ	σ(θ)	θ	σ(θ)
O(3)–P(1)–O(4)	104·02°	0·32°	102·22°	0·27°
–O(5)	112·17	0·30	110·09	0·26
–O(6)	105·68	0·30	105·48	0·25
O(4)–P(1)–O(5)	104·15	0·27	104·75	0·23
–O(6)	109·01	0·22	109·91	0·21
O(5)–P(1)–O(6)	120·62	0·38	122·62	0·31
C(5)–N(1)–C(6)	113·14	0·50	113·52	0·51
–C(7)	109·92	0·60	112·86	0·66
–C(8)	106·34	0·50	107·16	0·56
C(6)–N(1)–C(7)	111·01	0·52	107·03	0·57
–C(8)	107·70	0·61	105·58	0·67
C(7)–N(1)–C(8)	108·50	0·49	110·46	0·58
P(1)–O(3)–C(3)	115·80	0·49	118·56	0·37
P(1)–O(4)–C(4)	118·27	0·37	119·13	0·34
O(1)–C(1)–C(2)	111·65	0·56	107·58	0·45
O(2)–C(2)–C(1)	107·50	0·53	111·47	0·46
–C(3)	107·57	0·47	106·96	0·46
C(1)–C(2)–C(3)	109·62	0·58	114·01	0·51
O(3)–C(3)–C(2)	109·13	0·58	108·44	0·45
O(4)–C(4)–C(5)	112·69	0·65	110·78	0·57
N(1)–C(5)–C(4)	115·33	0·47	115·04	0·47

in the phosphate groups of the two compounds as one of the remaining oxygen atoms in adenosine 5′-phosphate is bonded to a hydrogen atom.

The molecular packing is illustrated in Figs. 5 and 6. There are no intramolecular hydrogen bonds. In both independent molecules the glycerol oxygen atom O(1) forms a hydrogen bond of 2·70 Å with O(6) of the phosphate group of a symmetry-related molecule. The other hydroxyl oxygen atom O(2) of the two glycerol residues takes part in a hydrogen bond (2·70 Å) almost parallel to the *b* axis with O(5) of a *b*-translated molecule. These hydrogen bonds link together equivalent molecules into infinite spirals in the **b** direction. This also conforms with **b** being the needle direction. There are no hydrogen bonds between the two molecules constituting the asymmetric unit.

The structure can also be described as being built up of bimolecular layers parallel to the *ab* plane of one type of molecule alternating with double layers of molecules of the other type. These layers show fairly smooth boundary surfaces towards each other. Some of the shorter interlayer distances are indicated in Fig. 6.

The positively charged nitrogen atom is roughly tetrahedrally surrounded by oxygen atoms. The two shortest N–O distances are between N(1) and the negatively charged oxygen atoms O(6) and O(5′) (3·81 Å and 3·88 Å). These atoms lie very close to triad axes of the tetramethylammonium tetrahedron. One hydroxyl oxygen atom O(1) is also fairly close to N(1) (3·90 Å), whereas the fourth oxygen atom O(6) of a symmetry-related molecule is further away (4·44 Å). The packing around N(1′) seems less effective as the corresponding shortest N–O distances are about 0·3 Å longer here.

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