

Fig. 3. Amine location relative to the sodium and chlorine ions. Ionic radii are used for Na and Cl; neutral radii are used for N and H.

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Acta Cryst. (1972). **B28**, 2514

A Neutron Diffraction Study of the Structure of L-Glutamic⁻Acid.HCl

BY A. SEQUEIRA, H. RAJAGOPAL AND R. CHIDAMBARAM

Nuclear Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay-85, India

(Received 6 December 1971)

A neutron diffraction study of L-glutamic acid hydrochloride, $C_5H_{10}O_4N.Cl$, has been carried out. The structure is orthorhombic, space group $P2_12_12_1$, with four molecules per unit cell. The cell parameters are: $a=5.151$ (6), $b=11.79$ (2) and $c=13.35$ (2) Å. Intensities of 639 (606 non-zero) independent reflexions have been measured at a wavelength of 1.406 Å, using the diffractometer in symmetrical setting. The positions of the ten hydrogen atoms in the asymmetric unit have been determined from a Fourier map of the nuclear scattering density computed using the phases from the X-ray heavy-atom positions. The structure has been refined to a final conventional R value of 4.3% by the method of least-squares. It consists of molecules hydrogen-bonded in zigzag chains along the c direction. Details of hydrogen bonding and molecular conformation are discussed. The average C-H bond length is 1.090 (11) Å. The average values of the C-C-H and H-C-H angles are 109.4 (7) and 106.0 (12)°, while those of the C-N⁺-H and H-N⁺-H angles are 109.9 (7) and 109.0 (9)°.

Introduction

A detailed knowledge of the hydrogen atom positions and the side group conformations in amino acids is of considerable interest in the calculation of the configuration of the side groups associated with polypeptide chains. This paper reports a precision neutron diffraction study of the structure of L-glutamic acid.HCl as part of the program of studies currently in progress in our laboratory on the structure and hydrogen-bond-

ing properties of amino-acids. A two-dimensional X-ray study of this structure was carried out by Dawson (1953) but the hydrogen atom positions were not determined.

Experimental

Large, clear and well formed crystals of L-glutamic acid.HCl, $C_5H_9O_4N.HCl$, were easily obtained by slow evaporation from a saturated aqueous solution with excess 20% hydrochloric acid. The crystals were

generally of tabular shape and deliquesced slightly on exposure to air. The principal faces were $\{001\}$ and the bounding faces were of the forms $\{011\}$ and $\{101\}$. The density of the crystals, measured by flotation in a mixture of carbon tetrachloride and ethylacetate, was 1.524 g.cm^{-3} .

Neutron intensity data were recorded using the 4-circle diffractometer, 3D-FAD (Momin, Sequeira & Chidambaram, 1969), at the CIRUS reactor in Trombay. The specimen crystal used was in the shape of a five-sided prism (volume = 27 mm^3) with height = 5.1 mm along the a direction and with four of its side faces being (001) , $(00\bar{1})$, $(0\bar{1}1)$ and $(01\bar{1})$ and the fifth one cut roughly parallel to (010) . The widths of these faces were 2.5 , 2.3 , 0.9 , 1.4 and 1.9 mm respectively. The crystal was given a thin coating of an adhesive (brand name: Stickfast) to prevent exposure to air, and mounted on the diffractometer with its a axis parallel to the φ axis. The cell parameters and crystal orientation were refined on the basis of the optimized 2θ , χ and φ values for some 25 strong reflexions, using the program *REFINE* (Srikanta & Sequeira, 1968). The refined values of the cell constants are listed in Table 1 along with other crystal data. The systematic absences were consistent with the space group $P2_12_12_1$.

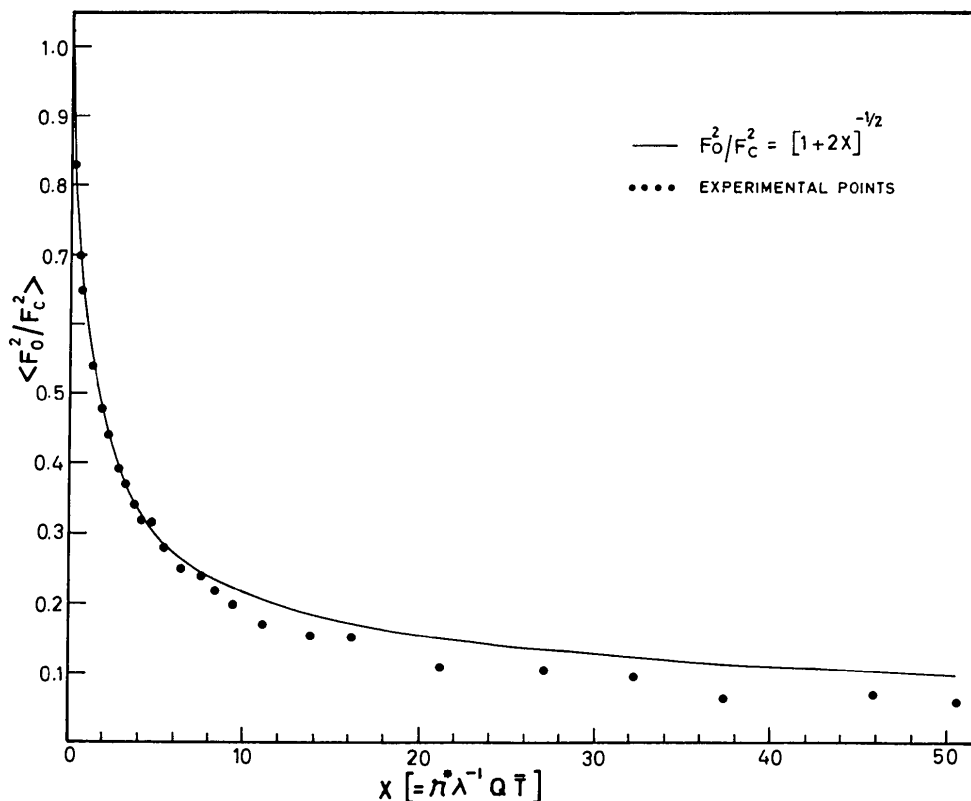
The integrated intensities of 639 independent reflexions within the limit $\sin \theta/\lambda = 0.57$ [$\lambda = 1.406(1) \text{ \AA}$] were recorded in the 'bisecting position' using the θ - 2θ coupled step-scanning technique. Two standard reflex-

Table 1. *Crystal data for L-glutamic acid.HCL*

Space group	$P2_12_12_1$
a	$5.151(6) \text{ \AA}$
b	$11.789(19)$
c	$13.347(20)$
V	810.5 \AA^3
Z	4
D_m	1.524 g.cm^{-3}
D_c	1.509

ions were recorded after every 20 reflexions to keep a check on the stability of the crystal and that of the counting equipment. The reproducibility of the standard intensities was within 4%, and there was no deterioration of the crystal quality. The second order contamination in the beam was avoided by using germanium (331) as the monochromator. The effects of multiple reflexions were checked for the $h00$ reflexions by examining their peak intensities as function of the rotation about the scattering vectors and found to be negligible.

The integrated intensities were reduced to F_0^2 by applying the standard Lorentz and absorption corrections using our program *DATARED* (Srikanta, 1968) which includes the absorption correction program *ORABS* (Wehe, Busing & Levy, 1962) as a subroutine. An absorption coefficient of 2.75 cm^{-1} (measured) was used. The transmission factors ranged from 0.448 to 0.608.

Fig. 1. Variation of observed and estimated extinction factors as a function of the parameter X .

Refinement

The positions of the ten hydrogen atoms in the asymmetric unit were obtained from a three-dimensional Fourier synthesis of the nuclear scattering density computed using the program *FORADP* (Zalkin, 1962) with the observed F_o 's and phases as calculated from Dawson's (1953) heavy-atom positions. All the structural parameters were then subjected to a series of full-matrix least-squares refinements (on F^2), first with isotropic and then with anisotropic temperature factors, using the program *XFLS* (Busing, Martin &

Levy, 1962). In the anisotropic refinement the parameters of the heavy atoms and the hydrogen atoms were refined in alternate cycles as it was not possible to refine all the parameters in the same cycle. The function minimized was $\sum \omega (F_o^2 - |F_c|^2)^2$ with initial weights $\omega = [\sigma_s^2(F_o^2) + (0.1F_o^2)^2]^{-1}$ where $\sigma_s(F_o^2)$ are the standard errors based on counting statistics. Reflexions for which $|F_c|^2/\sin 2\theta > 100$ were not used initially.

Extinction

Severe extinction effects became apparent during the refinement, resulting in unreasonable values for some

Table 2. Final positions and thermal parameters

All the values are multiplied by 10⁴ and their standard deviations (in units of the last digit) are given in parentheses. The form of the anisotropic temperature factor is

$$\exp [-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$$

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	3866 (9)	3565 (4)	9105 (3)	154 (18)	37 (4)	21 (2)	-15 (7)	31 (5)	6 (2)
C(2)	5690 (9)	3038 (4)	8324 (3)	67 (14)	36 (3)	13 (2)	1 (7)	2 (5)	2 (2)
C(3)	4807 (8)	3450 (4)	7285 (3)	108 (14)	24 (3)	21 (2)	26 (6)	7 (5)	-7 (2)
C(4)	6619 (9)	3166 (4)	6416 (3)	165 (17)	27 (3)	20 (2)	17 (7)	-8 (6)	4 (3)
C(5)	5784 (10)	3709 (4)	5474 (4)	183 (16)	21 (3)	27 (3)	9 (7)	-7 (7)	7 (2)
O(1)	4369 (14)	4626 (5)	9271 (5)	250 (22)	39 (5)	56 (4)	-12 (10)	73 (10)	-15 (4)
O(2)	2098 (14)	3027 (5)	9486 (4)	297 (25)	47 (5)	27 (3)	26 (10)	29 (9)	0 (3)
O(3)	195 (16)	4481 (6)	5449 (4)	411 (29)	55 (5)	18 (3)	29 (12)	-1 (9)	9 (3)
O(4)	6935 (14)	3324 (6)	4663 (4)	314 (25)	51 (5)	20 (3)	30 (11)	4 (8)	-2 (3)
N	5599 (6)	1787 (3)	8423 (2)	125 (11)	31 (2)	26 (2)	17 (5)	-19 (4)	3 (2)
Cl	543 (6)	718 (3)	7386 (3)	154 (11)	42 (2)	34 (2)	24 (5)	16 (5)	6 (2)
H(1)	2916 (21)	4977 (8)	9683 (8)	303 (43)	49 (8)	56 (6)	64 (15)	73 (15)	-1 (6)
H(2)	6450 (24)	3716 (9)	4042 (6)	389 (44)	64 (8)	24 (4)	4 (17)	34 (13)	6 (5)
H(3)	5805 (25)	1560 (10)	9168 (6)	416 (43)	71 (8)	25 (4)	117 (19)	63 (13)	13 (5)
H(4)	7186 (21)	1434 (8)	8030 (8)	268 (38)	28 (7)	44 (6)	43 (14)	48 (13)	-1 (5)
H(5)	3796 (21)	1454 (11)	8137 (9)	186 (36)	79 (11)	60 (7)	-26 (16)	20 (13)	25 (7)
H(6)	7655 (15)	3316 (10)	8482 (8)	51 (26)	71 (8)	52 (6)	-19 (13)	7 (11)	8 (7)
H(7)	4575 (31)	4361 (8)	7319 (8)	700 (67)	34 (6)	43 (5)	-39 (20)	58 (20)	13 (6)
H(8)	2933 (23)	3103 (12)	7136 (9)	251 (37)	110 (12)	47 (6)	47 (21)	4 (15)	6 (8)
H(9)	8585 (18)	3460 (13)	6607 (8)	88 (29)	136 (13)	44 (5)	13 (17)	9 (12)	18 (8)
H(10)	6814 (34)	2236 (9)	6291 (8)	920 (91)	34 (7)	38 (5)	165 (23)	71 (20)	9 (5)

Table 3. Observed and calculated structure factors for L-glutamic acid. HCL

The five columns in each set contain the Miller indices h and l , 100 F_o^2 , 100 $|F_c|^2$ and 1000 Y . F_o^2 has been divided by the extinction factor Y .

h	l	100 F _o ²	100 F _c ²	1000 Y
0	0	1597	1533	477
0	0	1097	877	423
0	0	340	309	151
0	10	1922	2093	135
0	12	148	140	87
0	14	775	715	471
0	16	1008	1008	217
0	18	4524	4036	121
0	20	1010	945	582
0	22	1756	1756	295
0	24	598	511	805
0	26	1294	1294	245
0	28	4539	4697	230
0	30	139	139	813
0	32	1937	2073	136
0	34	1428	1410	100
0	36	233	209	787
0	38	1192	1198	106
0	40	1366	1366	204
0	42	5236	517	195
0	44	580	489	561
0	46	141	141	748
0	48	1100	1100	330
0	50	2789	2718	215
0	52	14	101	888
0	54	1325	1319	485
0	56	1048	1021	485
0	58	117	122	745
0	60	2192	2192	100
0	62	1622	1622	206
0	64	5236	517	195
0	66	580	489	561
0	68	141	141	748
0	70	1100	1100	330
0	72	2789	2718	215
0	74	14	101	888
0	76	1325	1319	485
0	78	1048	1021	485
0	80	117	122	745
0	82	2192	2192	100
0	84	1622	1622	206
0	86	5236	517	195
0	88	580	489	561
0	90	141	141	748
0	92	1100	1100	330
0	94	2789	2718	215
0	96	14	101	888
0	98	1325	1319	485
0	100	1048	1021	485
0	102	117	122	745
0	104	2192	2192	100
0	106	1622	1622	206
0	108	5236	517	195
0	110	580	489	561
0	112	141	141	748
0	114	1100	1100	330
0	116	2789	2718	215
0	118	14	101	888
0	120	1325	1319	485
0	122	1048	1021	485
0	124	117	122	745
0	126	2192	2192	100
0	128	1622	1622	206
0	130	5236	517	195
0	132	580	489	561
0	134	141	141	748
0	136	1100	1100	330
0	138	2789	2718	215
0	140	14	101	888
0	142	1325	1319	485
0	144	1048	1021	485
0	146	117	122	745
0	148	2192	2192	100
0	150	1622	1622	206
0	152	5236	517	195
0	154	580	489	561
0	156	141	141	748
0	158	1100	1100	330
0	160	2789	2718	215
0	162	14	101	888
0	164	1325	1319	485
0	166	1048	1021	485
0	168	117	122	745
0	170	2192	2192	100
0	172	1622	1622	206
0	174	5236	517	195
0	176	580	489	561
0	178	141	141	748
0	180	1100	1100	330
0	182	2789	2718	215
0	184	14	101	888
0	186	1325	1319	485
0	188	1048	1021	485
0	190	117	122	745
0	192	2192	2192	100
0	194	1622	1622	206
0	196	5236	517	195
0	198	580	489	561
0	200	141	141	748
0	202	1100	1100	330
0	204	2789	2718	215
0	206	14	101	888
0	208	1325	1319	485
0	210	1048	1021	485
0	212	117	122	745
0	214	2192	2192	100
0	216	1622	1622	206
0	218	5236	517	195
0	220	580	489	561
0	222	141	141	748
0	224	1100	1100	330
0	226	2789	2718	215
0	228	14	101	888
0	230	1325	1319	485
0	232	1048	1021	485
0	234	117	122	745
0	236	2192	2192	100
0	238	1622	1622	206
0	240	5236	517	195
0	242	580	489	561
0	244	141	141	748
0	246	1100	1100	330
0	248	2789	2718	215
0	250	14	101	888
0	252	1325	1319	485
0	254	1048	1021	485
0	256	117	122	745
0	258	2192	2192	100
0	260	1622	1622	206
0	262	5236	517	195
0	264	580	489	561
0	266	141	141	748
0	268	1100	1100	330
0	270	2789	2718	215
0	272	14	101	888
0	274	1325	1319	485
0	276	1048	1021	485
0	278	117	122	745
0	280	2192	2192	100
0	282	1622	1622	206
0	284	5236	517	195
0	286	580	489	561
0	288	141	141	748
0	290	1100	1100	330
0	292	2789	2718	215
0	294	14	101	888
0	296	1325	1319	485
0	298	1048	1021	485
0	300	117	122	745
0	302	2192	2192	100
0	304	1622	1622	206
0	306	5236	517	195
0	308	580	489	561
0	310	141	141	748
0	312	1100	1100	330
0	314	2789	2718	215
0	316	14	101	888
0	318	1325	1319	485
0	320	1048	1021	485
0	322	117	122	745
0	324	2192	2192	100
0	326	1622	1622	206
0	328	5236	517	195
0	330	580	489	561
0	332	141	141	748
0	334	1100	1100	330
0	336	2789	2718	215
0	338	14	101	888
0	340	1325	1319	485
0	342	1048	1021	485
0	344	117	122	745
0	346	2192	2192	100
0	348	1622	1622	206
0	350	5236	517	195
0	352	580	489	561
0	354	141	141	748
0	356	1100	1100	330
0	358	2789	2718	215
0	360	14	101	888
0	362	1325	1319	485
0	364	1048	1021	485
0	366	117	122	745
0	368	2192	2192	100
0	370	1622	1622	206
0	372	5236	517	195
0	374	580	489	561
0	376	141	141	748
0	378	1100	1100	330
0	380	2789	2718	215
0	382	14	101	888
0	384	1325	1319	485
0	386	1048	1021	485
0	388	117	122	745
0	390	2192	2192	100
0	392	1622	1622	206
0	394	5236	517	195
0	396	580	489	561
0	398	141	141	748
0	400	1100	1100	330
0	402	2789	2718	215
0	404	14	101	888
0	406	1325	1319	485
0	408	1048	1021	485
0	410	117	122	745

of the thermal parameters even though many strong reflexions were omitted. Hence, a correction for secondary extinction was applied in the following way (Zachariasen, 1967):

$$F_o^2 \text{ (corrected)} = F_o^2 / Y \\ Y = [1 + 2X]^{-1/2} \\ X = G Q_o \bar{T}$$

where $Q_o = (\lambda^3/v^2) |F_c|^2/\sin 2\theta$ is the reflectivity, $\bar{T} \left[= - (1/A) \frac{dA}{d\mu} \right]$ is the mean absorption weighted path length and $G = [\gamma/\lambda \{1 + (\gamma/\lambda g)^2\}^{-1/2}]$ is an isotropic extinction parameter. \bar{T} for each reflexion was computed by a modification of the program *ORABS* (Wehe, Busing & Levy, 1962) and transferred to the least-squares program. The extinction parameter G was refined along with other parameters (see, for example, Coppens & Hamilton, 1970) by suitable modifications of the program *XFLS*. Details of the extinction treatment will be given separately (Sequeira, Rajagopal & Chidambaram, 1972). The final value of G was $1.44(10) \times 10^5$, which corresponds to an equivalent mosaic spread of 0.4 sec of arc. Some 40 reflexions for which the extinction factor Y was less than 0.25 were omitted from the refinement as they were significantly undercorrected (see Fig. 1).

An error analysis based on F_o^2 values corrected for extinction indicated the suitability of the weighting scheme $\omega = 1/\sigma^2 = [0.35 + 0.04545|F_c|^2/\sin 2\theta]^{-2}$. This scheme used in the final stages of refinement resulted in the following values for the discrepancy factors:

No. obs.	R_1	R_2	R_w
636	0.0559	0.1096	—
566	0.0432	0.0683	0.0898

($F_o^2 > \sigma$; $Y > 0.25$)

where $R_1 = \sum |F_o| - |F_c| / \sum |F_o|$; $R_2 = \sum |F_o^2 - |F_c|^2| / \sum F_o^2$ and $R_w = [\sum \omega |F_o^2 - |F_c|^2|^2 / \sum \omega F_o^4]^{1/2}$. The values of the scattering amplitudes (in units of 10^{-12} cm) used were: H = -0.372, C = 0.6626, N = 0.94, O = 0.575 and Cl = 0.96 (Shull, 1971). The final positional and thermal parameters are listed in Table 2, and the observed and calculated structure factors are compared in Table 3.

Discussion of the structure

The X-ray structure of L-glutamic acid.HCl given by Dawson (1953) is basically correct. However, there are significant differences between Dawson's heavy atom parameters and those obtained in this study. For example, the systematic long-short-long type of variation in bond lengths along the carbon chain pointed out by Dawson is not observable. The distances and angles within the molecule, computed using the program *ORFFE* (Busing, Martin & Levy, 1964), are given in Table 4. The distances and angles involving the non-hydrogen atoms are compared in Table 5 with the weighted average values for un-ionized amino acids reported by Sundaralingam & Putkey (1970). The two

seem to agree fairly well. The bond distances except C(4)–C(5) in the side chain are close to their normal values. The value of C(4)–C(5) (1.476 Å), however, is somewhat shorter than the value of 1.50 Å normally associated with C_{sp^2} – C_{sp^3} single bonds.

Table 4. Bond distances (Å) and angles (°) within the molecule

The standard deviations are given in parentheses.

Bond distances			
C(1)–O(1)	1.296 (8)	C(2)–H(6)	1.085 (10)
C(1)–O(2)	1.221 (9)	N—H(3)	1.036 (11)
C(1)–C(2)	1.535 (7)	N—H(4)	1.056 (11)
C(2)–N	1.482 (6)	N—H(5)	1.078 (12)
C(2)–C(3)	1.537 (6)	C(3)–H(7)	1.082 (11)
C(3)–C(4)	1.526 (7)	C(3)–H(8)	1.067 (13)
C(4)–C(5)	1.476 (7)	C(4)–H(9)	1.101 (12)
C(5)–O(3)	1.225 (9)	C(4)–H(10)	1.113 (12)
C(5)–O(4)	1.315 (8)	O(1)–H(1)	1.017 (13)
		O(4)–H(2)	0.981 (11)
Bond angles			
C(1)–O(1)–H(1)	109.8 (8)	C(2)–C(3)–C(4)	115.8 (4)
O(1)–C(1)–O(2)	125.4 (6)	C(2)–C(3)–H(7)	108.0 (7)
O(1)–C(1)–C(2)	112.6 (5)	C(2)–C(3)–H(8)	108.4 (8)
O(2)–C(1)–C(2)	122.0 (5)	C(4)–C(3)–H(7)	108.4 (8)
C(1)–C(2)–N	108.8 (4)	C(4)–C(3)–H(8)	109.1 (8)
C(1)–C(2)–C(3)	107.7 (4)	H(7)–C(3)–H(8)	106.7 (12)
C(1)–C(2)–H(6)	108.4 (7)	C(3)–C(4)–C(5)	112.0 (4)
N—C(2)–C(3)	112.6 (3)	C(3)–C(4)–H(9)	108.5 (7)
N—C(2)–H(6)	108.2 (7)	C(3)–C(4)–H(10)	112.7 (8)
C(3)–C(2)–H(6)	110.9 (7)	C(5)–C(4)–H(9)	109.2 (8)
C(2)–N—H(3)	109.8 (7)	C(5)–C(4)–H(10)	109.0 (7)
C(2)–N—H(4)	108.9 (6)	H(9)–C(4)–H(10)	105.2 (13)
C(2)–N—H(5)	111.0 (8)	C(4)–C(5)–O(3)	122.7 (5)
H(3)–N—H(4)	107.2 (9)	C(4)–C(5)–O(4)	114.9 (5)
H(3)–N—H(5)	109.5 (10)	O(3)–C(5)–O(4)	122.4 (5)
H(4)–N—H(5)	110.4 (9)	C(5)–O(4)–H(2)	114.7 (9)

Table 5. Comparison of bond distances and angles

	Present value	Weighted average value* for un-ionized amino acid residues
Distance (Å)		
C(1)–O(1)	1.296 (8)	1.306 (11)
C(1)–O(2)	1.221 (8)	1.203 (9)
C(1)–C(2)	1.535 (6)	1.524 (7)
C(2)–N	1.482 (6)	1.482 (4)
C(2)–C(3)	1.537 (6)	1.523 (13)
Angle (°)		
O(1)–C(1)–O(2)	125.4 (6)	126.1 (9)
C(2)–C(1)–O(1)	112.6 (5)	111.1 (10)
C(2)–C(1)–O(2)	122.0 (5)	122.8 (15)
C(1)–C(2)–N	108.0 (4)	108.4 (12)
C(1)–C(2)–C(3)	107.7 (4)	110.2 (21)
N—C(2)–C(3)	112.6 (3)	110.4 (6)

* Sundaralingam & Putkey (1970).

The average distances and angles involving the hydrogen atoms are in good agreement with the values observed in other amino acid crystals. For example, the average C–H distance of 1.090 (11) Å obtained here is close to 1.096 Å observed in L-alanine (Lehmann, Koetzle & Hamilton, 1972); the average values of 109.4 (7)° for the C–C–H angle, 106.0 (12)° for the H–C–H angle, 109.9 (7)° for the C–N⁺–H angle and

109.0 (9)° for the H–N⁺–H angle also compare fairly well with the corresponding values of 110.2, 108.7, 109.8 and 109.1° observed in L-alanine.

Molecular conformation

A stereoscopic picture of the molecule drawn using the program *ORTEP* (Johnson, 1965) is shown in Fig. 2 and its conformation in Fig. 3. The torsion angles about various bonds are also given in Fig. 3 following the nomenclature recommended by the IUPAC-IUB Commission (1970).

The α -carbon atom [C(2)] is planar with the carboxyl group C(1) O(1) O(2), and the least-squares plane through these is

$$3.197X - 3.233Y + 9.804Z - 9.000 = 0,$$

the maximum deviation from the plane being 0.01 Å for C(1). The ammonium nitrogen is displaced from this plane by 0.47 Å, such that the value of the torsion angle $\psi(1)$, {N–C(2)–C(1)–O(2)}, is negative as is usually observed (Lakshminarayanan, Sasisekharan & Ramachandran, 1967) in L-amino acids. The α -NH₃⁺ group is staggered relative to the substituents on C(2) as shown in Fig. 3(b).

The side chain conformation is normal, with C(4) taking the most favourable staggered position *trans* to C(1) [Figure 3(c)] and C(5) being *trans* to C(2) across C(3)–C(4) [Fig. 3(d)]. The end carboxyl group C(5) O(3) O(4) is planar with C(4), and the corresponding least-squares plane is

$$3.760X + 7.964Y + 1.390Z - 5.899 = 0.$$

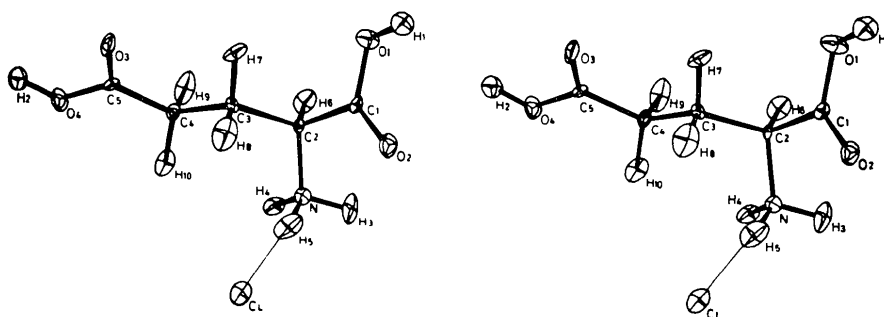


Fig. 2. A stereoscopic drawing of the molecule.

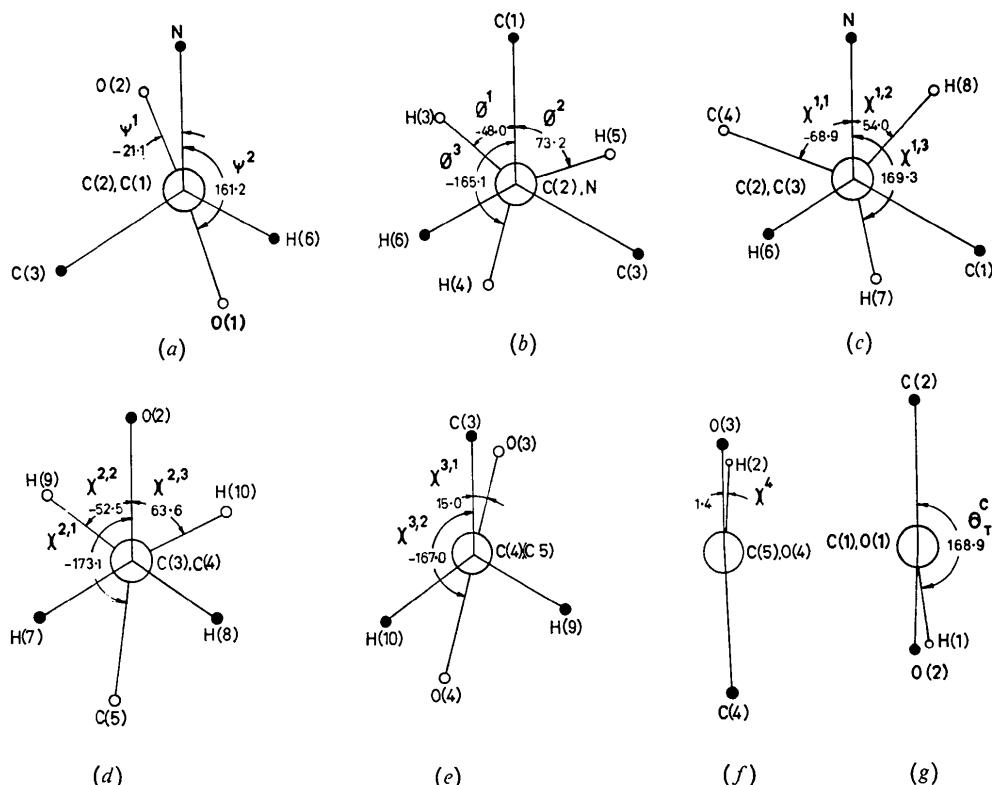


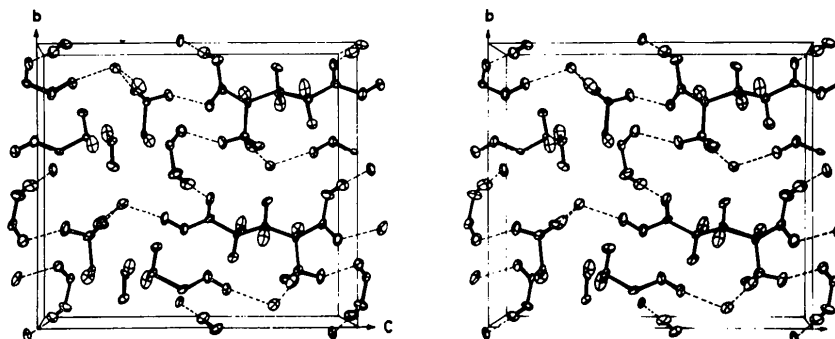
Fig. 3. Torsional conformations looking down bonds: (a) C(2)–C(1); (b) C(2)–N; (c) C(2)–C(3); (d) C(3)–C(4); (e) C(4)–C(5); (f) C(5)–O(4); (g) C(1)–O(1).

Table 6. *Hydrogen bonds in L-glutamic acid.HCl*

Bond description	d_{X-H}	$d_{H...Y}$	$d_{X...Y}$	$\angle H-X...Y$
$X-H...Y$				
O(1)-H(1)···O(3 ^{III})	1.017 (13) Å	1.624 (13) Å	2.637 (10) Å	4.0 (7)°
O(4)-H(2)···Cl ^{IV}	0.981 (11)	2.072 (10)	3.043 (8)	6.6 (7)
N—H(3)···O(2 ^V)	1.036 (10)	1.977 (11)	2.904 (8)	21.4 (7)
N—H(4)···Cl ^{II}	1.056 (11)	2.107 (11)	3.160 (6)	3.8 (6)
N—H(5)···Cl ^I	1.078 (12)	2.137 (12)	3.208 (6)	5.6 (6)

Code for symmetry-related atoms:

I	x	y	z	IV	$\frac{1}{2}+x$	$\frac{1}{2}-y$	$1-z$
II	$x+1$	y	z	V	$\frac{1}{2}+x$	$\frac{1}{2}-y$	$2-z$
III	$\frac{1}{2}-x$	$1-y$	$\frac{1}{2}+z$				

Fig. 4. A stereoscopic drawing of the unit cell viewed along the a axis.

This plane is tilted by 13.9° from the plane defined by the previous adjacent three atoms C(5) C(4) C(3) while the corresponding tilt in *L*-aspartic acid is about 50° (Derissen, Endeman & Peerdeman, 1968).

The dihedral angles 89.6 (4), 89.9 (5) and 88.5 (5)° between the H-C-H and C-C-C planes through the tetrahedral carbon atoms C(2), C(3) and C(4) respectively are close to the expected value of 90° .

Hydrogen bonding

The structure is strongly hydrogen-bonded. Each molecule is involved in five hydrogen bonds, two from the carboxyl hydrogens H(1) and H(2) and three from the amino hydrogens H(3), H(4) and H(5). The distances and angles characterizing these hydrogens bonds are listed in Table 6. Adjacent molecules are linked into zigzag chains along the direction of the c axis by means of strong hydrogen bonds of the type O(1)-H(1)···O(3) between the carboxyl groups. These chains are then held together by the N-H···O bonds, while the N-H···Cl and the O-H···Cl bonds provide additional links between them. A stereoscopic drawing of the unit cell is shown in Fig. 4.

Technical assistance given by Shri S. N. Momin during the data collection is gratefully acknowledged.

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