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X-RAY CRYSTALLOGRAPHIC STUDIES OF THE AMINO ACID SERINE

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A dissertation submitted to the Faculty of Science, University of the Witwatersrand, in fulfilment of the requirements for the degree of Master of Science

Johannesburg, 1998

I declare that this dissertation is my own, unaided work. It is being submitted for the degree of Master of Science in the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination in any other University.



31st day of March 1998

Abstract

X-ray diffraction data has been measured for DL-serine at 298K and 123K as well as for D-serine.H_2O and L-serine.H_2O at 298K. The cell parameters for DL-serine (space group $P2_1/a$) are; at 298K, a=10.7332(11)Å, b=9.1443(8)Å, c=4.8286(7)Å and β=106.42(1)° and at 123K, a=10.7720(5)Å, b=9.1835(4)Å, c=4.87956(2)Å and β=106.73(1)°.The low temperature data set was used to further examine residual electron density that was observed at room temperature. The cell parameters for the orthorhombic crystals (space group $P2_12_12_1$) L-serine.H_2O and D-serine.H_2O are a=4.8189(6)Å, b=9.3566(15)Å and c=12.2253(12)Å and a=4.8195(6)Å, b=9.3584(17)Å and c=12.2183(14)Å respectively. The absolute structures for both enantiomers were accurately determined by refinement of the Flack parameter in SHELX.

To Emily-George

For making this a bit more of a challenge

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Chapter 1

Introduction

Amino acids are the building blocks of proteins. They are the monomers that, when linked through hydrolysis form a sequence known as the primary structure. This structure then folds in the aqueous environment of the cell to form a macromolecule with a unique shape. This shape is directly related to the function of the protein and is largely dependent on the amino acid composition.

1. Chemical structure of the twenty naturally occurring amino acids

The first amino acid to be isolated was glycine, in 1820, from a gelatin hydrolysate by H. Braconnot. There are 20 L-α amino acids found in proteins referred to as standard amino acids (table 1.1). All, with the exception of proline, have a free carboxyl and a free unsubstituted amino group on the α carbon. They differ from one another in the structure of the side chain, R. (Lehninger, 1975). The absolute configuration at the α carbon atom of α amino acids is identical with that of glyceraldehyde .

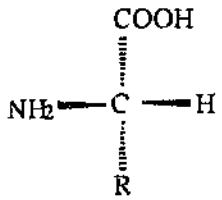
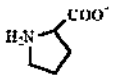
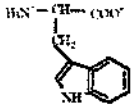
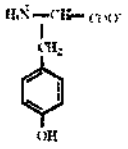
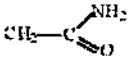
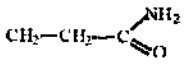
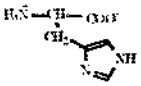


Figure 1.1: The structure of an L-amino acid

Table 1.1: The twenty standard amino acid symbols and side chains.

Name	Symbol	R
Glycine	Gly	H
Alanine	Ala	CH_3
Leucine	Leu	$CH_2CH(CH_3)_2$

Isoleucine	Ile	$CH(CH_3)CH_2CH_3$
Valine	Val	$CH(CH_3)_2$
Proline	Pro	
Phenylalanine	Phe	CH_2Ar
Tryptophan	Trp	
Methionine	Met	$CH_2CH_2SCH_3$
Serine	Ser	CH_2OH
Threonine	Thr	CH_2CH_2OH
Tyrosine	Tyr	
Asparagine	Asn	
Glutamine	Gln	
Cysteine	Cys	CH_2SH
Lysine	Lys	$(CH_2)_3NH_2$
Arginine	Arg	$(CH_2)_3NHC(NH_2)_2$
Histidine	His	
Aspartic acid	Asp	CH_2COOH
Glutamic acid	Glu	CH_2CH_2COOH

Amino acids other than the 20 standard forms exist. Rare amino acids may be found in some proteins, such as hydroxyproline in collagen and desmosine in elastin. In addition to the standard and few rare amino acids there are over 150 other amino acids known to occur

biologically free or in a combined form but never in proteins. Some have the D configuration such as D-glutamic acid found in the cell walls of bacteria, D-alanine found in some insect pupae and D-serine in earthworms.

1.2 Amino acid properties

1.2.1 Polarity

Amino acids can be classified on the basis of the polarity of the side chain dividing them into four groups: non-polar (hydrophobic), polar (neutral), positively charged and negatively charged. Non-polar amino acids have aliphatic side chains and include alanine, leucine, isoleucine, valine, and proline. Also hydrophobic are phenylalanine and tryptophan which contain aromatic rings and methionine which is sulphur containing. The uncharged polar amino acids include serine, threonine and tyrosine having a hydroxyl functional group; asparagine and glutamine having amide groups and cysteine having a sulphydryl group. Cysteine and tyrosine have the most polar substituents. The positively charged amino acids are basic at pH=7 and all have 6 carbon atoms. They include lysine, arginine and histidine The negatively charged amino acids are acidic pH=7 with a second carboxyl group that is fully ionised at pH 6-7. They are aspartic acid and glutamic acid.

The polarity of the amino acids is biologically important in that it affects the three dimensional structure that the protein assumes. Hydrophobic amino acids are found on the interior of a protein while the hydrophilic amino acids are exposed to the aqueous environment on the surface.

1.2.2 In the crystal

The co. . nic species of crystalline amino acids have a relatively high melting point (>200°C) and are much more solubie in water than in non polar solvents. This is to be expected as the crystal lattice is stabilised by e'ectrostatic interactions between charged carboxylate groups and ammonium group analogs. Most amino acids occur in, and crystallise

from neutral aqueous solutions as dipolar ions or Zwitterions.

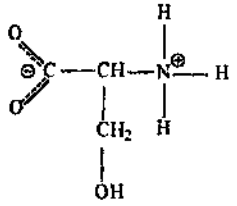


Figure 1.2: Serine as a Zwitterion.

Amino acids that crystallise with halide inclusions usually do not crystallise as Zwitterions but as $COOH\text{-}CHR\text{-}NH_3^+$. L-alanine, L-histidine, L-leucine, L-tyrosine, L-phenylalanine, L-tryptophan, L-valine and DL-valine have all been crystallised from an acidic environment with HX (X=Cl, Br) and have protonated carboxyl groups.

1.2.3 Acid Base Properties of Amino Acids

Amino acids are amphoteric in that they can act as acids (*COOH* is a proton donor) or bases (NH_2 is a proton acceptor). In its fully protonated form, an amino acid is a dibasic acid and can donate two protons during a complete titration with a base. The two stage titration yields two points at which equimolar amounts of proton donor and proton acceptor are present, one at the deprotonation of COOH and the other at the deprotonation of NH_3^+. Equivalence points are described with pK values.

pK_1: $NH_3^+\text{-}CHR\text{-}COOH + OH^- \rightleftharpoons NH_3^+\text{-}CHR\text{-}COO^- + H_2O$

pK_2: $NH_3^+\text{-}CHR\text{-}COO^- + OH^- \rightleftharpoons NH_2\text{-}CHR\text{-}COO^- + H_2O$

Table 1.2: The pK' values for selected amino acids (Lehninger, 1975)

	pK_1 $\alpha COOH$	pK_2 αNH_3
Alanine	2.34	9.69
Serine	2.21	9.15
Threonine	2.63	10.43
Histidine	1.82	9.17

The pH of a solution of amino acids is therefore an important factor when growing crystals and should lie in the region of pH 6-7 for the Zwitterion to be the dominant species. Structures that crystallise with HX and have a protonated carboxyl group are grown from strongly acidic solutions (pH≈ 2).

1.2.4 Stereochemistry

With the exception of glycine, all naturally occurring amino acids show optical activity, that is, they rotate plane polarised light. Because of the nature of the sp^3 orbitals of the α-carbon atom, four different groups can occupy two different arrangements in space to yield two different chiral configurations or enantiomers. The prefixes D and L describe the absolute configuration or structure of the molecule.

1.2.4.1 Absolute Structure

The absolute structure of a molecule or crystal is its structure expressed in an absolute frame of reference. This means that the parameters that serve to define the structure must contain not only the coordinates of each atom in the structure, but also a firm indication of the handedness of the structure (Glusker, 1994). In 1951 Bijvoet showed that it is possible to determine the absolute configuration of an optically active molecule from the effects of anomalous scattering. Anomalous scattering occurs when the scattering atom, usually a heavy atom (particularly those with Z close to that of the element used to generate the incident X-rays), absorbs X-rays. A phase change occurs for the X-rays scattered by the absorbing atom

relative to the phases of the X-rays scattered by other atoms. The scattering is anomalous in that correction must be applied to the normal scattering factors (the scattering power of a given atom for a given reflection). The scattering factor (f_n) corrected for anomalous dispersion is represented by the following expression:

$$f_n^{anom} = f_n \cdot \Delta f' + i\Delta f'' = f' - i\Delta f''$$

where f_o = the normal scattering factor

$\Delta f'$ = the real correction term

$i\Delta f''$ = the imaginary component

The increase of anomalous scattering with the increase in atomic mass is shown in table 1.3.

Table 1.3: Dispersion effects on scattering factors using MoK_α incident radiation (Glusker, 1994)

	$\Delta f'$	$\Delta f''$
H	0	0
C	0.0033	0.0016
N	0.0061	0.0033
P	0.1023	0.0942
Br	-0.2901	2.4595

Friedel's law states that , $Fhkl = F\bar{h}\bar{k}\bar{l}$[1]. This is true for centrosymmetric crystals but does not hold for non centrosymmetric structures if there is an anomalous scatterer present in the structure. Anomalous scattering therefore enables the determination of absolute configuration. Put simply, the $Fhkl$ and $F\bar{h}\bar{k}\bar{l}$ values that are observed are compared to those that are calculated in order to determine whether the correct configuration has been chosen.

---

[1] $F_{hkl} = \sum f_r\{\cos 2(hx+ky+z) + i\sin 2(hx+ky+lz)\}$ ie. the structure factor. See section 1.6.1.1

This method has been incorporated into the SHELX refinement method to produce an additional parameter known as the Flack parameter (x) which gives an indication of the absolute configuration (Flack, 1983). Formally the x parameter is defined by

$$|F(\mathbf{h},x)|^2 = (1-x)|F(\mathbf{h})|^2 + x\,|F(-\mathbf{h})|^2$$

where $F(\mathbf{h},x)$ is the structure factor for the reflection **h**, including the Flack parameter x.
$F(\mathbf{h})$ and $F(-\mathbf{h})$ are the structure factors of the Friedel pairs of reflection **h**.

When the atomic coordinate set of the calculated model and the observed structure have the same chirality, x takes the value of 0, whereas when they are opposed x becomes 1. For a centrosymmetric crystal in which Friedel's law holds true, x is clearly undefined.

The effect of anomalous scattering primarily involves the inner electrons of the atom (hence the heavier the atom the greater the effect). For a given atom, the effects of dispersion are relatively greater at a high sinθ than at low ones (Stout and Jensen, 1989). If the molecule under study contains no strong scatterers, collection of high angle data will assist in absolute structure determination.

In this project, the structures of both D and L-serine.H_2O were solved in order to ascertain to what extent the refinement of small molecules containing atoms no heavier than oxygen, can give an accurate absolute structure determination.

1.3 Crystal studies of Amino Acids

R.E. Marsh was involved in the early crystal structure determination of many amino acids. In 1967 he reviewed all the amino acid structures that had been solved at that time. For structures with three-dimensional structural data, he compared bond distances and angles of the amino acid groupings as well as conformation about the C-Cα bond. He also briefly commented on hydrogen bond distances. Since then, accurate structural data has been collected for all of the L, most of the DL and a few D-amino acids.

Amino acids have been extensively studied by diffraction techniques and structural data are available for all twenty of the genetically coded amino acids. Neutron structural data are available for 16 of the 20 (Koritsanzky, 1996). Most of these are room temperature measurements, but increasing numbers are being studied at low temperature for more accurate bond structural parameters and often in order to determine the electron density. Those that have been studied at low temperature are L-threonine at 12K (Janczak 1997), L-asparagine monohydrate at 15K (Weisinger, 1982), glycine at 77K (Kozhin, 1978), L- alanine at 23K (Destro, 1988) and L-cysteine (G[illegible] 1996), L-leucine (Gorbitz, 1996), L-methionine (Dalhus, 1996), DL-valine [illegible] L-valine (Dalhus, 1996) all at 120K. The racemate has been studied [illegible]e, DL-isoleucine, DL-arginine, DL-phenylalanine and DL-tryptophan. Beca[illegible] of D amino acids is essentially identical to L amino acids, few studies of [illegible] structures [illegible]n done. Those structures that have been determined are D-methionine (Khawas, 1986), D-tyrosine (Khawas, 1986) and D-isoleucine hydrobromide monohydrate (Trommel, 1954).

Amino acids often crystallize with inclusions of ions or solvent molecules. Those that have water in the crystal lattice are of particular interest as both serine enantiomers crystallize as hydrates. Apart from DL-proline monohydrate, all of the hydrated amino acid crystals are composed of a single enantiomer. These include L-arginine hydrobromide monohydrate, L-asparagine monohydrate, L-cysteine hydrochloride monohydrate, L-histidine hydrochloride monohydrate, D-isoleucine hydrobromide monohydrate, L-lysine hydrochloride dihydrate and L-serine monohydrate.

1.3.1 The Cambridge Crystallographic Database

Information on the molecular structures of amino acids was found by searching the Cambridge Crystallographic Database (CSD) (V5.13, April 1997) (Kenard, 1992). The CSD contains results derived from the X-ray and neutron diffraction analysis of organic and organometallic compounds. The current version of the database contains 175093 entries and can be searched with crystallographic information such as unit cell parameters, symmetry, space group or three dimensional coordinates. Authors, journals, publication year and other

'text' based information can also be used as a search. Parameters were specified and search data were then analysed with the statistical package, VISTA.

1.4 Serine

The amino acid under study is serine or 2-amino-3-hydroxypropanoic acid denoted by the symbol ser or s. The molecular formula of serine is $C_3H_7NO_3$, it has a molecular weight of 105.09 and an isoelectric point of 5.68 [1] contains a terminal hydroxyl group and is a hydrophilic amino acid. It was chosen reasons of availability, ease of crystallisation and simplicity of structure. L-serine ((S)-2-amino-3-hydroxypropanoic acid) is a genetically coded amino acid found in peptide linkages in proteins and encoded by the codons AGC or AGU. In mammals it is a nonesssential dietary amino acid. D-serine ((R)-2-amino-3-hydroxypropanoic acid) occurs in silkworms and earthworms and residues of D-serine occur in certain peptide antibiotics (Oxford dictionary of Biochemistry, 1997).

1.4.1 Serine function

The hydroxyl group of serine plays an important role at the active site of a group of enzymes know as the serine peptidases. Peptidases are a group of digestive enzymes that hydrolyse peptide bonds. During catalysis by a serine peptidase an acyl enzyme intermediate is formed by esterification of the hydroxyl group of the reactive serine with the carbonyl group of a peptide bond of the substrate.

1.4.2 Crystal Studies of Serine

A number of crystal structures of serine have been reported. X-ray diffraction experiments have been performed on DL-serine by Shoemaker (1953) and Kistenmacher (1974) and on L-serine by Kistenmacher (1974) and Benedetti (1973). A neutron study by Frey et al. (1973) looked at the structures of DL-serine and L-serine.H_2O. A recent X-ray diffraction experiment at 100K on DL-serine by Koritsanszky (1998) is in press but crystal data were kindly made available for comparison.

1.5 Electron density of DL serine

The refinement of the crystal structure of DL-serine by Kistenmacher et al. (1974) showed significant amounts of electron density between various pairs of bonded atoms. They referred these as 'bonding electrons' but did not investigate them further. Part of this study therefore involves the electron density determination of DL-serine from a low temperature data set in order to get a more accurate picture of this unusual electron density distribution.

1.5.1 Electron density determination

It is one of the basic tenets of quantum mechanics that the location of an electron cannot be specified at a particular time. The position must be discussed with respect to the probability of finding it in a volume element which is related to the square of the wave function. The ability to measure this probability density, otherwise called charge or electron density, would provide a great deal of information on chemical bonding (Coppens, 1984). Using X-ray diffraction methods electron density studies have become possible which have applications to chemical and physical problems. These include comparison with theoretical results, calculation of intermolecular interactions and the determination of the ground state in metal coordination complexes .

The success of the method depends on the experimental conditions. The data collection should be performed at a very low temperature in order to minimize the effect of thermal smearing (Boeyens, 1995) . Because there is a limit to the number of measurable reflection intensities it is also necessary to collect as many independent Bragg reflections as possible. High angle reflections are particularly important for obtaining parameters associated with the core electron density. By lowering the temperature the background scattering associated with high angle reflections is reduced (Coppens, 1989).

1.5.1.1 The phase problem

In order to calculate the electron density at a point, (x,y,z), in the unit cell, knowledge of the amplitudes and the phases of the diffracted wave in reciprocal space is needed. The amplitude of the Fourier term in a series that describes (x,y,z) is calculated from the measurable intensity ,I_{hkl}, of the diffracted ray. The phase is not as obviously recorded. The structure factor, F_{hkl}, the computed series for the reflection *hkl*, is calculated by summing the waves diffracted by each of N atoms in the cell. Each term in the summation represents one diffracted wave (Dent-Glasser, 1977).

$$F_{hkl} = \sum f_r \{\cos 2(hx+ky+lz) + i\sin 2(hx+ky+lz)\}$$

f_r=scattering factor for the rth atom and the relative phase is described by the rest of the term.

i. The centrosymmetric crystal

In the case of a structure that packs into a space group with a centre of symmetry, the phase problem is somewhat simplified. For every atom (x, y, z), there is an identical atom at (-x,-y,-z) and since sin(-x)=-sin(x), the structure factor equation reduces to

$$F_{hkl} = \sum f_r \{\cos 2(hx+ky+lz)\}$$

ie. the phase is restricted to two values and the atoms may be treated spherically when calculating the phase.

ii. The non centrosymmetric crystal

For the acentric crystal the imaginary term, $i\sin 2(hx+ky+lz)\}$, is retained and the values of the phases are thus continuous variables. The model used to calculate phases must therefore include the deviation from spherical symmetry of the atom densities ie. a non-spherical least squares refinement is to be used to determine model parameters.

For this reason, electron density studies are preferentially performed on centrosymmetric

structures, in this case DL-serine.

1.6 A Low Temperature (23K) Study of L-Alanine (Destro, Marsh and Bianchi)

Although there are many low temperature structures of amino acids, this study of alanine has been selected as a particularly good example of a thorough X-ray diffraction study of an amino acid. Results from this study give an indication of the amount of information that can be deduced from an accurate low temperature data set.

The limitations of room temperature studies are discussed, the three main ones being:

1. Thermal smearing
2. The subsequent difficulty in estimating true interatomic distances
3. Valence electron scattering being poorly represented by the widely used spherically symmetric atom model.

Effects (1) and (2) can be minimised by cooling the crystal and effect (3) by modelling the outer electrons differently.

Intensity data at 23 K were collected three times from the same crystal and the weighted average of the three sets was used. Intensities were collected to a 2θ value of 100° with background measurements made before and after each scan. Corrections were made for Lorentz and polarisation effects but not for absorption which was considered negligible.

Least squares refinement was carried out on five different models, those being:

A. The spherical atom model
B. As (A) but using only reflections with $2\theta > 40°$
C. As (A) but with hydrogen atoms polarised in the direction of the atom to which they are bonded.
D. Multipole model in which the electronic charge density of the molecule was analysed by a spherical-atom formalism.
E. A restricted multipole model in which the smallest multipoles of (D) were held constant at zero

Table 1.4: The five different models used to refine alanine.

	A	B	C	D	E
no. of data	2515	2283	2515	2519	2519
no. of parameters	83	83	83	186	159
R	0.032	0.03	0.032	0.0203	0.0206
goodness of fit	2.35	1.44	2.39	1.166	1.192
scale factor	1.006(1)	0.986(1)	1.006(1)	0.986(2)	0.990(2)

The results found models A and C to be essentially identical indicating that modelling the poles of the hydrogen atoms had no effect on the overall refinement. Refinement B which ignored low angle data (those reflections sensitive to the valence electron density) was predictably found to have a different scale factor to those for A and C. Reliable scale and temperature parameters are best obtained by either ignoring low-angle data or by appropriately modelling the valence electrons as in D and E. The multipole models were found to best fit the experimental data as evidenced by the R index and goodness of fit values.

This study shows that X-ray diffraction intensities that are accurately measured at a low temperature and properly corrected allow for a reliable deconvolution of the electron distribution from thermal motion, particularly when interpreted by a multipole model. Non hydrogen atom bond distances and angles were more accurate and precise than those obtained in previous room temperature and neutron studies. C-H and N-H bond lengths were in agreement with those obtained from neutron diffraction work and features of the hydrogen bonding network were found in the deformation density maps.

As extensive a treatment of serine is not possible in this particular study given that the quality and number of data at hand does not match that described. This said, the low temperature data collected certainly suffices in making valid comparisons with the room temperature structure and previous neutron studies, give more accurate bond lengths and angles as well as supply some insight into the electron density distribution of the serine molecule.

1.7. Aim

The main objective of this project is to collect good quality X-ray diffraction data for DL-serine, L-serine.H_2O and D-serine.H_2O for purposes of comparison. The aim is fourfold.

1. To determine the accuracy of refinement of an absolute structure parameter for D and L-serine.H_2O using Friedel pairs collected to a high 2θ.
2. To compare the configuration of both enantionmers in order to determine the extent of the similarity of two structures that are expected to be identical.
3. To further examine electron density found along the C-C bonds at room temperature using a data set collected at 123K.
4. To compare the racemic and enantiomeric crystal structures.

Chapter 2

Experimental

2.1 Crystal Growth and Mounting

It is relatively easy to grow good quality amino acid crystals from aqueous solution (Black, 1988). The solubility and the assumed form of the amino acid is highly sensitive to pH.

2.1.1 L-serine.H_2O

L-serine crystals were purchased from Sigma chemical company and recrystallised from aqueous solution. Initially it was presumed that the crystals formed were pure L-serine as per Kistenmacher *et al.* (1974). It was soon realised from a Weissenberg photograph that the crystals were dehydrating and becoming opaque at room temperature. This efflorescence indicated that the crystal was more likely the mono-hydrated serine structure.
Attempts to crystallize pure L-Serine from non-aqueous solvents such as ether and ethanol were unsuccessful due to the limited solubility of serine in these substances.
Large, flat, prisms of good quality L-serine.H_2O formed from a slow cooled solution saturated at 65°C. The crystals were selected according to their ability to extinguish polarised light under a microscope and were subsequently cut to size (0.2 mm × 0.3 mm × 0.3 mm) with a blade. The crystal was mounted in a Linderman tube (0.5mm diameter) with a small amount of water placed at the end of the tube to ensure a moist atmosphere. The tube was sealed with cyanoacrylate, as dehydration of the crystal was unavoidable when sealing with a flame.

2.1.2. D-serine.H_2O

Crystals of D-serine.H_2O were prepared in the same way as L-serine.H_2O as, being enantiomers, they exhibited the same properties. Two crystals were selected for the two data

collections; one of dimensions 0.2mm×0.25mm × 0.4mm for the CAD4 and another of dimensions 0.3mm×0.3mm×0.2mm for the SMART.

2.1.3 DL-serine

DL-serine crystals were recrystallised by slow cooling from an aqueous solution of 0.5 g of D-serine and 0.5 g of L-serine in enough solvent to result in a saturated solution at 65°C. Clusters of rectangular prisms of good quality formed. DL-serine does not crystallise with the inclusion of water so no special treatment of the crystal was required. Two crystals were selected for the two data collections at different temperatures; one of dimensions 0.2mm×0.3mm×0.3mm for the CAD4 room temperature data collection and another of dimensions 0.4mm×0.2mm×0.4mm for the SMART low temperature data collection.

2.2 X-ray photographs

Oscillation, zero and first layer Weissenberg photographs were taken of all crystals prior to data collection on the diffractometer. This was done in order to determine the cell parameters and space group as well as to confirm that the crystal was not twinned and had not dehydrated as in the case of L and D-serine.H_2O.

2.3 Data collection

2.3.1 Data collection on DL-serine, D and L-serine.H_2O at room temperature on the Enraf Nonius CAD4 diffractometer.

Data were collected on an Enraf-Nonius CAD-4 diffractometer, on a Phillips generator, with graphite monochromated, molybdenum Kα radiation (λ=0.71069Å) from a fine focus sealed tube set at 50 kV and 30 mA as X-ray source. Cell parameters were refined by least squares calculations from 25 centered reflections. Peak profiles were collected.

Table 2.1 :Crystal data collected on DL-serine, D and L-serine.H_2O using the Enraf Nonius CAD4 diffractometer

	DL-serine	L-serine.H_2O	D-serine.H_2O
Identification code	sc53	sc54	sc55
Empirical formula	$C_3H_7NO_3$	$C_3H_9NO_4$	$C_3H_9NO_4$
Formula weight	105.1	123.11	123.11
Temperature (K)	293(2)	293(2)	293(2)
Absorption coefficient (mm^{-1})	0.137	0.138	0.138
F(000)	224	264	264
Theta range (°)	2.98 to 29.97	2.74 to 29.95	2.74 to 29.95
Index range	$-15 \geq h \geq 15$ $-12 \geq k \geq 12$ $-6 \geq l \geq 6$	$-6 \geq h \geq 6$ $-13 \geq k \geq 13$ $-17 \geq l \geq 17$	$-6 \geq h \geq 6$ $-13 \geq k \geq 13$ $-17 \geq l \geq 17$
Reflections collected	2928	2845	3079
Independent reflections	1323 [R(int)=0.0159]	1192 [R(int)=0.0217]	1596 [R(int)=0.0269]
Data collection method	ω-2θ	ω-2θ	ω-2θ

Three strong reflections were monitored periodically during the data collection (table 2.2). The crystals were stable in X-rays and did not undergo any structural change. This was particularly important in the case of the hydrated crystals as dehydration would be evident in the decay of the intensity of the control reflections.

Table 2.2: Intensity controls for DL-serine, D and L-serine.H_2O

	DL-serine	L-serine.H_2O	D-serine.H_2O
Intensity controls *h k l*	*3 5 1* *-2 7 1* *6 -1 2*	*-3 2 0* *1 4 0* *3 2 0*	*0 -4 -5* *0 -2 -7* *2 2 4*

Unique reflections were considered observed for $I > 2\sigma(I)$.

The final data were reduced with the data reduction program PROFIT (Strel'stov & Zavodnik, 1989) which corrected for Lorentz polarisation effects and scaled the data. Structures were solved by direct methods using SHELXS86 (Sheldrick, 1990) and refined with SHELXL93 (Sheldrick, 1993). Method of refinement was full matrix least squares on F^2 with non-H atoms refined anisotropically and H atoms isotropically to convergence. The atomic scattering factors used were from the International Tables Volume C (Wilson, 1992).

2.3.2 Data collection on DL-serine at 123K and D-serine.H_2O at 273K on the SMART CCD diffractometer

2.3.2.1. D-serine.H_2O

Due to the tendency of the enantiomeric crystals to dehydrate, a small data set was collected at room temperature over 1 hour on D-serine.H_2O on the SMART CCD diffractometer to compare with data collected over 3 days on the Enraf Nonius diffractometer. Any crystal decomposition due to dehydration over time would be minimised with the shorter data collection time.

Data were collected on a Siemens SMART CCD diffractometer, on a Phillips generator, with graphite monochromated, molybdenum Kα radiation (λ=0.71069Å) from a fine focus sealed tube set at 50 kV and 30 mA as X-ray source. The detector was set at a distance of 4.50 cm from the crystal. Data were collected by rotation about the ω axis. The rotation width was 0.3°. The frame size was 512×512 pixels and exposure time per frame was 10 seconds. The final data were then reduced using the reduction program SAINT (Siemens, 1995b). Structures were solved by direct methods using SHELXTL Version 5 (Siemens, 1995a) and refined with SHELXTL (Siemens, 1995a). Method of refinement was full matrix least squares on F^2 with non-H atoms refined anisotropically and H atoms isotropically to convergence. The atomic scattering factors used were from the International Tables Volume C (Wilson, 1992).

2.3.2.2. DL-serine

Data for DL-serine were collected at 123K for purposes of examining the electron density and determining the atomic coordinates more accurately.

Data were collected on a Siemens SMART CCD diffractometer, on a Phillips generator, with graphite monochromated, molybdenum Kα radiation (λ=0.71069Å) from a fine focus sealed tube set at 50 kV and 30 mA as X-ray source. The detector was set at a distance of 4.50 cm from the crystal. 37 reflections were used to determine cell parameters. Data were collected by rotation about the ω axis. The rotation width was 0.3°. The frame size was 512 × 512 pixels and exposure time per frame was 10 seconds. To check for intensity decay, 50 frames of the first exposure set were repeated at the end of the data collection. Crystal decay was found to be negligible after analysing the duplicate reflections. Unique reflections were considered observed for $I>2\sigma(I)$. Empirical absorption corrections were performed by SADABS (Sheldrick, 1996b). The final data was then reduced using the reduction program SAINT (Siemens, 1995b). Structures were solved by direct methods using SHELXS86 (Sheldrick, 1990) and refined with SHELXL93 (Sheldrick, 1993). The method of refinement was full matrix least squares on F^2. Non-H atoms refined anisotropically and H atoms isotropically to convergence. Atomic scattering factors used were from the International Tables Volume C (Wilson, 1992).

Table 2.3: Crystal data collected on DL-serine, D and L-serine.H_2O using the Siemens SMART CCD diffractometer

	DL-serine	D-serine.H_2O
Identification code	serine_1	sc56
Empirical formula	$C_3H_7NO_3$	$C_3H_9NO_4$
Formula weight	105.1	123.11
Temperature (K)	123(2)	298(2)
Maximum theta (°)	70.23	24.73
Index range	$-17>h>17$ $-14\geq k>14$ $-7>l>7$	$-2\geq h\geq 5$ $-4>k>10$ $-13>l>4$
Total frames	2169	252
Total data collection time	6 hours	1 hour
Spot spread XY (°)	1.6	1.6
Spot spread Z (°)	0.6	0.6
Reflections collected	6892	858
Independent reflections	1940 [R(int)=0.0162]	680 [R(int)=0.0239]

Chapter 3

Results and discussion

3.1 Crystal data, structure solution and refinement for DL-serine, D-serine.H_2O and L-serine.H_2O

Table 3.1: Results of data collection and refinement

	DL-serine	L-serine.H_2O	D-serine.H_2O	D-serine.H_2O	DL-serine
Identification code	sc53	sc54	sc55	sc56	serine_1
a (Å)	10.7332(11)	4.8189(4)	4.8195(6)	4.8176(10)	10.7720(5)
b (Å)	9.1443(8)	9.3566(15)	9.3584(17)	9.3466(19)	9.1835(4)
c (Å)	4.8286(7)	12.2253(12)	12.2183(14)	12.207(3)	4.7956(2)
β (°)	106.42(1)	not applicable	not applicable	not applicable	106.73(1)
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic
Space group	$P2_1/a$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_1/a$
Volume ($Å^3$)	454.57(9)	551.22(11)	551.08(14)	549.6(2)	454.31(3)
Z	4	4	4	4	4
Density (calc) (g/m^3)	1.536	1.483	1.484	1.488	1.537
Absorption coefficient (mm^{-1})	0.137	0.138	0.138	0.138	0.137
Temperature (K)	298	298	298	298	123
Diffractometer type	CAD4	CAD4	CAD4	SMART	SMART
Refinement method	Full-matrix least-squares on F^2				
data/restraints/parameters	1323/0/92	1192/0/109	1596/0/109	680/0/101	1940/0/92
Goodness of fit on F^2	1.078	0.837	1.065	1.137	1.375
Final R indices [I>2σ(I)]	R1=0.0365 wR2=0.106	R1=0.0331 wR2=0.086	R1=0.0360 wR2=0.098	R1=0.0275 wR2=0.0713	R1=0.0323 wR2=0.1467
R indices (all data)	I =0.0402 wR2=0.110	R1=0.0333 wR2=0.086	R1=0.0397 wR2=0.102	R1=0.0293 wR2=0.0734	R1=0.0340 wR2=0.1503
Flack parameter	not applicable	0.30(13)	0.20(12)	not calculated	not applicable
Largest difference peak and hole ($e.Å^{-3}$)	0.409 and -0.179	0.135 and - 0.183	0.315 and -0.201	0.125 and -0.111	0.481 and -0.259

Structures may be referred to by their identification codes in order that different structure determinations of the same compound not be confused.

3.1.1 Crystal data

3.1.1.1 DL-serine



Figure 3.1: ORTEP (Johnson, 1970) diagram of DL-serine at room temperature (sc53)



Figure 3.2: ORTEP (Johnson, 1970) diagram of DL-serine at 123K (serine_l)

Table 3.2: A comparison of DL-serine crystal data with literature values

	KRM [a]	FLKH [b]	sc53	serine_1	TK[c]
a (Å)	10.739(2)	10.719(3)	10.7332(11)	10.7720(5)	10.7626
b (Å)	9.149(2)	9.136(4)	9.1443(8)	9.1835(4)	9.1752
c (Å)	4.830(1)	4.833(2)	4.8286(7)	4.7956(2)	4.7889
β (°)	106.42(1)	106.43(3)	106.427(12)	106.7340(10)	106.7

The unit cell dimensions of the three room temperature structures (KRM, FLKH, sc53 (figure 3.1)) compare favourably for the short axis *c* and for β, but for *a* and *b* the FLKH values are significantly smaller. Kistenmacher et al. also noted that cell constants were only in moderate agreement with those found by Frey et al. Differences in cell constants are difficult to account for as they are a result of the reflections selected for calculation of the cell parameters and the orientation matrix. The intensity , 2θ value, distribution in the octants of the reciprocal lattice and number of reflections all play a role in the determination of the cell constants but are usually not fully described in literature accounts. In the case of the respective DL-serine cell constants, they were obtained by least squares techniques from 21 (FLKH), 11 (KRM) and 25 (sc53) centred reflections.

Data were collected at 123K for serine_1 (figure 3.2) and at 100K for TC. The cell constants for the two low temperature structures were similar. There was an increase in *a* and *b* and an overall volume shrinkage on cooling of only 0.05% for serine_1 and 0.35% for TC compared to sc53. This indicates that contraction of the cell constants need not necessarily occur at low temperatures.

For both data collections the cell parameters were initially found to be *a*=4.828Å, *b*=9.144Å, *c*=10.450Å, β=99.88°. These cell constants were close to those reported in the literature except that the *a* and *c* axis had been reversed, the *β* angle was smaller and the space group was $P2_1/n$ as opposed to $P2_1/a$. In a standard setting the *a* axis is chosen to be the shortest axis

[a] T.J. Kistenmacher, G.A.Rand, R.E.Marsh, *Acta Cryst., B30* (1974) 248
[b] M.N. Frey, M.S. Lehman, T.F. Koetzle, W.C. Hamilton, *Acta Cryst., B29* (1973) 876
[c] Tibor Koritsanzansky, *Written communication, 1998.*

but in this case a transformation was required in order to compare to literature values. The following matrices were used to transform the cell parameters.

i.

$$\begin{vmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

ii.

$$\begin{vmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$

The transformation resulted in a cell having space group $P2_1/c$ as the diffractometer software did not recognise $P2_1/a$.

iii. A further transformation was performed in the structure refinement using an HKLF 4 1 0 0 1 0 -1 0 1 0 0 in the instruction file ie. the transformation matrix was

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

The final transformation resulted in the desired space group and cell constants

3.1.1.2 D and L-serine.H_2O



Figure 3.3: ORTEP (Johnson, 1970) diagram of L-serine.H_2O (sc54)



Figure 3.4: ORTEP (Johnson, 1970) diagram of D-serine.H_2O (sc55)

Table 3.3: A comparison of L-Serine.H_2O and D-Serine.H_2O crystal data with literature values

	L-serine.H_2O FLKH	L-serine.H_2O (sc54)	D-serine.H_2O (sc55)	D-serine.H_2O (sc56)
a (Å)	9.365(7)	4.8189(4)	4.8195(6)	4.8176(10)
b (Å)	12.239(9)	9.3566(15)	9.3584(17)	9.3466(19)
c (Å)	4.835(7)	12.2253(12)	12.2183(14)	12.207(3)

The cell constants found are inverted with respect to the literature values with no consequence because the cell is orthorhombic. The literature values are higher for all axis but this is of little concern because the standard deviations for these values are also high. The values for D (sc55, figure 3.4) and L-serine.H_2O (sc54, figure 3.3) in this study compare favorably to one another although the *c* axis is slightly longer for L-serine.H_2O

Comparing the D-serine.H_2O structures, sc55 and sc56, it can be seen that the *a* axes are the same but the *b* and *c* are significantly shorter for data collected on the SMART CCD. This is probably a result of the different methods used in determining the cell parameters on the two diffractometers. The calculation of the cell constants using the SMART CCD is generally considered more accurate than for the CAD4. In the former 'frames' of intensity peaks give a higher number and 2θ spread of reflections than the 25 individual reflections selected on the CAD4. This said, the high standard deviation on the *c* axis may be an indication that too few 00*l* reflections were selected in the initial determination of the cell constants. This would subsequently affect further crystal data including the atomic parameters.

3.2.1 Absolute structure

Friedel opposites were collected for the D (sc55) and L-serine.H_2O (sc54) data collections in order that any anomalous scattering be detected and used in the determination of the correct absolute structure. Data collected for D-serine.H_2O (sc56) were small (680 reflections) and did not include Friedel pairs so there was no information for absolute structure calculation. As this structure was known to be the D-enantiomer, it was simply compared to D-serine.H_2O (sc55) to ensure that the correct absolute structure had been refined.

The absolute structure parameter was refined as a separate parameter in the SHELXL

refinement for D and L-serine.H_2O. This particular absolute structure parameter is called the Flack parameter and numerically lies between 0 and 1. A value close to zero indicates that the correct absolute structure has been allocated, whereas if it lies close to one, the structure needs to be inverted. This was the case with the initial refinement of L-serine.H_2O. A Flack parameter of 0.70(13) was found as opposed to that of 0.20(12) for D-serine.H_2O. A MOVE 1 1 1 -1 card was inserted into the L-serine.H_2O SHELX instruction file to invert the structure. The resulting parameter was 0.30(13) indicating that the correct absolute structure had indeed been assigned.

In this study the high angle data collection (2θ to 29.95° for both structures) accentuated any weak anomalous dispersion so, although serine is an organic molecule with no atoms heavier than oxygen, the absolute structure was accurately determined with no strong scatterers present. This indicates that the anomalous scattering of carbon, nitrogen and oxygen is sufficiently detectable in the refinement and can therefore be relied upon for an accurate absolute structure determination.

3.2 Molecular configurations

Bond lengths of organic compounds have been determined from structures in the CSD (Allen, 1987), using the weighted mean values of bond lengths of a certain type. Mean lengths of the bond types present in serine are given in table 3.4.

Table 3.4: Mean values of bond length types found in serine

Bond type	Bond length (Å)
C-COO^- in carboxylate anions	1.520(11)
Csp^3-Csp^3	1.524(14)
C-NH_3^+	1.488(13)
CH_2-OH	1.426(11)
C-C=O delocalised double bonds in carboxylate anions	1.254(10)

3.2.1 DL-Serine

Table 3.5: A comparison of non hydrogen bond lengths for DL-serine

Bond Length (Å)	KRM esd: 0.002-3 Å	FLKH esd: 0.001-2 Å	sc53 esd: 0.0011-13 Å	serine_1 esd: 0.0007-9 Å
C(1)-C(2)	1.531	1.531	1.5295	1.5329
C(2)-C(3)	1.518	1.518	1.5178	1.5241
C(2)-N	1.491	1.487	1.4910	1.4908
C(1)-O(1)	1.245	1.248	1.2477	1.2549
C(1)-O(2)	1.260	1.257	1.2600	1.2680
C(3)-O(3)	1.419	1.414	1.4192	1.4223

Table 3.6 : A comparison of non hydrogen bond angles for DL-serine

Bond Angle (°)	KRM esd: 0.1-2°	FLKH esd: 0.1°	sc53 esd: 0.07 -8°	serine_1 esd: 0.05 °
O(1)-C(1)-O(2)	126.0	125.8	125.89	125.94
O(1)-C(1)-C(2)	117.9	117.9	117.94	117.83
O(2)-C(1)-C(2)	116.1	116.3	116.16	116.22
C(1)-C(2)-N	109.5	109.6	109.48	109.72
C(3)-C(2)-N	111.7	111.7	111.64	111.47
C(1)-C(2)-C(3)	111.8	111.5	111.75	111.42
C(2)-C(3)-O(3)	111.4	111.4	111.39	111.28

The distances (table 3.5) and angles (table 3.6) for the room temperature structure of DL-serine compare favourably with those found by Kistenmacher and Frey. The values from this study agree most strongly with KRM but any deviation from FLKH values is not significant. All DL-serine bonds fall within the range described by Allen (1987).

Aside from the C-N bond which remains unchanged, a comparison of the room and low temperature structures reveals an overall increase in the bond lengths for the low temperature structure. This is most likely a result of the elongation of the *a* and *b* cell axes on cooling. The standard deviations for bonds and angles have decreased for the low temperature structure which is to be expected with the relative reduction in thermal motion at 123K.

The C1-O1 bond of the carboxylic acid group is substantially shorter than the C1-O2 by 0.010-15Å for all structures. The carboxyl group is anionic in the solid form with charge being unevenly distributed across the functional group. The cause of this uneven distribution is the hydrogen bonding of the carbonyl oxygens with O2 having two (to H2 and H3) and O1 having one hydrogen bond (to H7). The increased hydrogen bonding to O2 reduces the electron density available for bonding thereby elongating the C-O2 bond giving it more single bond character. A single hydrogen bond to O1 leaves more electron density available for the covalent bond and results in a shorter, stronger C-O bond. The structures of most Zwitterionic amino acids show the same feature. In the multipole analysis of the 23K study of alanine (Destro, 1988), the O2 was found to have a slightly larger negative charge than O1.

The C1-C2 bond for all structures is unexpectedly and significantly longer than the C2-C3 bond. From a statistical analysis of 69 amino acids found on the Cambridge structural database (CSD), the mean length of the C-COO$^-$ was found to be 1.533Å (Appendix C, figure C3) which falls at the high end of the range of 1.520(11)Å described by Allen (1987). Not satisfied that Allen's value appropriately described the bond, a further search for this bond was performed over the entire database. A search for any structure that contained the Zwitterion group resulted in 312 hits and a mean bond length of 1.534Å (Appendix C, figure C4), leading to the conclusion that this elongated bond length appears to be a feature common to all Zwitterionic structures. The long C1-C2 distance was commented on in a topological analysis of the experimental electron density of DL- aspartic acid (Flaig et al., 1997). It was reported to be due to the net atomic charges of C1 and C2, calculated to be -0.4 and 0.2 respectively.

3.2.2 L-serine.H_2O and D-serine.H_2O

Table 3.7: A comparison of non hydrogen bond lengths for L-serine.H_2O and D-serine.H_2O

Bond Length (Å)	FLKH esd: 0.002-4 Å	L-serine.H_2O (sc54) esd: 0.002 Å	D-serine.H_2O (sc55) esd: 0.002 Å	D-serine.H_2O (sc56) esd: 0.002-3Å
C(1)-C(2)	1.527	1.533	1.533	1.516
C(2)-C(3)	1.519	1.517	1.518	1.519
C(2)-N	1.488	1.484	1.489	1.491
C(1)-O(1)	1.248	1.248	1.244	1.246
C(1)-O(2)	1.251	1.251	1.251	1.250
C(3)-O(3)	1.413	1.417	1.418	1.417

Table 3.8: A comparison of non hydrogen bond angles for L-serine.H_2O and D-serine.H_2O

Bond Angle (°)	L-serine.H_2O FLKH esd: 0.2°	L-serine.H_2O (sc54) esd: 0.11-14°	D-serine.H_2O (sc55) esd: 0.1°	D-serine.H_2O (sc56) esd: 0.1-2°
O(1)-C(1)-O(2)	125.1	125.2	125.3	124.8
O(1)-C(1)-C(2)	118.6	118.7	118.8	119.0
O(2)-C(1)-C(2)	116.3	116.1	115.8	116.1
C(1)-C(2)-N	110.6	110.7	110.4	110.9
C(3)-C(2)-N	111.2	111.5	111.4	111.0
C(1)-C(2)-C(3)	110.9	111.3	111.3	111.8
C(2)-C(3)-O(3)	111.8	111.3	111.3	110.7

Bond lengths (table 3.7) and angles (table 3.8) all compare favourably and fall within the range of standard deviation. As for DL-serine, the C2-C3 bond for FLKH, sc54 and sc55 is longer than the C1-C2 bond. However, the C1-C2 bond for D-serine.H_2O (sc56) is 0.015Å shorter than for the other structures. It is likely that this difference in bond length is a result of the shorter cell parameters found for sc56. It could also be due to the low number of data collected on the SMART CCD. This bond length is inconsistent with that obtained from the CSD search on the C1-C2 bond (Appendix C, figure C4), and with the other three serine.H_2O structures.

3.2.3 A comparison of the geometries of DL-serine and L/D-serine.H_2O

On comparison of the bond lengths and angles of the racemic and enantiomeric structures, it was apparent that the two structures assume similar configurations in the crystal. A comparison of torsion angles (table 3.9) further indicated that D/L-serine.H_2O and DL-serine assume nearly identical geometries. The C-N bond and the carboxylate group are planar to one another, the conformation is staggered down the C2-C3 bond (figure 3.5) and the ammonium hydrogens are also staggered with respect to the groups attached to C2 (figure 3.6). Anhydrous L-serine (Kistenmacher, 1974) also assumes a similar geometry although there are significant differences in the conformational angles about the C2-C3 and O3-C3 bonds. These differences result from the differences in the O3-H7...O hydrogen bond (see tables 3.11 and 3.12).

Table 3.9: Selected torsion angles for D-serine.H_2O, L-serine.H_2O, DL-serine and L-serine

Torsion angle (°)	D-serine.H_2O sc55	L-serine.H_2O sc54	DL-serine sc53	L-serine (KRM)
O1-C1-C2-C3	125.87	126	125.71	124
O2-C1-C2-C3	54.95	54.6	55.47	56
N-C2-C1-O1	1.64	1.36	1.5	2
N-C2-C1-O2	179.17	179.3	179.68	179
O3-C3-C2-N	70.82	71.3	70.21	60
O3-C3-C2-C1	52.86	52.68	52.77	63
H1-N-C2-C3	64.61	64.39	60.88	60
H2-N-C2-C3	49.8	49.78	56.48	60
H3-N-C2-C3	178.09	172.57	179.35	180

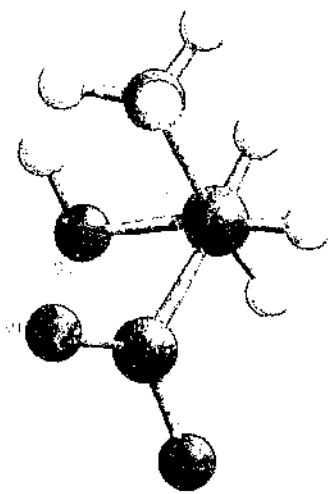


Figure 3.5: The staggered conformation down the C2-C3 bond of DL-serine (sc53)

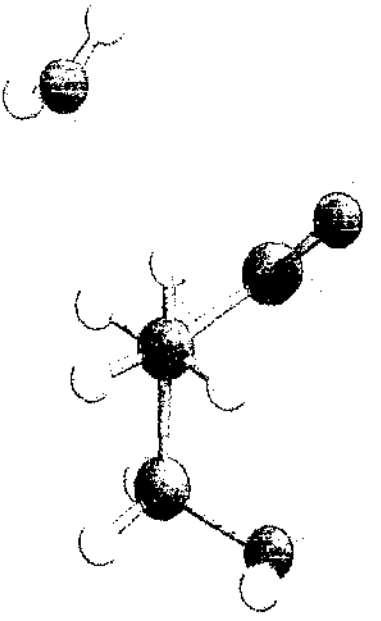


Figure 3.6: The staggered conformation down the N-C2 bond of D-serine.H_2O (sc55)

3.3. Hydrogen Bonding

According to Jeffrey (1997) hydrogen bonds can be classified as strong, moderate or weak depending on their bond lengths (table 3.10) . Most biomolecules have moderate hydrogen bonds, but weak hydrogen bonds may also be present as the minor component of a three-centre hydrogen bond. Weak C-H...O hydrogen bonds also occur in amino acid structures.

Table 3.10: Interatomic distances and hydrogen bond strengths for the A-H....B bond

A-H...B	Strong (15-40 kcal mol^{-1})	Moderate (4 15 kcal mol^{-1})	Weak (1-4 kcal mol^{-1})
H.....B (Å)	1.2-1.5	1.5-2.2	2.2-3.2
A....B (Å)	2.2-2.5	2.5-3.2	3.2-4.0

Hydrogen bonds are usually linear with a single acceptor. Hydrogen atoms with two acceptors that form non linear bonds are found in approximately 75% of Zwitterionic amino acid crystal structures. These bonds are referred to as three-centred since the hydrogen is bonded to three atoms: one covalent and two hydrogen bonds (figure 3.7).

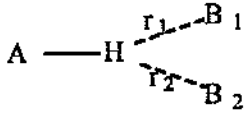


Figure 3.7: A three-centre hydrogen bond.

Three centred hydrogen bonds occur because the COO^- group prefers to accept four hydrogen bonds, *ie.* two per oxygen atom. The NH_3^+ group has only three protons so sharing becomes necessary in order to satisfy the strong potential of the carboxyl group as hydrogen bond acceptors. The three-centre bond is usually unsymmetrical with a shorter major and a longer minor component (r1>r2). A study by Jeffrey and Mitra (1984) showed the hydrogen bond configuration of 49 amino acid structures to be that depicted in figure 3.8. The three-centred bond is found in 39 of the 49 structures.

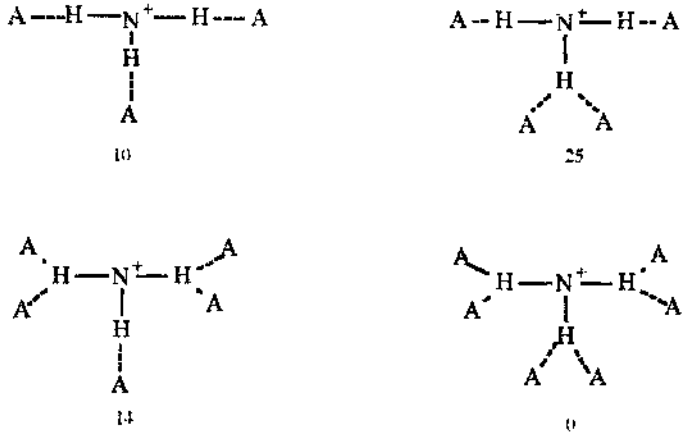


Figure 3.8: The hydrogen bond configurations found in 49 amino acids (numbers of examples are given below structures).

The following tables note all H...O bonds under 3Å long. Most of the bonds are weak but all contribute to the assumed geometry of the molecules in the crystal.

3.3.1. DL-serine

Table 3.11: Hydrogen bond distances for dl serine at room and low temperature (i indicates an intramolecular bond distance)

	DL-serine (sc53)			DL-serine (serine_l)		
A-H...B	H...B (Å)	A...B (Å)	∠AH..B(°)	H...B (Å)	A...B (Å)	∠AH..B(°)
N-H1...O3	1.895	2.773	158.42	1.899	2.766	160.33
N-H2...O2	1.946	2.822	161.55	1.929	2.800	162.23
N-H3...O2	1.916	2.874	171.48	2.063	2.860	164.93
N-H3...O1 i	2.644	2.629	81.06	2.630	2.638	81.63
N-H3...O3 i	2.807	3.018	93.16	2.707	3.011	104.02
N-H3...O1	2.755	3.397	124.68	2.816	3.421	132.55
O3-H7...O1	1.778	2.673	175.73	1.742	2.666	172.26
O3-H7...O2	2.833	3.273	127.56	2.846	3.410	120.21
C2-H4...O1	2.346	3.294	173.62	2.333	3.288	173.74

Discrepancies in the hydrogen bond lengths are due to the difficulty in accurately placing a hydrogen atom in an X-ray diffraction experiment. The positions of hydrogens in this study are significant within 0.05Å.

There are four moderate strength H...O hydrogen bonds per asymmetric unit. Two of the NH_3^+ hydrogen atoms bond with neighbouring carbonyl oxygens; both H2 and H3 bond to O2 atoms of adjacent serine molecules of the same chirality. Hydrogen bonds to O2 hold the layers of serine molecules together so that they appear to stack upon on another (fig 3.9). H1 bonds to O3 and it is this hydrogen bond that holds the columns of D and L-serine molecules together (fig 3.11). The O3-H7...O1 bond is the strongest hydrogen bond as indicated by its short bond length of 1.778Å. The O3-H7-O1 bond angle is 175.73°, *ie.* close to linear as expected for a strong hydrogen bond.

Atom H3 is involved in a three centre hydrogen bond (fig 3.10). The major component is the H3...O2 bond (1.916 Å) and the minor component is the intramolecular H3...O1 (2.644 Å). The C1-O2-H3 bond angle is 108.72° and the O1-C1-H3 angle is 81.06° owing to the three centre arrangement. A short distance of 2.346Å was found between H4 and O1 indicating the presence of a C-H hydrogen bond. The C2-H4-O1 angle is 173.62°.

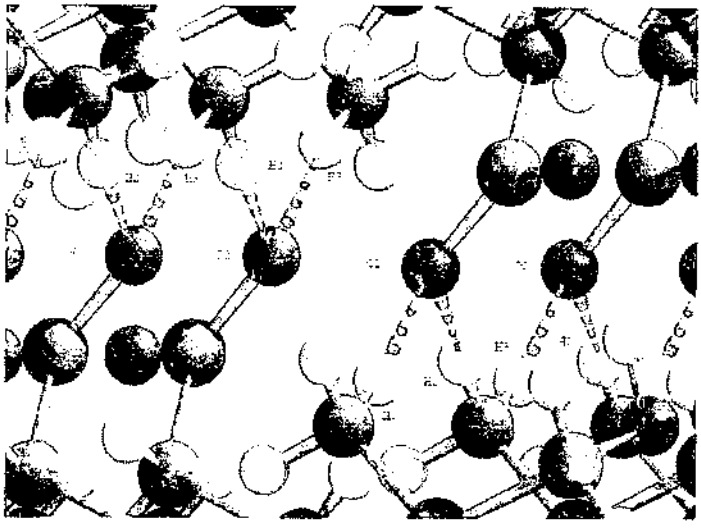


Figure 3.9 : A detail of a packing diagram showing hydrogen bonds from H2 and H3 to O2.

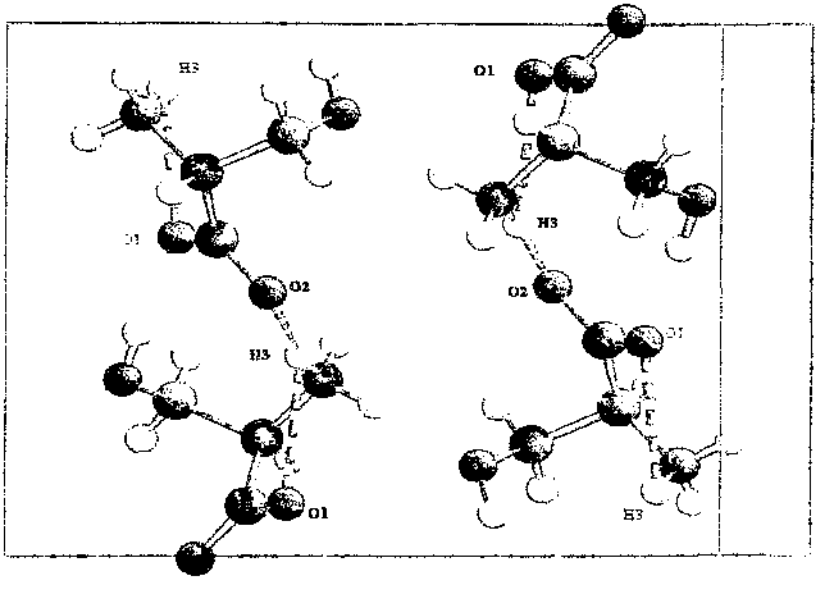


Figure 3.10: H3 involved in a three centre hydrogen bond with O1 and O2.

3.3.2. D and L-serine.H_2O

Table 3.12: Hydrogen bond distances for D and L-serine.H_2O (*i* indicates an intramolecuar bond distance)

	D-serine.H_2O (sc55)			L-serine.H_2O (sc54)		
A-H...B	H...B (Å)	A...B (Å)	∠AH..B(°)	H...B (Å)	A...B (Å)	∠AH..B(°)
N-H1...O1 *i*	2.495	2.670	92.05	2.487	2.672	91.38
N-H1...O4	2.203	2.906	135.78	2.178	2.906	135.35
N-H1. .O4	2.764	2.966	94.16	2.769	2.966	93.18
N-H2...O3 *i*	2.764	3.017	98.82	2.693	3.021	104.06
N-H2...O1 *i*	2.638	2.670	82.67	2.680	2.672	79.65
N-H2...O2	2.065	2.911	158.95	2.071	2.910	163.99
N-H2...O4	2.793	2.966	91.80	2.847	2.966	89.34
N-H3...O2	1.839	2.758	158.95	1.835	2.758	155.16
N-H3...O4	2.883	2.966	85.02	2.850	2.966	87.85
O3-H7...O1	1.956	2.784	169.72	1.900	2.782	170.28
O3-H7...O2	2.612	3.247	133.64	2.633	3.246	129.53
O4-H8...O1	1.987	2.813	173.09	1.952	2.811	173.6
O4-H9...O3	2.027	2.866	176.95	2.032	2.867	177.72
O4-H9...O2	2.965	3.158	97.96	2.885	3.159	100.29

There are 6 hydrogen bonds per asymmetric unit. Atom H1 of the NH_3^+ group is bonded to O4 of the water molecule; the two remaining hydrogen atoms of the NH_3^+ group hydrogen bond to carboxyl oxygens (O2) of neighbouring serines; the hydroxyl hydrogen bonds to a neighbouring carboxyl oxygen (O1) and the hydroxyl oxygen accepts a hydrogen bond from a water molecule. A short intramolecular contact worth noting is the N·O1 distance of 2.670Å.

The strongest H bond is between the carbonyl oxygen O2 and H3.

3.4 Packing

An interesting part of this investigation lies in the close relationship between the structures of the enantiomeric and racemic crystal. Both structures are made up of sheets of serine stacked upon one another.

3.4.1 DL-serine

Columns of serine molecules appear to lie parallel to the (100) face (Shoemacher, 1953). A column of L-serine is bonded to a column of D-serine by H(1)....O3 hydrogen bonds. The three remaining H bonds; O3-H7...O1, N-H3...O2 and N-H2 ..O2, bind the molecules within each column. The repeat period along the *a* axis therefore consists of alternating layers of L and D serine molecules (figure 3.11).

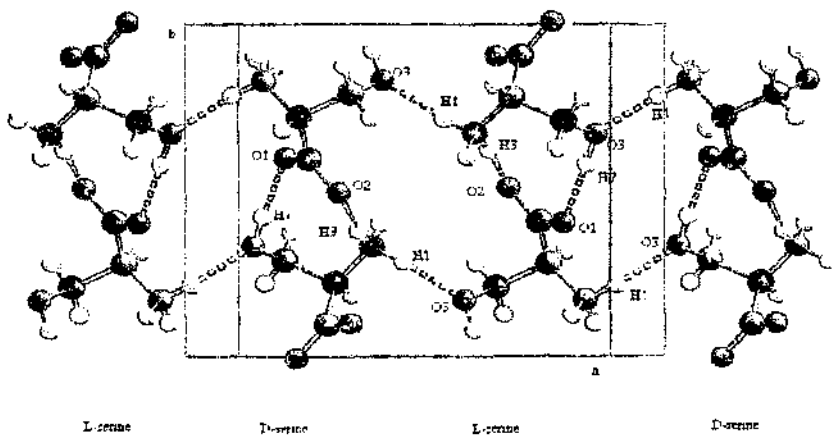


Figure 3.11: The repeat period along the *a* axis of DL-serine showing the alternating columns of D and L-serine.

3.4.2 D and L-serine.H_2O

Packing in the enantiomeric crystal is similar to that of DL-serine except that the columns of serine lie parallel to the (001) face. The serine columns are linked together by hydrogen bonds through the water molecules. The repeat period along the *c* axis therefore consists of layers of serine molecules separated by layers of H_2O molecules (figure 3.12).

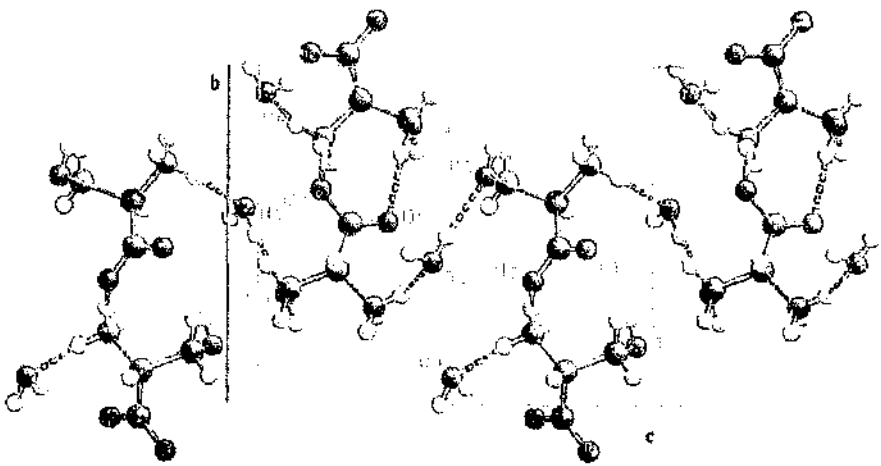


Figure 3.12: The repeat period along the *c* axis of D-serine.H_2O showing the columns of serine linked through water molecules.

3.4.3 L-serine (Kistenmacher, 1974)

The non hydrated L-serine structure proves to be completely different from the hydrated and racemic crystals. The hydroxyl groups are exclusively bonded to neighbouring hydroxyl groups and all N-H hydrogens are donated to neighbouring carboxyl oxygen atoms.

3.4.4 Alanine (Destro, 1988)

The stacking feature is also seen in the structure of alanine where N-H...O2 hydrogen bonds link molecules together to form columns along the x axis. The other two N-H...O bonds link the columns together in a three-dimensional network

3.5 Residual Electron Density

The refined room temperature structure of DL-serine was found to have residual electron density almost coplanar with and half way along the C1-C2 and C2-C3 bonds. These features were noted by Kistenmacher et al. and referred to as 'bonding electron' density but were not further investigated. It was hoped that a low temperature study would give more insight into the nature of this electron density which, given its presence in two separate studies, did not appear to be artifactual. On further investigation it was noted that residual electron density was present along most non hydrogen atom bonds. The residual electron density peaks are denoted by E.

Table 3.13: Details of interbond residual electron density for DL-serine 298K

Bond A-B	Inter-bond electron density, E (e.Å^{-3})	Angle A-E-B (°)	Distance A-B (Å)	Distance A-E (Å)	Distance B-E (Å)
C2-C3	0.41	173.4	1.517	0.761	0.759
C1-C2	0.39	173	1.529	0.755	0.778
C3-O3	0.27	161.4	1.419	0.784	0.654
C2-N	0.25	173.1	1.491	0.773	0.720

Table 3.14: Details of interbond residual electron density for DL-serine at 123K.

Bond A-B	Inter-bond electron density, E (e.Å^{-3})	Angle A-E-B (°)	Distance A-B (Å)	Distance A-E (Å)	Distance B-E (Å)
C2-C3	0.48	167.7	1.522	0.777	0.756
C1-C2	0.45	171.8	1.533	0.795	0.742
C2-N	0.34	175.4	1.490	0.677	0.815
C1-O1	0.32	171.0	1.268	0.636	0.635
C1-O2	0.30	161.1	1.255	0.671	0.601

The largest electron density peaks are present half way along the C2-C3 and C1-C2

internuclear axes with densities equivalent to less than half an electron per Å^3. In any X-ray diffraction experiment the single electron of the hydrogen atom is difficult to locate and the apparent position will be shifted towards the atom X of the X-H bond by up to 0.1Å (Jeffrey, 1997). Considering this difficulty it seems unlikely that a smaller amount of electron density could be accurately placed on a Fourier map. Nevertheless, the above results show a strong correlation with one another and the literature observation, suggesting that this electron density is not artifactual but real and observed. If these peaks were not real, it would be expected that they would disappear in the low temperature study

In a room temperature structure thermal motion of atoms is modeled using anisotropic thermal parameters. Thermal parameters that are unsuitable contribute to residual electron density. When temperature is lowered, thermal libration is greatly reduced and electron density becomes more spherical in nature and is positioned closer to the core of the atom. This normally eliminates any residual electron density due to libration effects that may be present in the room temperature structure. In the case of DL-serine, thermal motion was halved on cooling (see ORTEP diagrams (figures 3.1 and 3.2) and thermal parameters (Appendix A, Tables A3 and A7)), yet the residual density is still present in the same amount at similar coordinates.

The electron density has moved further from the plane of the bond at 123K yet is still visible in a Fourier difference map through the plane of the C1, C2 and C3 atoms. The anomalous shifts in the electron density away from the bonds may be due to the limited scattering power of the peak. This could mean that the placement of this non artifactual electron density, like in the placement of hydrogen atoms, is significant within 0.1Å.

The peak between the C3-O3 nuclei disappeared on cooling indicating that it was due to the libration of the terminal oxygen atom. A small amount of electron density is also present on the C-N bond for both structures. Electron density occurs midway along the C-O bonds of the carbonyl group in the low temperature refinement. It is possible that these small peaks of electron density are visible at low temperature because high angle reflections were collected. The 123K data were collected to $2\theta=35°$, 5° more than the 298K data giving 667 extra

reflections. Further information about the topology of the electron density of DL-serine is contained in the high angle reflections.

The question then arose as to whether the peaks play a role in bonding. These effects were not encountered for L and D-serine.H_2O, nor for any other amino acid structures in the literature. There does not appear to be any other structural feature unique to DL-serine that may help account for this observation. The fact that the electron density was midway along a bond, real and reproducible implies that it is electron density due to bonding. These features, if they exist, don't normally appear in a Fourier difference map. Images of bonding density, lone pairs and the like are usually visualised with a deformation density map (The 'standard deformation density' is the difference between the total density and the density corresponding to superimposed spherical atoms (Coppens, 1989)). For further insight into this bonding density, treatment with a charge density program (eg. Multipole refinement and deformation density map with XD (Koritsanszky, 1995) would be required.

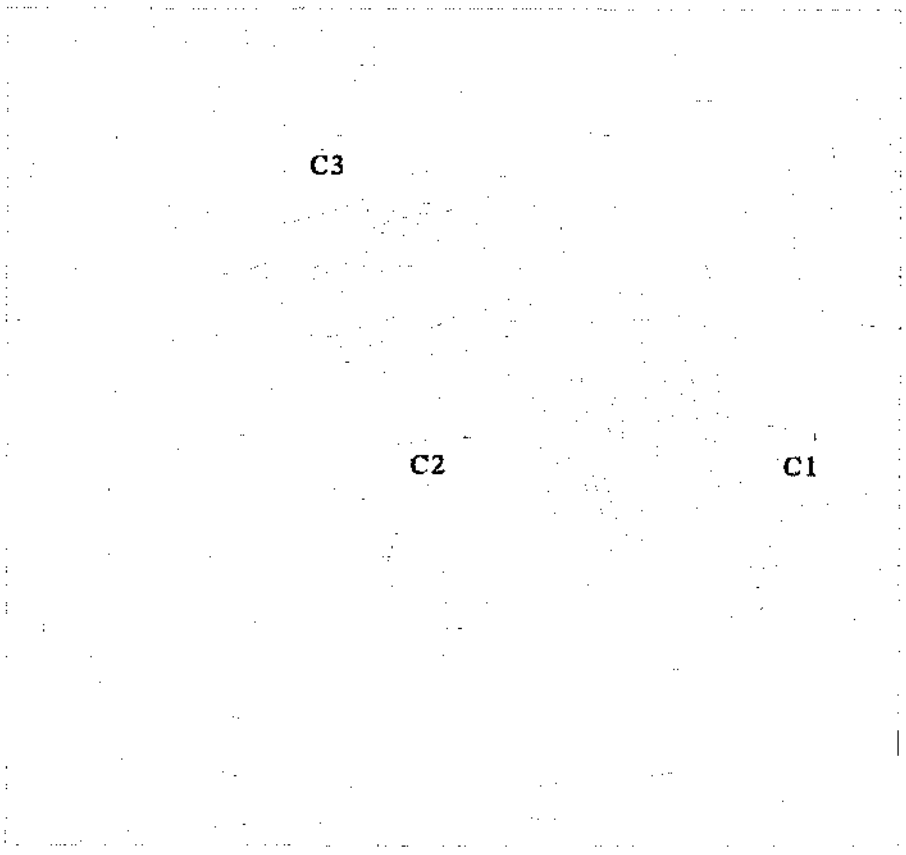


Figure 3.13: Fourier difference map through the zero layer of the plane defined by C1, C2 and, C3 of DL-serine at 298K. Contour intervals at 0.06 e.A^{-3}. Negative contours represented by dotted lines

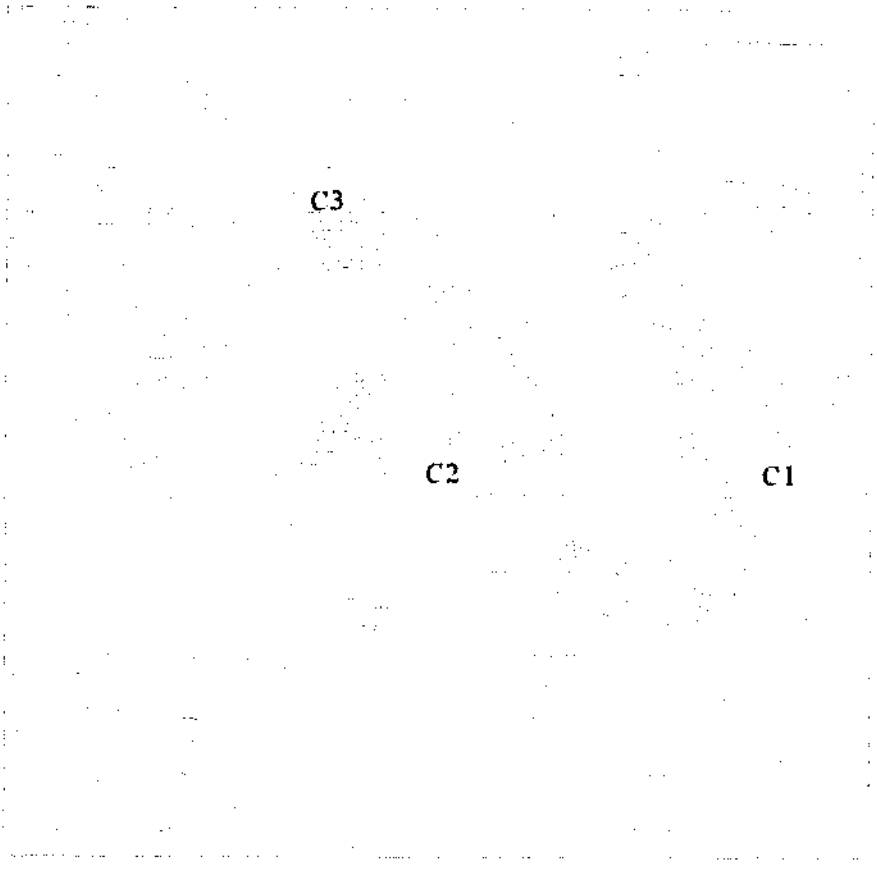


Figure 3.14: Fourier difference map through the zero layer of the plane defined by C1, C2 and, C3 of DL-serine at 123K. Contour intervals at 0.06 e.Å^{-3}. Negative contours represented by dotted lines

Chapter 4

Conclusion

From the analysis of the X-ray diffraction structure solutions of DL-serine, D-serine.H_2O and L-serine.H_2O the following points have emerged.

Lowering the temperature of the data collection has a considerable effect on the cell parameters relative to data collected at room temperature. Expansion of the *a* and *b* axes and contraction of *c* resulted for DL-serine at 123K with minimal change in total cell volume. There was also a significant change in bond lengths, notably the elongation of the C-O carbonyl bonds.

Aside from attaining more accurate cell parameters, the main reason for the low temperature data collection was to further examine residual electron density present in the room temperature structure. Electron density at 123K was present in similar concentrations to that found in the room temperature structure, particularly along the C-C internuclear axes. This indicated that it was not artifactual nor due to inadequate modelling of the atom density, but real and most likely part of the bond. The data set collected at 123K is large and of good quality. With XD, a computer program package for multipole refinement and analysis of electron densities from diffraction data (Koritsanszky, 1995), it would be possible to thoroughly analyse the nature and topology of the residual electron density.

The elongation of the C1-C2 bond with respect to the C2-C3 bond was earlier discussed. It could be that the 'bonding' density is in fact a product of this feature of the Zwitterion group. Selected Zwitterionic structures need to be analysed by crystallographic methods with the sole purpose of analysing the residual electron density in order to confirm this.

Data were collected for D and L-serine.H_2O for the purposes of comparing the two structures and to ascertain whether the absolute structure of small organic molecules can be determined with the collection of Friedel pairs. As expected, the structures were essentially found to be identical. With the assistance of the Flack parameter that refines as part of the SHELX refinement for

acentric structures, the correct absolute structure was assigned for both enantiomers. This confirms that chiralty of structures without heavy atoms can be accurately assigned if Friedel pairs are collected to a relatively high 2θ angle.

All structures were found to be stabilised by extensive hydrogen bond networks with most of the bonds being weak in nature. The racemic and enantiomeric crystal structure pack together similarly with columns of serine linked together through hydrogen bonds.

X-ray crystallographic studies of amino acids are ongoing, particularly at low temperatures and using synchrotron radiation sources The aim of such detailed studies is to derive methodically self-consistent experimental electronic properties of these molecules. Topological descriptions of the electron densities of amino acids could ultimately lead the modelling of proteins from their primary sequence alone.

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CRYSTAL DATA FOR DL-SERINE

DL-serine at room temperature (sc53)

Table A1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sc53. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	3362(1)	977(1)	5691(2)	32(1)
O(2)	1679(1)	-59(1)	2472(2)	34(1)
N	3476(1)	4299(1)	2561(2)	24(1)
O(3)	685(1)	3311(1)	2710(2)	34(1)
C(1)	2504(1)	944(1)	3328(2)	23(1)
C(2)	2449(1)	2209(1)	1225(2)	22(1)
C(3)	1112(1)	2906(1)	293(2)	28(1)

Table A2. Bond lengths [A] and angles [deg] for sc53.

O(1)-C(1)	1.2477(12)
O(2)-C(1)	1.2605(11)
N-C(2)	1.4910(11)
N-H(1)	.921(14)
N-H(2)	.91(2)
N-H(3)	.97(2)
O(3)-C(3)	1.4192(13)
O(3)-H(7)	.90(2)
C(1)-C(2)	1.5295(12)
C(2)-C(3)	1.5178(12)
C(2)-H(4)	.952(14)
C(3)-H(6)	.99(2)
C(3)-H(5)	.97(2)
C(2)-N-H(1)	109.7(9)
C(2)-N-H(2)	108.5(10)
H(1)-N-H(2)	107.7(13)
C(2)-N-H(3)	115.0(10)
H(1)-N-H(3)	106.3(12)
H(2)-N-H(3)	109.4(14)
C(3)-O(3)-H(7)	109.6(11)
O(1)-C(1)-O(2)	125.89(8)
O(1)-C(1)-C(2)	117.95(8)
O(2)-C(1)-C(2)	116.16(8)
N-C(2)-C(3)	111.64(7)
N-C(2)-C(1)	109.48(7)
C(3)-C(2)-C(1)	111.75(7)
N-C(2)-H(4)	107.2(8)
C(3)-C(2)-H(4)	108.4(8)
C(1)-C(2)-H(4)	108.2(8)
O(3)-C(3)-C(2)	111.39(8)
O(3)-C(3)-H(6)	112.0(9)
C(2)-C(3)-H(6)	110.1(8)
O(3)-C(3)-H(5)	108.5(9)
C(2)-C(3)-H(5)	108.4(9)
H(6)-C(3)-H(5)	106.2(12)

Table A3. Anisotropic displacement parameters ($A^2 \times 10^3$) for se53. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
O(1)	39(1)	27(1)	26(1)	-4(1)	4(1)	0(1)
O(2)	44(1)	26(1)	31(1)	-3(1)	10(1)	-9(1)
N	23(1)	22(1)	27(1)	-4(1)	8(1)	2(1)
O(3)	27(1)	32(1)	48(1)	-12(1)	19(1)	-6(1)
C(1)	30(1)	20(1)	22(1)	-1(1)	11(1)	2(1)
C(2)	25(	23(1)	19(1)	3(1)	8(1)	1(1)
C(3)	24(1)	31(1)	27(1)	1(1)	5(1)	1(1)

Table A4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($A^2 \times 10^3$) for se53.

	x	y	z	U(eq)
H(6)	1113(13)	3743(18)	-995(35)	37(4)
H(1)	4276(13)	2847(16)	3087(30)	34(3)
H(4)	2643(13)	1833(15)	-446(31)	29(3)
H(5)	502(14)	2198(18)	-849(32)	38(4)
H(2)	3493(15)	3989(18)	1221(36)	41(4)
H(3)	3379(15)	3768(19)	4279(35)	41(4)
H(7)	979(15)	4206(21)	3307(36)	48(4)

DL-serine at 123K (serine_l)

Table A5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for serine_l. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N	3470(1)	8276(1)	-2443(1)	11(1)
O(1)	1699(1)	4902(1)	-2521(1)	15(1)
C(1)	2528(1)	5908(1)	-1665(1)	11(1)
O(2)	3402(1)	5943(1)	720(1)	14(1)
C(2)	3455(1)	7176(1)	-3784(1)	10(1)
O(3)	702(1)	8264(1)	-2240(1)	15(1)
C(3)	1108(1)	7855(1)	-4702(1)	13(1)

Table A6. Bond lengths [A] and angles [deg] for serine_l.

N-C(2)	1.4908(8)
N-H(3)	0.903(13)
N-H(2)	0.816(16)

N-H(1)	0.900(12)
O(1)-C(1)	1.2680(7)
C(1)-O(2)	1.2549(7)
C(1)-C(2)	1.5329(8)
C(2)-C(3)	1.5241(9)
C(2)-H(4)	0.959(13)
O(3)-C(3)	1.4223(8)
O(3)-H(7)	0.930(17)
C(3)-H(6)	0.956(13)
C(3)-H(5)	0.964(15)
C(2)-N-H(3)	110.4(8)
C(2)-N-H(2)	109.1(10)
H(3)-N-H(2)	113.4(13)
C(2)-N-H(1)	108.8(8)
H(3)-N-H(1)	104.9(11)
H(2)-N-H(1)	110.1(13)
O(2)-C(1)-O(1)	125.94(5)
O(2)-C(1)-C(2)	117.83(5)
O(1)-C(1)-C(2)	116.22(5)
N-C(2)-C(3)	111.47(5)
N-C(2)-C(1)	109.72(5)
C(3)-C(2)-C(1)	111.42(5)
N-C(2)-H(4)	104.7(8)
C(3)-C(2)-H(4)	109.1(8)
C(1)-C(2)-H(4)	110.3(8)
C(3)-O(3)-H(7)	107.6(11)
O(3)-C(3)-C(2)	111.28(5)
O(3)-C(3)-H(6)	109.5(8)
C(2)-C(3)-H(6)	107.4(7)
O(3)-C(3)-H(5)	109.3(9)
C(2)-C(3)-H(5)	107.0(9)
H(6)-C(3)-H(5)	112.4(12)

Table A7. Anisotropic displacement parameters (A^2 x 10^3) for serine_1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N	13(1)	10(1)	12(1)	1(1)	-1(1)	0(1)
O(1)	19(1)	12(1)	13(1)	-1(1)	-4(1)	-4(1)
C(1)	14(1)	9(1)	10(1)	-1(1)	5(1)	1(1)
O(2)	17(1)	12(1)	11(1)	2(1)	1(1)	0(1)
C(2)	11(1)	10(1)	9(1)	0(1)	3(1)	0(1)
O(3)	13(1)	14(1)	20(1)	-6(1)	8(1)	-3(1)
C(3)	11(1)	14(1)	12(1)	0(1)	2(1)	0(1)

Table A8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for serine_1.

	x	y	z	U(eq)
H(4)	2671(13)	6848(14)	-5490(3)	22(3)
H(7)	944(16)	9229(19)	-1810(4)	40(4)
H(6)	1150(12)	8701(15)	-5830(3)	19(3)
H(5)	524(13)	7128(19)	-5800(3)	29(3)
H(3)	4264(13)	7861(14)	-1960(3)	23(3)
H(2)	3292(14)	8660(17)	-1070(3)	25(3)
H(1)	3491(11)	8950(12)	-379(3)	13(2)

CRYSTAL DATA FOR D AND L-SERINE.H_2O

L-serine.H_2O (sc54)

Table B1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sc54.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(2)	7331(3)	6356(1)	7025(1)	31(1)
C(1)	6889(3)	5353(1)	7678(1)	23(1)
N	7854(3)	2885(1)	8318(1)	25(1)
C(2)	8603(3)	3993(1)	7501(1)	22(1)
C(3)	8293(4)	3438(2)	6341(1)	28(1)
O(3)	5462(3)	3270(1)	6054(1)	37(1)
O(4)	11415(3)	4207(2)	9949(1)	42(1)
O(1)	5208(3)	5388(1)	8454(1)	42(1)

Table B2. Bond lengths [A] and angles [deg] for sc54.

O(2)-C(1)	1.2504(18)
C(1)-O(1)	1.248(2)
C(1)-C(2)	1.533(2)
N-C(2)	1.4847(18)
N-H(1)	0.92(3)
N-H(2)	0.87(3)
C(2)-C(3)	1.517(2)
C(2)-H(4)	0.98(3)
C(3)-O(3)	1.417(2)
C(3)-H(5)	0.99(3)
C(3)-H(6)	0.99(2)
O(3)-H(7)	0.88(5)
O(1)-C(1)-O(2)	125.20(13)
O(1)-C(1)-C(2)	118.65(12)
O(2)-C(1)-C(2)	116.14(13)
C(2)-N-H(1)	107.9(17)
C(2)-N-H(2)	108.3(16)
H(1)-N-H(2)	114(3)
N-C(2)-C(3)	111.52(12)
N-C(2)-C(1)	110.68(11)
C(3)-C(2)-C(1)	111.31(12)
N-C(2)-H(4)	108.1(12)
C(3)-C(2)-H(4)	106.6(12)
C(1)-C(2)-H(4)	108.4(12)
O(3)-C(3)-C(2)	111.36(14)
O(3)-C(3)-H(5)	110.2(16)
C(2)-C(3)-H(5)	108.0(13)
O(3)-C(3)-H(6)	108.6(15)
C(2)-C(3)-H(6)	107.5(14)
H(5)-C(3)-H(6)	111(2)
C(3)-O(3)-H(7)	104(3)

Table B3. Anisotropic displacement parameters (A^2 x 10^3) for sc54.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(2)	28(1)	22(1)	42(1)	7(1)	2(1)	0(1)
C(1)	20(1)	18(1)	31(1)	-2(1)	-1(1)	-1(1)
N	27(1)	20(1)	28(1)	1(1)	0(1)	2(1)
C(2)	20(1)	19(1)	26(1)	0(1)	2(1)	0(1)
C(3)	32(1)	26(1)	26(1)	-1(1)	3(1)	0(1)
O(3)	43(1)	30(1)	39(1)	5(1)	-15(1)	-9(1)
O(4)	46(1)	44(1)	36(1)	-5(1)	8(1)	-5(1)
O(1)	49(1)	29(1)	48(1)	4(1)	21(1)	9(1)

Table B4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sc54.

	x	y	z	U(eq)
H(4)	10570(5)	4230(2)	7598(17)	35(6)
H(5)	9270(6)	2510(3)	6291(18)	39(6)
H(1)	8040(6)	3280(3)	9000(2)	52(7)
H(7)	5080(10)	2370(5)	6210(3)	77(15)
H(6)	9130(5)	4150(2)	5847(19)	35(6)
H(2)	6190(6)	2590(3)	8180(2)	41(6)
H(3)	10750(8)	7120(4)	6720(3)	59(10)
H(8)	830(6)	4940(3)	10260(2)	55(8)
H(9)	2650(7)	4520(3)	9510(2)	44(7)

D-serine.H_2O (sc55)

Table B5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sc55.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(2)	2663(2)	1354(1)	7025(1)	32(1)
C(1)	3113(2)	353(1)	7679(1)	24(1)
C(2)	1390(2)	-1003(1)	7498(1)	22(1)
O(3)	4538(3)	-1730(1)	6054(1)	37(1)
N	2150(3)	-2115(1)	8317(1)	26(1)
C(3)	1705(3)	-1558(1)	6337(1)	29(1)
OW	-1412(3)	-793(1)	9949(1)	42(1)
O(1)	4792(3)	387(1)	8452(1)	43(1)

Table B6. Bond lengths [A] and angles [deg] for sc55.

O(2)-C(1)	1.2307(15)
C(1)-O(1)	1.2442(18)
C(1)-C(2)	1.5326(16)
C(2)-N	1.4891(15)
C(2)-C(3)	1.5183(17)
C(2)-H(4)	0.96(2)

O(3)-C(3)	1.4176(19)
O(3)-H(7)	0.85(3)
N-H(1)	0.885(19)
N-H(2)	0.88(3)
N-H(3)	0.97(3)
C(3)-H(5)	0.97(2)
C(3)-H(6)	1.00(3)
OW-H(8)	0.82(3)
OW-H(9)	0.85(3)
O(1)-C(1)-O(2)	125.36(11)
O(1)-C(1)-C(2)	118.86(10)
O(2)-C(1)-C(2)	115.76(11)
N-C(2)-C(3)	111.38(10)
N-C(2)-C(1)	110.40(10)
C(3)-C(2)-C(1)	111.31(10)
N-C(2)-H(4)	107.9(11)
C(3)-C(2)-H(4)	107.0(11)
C(1)-C(2)-H(4)	108.7(11)
C(3)-O(3)-H(7)	103.5(19)
C(2)-N-H(1)	108.2(13)
C(2)-N-H(2)	110.8(15)
H(1)-N-H(2)	107(2)
C(2)-N-H(3)	105.2(16)
H(1)-N-H(3)	107(2)
H(2)-N-H(3)	118(2)
O(3)-C(3)-C(2)	111.30(11)
O(3)-C(3)-H(5)	111.1(14)
C(2)-C(3)-H(5)	106.4(12)
O(3)-C(3)-H(6)	107.5(15)
C(2)-C(3)-H(6)	112.6(13)
H(5)-C(3)-H(6)	108.0(18)
H(8)-OW-H(9)	103(2)

Table B7. Anisotropic displacement parameters (A^2 x 10^3) for sc55. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(2)	29(1)	19(1)	47(1)	6(1)	-1(1)	0(1)
C(1)	21(1)	16(1)	34(1)	-2(1)	1(1)	1(1)
C(2)	20(1)	17(1)	30(1)	0(1)	-1(1)	0(1)
O(3)	43(1)	25(1)	42(1)	6(1)	13(1)	9(1)
N	28(1)	18(1)	31(1)	1(1)	0(1)	-2(1)
C(3)	34(1)	24(1)	30(1)	-2(1)	-3(1)	-1(1)
OW	47(1)	41(1)	38(1)	-4(1)	-8(1)	5(1)
O(1)	49(1)	26(1)	54(1)	5(1)	-22(1)	-10(1)

Table B8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sc55.

	x	y	z	U(eq)
H(1)	1990(4)	-1740(2)	8978(14)	31(4)
H(4)	-540(4)	-776(19)	7599(15)	31(4)
H(2)	3900(5)	-2390(3)	8237(18)	37(5)
H(5)	800(5)	-860(2)	5864(16)	40(5)
H(7)	4900(6)	-2580(3)	6258(19)	63(8)
H(6)	770(6)	-2500(3)	6226(18)	47(6)
H(3)	740(6)	-2840(3)	8250(2)	58(7)
H(8)	-2600(6)	-510(2)	9516(17)	44(5)
H(9)	-360(6)	-30(3)	10250(2)	65(8)

D-serine.H_2O (sc56)

Table B9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for sc56. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8107(4)	4653(2)	2323(2)	33(1)
O(1)	9791(4)	4612(2)	1548(1)	53(1)
O(2)	7667(3)	3646(2)	2974(1)	40(1)
C(2)	6409(4)	5998(2)	2502(2)	31(1)
N	7156(4)	7120(2)	1685(2)	35(1)
C(3)	6703(5)	6560(3)	3663(2)	40(1)
O(3)	9537(4)	6731(2)	3943(1)	48(1)
O(4)	13580(4)	5798(2)	52(1)	53(1)

Table B10. Bond lengths [A] and angles [deg] for sc56.

C(1)-O(1)	1.246(3)
C(1)-O(2)	1.250(2)
C(1)-C(2)	1.516(3)
C(2)-N	1.491(3)
C(2)-C(3)	1.519(3)
C(2)-H(4)	0.99(3)
N-H(3)	1.12(3)
N-H(2)	0.93(3)
N-H(1)	0.93(2)
C(3)-O(3)	1.417(3)
C(3)-H(5)	1.04(3)
C(3)-H(6)	1.04(3)
O(3)-H(1)	0.98(4)
O(4)-H(8)	0.94(4)
O(4)-H(9)	0.78(3)
O(1)-C(1)-O(2)	124.8(2)
O(1)-C(1)-C(2)	119.06(19)
O(2)-C(1)-C(2)	116.17(17)
N-C(2)-C(1)	110.91(16)
N-C(2)-C(3)	110.99(19)
C(1)-C(2)-C(3)	111.80(19)
N-C(2)-H(4)	109.8(14)
C(1)-C(2)-H(4)	108.3(13)
C(3)-C(2)-H(4)	104.8(13)
C(2)-N-H(3)	105.1(14)
C(2)-N-H(2)	111.2(18)
H(3)-N-H(2)	116(2)
C(2)-N-H(1)	110.4(15)
H(3)-N-H(1)	102(2)
H(2)-N-H(1)	112(2)
O(3)-C(3)-C(2)	110.74(19)
O(3)-C(3)-H(5)	111.7(16)
C(2)-C(3)-H(5)	105.9(14)
O(3)-C(3)-H(6)	110.8(16)
C(2)-C(3)-H(6)	110.7(14)
H(5)-C(3)-H(6)	107(2)
C(3)-O(3)-H(1)	111.1(18)
H(8)-O(4)-H(9)	97(3)

Table B11. Anisotropic displacement parameters (A^2 x 10^3) for sc56.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	31(1)	28(1)	40(1)	-3(1)	-2(1)	-3(1)
O(1)	60(1)	40(1)	58(1)	5(1)	23(1)	11(1)
O(2)	39(1)	29(1)	53(1)	7(1)	3(1)	-1(1)
C(2)	28(1)	29(1)	37(1)	2(1)	2(1)	0(1)
N	39(1)	30(1)	36(1)	2(1)	0(1)	1(1)
C(3)	42(1)	39(2)	38(1)	0(1)	3(1)	2(1)
O(3)	54(1)	41(1)	48(1)	6(1)	-14(1)	-10(1)
O(4)	59(1)	55(1)	46(1)	-5(1)	7(1)	-7(1)

Table B12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for sc56.

	x	y	z	U(eq)	
H(4)	4430(6)	5750(2)	2429(19)	47	
H(3)	5470(6)	7940(3)	1750(2)	53	
H(2)	8960(6)	7460(3)	1800(2)	53	
H(1)	6900(6)	6780(3)	980(2)	53	
H(5)	5730(6)	5820(3)	4160(2)	60	
H(6)	5630(6)	7520(3)	3760(2)	60	
H(1)	10180(7)	7700(4)	3780(2)	71	
H(8)	12210(8)	5410(3)	510(2)	80	
H(9)	14050(8)	5080(4)	-220(3)	80	

CSD SEARCH RESULTS FOR BONDS FOUND IN ZWITTERIONS

The CSD was searched in order to collect all available information on amino acid structures that have been solved. The most obvious search was for the fragment common to all amino acids, COO-CH-NH_2. The database contains 175 093 entries and, when searched for, this fragment had over 600 'hits'. All amino acid structures were contained in these hits so the results were treated as a small database. Each of the twenty naturally occurring amino acids were searched for individually by 'building' the exact structure required. In most instances there was more than one hit per structure.

Once all of the amino acids had been found, they were combined to form a database of amino acid structures containing 123 entries. The number was reduced by insisting on coordinates, no disorder, R factor <10% and no errors. This amino acid database contained all L, D and DL structures, some of which have solvent or ion inclusions. A structure was present more than once if it has been solved a number of times and fulfilled the requirements listed above. The next search was for $^{+}H_3N$-C-COO^{-} in order to exclude any amino acids that do not crystallise as Zwitterions. The statistical package VISTA was used to examine the lengths of the bonds that are common to all amino acids .ie. C=O, C-N and Cα-COO^{-}.

4.1 The C=O bond of the carboxylate anion

The mean of the CO bond was found to be 1.250 Å which falls in the range described by Allen (1987). The spread is quite wide due to the difference in length of the two delocalised C-O bonds in Zwitterionic amino acids (figure C1).

4.2 The C-N bond

The mean of the CN bond was found to be 1.487Å which falls in the range described by Allen (figure C2). Short bonds are found in γ-glycine (GLYCIN16, 1.461Å [1] and GLYCIN18,

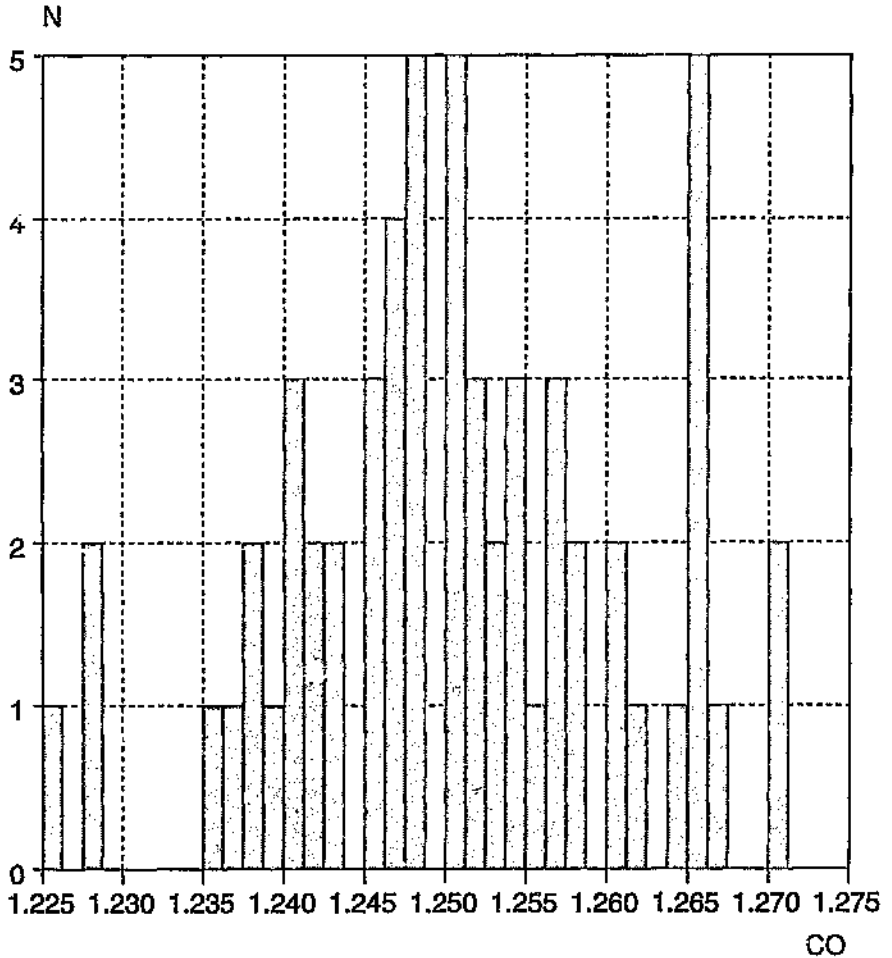
[1] The amino acid referred to by its CSD REFCODE and the relevant bond length.

1.467Å) and L-methionine (LMETON10, 1.465Å). Long bonds are found in L-histidine, (LHISTD02, 1.510Å) and L-leucine (LEUCIN01, 1.530Å)

4.3 The Cα-COO⁻bond

The mean of the C-C bond was found to be 1.533Å which falls in the range described by Allen but would be considered long for this type of bond (figure C3). It was felt that Allen's bond length did not appropriately describe the C-C bond in the Zwitterionic group. A search was therefore performed for any molecule, not necessarily an amino acid, in the database that was Zwitterionic. 312 structures were found and 4 were suppressed giving a mean bond length of 1.534Å confirming that a C-C bond found between an ammonium and a carboxylate group is longer than 'standard' C-COO⁻bond (figure C4).

Figure C1: CSD results for the CO bond

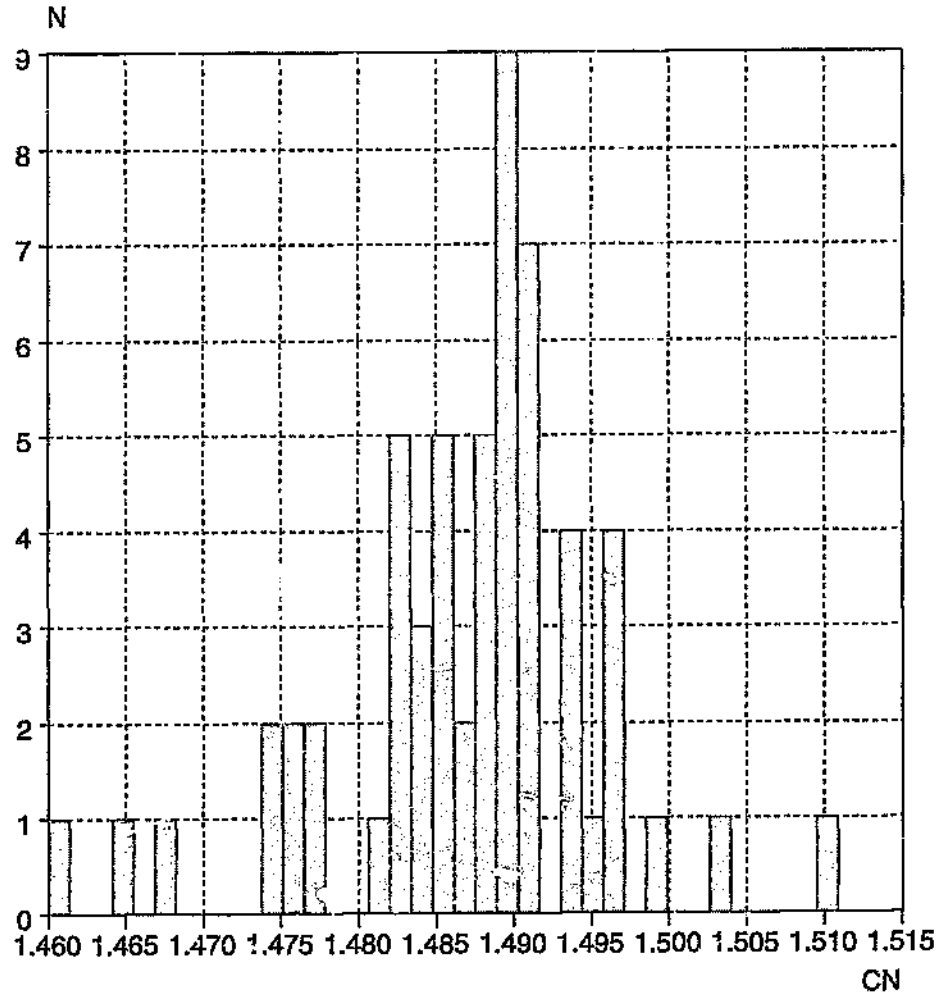


Plot Data
File=co
Test=1
Tot.Obs.=58
Obs.=58
Supp.=0

X-axis
Min.=1.226
Max.=1.271
Range=0.045
Mean=1.250
Mean SE=0.001
Sample SD=0.010

Histogram
Median=1.250
Skew=-0.135
Quantile=10.000
LQ=1.237
HQ=1.265
Bin Width=0.001
Max. Bin =5.000

Figure C2: CSD re'lt. or the CN bond



Plot Data
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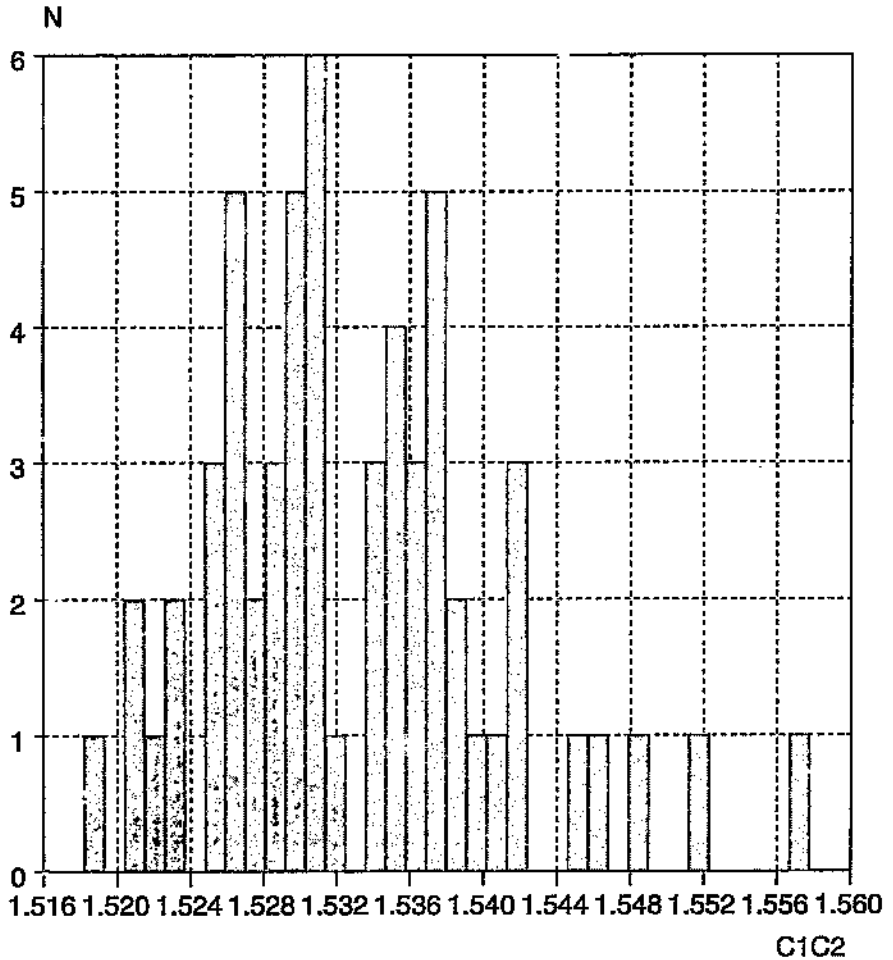
Test=1
Tot.Obs.=58
Obs.=58
Supp.=0

X-axis
Min.=1.461
Max.=1.510
Range=0.049
Mean=1.487
Mean SE=0.001
Sample SD=0.009

Histogram
Median=1.488
Skew=-0.595
Quantile=10.000
LQ=1.475
HQ=1.497
Bin Width=0.001
Max. Bin =9.000

Figure C3: CSD results for the C1C2 bond

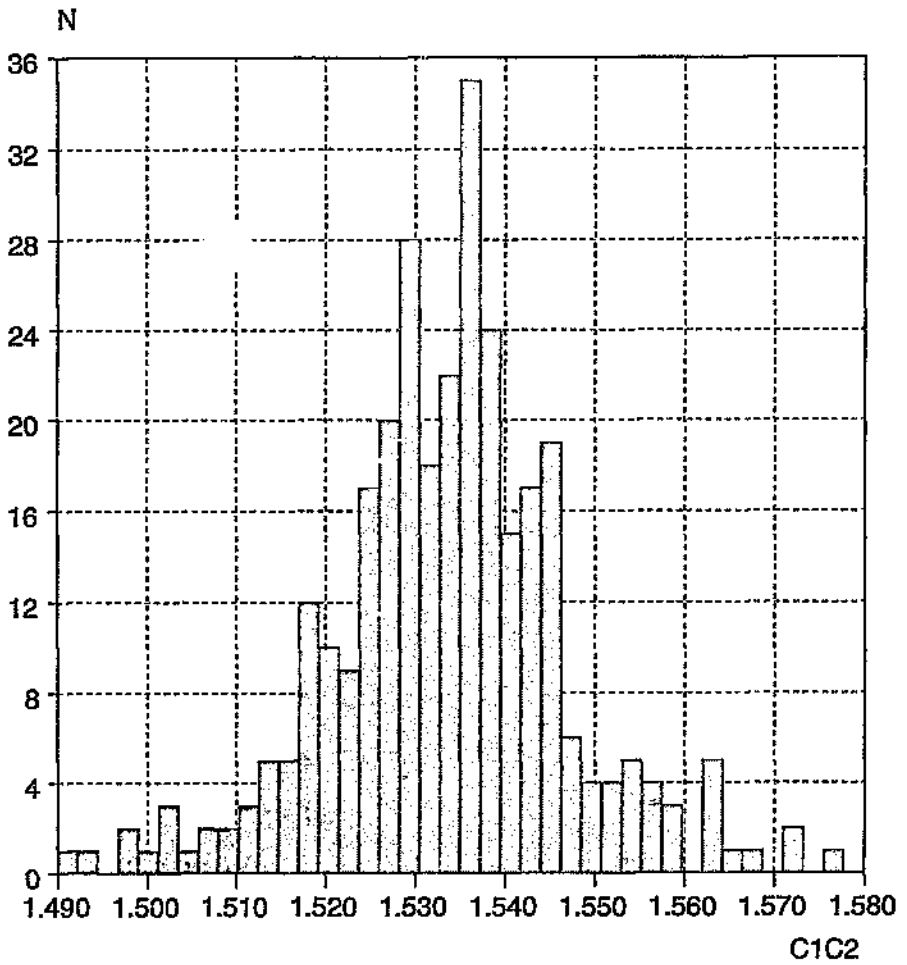


Plot Data
File=cc
Test=1
Tot.Obs.=58
Obs.=58
Supp.=0

X-axis
Min.=1.519
Max.=1.557
Range=0.038
Mean=1.533
Mean SE=0.001
Sample SD=0.008

Histogram
Median=1.531
Skew=0.687
Quantile=10.000
LQ=1.523
HQ=1.542
Bin Width=0.001
Max. Bin =6.000

Figure C4: CSD results for the C1C2 bond found in Zwitterions



Plot Data
File=c1c2
Test=1
Tot.Obs.=312
Obs.=308
Supp.=4

X-axis
Min.=1.490
Max.=1.576
Range=0.086
Mean=1.534
Mean SE=0.001
Sample SD=0.013

Histogram
Median=1.534
Skew=-0.048
Quantile=10.000
LQ=1.518
HQ=1.548
Bin Width=0.002
Max. Bin =35.000

REFCODES OF THE 123 AMINO ACIDS STRUCTURES FOUND IN THE CSD

ALAHCL	GLYCIN	LHISTD01
ARGBRH01	GLYCIN01	LHISTD02
ARGBRH02	GLYCIN02	LHISTD04
ARGBRH10	GLYCIN03	LHISTD10
ASPARM	GLYCIN04	LHISTD13
ASPARM01	GLYCIN05	LMETON01
ASPARM02	GLYCIN06	LMETON02
ASPARM03	GLYCIN07	LMETON10
ASPARM04	GLYCIN08	LNLEUC10
ASPARM05	GLYCIN09	LSERIN01
ASPARM06	GLYCIN10	LSERIN02
ASPARM07	GLYCIN11	LSERIN03
ASPART10	GLYCIN12	LSERIN10
CYSCLM10	GLYCIN13	LTHREO
DLALNI	GLYCIN14	LTHREO01
DLGLAC	GLYCIN15	LTHREO02
DLHIST	GLYCIN16	LTYRHC10
DLLEUC	GLYCIN17	LTYROS02
DLLEUC01	GLYCIN18	LTYROS03
DLLYSC	HISTCM	LTYROS10
DLLYSC10	HISTCM01	LTYROS11
DLMETA	HISTCM12	LVALIN
DLMETA01	HISTDC10	LVALIN01
DLMETA02	HOPROL	LYSCLH
DLMETA03	HOPROL01	LYSCLH02
DLMETA04	HOPROL12	LYSCLH03
DLNLUA	LALNIN	LYSCLH11
DLNLUA01	LALNIN01	PHALNC01
DLNLUA02	LALNIN03	PHALNC10
DLPROL	LALNIN12	PROLIN
DLPROM	LCYSTN	TACQUI
DLPROM01	LCYSTN03	TRYPTC
DLSERN	LCYSTN04	TRYPTC01
DLSERN02	LCYSTN12	TRYPTD01
DLSERN11	LCYSTN21	TRYPTD10
DLTYRS	LEUCBH	VALEHC10
DLTYRS01	LEUCHI	VALEHC11
DLVALC	LEUCIN	VALIDL
FAZHAP	LEUCIN01	VALIDL01
FAZHET	LEUCIN02	VALIDL02
GLUTAM	LEUCNB10	
GLUTAM01		

STRUCTURE FACTOR TABLES FOR DL-SERINE

DL-serine (sc53)

Table E1. Observed and calculated structure factors for sc53

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	500	537	1	1	7	0	79	78	1	5	1	1	49	50	1	11	4	1	82	84	1
2	8	1	49	50	1	4	0	0	287	278	1	2	7	0	50	59	1	6	1	1	176	184	1
12	4	1	30	30	1	3	8	1	28	31	1	6	0	0	5	4	1	3	7	0	168	171	1
7	1	1	50	48	1	-13	5	1	39	58	1	4	8	1	113	115	1	8	0	0	17	18	1
4	7	0	65	66	1	8	1	1	22	23	1	-12	5	1	13	10	1	5	8	1	72	71	1
10	0	0	170	175	1	5	7	0	6	5	1	9	1	1	77	75	1	-11	5	1	9	5	1
6	8	1	14	12	1	12	0	0	132	129	1	6	7	0	27	26	1	10	1	1	64	63	1
-10	5	1	32	29	1	7	8	1	61	60	1	14	0	0	33	32	1	7	7	0	89	88	1
11	1	1	7	8	1	-9	5	1	2	4	2	8	8	1	70	70	1	1	1	0	93	83	1
8	7	0	24	23	1	12	1	1	64	62	1	-8	5	1	94	98	1	9	8	1	17	17	1
2	1	0	31	24	1	9	7	0	17	17	1	13	1	1	17	17	1	-7	5	1	31	31	1
10	8	1	5	4	5	3	1	0	181	168	1	10	7	0	28	30	1	-14	2	1	68	67	1
-6	5	1	48	52	1	-10	9	1	13	13	1	4	1	0	443	436	1	11	7	0	26	26	1
-13	2	1	43	44	1	-5	5	1	120	124	1	-9	9	1	11	11	1	5	1	0	125	125	1
12	7	0	5	2	2	-12	2	1	14	12	1	-4	5	1	94	95	1	-8	9	1	7	7	1
6	1	0	58	57	1	0	8	0	12	8	1	-11	2	1	28	29	1	-3	5	1	78	78	1
-7	9	1	11	12	1	7	1	0	90	91	1	1	8	0	206	214	1	-10	2	1	19	19	1
-2	5	1	104	101	1	-6	9	1	8	7	1	8	1	0	179	183	1	2	8	0	59	58	1
-9	2	1	12	12	1	-1	5	1	57	57	1	-5	9	1	60	59	1	9	1	0	22	21	1
3	8	0	75	76	1	-8	2	1	55	54	1	0	5	1	165	164	1	-4	9	1	40	39	1
10	1	0	23	25	1	4	8	0	19	18	1	-7	2	1	203	206	1	5	5	1	142	146	2
-3	9	1	26	26	1	11	1	0	3	4	2	5	8	0	40	41	1	-6	2	1	14	16	1
2	5	1	31	32	1	-2	9	1	79	82	1	12	1	0	21	20	1	6	8	0	59	58	1
-5	2	1	33	29	1	3	5	1	193	194	1	-1	9	1	129	133	1	13	1	0	8	9	1
7	8	0	24	23	1	-4	2	1	304	294	1	4	5	1	94	102	1	0	9	1	58	59	1
14	1	0	34	33	1	8	8	0	9	9	1	-3	2	1	264	257	1	5	5	1	127	130	1
1	9	1	133	139	1	0	2	0	239	232	2	9	8	0	61	59	1	-2	2	1	408	387	3
6	5	2	41	45	1	2	9	1	4	5	4	1	2	0	85	65	1	10	8	0	5	3	2
-1	2	1	199	188	1	7	5	1	139	121	1	3	9	1	26	24	1	2	2	0	171	158	1
11	8	0	121	117	1	0	2	1	375	358	3	8	5	1	51	54	1	4	9	1	3	0	2
3	2	0	522	512	1	1	9	0	9	9	1	1	2	1	264	243	1	9	5	1	4	8	4
5	9	1	26	26	1	4	2	0	38	31	1	2	9	0	2	2	2	2	2	1	70	70	1
10	5	1	32	30	1	6	9	1	43	42	1	5	2	0	56	50	1	3	9	0	56	56	1
3	2	1	279	265	1	11	5	1	21	21	1	7	9	1	10	7	1	6	2	0	258	258	1
4	9	0	29	28	1	4	2	1	242	242	1	12	5	1	7	6	1	8	9	1	17	19	1
7	2	0	32	29	1	5	9	0	9	9	1	5	2	1	195	194	1	-13	6	1	8	5	2
9	9	1	58	56	1	8	2	0	71	76	1	6	9	0	4	4	4	6	2	1	93	96	1
-12	6	1	18	20	1	-9	10	1	11	12	1	9	2	0	77	72	1	7	9	0	73	73	1
7	2	1	130	130	1	-11	6	1	40	38	1	-8	10	1	51	49	1	10	2	0	5	6	1
8	9	0	39	39	1	8	2	1	174	181	1	-10	6	1	70	72	1	-7	10	1	50	49	1
11	2	0	20	19	1	9	9	0	17	18	1	9	2	1	32	31	1	-9	6	1	19	19	1
-6	10	1	48	46	1	12	2	0	8	10	1	10	9	0	9	10	1	10	2	1	40	42	1
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11	2	1	5	8	4	-7	6	1	30	28	1	-4	10	1	79	78	1	14	2	0	4	1	4
1	10	0	37	38	1	12	2	1	16	15	1	-6	6	1	116	124	2	-3	10	1	108	109	1
1	3	0	324	293	1	2	10	0	89	89	1	13	2	1	3	1	3	-5	6	1	42	44	1
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-13	3	1	47	46	1	-3	6	1	128	135	1	0	10	1	25	23	1	4	3	0	152	146	1
5	10	0	27	26	1	-12	3	1	11	8	1	-2	6	1	11	11	1	1	10	1	27	25	1
5	3	0	64	62	1	6	10	0	11	12	1	-11	3	1	90	93	1	-1	6	1	104	108	1
2	10	1	26	26	1	6	3	0	25	30	1	7	10	0	3	4	3	-10	3	1	46	49	1
0	6	1	82	83	1	3	10	1	7	9	2	7	3	0	100	101	1	8	10	0	33	32	1
-9	3	1	14	17	1	1	6	1	37	37	1	4	10	1	44	45	1	8	3	0	35	31	1
9	10	0	24	23	1	-8	3	1	53	56	1	2	6	1	101	102	1	5	10	1	8	4	1
9	3	0	85	88	1	1	11	0	6	1	1	-7	3	1	179	183	1	3	6	1	47	47	1
6	10	1	5	4	4	10	3	0	10	10	1	2	11	0	7	5	1	-6	3	1	85	84	1
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4	11	0	4	5	1	-4	3	1	228	226	2	6	6	1	19	17	1	-7	11	1	11	10	1
13	3	0	20	19	1	5	11	0	4	5	3	-3	3	1	279	269	2	7	6	1	10	13	1
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0	12	0	81	77	1	0	3	1	97	85	1	10	6	1	22	23	1	-3	11	1	59	59	1
2	4	0	32	27	1	1	12	0	4	2	1	1	3	1	345	328	1	11	6	1	76	74	1
-2	11	1	45	46	1	3	4	0	260	250	1	2	12	0	20	20	1	2	3	1	82	69	1
-12	7	1	3	5	3	-1	11	1	25	24	1	4	4	0	18	24	1	3	12	0	4	0	3
3	1	272	264	3	-11	7	1	41	42	1	0	13	1	50	50	1	5	4	0	89	83	1	4
12	0	23	22	2	-4	3	1	53	55	1	-10	7	1	30	49	1	1	11	1	26	27	1	6
4	0	4	5	1	5	12	0	6	7	1	5	3	1	92	88	1	-9	7	1	6	7	1	3
11	1	24	24	1	7	4	0	16	15	1	-14	0	1	38	35	1	6	3	1	33	30	1	-8
7	1	31	33	1	3	11	1	3	0	3	8	4	0	21	26	1	-12	0	1	45	46	1	7
3	1	118	114	1	-7	7	1	68	70	1	4	11	1	39	31	1	9	4	0	6	8	1	-10
0	1	38	39	1	8	3	1	95	97	1	-6	7	1	58	58	1	5	11	1	5	5	3	10
4	0	50	47	1	-8	0	1	70	72	1	9	3	1	60	58	1	-5	7	1	172	174	1	6
11	1	46	44	1	11	4	0	53	57	1	-6	0	1	43	45	1	10	3	1	50	51	1	-4
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3	2	75	75	1	-3	7	1	54	57	1	-4	12	1	21	23	1	13	4	0	6	6	1	-2
0	1	391	369	1	12	3	1	26	25	1	-2	7	1	139	143	1	-3	12	1	31	31	1	1
5	0	75	75	1	0	0	1	11	6	1	13	3	1	9	10	2	-1	7	1	13	6	1	-2
12	1	36	35	1	2	5	0	10	7	1	2	0	1	225	198	1	-14	4	1	4	4	4	0
7	1	93	94	1	-1	12	1	45	44	1	3	5	0	279	278	1	4	0	1	6	9	1	-13
4	1	6	9	3	1	7	1	17	19	1	0	13	1	57	56	1	4	5	0	119	115	1	5
0	1	245	246	1	-12	4	1	40	39	1	2	7	1	20	19	1	1	12	1	42	40	1	5
5	0	176	176	1	8	0	1	130	131	1	-11	4	1	61	61	1	3	7	1	30	31	1	2
12	1	8	7	1	6	5	0	78	82	1	10	0	1	110	110	1	-10	4	1	35	36	1	4
7	1	65	72	1	3	12	1	23	23	1	7	5	0	112	116	1	12	0	1	34	34	1	-9
4	1	28	25	1	5	7	1	54	58	1	4	12	1	10	10	1	8	5	0	35	32	1	-14
0	2	57	55	1	9	5	0	108	111	1	-13	1	1	73	71	1	-7	4	1	76	76	1	7
7	1	57	60	1	-12	0	2	70	73	1	10	5	0	47	49	1	-12	1	1	42	43	1	-6
4	1	51	54	1	8	7	1	72	71	1	-10	0	2	150	154	1	11	5	0	6	3	1	-11
1	1	2	5	2	-5	4	1	32	32	1	9	7	1	69	69	1	-8	0	2	44	49	1	1
5	0	4	4	3	-10	1	1	127	132	1	-4	4	1	205	205	1	10	7	1	5	0	5	-6
0	2	20	20	23	1	13	5	0	52	50	1	-9	1	1	22	25	1	-5	4	1	3	2	2
11	7	1	21	20	1	-4	0	2	38	46	1	0	6	0	108	106	3	-8	1	1	16	14	1
-2	4	1	24	24	1	-11	8	1	17	16	1	-2	0	2	102	104	2	1	6	0	81	82	1
-7	1	1	7	9	1	-1	4	1	240	227	1	-10	8	1	19	19	1	0	0	2	335	331	3
2	6	0	119	117	1	-6	1	1	93	91	1	0	4	1	290	282	3	-9	8	1	27	26	1
2	0	2	139	134	1																		

| | | |

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-10	4	2	16	14	1	7	7	2	33	31	1	10	0	3	14	13	1	-1	4	3	55	57	1	1	8	3	8	8	1
-9	4	2	49	50	1	8	7	2	81	82	1	-14	1	3	54	52	1	0	4	3	42	44	1	2	8	3	40	39	1
-8	4	2	64	65	1	9	7	2	45	44	1	-13	1	3	38	39	1	1	4	3	124	129	2	3	8	3	83	82	1
-7	4	2	34	33	1	10	7	2	7	5	2	-12	1	3	47	48	1	2	4	3	152	160	1	4	8	3	33	34	1
-6	4	2	181	183	1	-11	8	2	42	41	1	-11	1	3	4	4	4	3	4	3	123	124	1	5	8	3	50	49	1
-5	4	2	55	59	1	-10	8	2	26	25	1	-10	1	3	70	74	1	4	4	3	191	195	2	6	8	3	3	6	3
-4	4	2	4	3	1	-9	8	2	31	33	1	-9	1	3	15	14	1	5	4	3	72	75	1	7	8	3	50	50	1
-3	4	2	78	77	1	-8	8	2	18	18	1	-8	1	3	128	132	1	6	4	3	24	25	1	-10	9	3	13	14	1
-2	4	2	196	199	1	-7	8	2	45	46	1	-7	1	3	70	72	1	7	4	3	9	10	1	-9	9	3	9	14	2
-8	9	3	25	25	1	0	2	4	18	20	1	0	6	4	153	153	1	5	1	5	9	8	1	2	6	5	9	10	1
-7	9	3	83	80	1	1	2	4	161	167	1	1	6	4	63	65	1	6	1	5	6	4	4	3	6	5	30	27	1
-6	9	3	28	27	1	2	2	4	18	17	1	2	6	4	82	83	1	-12	2	5	8	7	1	-8	7	5	3	1	3
-5	9	3	92	90	1	3	2	4	34	37	1	3	6	4	4	1	3	-11	2	5	7	6	1	-7	7	5	31	31	1
-4	9	3	11	9	1	4	2	4	51	53	1	4	6	4	5	5	4	-10	2	5	59	60	1	-6	7	5	4	6	4
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-2	9	3	12	12	1	6	2	4	5	6	1	6	6	4	11	8	1	-8	2	5	56	57	1	-4	7	5	22	21	1
-1	9	3	84	84	1	7	2	4	3	3	2	7	6	4	36	34	1	-7	2	5	13	13	1	-3	7	5	41	42	1
0	9	3	33	33	1	8	2	4	5	4	4	-11	7	4	36	36	1	-6	2	5	8	7	1	-2	7	5	47	44	1
1	9	3	[illegible]	68	1	-13	3	4	23	23	1	-10	7	4	27	28	1	-5	2	5	78	81	1	-1	7	5	78	77	1
2	9	3	54	55	1	-12	3	4	70	72	1	-9	7	4	13	16	1	-4	2	5	57	58	1	0	7	5	82	80	1
3	9	3	78	77	1	-11	3	4	27	26	1	-8	7	4	24	20	1	-3	2	5	106	111	2	1	7	5	48	48	1
4	9	3	14	13	1	-10	3	4	54	57	1	-7	7	4	25	23	1	-2	2	5	19	17	1	2	7	5	16	15	1
5	9	3	65	65	1	-9	3	4	32	32	1	-6	7	4	41	38	1	-1	2	5	7	7	1	-6	8	5	4	0	3
6	9	3	42	41	1	-8	3	4	5	0	1	-5	7	4	8	10	1	0	2	5	28	30	1	-5	8	5	39	36	1
-8	10	3	16	16	1	-7	3	4	37	37	1	-4	7	4	37	38	1	1	2	5	8	7	1	-4	8	5	48	46	1
-7	10	3	3	2	2	-6	3	4	3	1	3	-3	7	4	33	35	1	2	2	5	51	51	1	-3	8	5	19	17	1
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-4	10	3	39	38	1	-3	3	4	50	53	1	0	7	4	40	41	1	5	2	5	9	7	4	0	8	5	12	11	1
-3	10	3	79	78	1	-2	3	4	70	68	1	1	7	4	55	55	1	6	2	5	11	13	2	-10	0	6	53	50	1
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0	10	3	29	29	1	1	3	4	44	45	1	4	7	4	32	32	1	-10	3	5	5	5	4	-4	0	6	76	76	1
1	10	3	27	29	1	2	3	4	74	77	1	5	7	4	4	5	3	-9	3	5	40	40	1	-2	0	6	10	8	1
2	10	3	24	23	1	3	3	4	43	44	1	6	7	4	4	1	4	-8	3	5	3	1	2	0	0	6	57	54	1
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4	10	3	3	1	3	5	3	4	15	17	1	-8	8	4	10	6	1	-6	3	5	40	38	1	-10	1	6	41	41	1
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2	0	4	75	81	1	0	4	4	22	25	1	-4	9	4	3	2	2	-7	4	5	25	24	1	-6	2	6	6	8	2
4	0	4	198	205	1	1	4	4	78	80	1	-3	9	4	3	6	3	-6	4	5	40	38	1	-5	2	6	41	41	1
6	0	4	76	78	1	2	4	4	59	59	1	-2	9	4	36	35	1	-5	4	5	8	6	1	-4	2	6	32	31	1
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0	1	4	127	130	2	-3	5	4	65	65	1	-4	0	5	89	85	1	-6	5	5	3	0	3	0	3	6	25	27	1
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3	1	4	33	35	1	0	5	4	3	1	2	2	0	5	38	39	1	-3	5	5	54	52	1	-8	4	6	17	17	1
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6	1	4	15	15	1	3	5	4	35	35	1	-12	1	5	54	54	1	0	5	5	66	65	1	-5	4	6	34	34	1
7	1	4	30	30	1	4	5	4	16	18	1	-11	1	5	40	42	1	1	5	5	22	21	1	-4	4	6	35	35	1
8	1	4	15	16	1	5	5	4	23	25	1	-10	1	5	5	2	3	2	5	5	28	27	1	-3	4	6	25	24	1
9	1	4	48	44	1	6	5	4	36	37	1	-9	1	5	37	37	1	3	5	5	24	22	1	-2	4	6	46	45	1
-13	2	4	6	3	3	7	5	4	18	20	1	-8	1	5	31	33	1	4	5	5	7	10	5	-1	4	6	6	6	1
-12	2	4	33	31	1	-12	6	4	50	49	1	-7	1	5	19	21	1	-10	6	5	27	24	1	0	4	6	8	2	2
-11	2	4	90	89	1	-11	6	4	4	6	1	-6	1	5	62	61	1	-9	6	5	4	5	4	1	4	6	3	2	3
-10	2	4	18	19	1	-10	6	4	109	108	1	-5	1	5	46	46	1	-8	6	5	9	8	2	-7	5	6	4	8	4
-9	2	4	67	68	1	-9	6	4	7	4	2	-4	1	5	95	95	1	-7	6	5	22	21	1	-6	5	6	10	0	2
-8	2	4	8	11	1	-8	6	4	5	5	1	-3	1	5	37	37	1	-6	6	5	5	4	4	-5	5	6	18	16	1
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-6	2	4	41	42	1	-6	6	4	23	24	1	-1	1	5	93	89	1	-4	6	5	74	74	1	-3	5	6	83	80	1
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-4	2	4	69	69	1	-4	6	4	23	28	1	1	1	5	36	38	1	-2	6	5	40	39	1	-1	5	6	72	71	1

-3 2 4 89 87 1 -3 6 4 22 21 1 2 1 5 51 53 1 -1 6 5 13 13 1 -1 6 6 29 29 1
-2 2 4 145 146 1 -2 6 4 20 16 1 3 1 5 16 14 1 0 6 5 7 4 2
-1 2 4 53 58 1 -1 6 4 38 38 1 4 1 5 57 60 1 1 6 5 52 51 1
E

DL-serine (serine_1)

Table 2 Observed and calculated structure factors for serine_1

h k l 10Fo 10Fc 10s	h k l 10Fo 10Fc 10s	h k l 10Fo 10Fc 10s	h k l 10Fo 10Fc 10s	h k l 10Fo 10Fc 10s
4 0 0 301 309 2	4 6 0 134 136 1	3 13 0 23 23 1	-13 3 1 50 49 1	12 5 1 21 22 1
6 0 0 13 12 1	5 6 0 116 121 1	4 13 0 114 114 1	-12 3 1 30 28 1	13 5 1 34 34 1
8 0 0 19 20 1	6 6 0 74 80 1	5 13 0 17 17 1	-11 3 1 121 126 1	14 5 1 48 48 1
10 0 0 229 234 1	7 6 0 33 35 1	6 13 0 52 53 1	-10 3 1 69 74 1	-15 6 1 14 13 1
12 0 0 213 216 2	8 6 0 146 157 1	7 13 0 9 6 1	-9 3 1 12 0 1	-14 6 1 27 27 1
14 0 0 61 60 1	9 6 0 44 44 1	0 14 0 17 3 1	-8 3 1 68 71 1	-13 6 1 11 10 1
16 0 0 18 18 1	10 6 0 5 5 2	1 14 0 27 26 1	-7 3 1 214 213 1	-12 6 1 47 47 1
3 1 0 159 158 1	11 6 0 19 18 1	2 14 0 35 35 1	-6 3 1 102 102 1	-11 6 1 57 57 1
4 1 0 458 469 1	12 6 0 8 4 1	3 14 0 54 55 1	-5 3 1 241 237 1	-10 6 1 126 127 1
5 1 0 157 155 1	13 6 0 10 7 4	4 14 0 26 27 1	-4 3 1 275 272 1	-9 6 1 13 14 1
6 1 0 63 59 1	14 6 0 82 82 1	5 14 0 39 37 1	-3 3 1 266 264 1	-8 6 1 57 58 1
7 1 0 82 83 1	15 6 0 7 8 1	-16 0 1 11 7 1	-2 3 1 59 58 1	-7 6 1 25 20 1
8 1 0 224 226 1	1 7 0 112 115 1	-14 0 1 55 54 1	-1 3 1 413 430 2	-6 6 1 166 172 1
9 1 0 45 43 1	2 7 0 48 49 1	-12 0 1 56 58 1	0 3 1 151 135 1	-5 6 1 45 45 1
10 1 0 19 22 1	3 7 0 199 207 1	-10 0 1 52 54 1	1 3 1 360 360 1	-4 6 1 82 79 1
11 1 0 22 24 1	4 7 0 102 106 1	-8 0 1 84 87 1	2 3 1 72 59 1	-3 6 1 140 148 1
12 1 0 47 43 1	5 7 0 10 12 1	-6 0 1 73 70 1	3 3 1 289 285 1	-2 6 1 31 30 1
13 1 0 14 12 1	6 7 0 47 44 1	-4 0 1 112 115 1	4 3 1 32 33 1	-1 6 1 131 137 1
14 1 0 58 60 1	7 7 0 102 99 1	2 0 1 241 224 2	5 3 1 114 112 1	0 6 1 92 90 1
15 1 0 20 21 1	8 7 0 45 43 1	4 0 1 18 10 1	6 3 1 54 51 1	1 6 1 10 9 1
16 1 0 21 21 1	9 7 0 38 36 1	6 0 1 255 260 2	7 3 1 144 142 1	2 6 1 119 119 1
2 2 0 183 180 2	10 7 0 37 39 1	8 0 1 111 116 1	8 3 1 136 133 1	3 6 1 55 49 1
3 2 0 487 500 2	11 7 0 39 40 1	10 0 1 183 186 1	9 3 1 90 89 1	4 6 1 95 99 1
4 2 0 22 16 1	12 7 0 20 29 1	12 0 1 61 61 1	10 3 1 51 50 1	5 6 1 62 56 1
5 2 0 67 58 1	13 7 0 8 7 1	14 0 1 57 55 1	11 3 1 117 120 2	6 6 1 34 29 1
6 2 0 301 304 1	14 7 0 9 6 1	-17 1 1 10 10 1	12 3 1 60 61 1	7 6 1 16 20 1
7 2 0 48 46 1	0 8 0 63 64 1	-16 1 1 80 86 1	13 3 1 34 33 1	8 6 1 61 59 1
8 2 0 92 93 1	1 8 0 256 265 1	-15 1 1 89 88 1	14 3 1 28 29 1	9 6 1 75 71 1
9 2 0 123 119 1	2 8 0 53 54 1	-14 1 1 3 1 1	15 3 1 56 54 1	10 6 1 15 17 1
10 2 0 5 4 1	3 8 0 99 103 1	-13 1 1 132 132 1	-16 4 1 32 30 1	11 6 1 121 120 1
11 2 0 39 37 1	4 8 0 9 9 1	-12 1 1 71 71 1	-15 4 1 65 62 1	12 6 1 23 24 1
12 2 0 24 26 1	5 8 0 25 28 1	-11 1 1 13 11 1	-14 4 1 7 7 1	13 6 1 27 29 1
13 2 0 78 79 1	6 8 0 91 90 1	-10 1 1 149 156 1	-13 4 1 20 20 1	14 6 1 15 17 3
14 2 0 11 13 1	7 8 0 43 40 1	-9 1 1 43 43 1	-12 4 1 62 62 1	-14 7 1 121 120 1
15 2 0 48 47 1	8 8 0 16 13 1	-8 1 1 11 7 1	-11 4 1 96 95 1	-13 7 1 55 55 1
16 2 0 28 29 1	9 8 0 98 97 1	-7 1 1 40 42 1	-10 4 1 65 64 1	-12 7 1 11 7 1
1 3 0 293 283 1	10 8 0 27 27 1	-6 1 1 97 93 1	-9 4 1 51 48 1	-11 7 1 39 38 1
2 3 0 352 350 1	11 8 0 206 210 1	-5 1 1 86 81 1	-8 4 1 120 122 1	-10 7 1 68 66 1
3 3 0 74 65 1	12 8 0 8 6 1	-4 1 1 60 50 1	-7 4 1 96 96 1	-9 7 1 10 7 1
4 3 0 133 145 1	13 8 0 62 62 1	-3 1 1 455 473 2	-6 4 1 28 35 1	-8 7 1 36 40 1
5 3 0 70 69 1	1 9 0 6 6 1	2 1 1 211 202 1	-5 4 1 82 66 1	-7 7 1 103 103 1
6 3 0 38 44 1	2 9 0 5 1 1	3 1 1 131 133 1	-4 4 1 240 234 1	-6 7 1 28 25 1
7 3 0 126 122 1	3 9 0 69 70 1	4 1 1 57 55 1	-3 4 1 27 29 1	-5 7 1 221 225 1
8 3 0 51 46 1	4 9 0 55 54 1	5 1 1 29 32 1	-2 4 1 6 4 1	-4 7 1 169 170 1
9 3 0 47 51 1	5 9 0 26 25 1	6 1 1 217 228 1	-1 4 1 275 268 1	-3 7 1 102 104 1
10 3 0 15 12 1	6 9 0 16 18 1	7 1 1 54 54 1	0 4 1 292 289 1	-2 7 1 176 180 1
11 3 0 79 77 1	7 9 0 107 108 1	9 1 1 89 91 1	1 4 1 102 104 1	-1 7 1 17 13 1
12 3 0 13 11 2	8 9 0 54 56 1	10 1 1 72 72 1	2 4 1 240 233 1	0 7 1 112 116 1
13 3 0 20 19 1	9 9 0 40 43 1	11 1 1 0 3 1	3 4 1 249 247 1	1 7 1 8 10 1
14 3 0 49 47 1	10 9 0 14 13 1	12 1 1 94 95 1	4 4 1 146 146 1	2 7 1 12 14 1
15 3 0 4 7 3	11 9 0 23 22 1	13 1 1 27 28 1	5 4 1 132 129 1	3 7 1 50 51 1
16 3 0 52 53 1	12 9 0 37 37 1	14 1 1 33 32 1	6 4 1 12 7 1	4 7 1 76 84 1
0 4 0 29 35 1	13 9 0 18 18 1	15 1 1 44 42 1	7 4 1 143 139 1	5 7 1 68 75 1
1 4 0 308 316 1	0 10 0 193 198 1	-16 2 1 38 39 1	8 4 1 1 2 1	6 7 1 27 32 1
2 4 0 32 29 1	1 10 0 12 9 1	-15 2 1 49 49 1	9 4 1 69 66 1	7 7 1 106 109 1
3 4 0 289 282 1	2 10 0 111 113 1	-14 2 1 112 111 1	10 4 1 36 37 1	8 7 1 94 91 1
4 4 0 20 23 1	3 10 0 26 26 1	-13 2 1 56 55 1	11 4 1 137 140 1	9 7 1 116 115 1
5 4 0 99 92 1	4 10 0 15 15 1	-12 2 1 14 13 1	12 4 1 38 37 1	10 7 1 13 15 1
6 4 0 6 7 1	5 10 0 60 62 1	-11 2 1 54 54 1	13 4 1 39 41 1	11 7 1 19 18 1
7 4 0 12 11 1	6 10 0 13 14 1	-10 2 1 33 33 1	14 4 1 16 16 1	12 7 1 34 34 1
8 4 0 8 9 1	7 10 0 4 1 2	-9 2 1 15 20 1	-15 5 1 17 14 1	13 7 1 55 54 1
9 4 0 7 12 1	8 10 0 43 44 1	-8 2 1 75 73 1	-14 5 1 68 69 1	-14 8 1 52 50 1
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-3	5	4	109	108	1	-8	9	4	26	26	1	5	1	5	17	20	1	-4	5	5	41	35	1	-7	10	5	84	83	1
-2	5	4	46	42	1	-7	9	4	25	27	1	6	1	5	14	13	1	-3	5	5	88	91	1	-6	10	5	29	28	1
-1	5	4	153	157	1	-6	9	4	23	23	1	7	1	5	73	73	1	-2	5	5	21	20	1	-5	10	5	4	1	1
0	5	4	18	16	1	-5	9	4	34	35	1	8	1	5	32	31	1	-1	5	5	59	60	1	-4	10	5	108	110	1
1	5	4	125	129	1	-4	9	4	6	1	1	9	1	5	56	53	1	0	5	5	99	98	1	-3	10	5	107	108	1
2	5	4	18	18	1	-3	9	4	7	2	1	-15	2	5	91	91	1	1	5	5	18	17	1	-2	10	5	78	80	1
3	5	4	39	40	1	-2	9	4	72	74	1	-14	2	5	83	84	1	2	5	5	52	51	1	-1	10	5	13	11	1
4	5	4	27	30	1	-1	9	4	50	50	1	-13	2	5	20	22	1	3	5	5	44	43	1	0	10	5	11	9	1
5	5	4	45	46	1	0	9	4	100	102	1	-12	2	5	17	16	1	4	5	5	30	28	1	1	10	5	76	75	1
6	5	4	51	49	1	1	9	4	30	30	1	-11	2	5	11	9	1	5	5	5	40	41	1	2	10	5	49	47	1
7	5	4	36	37	1	2	9	4	10	7	1	-10	2	5	107	106	1	6	5	5	12	11	1	-5	11	5	26	25	1
8	5	4	55	53	1	3	9	4	29	30	1	-9	2	5	2	1	2	7	5	5	47	48	1	-4	11	5	25	21	1
9	5	4	33	35	1	4	9	4	13	12	1	-8	2	5	83	86	1	-14	6	5	78	78	1	-3	11	5	21	20	1
10	5	4	22	24	1	5	9	4	6	8	1	-7	2	5	20	19	1	-13	6	5	42	41	1	-2	11	5	19	19	1
-15	6	4	47	46	1	6	9	4	12	10	1	-6	2	5	5	3	1	-12	6	5	21	20	1	-1	11	5	17	15	1
-14	6	4	37	37	1	7	9	4	49	50	1	-5	2	5	99	103	1	-11	6	5	15	13	1	0	11	5	55	54	1
-13	6	4	71	71	1	-11	10	4	43	45	1	-4	2	5	97	100	1	-10	6	5	46	46	1	-14	0	6	83	80	1
-12	6	4	68	69	1	-10	10	4	63	61	1	-3	2	5	159	158	1	-9	6	5	21	21	1	-12	0	6	2	0	2
-11	6	4	33	36	1	-9	10	4	29	28	1	-2	2	5	31	28	1	-8	6	5	12	13	1	-10	0	6	112	112	1
-10	6	4	162	162	1	-8	10	4	71	69	1	-1	2	5	4	3	1	-7	6	5	37	37	1	-8	0	6	96	96	1
-9	6	4	5	7	1	-7	10	4	63	61	1	0	2	5	48	50	1	-6	6	5	24	24	1	-6	0	6	209	211	1
-8	6	4	8	7	1	-6	10	4	44	42	1	1	2	5	13	13	1	-5	6	5	8	7	1	-4	0	6	100	102	1
-7	6	4	28	29	1	-5	10	4	22	21	1	2	2	5	67	69	1	-4	6	5	114	114	1	-2	0	6	13	13	1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
-6	6	4	91	53	1	-4	10	4	14	12	1	2	2	5	13	14	1	-3	6	5	24	24	1
-5	6	4	58	63	1	-3	10	4	44	46	1	4	2	5	124	127	1	-2	6	5	63	61	1
-4	6	4	36	44	1	-2	10	4	4	0	1	5	2	5	13	10	1	-1	6	5	9	8	1
-3	6	4	18	16	1	-1	10	4	24	24	1	6	2	5	20	21	1	0	6	5	35	34	1
-2	6	4	16	10	1	0	10	4	10	8	2	7	2	5	119	117	1	1	6	5	86	84	1
-1	6	4	72	71	1	1	10	4	7	2	1	8	2	5	82	79	1	2	6	5	15	13	1
0	6	4	205	209	1	2	10	4	38	38	1	9	2	5	60	59	1	3	6	5	49	49	1
-11	1	6	42	41	1	-12	3	6	63	63	1	-9	5	6	15	15	1	0	6	6	39	38	1
-10	1	6	67	69	1	-11	3	6	7	6	2	-8	5	6	5	3	1	1	7	6	61	60	1
-9	1	6	2	1	2	-10	3	6	24	24	1	-7	5	6	26	26	1	2	7	6	7	7	3
-8	1	6	49	52	1	-9	3	6	83	83	1	-6	5	6	11	13	1	-9	8	6	31	33	1
-7	1	6	14	15	1	-8	3	6	43	45	1	-5	5	6	25	25	1	-8	8	6	10	8	1
-6	1	6	113	112	1	-7	3	6	9	10	1	-4	5	6	73	71	1	-7	8	6	78	78	2
-5	1	6	42	45	1	-6	3	6	14	12	1	-3	5	6	144	145	1	-6	8	6	6	4	4
-4	1	6	11	10	1	-5	3	6	21	19	1	-2	5	6	22	22	1	-5	8	6	63	65	1
-3	1	6	60	60	1	-4	3	6	88	88	1	-1	5	6	110	110	1	-4	8	6	10	11	1
-2	1	6	35	34	1	-3	3	6	40	40	1	0	5	6	26	25	1	-3	8	6	87	88	1
-1	1	6	3	7	3	-2	3	6	74	74	1	1	5	6	2	4	1	-2	8	6	31	31	1
0	1	6	34	34	1	-1	3	6	4	6	2	2	5	6	34	33	1	-1	8	6	10	9	2
1	1	6	17	21	1	0	3	6	33	34	1	3	5	6	75	74	1	0	8	6	6	7	3
2	1	6	89	87	1	1	3	6	30	31	1	4	5	6	22	21	1	1	8	6	76	81	1
3	1	6	12	13	1	2	3	6	14	16	1	-12	6	6	59	59	1	-4	9	6	18	16	1
4	1	6	108	108	1	3	3	6	32	33	1	-11	6	6	31	31	1	-3	9	6	27	28	1
5	1	6	7	0	1	4	3	6	8	6	1	-10	6	6	72	74	1	-2	9	6	27	25	1
6	1	6	8	0	1	5	3	6	23	22	1	-9	6	6	36	36	1	-10	0	7	12	4	1
-14	2	6	45	45	1	-13	4	6	75	75	1	-8	6	6	28	29	1	-8	0	7	18	19	1
-13	2	6	7	3	1	-12	4	6	14	14	1	-7	6	6	61	61	1	-6	0	7	59	57	1
-12	2	6	41	41	1	-11	4	6	56	55	1	-6	6	6	8	6	1	-5	0	7	26	26	1
-11	2	6	67	67	1	-10	4	6	9	2	1	-5	6	6	65	63	1	-2	0	7	17	17	1
-10	2	6	60	60	1	-9	4	6	47	47	1	-4	6	6	61	59	1	0	0	7	82	80	1
-9	2	6	48	47	1	-8	4	6	12	12	1	-3	6	6	12	10	1	-11	1	7	33	35	1
-8	2	6	28	28	1	-7	4	6	100	100	1	-2	6	6	41	40	1	-10	1	7	65	66	1
-7	2	6	16	15	1	-6	4	6	5	2	1	-1	6	6	20	20	1	-9	1	7	69	69	1
-6	2	6	17	18	1	-5	4	6	81	80	1	0	6	6	96	93	1	-8	1	7	62	63	1
-5	2	6	65	65	1	-4	4	6	44	47	1	1	6	6	6	4	2	-7	1	7	46	47	1
-4	2	6	61	59	1	-3	4	6	42	43	1	2	6	6	35	35	1	-6	1	7	39	39	1
-3	2	6	67	65	1	-2	4	6	80	81	1	3	6	6	17	16	1	-5	1	7	42	42	1
-2	2	6	20	19	1	-1	4	6	7	2	2	-10	7	6	0	0	2	-4	1	7	63	63	1
-1	2	6	42	43	1	0	4	6	4	5	4	-9	7	6	90	90	1	-3	1	7	14	14	1
0	2	6	21	20	1	1	4	6	16	16	1	-8	7	6	13	13	1	-2	1	7	22	22	1
1	2	6	30	30	1	2	4	6	8	5	1	-7	7	6	106	107	1	-1	1	7	28	27	1
2	2	6	26	27	1	3	4	6	60	60	1	-6	7	6	13	15	1	0	1	7	17	18	1
3	2	6	15	16	1	4	4	6	55	53	1	-5	7	6	10	11	2	1	1	7	24	26	1
4	2	6	33	34	1	5	4	6	55	52	1	-4	7	6	60	58	1	2	1	7	15	17	1
5	2	6	37	36	1	-12	5	6	25	22	2	-3	7	6	47	47	1	-10	2	7	37	37	1
6	2	6	80	78	1	-11	5	6	28	29	1	2	7	6	21	22	1	-9	2	7	26	26	1
-13	3	6	40	41	1	-10	5	6	35	33	1	-1	7	6	39	39	1	-8	2	7	52	52	1

E

STRUCTURE FACTOR TABLES FOR D AND L-SERINE.H_2O

L-serine.H_2O (sc54)

Table F1. Observed and calculated structure factors for sc54

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	183	185	1	0	3	1	111	111	1	-5	1	2	54	53	1	5	8	2	32	36	3
1	5	3	102	98	1	4	0	0	60	58	1	1	3	1	305	309	1	-4	1	2	74	71	1
-3	9	2	53	53	1	2	5	3	52	52	1	6	0	0	49	47	1	2	3	1	130	127	1
-3	1	2	115	112	1	-1	9	2	32	35	1	3	5	3	72	68	1	1	1	0	440	470	1
3	3	1	135	135	1	-2	1	2	279	269	2	0	9	2	73	74	1	4	5	3	73	73	1
2	1	0	135	132	1	4	3	1	116	117	1	-1	1	2	595	649	4	1	9	2	31	35	1
5	5	3	42	41	2	3	1	0	75	69	1	5	3	1	82	82	1	0	1	2	19	19	1
2	9	2	36	35	2	6	5	3	32	31	3	4	1	0	165	162	1	-5	4	1	32	27	1
1	1	2	594	647	3	3	9	2	49	53	1	-4	6	3	73	74	1	5	1	0	28	30	1
-5	4	1	22	18	3	2	1	2	280	269	1	-4	10	2	43	47	2	-3	6	3	96	103	1
6	1	0	25	26	3	-4	4	1	80	82	1	3	1	2	115	112	1	-3	10	2	64	64	1
-2	6	3	70	74	1	0	2	0	112	102	1	-3	4	1	56	55	1	4	1	2	75	71	1
-1	10	2	68	69	1	-1	6	3	31	32	2	1	2	0	327	336	1	-2	4	1	54	53	1
5	1	2	52	55	1	1	10	2	68	69	1	0	6	3	37	36	1	2	2	0	113	109	1
-1	4	1	203	204	1	-5	2	2	49	44	1	3	10	2	67	64	1	1	6	3	32	32	1
3	2	0	320	316	1	0	4	1	338	355	1	-4	2	2	83	83	1	4	10	2	47	47	2
2	6	3	70	74	1	4	2	0	39	42	1	1	4	1	205	204	1	-3	2	2	122	119	1
-3	11	2	62	61	1	3	6	3	101	103	1	5	2	0	61	61	1	2	4	1	84	53	1
-2	11	2	53	53	1	4	6	3	73	74	1	6	2	0	43	44	1	3	4	1	57	55	1
-1	11	2	42	42	1	5	6	3	51	29	2	1	3	0	419	435	1	4	4	1	82	82	1
0	2	2	9	11	3	0	11	2	48	49	1	-5	7	3	38	43	2	2	3	0	40	38	2
5	4	1	19	18	4	1	2	2	125	120	1	1	11	2	43	47	1	-4	7	3	52	53	1
3	3	0	46	46	1	3	4	1	30	27	4	3	2	2	93	88	1	2	11	2	55	53	1
-3	7	3	40	41	1	5	3	0	37	37	1	-6	5	1	34	36	2	3	2	2	122	119	1
3	11	2	60	61	2	-2	7	3	62	66	1	0	4	0	195	185	1	-5	5	1	40	39	1
4	2	2	84	83	1	-2	12	2	42	44	2	-1	7	3	114	116	1	1	4	0	417	429	1
-4	5	1	51	52	1	5	2	2	47	44	1	-1	12	2	53	51	1	0	7	3	152	153	1
2	4	0	140	135	2	-3	5	1	106	108	1	6	2	2	35	36	2	0	12	2	84	83	2
1	7	3	119	118	1	3	4	0	57	61	1	-2	5	1	79	75	1	-6	3	2	33	34	2
1	12	2	51	51	1	2	7	3	67	66	1	4	4	0	46	44	1	0	5	1	120	119	1
-4	3	2	83	82	1	2	12	2	46	44	2	3	7	3	40	41	1	5	4	0	21	17	3
2	5	1	78	75	1	-3	3	2	118	120	1	0	13	2	45	46	1	4	7	3	50	54	1
5	0	1	132	133	1	3	5	1	106	108	1	-2	3	2	295	289	1	1	0	3	237	231	1
5	7	3	45	43	2	4	5	0	60	62	1	4	5	1	52	52	1	-1	3	2	122	111	1
2	0	3	135	139	1	-3	8	3	28	30	2	5	5	0	24	26	2	5	5	1	40	39	2
0	3	2	508	517	1	3	0	3	146	149	2	-2	8	3	60	63	1	6	5	0	41	41	2
6	5	1	39	36	2	1	3	2	122	111	1	4	0	3	44	44	1	-1	8	3	119	119	1
0	6	0	61	60	1	-6	6	1	67	63	1	2	3	2	298	290	1	5	0	3	63	67	1
0	8	3	179	182	1	1	6	0	89	89	1	-4	6	1	75	72	1	3	3	2	121	120	1
-6	1	3	56	61	2	1	8	3	119	119	1	2	6	0	24	26	1	-3	6	1	40	37	1
4	3	2	83	82	1	-5	1	3	55	56	1	2	8	3	60	63	1	3	6	0	27	29	2
4	1	3	122	122	1	3	8	3	28	31	2	4	6	0	90	89	1	-1	6	1	115	112	1
5	3	2	34	34	2	-3	1	3	31	30	1	-4	9	3	56	57	1	5	6	0	64	64	1
0	6	1	30	30	1	-6	4	2	21	25	4	-2	1	3	254	247	1	-3	9	3	61	62	1
1	7	0	98	95	1	1	6	1	115	112	1	-5	4	2	34	30	2	-1	1	3	389	389	1
-2	9	3	50	49	1	4	7	0	68	66	1	2	6	1	169	169	1	-4	4	2	28	29	2
0	1	3	27	25	1	-1	9	3	96	100	1	0	8	0	64	66	1	3	6	1	40	37	1
-3	4	2	54	57	1	1	1	3	387	390	1	6	9	3	19	17	3	2	8	0	73	78	1
4	6	1	74	72	1	-2	4	2	75	73	1	2	1	3	255	247	2	1	9	3	95	100	1
5	8	0	43	43	1	6	6	1	65	63	1	-1	4	2	267	257	3	3	1	3	29	30	2
2	9	3	50	49	1	2	9	0	71	70	1	-5	7	1	45	43	1	1	4	2	268	257	1
4	1	3	120	122	1	3	9	3	64	63	1	3	9	0	44	43	1	-4	7	1	42	38	1
2	4	2	73	73	1	5	1	3	57	56	1	4	9	3	57	57	1	0	10	0	50	48	1
-3	7	1	79	81	1	3	4	2	57	57	1	6	1	3	60	61	1	-3	10	3	81	84	1
1	10	0	66	64	1	-2	7	1	54	56	1	4	4	2	29	28	2	-6	2	3	56	54	1
-2	10	3	77	81	1	4	10	0	42	44	1	-4	7	1	52	55	1	5	4	2	29	30	2
-5	2	3	30	30	2	-1	10	3	51	52	4	1	11	0	78	76	1	0	7	1	166	170	1
6	4	2	25	25	3	-4	2	3	87	86	1	3	10	3	49	52	1	2	11	0	47	47	1
1	7	1	52	55	1	-5	5	2	61	63	1	-3	2	3	112	110	1	2	10	3	78	81	1
3	11	0	66	65	1	2	7	1	53	56	1	-4	5	2	60	61	1	-2	2	3	64	70	1
3	10	3	84	84	1	0	12	0	46	45	1	3	7	1	78	81	1	-3	5	2	86	90	1
-1	2	3	257	253	1	-1	11	3	73	72	1	2	12	0	51	51	1	4	7	1	39	38	2
-2	5	2	136	133	1	0	2	3	331	334	2	-1	11	3	32	31	1	1	13	0	29	27	2
5	7	1	46	45	1	-1	5	2	131	128	1	1	2	3	258	253	1	0	11	3	62	63	1
1	0	1	199	191	1	-4	8	1	31	29	1	0	5	2	94	87	1	2	3	3	65	70	1
1	11	3	34	31	1	2	0	1	193	188	2	-2	8	1	69	76	1	1	5	2	131	128	1
3	2	3	113	1	1	3	11	3	74	72	1	3	0	2	209	198	1	-1	8	1	57	57	1
2	5	2	141	133	1	4	2	3	85	86	1	3	11	3	42	41	2	4	0	1	43	44	1
0	8	1	187	191	1	3	5	2	69	90	1	5	2	3	34	30	2	-1	12	3	35	32	1
5	0	1	58	59	1	1	8	1	57	57	1	4	5	2	61	61	1	6	2	3	50	54	2
0	12	3	32	32	1	6	0	1	42	38	1	2	8	1	69	76	1	5	5	2	63	63	1
-6	3	3	34	31	2	1	12	3	35	32	1	-6	1	1	65	67	1	4	8	1	31	29	2
-5	6	2	52	50	1	-5	3	3	61	61	1	0	0	4	45	45	1	-5	1	1	44	42	1
-3	9	1	52	56	2	-4	6	2	35	36	2	-4	3	3	36	37	1	1	0	4	71	79	1
-3	1	1	129	132	1	-2	9	1	66	63	1	-2	6	2	117	116	1	-3	2	3	112	112	1
2	0	4	285	280	1	-2	1	1	250	248	1	-1	9	1	132	134	1	-1	6	2	100	102	1
-2	3	3	76	72	1	3	0	4	87	90	1	-1	1	1	217	234	1	0	9	1	71	69	1
0	6	2	64	63	1	-1	3	3	222	212	1	4	0	4	121	123	1	0	1	1	44	41	1
1	9	1	132	134	1	1	6	2	101	102	1	0	3	3	405	414	1	-5	1	4	37	36	1
1	1	1	216	234	1	2	9	1	64	63	1	2	6	2	120	116	1	1	3	3	222	212	1
-4	1	4	61	65	2	2	1	1	249	248	1	3	9	1	53	57	1	4	6	2	38	36	2
2	3	3	73	72	1	-3	1	4	119	113	1	3	1	1	130	132	1	-4	10	3	24	27	4
5	6	2	52	50	1	3	3	3	115	112	1	-2	1	4	187			5	1	1	44	42	1
-3	10	1	53	54	2	-5	7	2	41	41	2	4	5	3	35	37	1	-1	1	4	69	71	1
6	1	1	66	67	1	-2	10	1	39	25	4	-4	7	2	37	39	2	5	3	3	62	61	1
0	1	4	123	119	1	-6	2	1	43	43	1	-1	10	1	90	90	1	-3	7	2	80	85	1
6	3	3	31	31	2	1	1	4	68	71	1	-5	2	1	93	93	1	0	10	1	111	110	1
-2	7	2	90	87	1	-5	4	3	52	52	1	2	1	4	184	186	1	-4	2	1	116	118	1
1	10	1	90	90	1	-1	7	2	154	154	3	-3	4	3	92	1	3	1	4	118	113	1	
-3	2	1	162	162	2	2	10	1	23	25	2	0	7	2	197	203	1	-2	4	3	98	101	1
4	1	4	60	63	1	-2	2	1	212	207	1	3	10	1	35	34	2	1	7	2	156	154	2
-1	4	3	72	67	1	5	1	4	34	36	1	-1	2	1	239	232	1	4	10	1	28	27	2
2	7	2	90	87	1	0	4	3	232	216	1	-3	2	4	28	29	2	0	2	1	143	154	1
-2	11	1	42	44	1	3	7	2	83	85	1	1	4	3	72	67	1	-3	2	4	61	60	1
1	2	1	249	252	1	-1	11	1	49	48	1	4	7	2	42	39	2	2	4	3	102	101	1
-2	2	4	135	130	1	2	2	1	214	207	1	0	11	1	30	27	1	5	7	2	42	41	2
3	4	3	93	92	1	-1	2	4	217	208	2	3	2	1	169	162	2	1	11	1	50	48	1
-4	8	2	67	68	1	4	4	3	21	15	2	0	2	4	409	421	1	4	2	1	116	118	2
2	11	1	45	44	1	-3	8	2	52	49	1	5	4	3	53	52	1	1	2	4	214	208	2

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| | | |

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	5	12	65	63	1	4	1	13	4	2	4	2	6	13	6	11	5	0	4	14	9	9	1	2	3	15	34	33	1

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