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# The crystal structure of bis-(L-threonine) copper(II).$H_2O$

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**Abstract.** The crystal structure of bis-(L-threonine) copper (II).$H_2O$, Cu $(C_4H_8NO_3)_2.H_2O$ has been determined by heavy atom and Fourier methods and refined by least-squares using visually estimated three-dimensional x-ray data of 893 reflections. The blue crystals are monoclinic, space group $P2_1$ with $a = 11{\cdot}02$, $b = 4{\cdot}90$, $c = 11{\cdot}16$Å and $\beta = 93{\cdot}5°$, $Z = 2$. The final $R$ is 0·10. Coordination of copper is distorted square pyramidal with ligands in *trans* configuration. The conformation of one of the aminoacid ligand is identical with $L_s$-Threonine while the other has a conformation with torsional angle $\chi^{1,2} = -74(1)°$.

**Keywords.** Bis-(L-threonine) Cu(II)$H_2O$.

## 1. Introduction

In the plasma protein ceruloplasmin, copper is bound to the aminoacids, threonine, histidine and glutamine (Sarkar and Kruck 1966). The present work was undertaken in order to elucidate the nature of copper coordination with the aminoacid threonine.

## 2. Experimental

The details of the preparation of Cu $(L\text{-Thr})_2$, $H_2O$ and the unit cell data have been published (Amirthalingam and Muralidharan 1973). The blue crystals belonging to the monoclinic system have cell parameters $a = 11{\cdot}02\,(2)$, $b = 4{\cdot}90\,(1)$, $c = 11{\cdot}16\,(2)$ Å and $\beta = 93{\cdot}5°\,(5)$. The values obtained from Weissenberg photographs using Cu $K_\alpha$ radiation were further refined by least-squares method using the powder data obtained from a Philips diffractometer. The space group is $P2_1$ with two molecules in the unit cell. The calculated density, 1·75 g/cc compares well with the observed value of 1·73 g/cc (obtained by floatation method using bromoform-carbon tetrachloride mixture). The composition as a monohydrate was well established after the completion of the structure analysis as well as by thermogravimetric analysis.

X-ray intensities were collected with Cu $K_\alpha$ radiation by the equi-inclination Weissenberg technique. The reflection $hkl$ ($k = 0$ to 3) and $0kl$ were recorded. and a total of 893 unique reflections were measured visually. The data were corrected for (*a*) Lorentz and polarisation effects, (*b*) spot size, and (*c*) absorption. The crystal used was almost cylindrical with a cross-section of 0·7 mm. $\mu = 28{\cdot}6\ cm^{-1}$. Initially the scale factors were determined by Wilson plots as well as by cross checking with common reflections.

**Table 1.** Atomic parameters with E.s.d.'s in parenthesis

| No. | Atom | $x/a$ | $y/b$ | $z/c$ | $B$ (Å)$^2$ |
|---|---|---|---|---|---|
| 1 | Cu | 0·4667 (1) | 0·3270 (1) | 0·2592 (1) | .. |
| 2 | C1 | 0·335 (1) | 0·797 (5) | 0·215 (1) | 3·3 (2) |
| 3 | C2 | 0·290 (1) | 0·700 (4) | 0·334 (1) | 2·3 (3) |
| 4 | C3 | 0·165 (1) | 0·579 (4) | 0·309 (1) | 3·1 (3) |
| 5 | C4 | 0·075 (1) | 0·788 (4) | 0·259 (1) | 5·0 (4) |
| 6 | C5 | 0·620 (1) | −0·104 (4) | 0·315 (1) | 3·0 (3) |
| 7 | C6 | 0·672 (1) | 0·055 (4) | 0·211 (1) | 2·6 (3) |
| 8 | C7 | 0·744 (1) | −0·150 (6) | 0·133 (1) | 3·8 (2) |
| 9 | C8 | 0·830 (2) | 0·015 (6) | 0·055 (2) | 4·4 (4) |
| 10 | 01 | 0·405 (1) | 0·638 (3) | 0·164 (1) | 2·9 (2) |
| 11 | 02 | 0·304 (1) | 0·020 (3) | 0·178 (1) | 3·1 (2) |
| 12 | 03 | 0·130 (1) | 0·460 (3) | 0·421 (1) | 3·8 (2) |
| 13 | 04 | 0·532 (1) | 0·018 (3) | 0·357 (1) | 3·2 (2) |
| 14 | 05 | 0·663 (1) | −0·319 (3) | 0·358 (1) | 4·2 (2) |
| 15 | 06 | 0·661 (1) | −0·298 (3) | 0·054 (1) | 3·8 (2) |
| 16 | 07 | 0·873 (1) | 0·350 (5) | 0·408 (1) | 5·0 (3) |
| 17 | N1 | 0·375 (1) | 0·491 (4) | 0·389 (1) | 2·6 (2) |
| 18 | N2 | 0·576 (1) | 0·203 (3) | 0·140 (1) | 2·3 (2) |

Anisotropic temperature factors for Cu of the form

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

| $\beta_{11}$ | $\beta_{22}$ | $\beta_{33}$ | $\beta_{12}$ | $\beta_{13}$ | $\beta_{23}$ |
|---|---|---|---|---|---|
| 0·0057 (1) | 0·0285 (16) | 0·0058 (1) | 0·0025 (1) | 0·0038 (2) | −0·0016 (10) |

## 3. Structure determination*

The *h*0*l* projection was solved first by locating the copper atom from the Patterson map and subsequent location of the lighter atoms from minimum function maps and successive Fourier maps. Then the '*y*' coordinate of copper (which can be chosen arbitrarily) and those of the 2 oxygen and 2 nitrogen atoms (which coordinate with coppper) were assigned assuming an approximate square-planar coordination, using their *x*, *z* coordinates with Cu–N and Cu–O distances as 2Å and Cu–ligand atoms angle as 90°. A 3-D Fourier map was then computed. This process destroyed to a great extent the spurious peaks which can arise due to the false mirror normal to '*b*' axis. Iterative Fourier methods revealed the entire structure together with the fact that there is only one water molecule and not two as was erroneously concluded from the (*h*0*l*) map and reported earlier. The parameters were refined by full-matrix least-squares method minimising $\Sigma w \,||\, KF_o \,| - |\, F_c \,||^2$ and with anisotropic thermal factors for the heavy copper atom only. Cruickshank's weighting scheme with $A = 5{\cdot}0$ and $C = 0{\cdot}01$ was used. The form factors for $Cu^{+2}$, N, C and O were taken from International Tables for x-ray crystallography (1962). $F_c$ values were corrected for anamolous dispersion of copper during this refinement. Hydrogen atoms were ignored. The final $R$ for all observed reflections was 0·10.

The structure projected down '*b*' and '*c*' axes are shown in figures 1 and 2.

* While this work was being prepared for publication we learned (from personal communication) that an independent structure of the same compound using counter data has been carried out by Professor H C Freeman at the University of Sydney, Australia. No details regarding the structure were furnished to us for comparison.

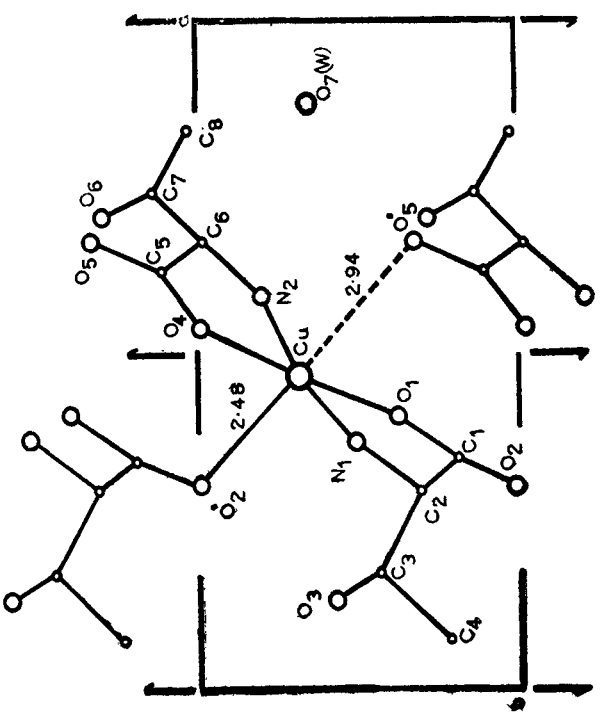


**Figure 2.** Structure projected down '*c*' axis. Overlapping molecule is not drawn for clarity.

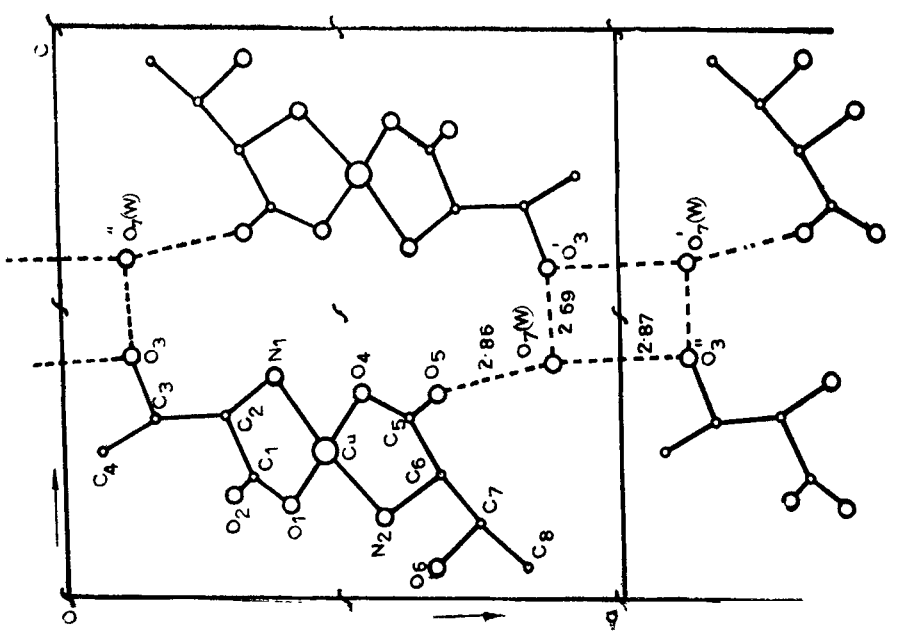


**Figure 1.** Structure projected down '*b*' axis, showing possible hydrogen bonding from water molecule.

The final parameters are given in table 1 and the structure factors in table 2. The final bond lengths and angles are shown in figure 3.

## 4. Description of the structure

The copper coordination as square pyramidal is clearly seen in figure 2, the apical atom being the carboxyl oxygen of one threonine molecule obtained by unit translation of the asymmetric unit along '*b*' axis. The distance Cu-O (apical) is 2·48 Å as compared to value of 2·391 Å found in bis (*L*-tyrosinato) copper where a similar coordination is found (Dick van der Helm and Tatsch 1972). The Cu-N distances [1·979 (5) and 1·936 (5) Å] in the basal plane differ significantly while the Cu–O distances [1·975 (5) and 1·979 (5) Å] compare well with the average value (1·98 ± 0·012 Å) given by Freeman (1967). The 'basal plane is' nearly planar, Cu atom being out of the mean plane containing the four coordination atoms by 0·08 Å (see table 3). The two threonine ligands are *trans* coordinated with copper. The bond lengths of the threonine molecules are comparable with *L*-threonine (Shoemaker *et al* 1950; Ramanadham *et al* 1973). A significant difference is found only in the C=O distances in the carboxyl groups. The two planar carboxyl groups are not coplanar with the basal plane (plane 1 in table 3). The deviations of the nitrogen atoms from the planar carboxyl groups are 0·55 and 0·72 Å, comparable with values obtained in similar structures

The two threonine ligands do not have the same conformation. The conformation of the ligand which has a water molecule near the carboxyl group has its torsion angle $\chi^{1,2} = -74\,(1)^\circ$ while the value for the other ligand $\chi^{1,2} = -177\,(1)^\circ$ which is nearly identical with $L_s$-threonine (see table 4). The difference in conformation of one of the threonine molecule is likely due to the formation of

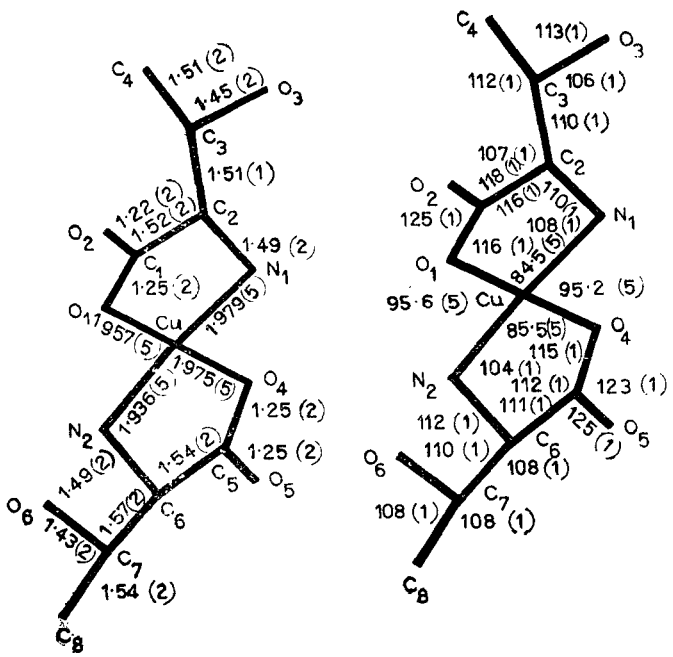


**Figure 3.** Bond lengths and angles of the molecule bis-(*L*-threonine) Cu(II)

**Table 2.** Structure factors.

| H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0 | 0 | 7·29 | 9·83 | 2 | 0 | 4 | 2·80 | 4·09 | 5 | 0 | 12 | 9·89 | 7·40 | 10 | 0 | 8 | 2·40 | 1·35 |
| 3 | 0 | 0 | 7·79 | 5·95 | 2 | 0 | 5 | 5·59 | 3·40 | 6 | 0 | 1 | 22·37 | 21·93 | 10 | 0 | 9 | 5·89 | 4·60 |
| 4 | 0 | 0 | 29·46 | 27·38 | 2 | 0 | 6 | 22·27 | 19·69 | 6 | 0 | 2 | 4·49 | 4·97 | 11 | 0 | 1 | 11·19 | 14·38 |
| 5 | 0 | 0 | 32·56 | 34·57 | 2 | 0 | 8 | 31·96 | 35·37 | 6 | 0 | 3 | 10·99 | 10·32 | 11 | 0 | 2 | 10·99 | 10·42 |
| 6 | 0 | 0 | 27·36 | 25·82 | 2 | 0 | 9 | 6·49 | 7·09 | 6 | 0 | 4 | 20·87 | 22·38 | 11 | 0 | 3 | 10·79 | 9·60 |
| 7 | 0 | 0 | 7·69 | 5·80 | 2 | 0 | 10 | 24·47 | 22·78 | 7 | 0 | 4 | 15·48 | 14·03 | 11 | 0 | 4 | 7·29 | 6·36 |
| 8 | 0 | 0 | 5·19 | 4·63 | 2 | 0 | 11 | 7·89 | 6·44 | 7 | 0 | 5 | 16·58 | 13·38 | 11 | 0 | 5 | 11·88 | 8·18 |
| 9 | 0 | 0 | 8·99 | 6·76 | 2 | 0 | 12 | 10·69 | 8·59 | 7 | 0 | 6 | 26·17 | 24·50 | 11 | 0 | 6 | 4·89 | 4·50 |
| 10 | 0 | 0 | 11·58 | 9·16 | 3 | 0 | 1 | 2·60 | 1·97 | 7 | 0 | 7 | 17·88 | 18·63 | 11 | 0 | 7 | 2·20 | 2·23 |
| 11 | 0 | 0 | 5·59 | 4·49 | 3 | 0 | 2 | 3·10 | 3·10 | 7 | 0 | 8 | 10·69 | 9·79 | 12 | 0 | 1 | 15·88 | 16·25 |
| 12 | 0 | 0 | 4·09 | 5·20 | 3 | 0 | 3 | 11·78 | 8·62 | 6 | 0 | 5 | 26·86 | 26·52 | 12 | 0 | 2 | 7·49 | 8·43 |
| 13 | 0 | 0 | 8·39 | 7·41 | 3 | 0 | 4 | 13·08 | 13·51 | 6 | 0 | 7 | 19·77 | 16·19 | 12 | 0 | 3 | 9·39 | 8·83 |
| 14 | 0 | 0 | 5·59 | 6·93 | 3 | 0 | 5 | 11·09 | 11·24 | 6 | 0 | 12 | 3·00 | 1·98 | 12 | 0 | 5 | 3·20 | 2·15 |
| 0 | 0 | 2 | 82·29 | 85·01 | 3 | 0 | 6 | 36·85 | 37·09 | 7 | 0 | 1 | 21·37 | 20·02 | 13 | 0 | 1 | 1·90 | 3·46 |
| 0 | 0 | 3 | 20·77 | 20·85 | 3 | 0 | 8 | 29·16 | 25·64 | 7 | 0 | 3 | 17·68 | 20·06 | 13 | 0 | 2 | 13·38 | 9·85 |
| 0 | 0 | 4 | 9·69 | 9·44 | 3 | 0 | 10 | 15·28 | 14·88 | 7 | 0 | 9 | 3·10 | 1·97 | 13 | 0 | 3 | 10·89 | 9·13 |
| 0 | 0 | 5 | 16·98 | 15·04 | 3 | 0 | 11 | 1·80 | 0·20 | 8 | 0 | 1 | 3·10 | 4·89 | 13 | 0 | 4 | 6·09 | 5·45 |
| 0 | 0 | 6 | 14·58 | 16·81 | 3 | 0 | 12 | 11·68 | 9·26 | 8 | 0 | 2 | 18·28 | 16·20 | 13 | 0 | 5 | 0·50 | 3·23 |
| 0 | 0 | 7 | 5·49 | 6·54 | 4 | 0 | 1 | 25·27 | 28·93 | 8 | 0 | 3 | 21·07 | 16·39 | 12 | 0 | 6 | 0·50 | 1·55 |
| 0 | 0 | 8 | 12·68 | 11·25 | 4 | 0 | 2 | 36·55 | 35·24 | 8 | 0 | 4 | 10·29 | 7·79 | 14 | 0 | 1 | 1·30 | 1·55 |
| 0 | 0 | 9 | 11·09 | 14·49 | 4 | 0 | 3 | 24·17 | 22·40 | 8 | 0 | 5 | 26·37 | 23·74 | 14 | 0 | 2 | 6·19 | 6·73 |
| 0 | 0 | 10 | 17·78 | 17·57 | 4 | 0 | 4 | 36·65 | 34·37 | 8 | 0 | 6 | 14·18 | 14·58 | −1 | 0 | 1 | 5·09 | 5·36 |
| 0 | 0 | 11 | 2·60 | 0·71 | 4 | 0 | 5 | 6·39 | 4·25 | 8 | 0 | 7 | 16·08 | 11·23 | −1 | 0 | 2 | 52·73 | 52·66 |
| 0 | 0 | 12 | 5·99 | 7·20 | 4 | 0 | 6 | 8·79 | 8·35 | 8 | 0 | 8 | 8·79 | 6·38 | −1 | 0 | 3 | 37·95 | 40·52 |
| 0 | 0 | 13 | 6·19 | 4·75 | 4 | 0 | 8 | 24·87 | 22·70 | 8 | 0 | 9 | 7·99 | 6·06 | −1 | 0 | 4 | 31·36 | 33·48 |
| 1 | 0 | 1 | 30·46 | 32·04 | 4 | 0 | 9 | 6·69 | 6·23 | 8 | 0 | 10 | 2·40 | 2·61 | −1 | 0 | 5 | 5·29 | 4·72 |
| 1 | 0 | 2 | 86·19 | 83·02 | 4 | 0 | 10 | 15·78 | 14·20 | 9 | 0 | 1 | 8·59 | 6·85 | −1 | 0 | 6 | 7·69 | 7·90 |
| 1 | 0 | 3 | 29·96 | 33·60 | 4 | 0 | 11 | 5·19 | 6·28 | 9 | 0 | 3 | 10·49 | 8·15 | −1 | 0 | 7 | 3·89 | 2·83 |
| 1 | 0 | 4 | 17·58 | 15·58 | 4 | 0 | 12 | 7·79 | 4·93 | 9 | 0 | 4 | 4·79 | 4·37 | −1 | 0 | 8 | 16·08 | 18·03 |
| 1 | 0 | 5 | 3·80 | 3·29 | 5 | 0 | 1 | 10·79 | 12·66 | 9 | 0 | 5 | 11·48 | 10·04 | −1 | 0 | 9 | 6·39 | 5·41 |
| 1 | 0 | 6 | 7·59 | 7·14 | 5 | 0 | 2 | 20·67 | 21·37 | 9 | 0 | 6 | 4·59 | 3·17 | −1 | 0 | 10 | 16·28 | 13·51 |
| 1 | 0 | 7 | 3·89 | 3·28 | 5 | 0 | 3 | 19·27 | 20·21 | 9 | 0 | 7 | 9·69 | 8·82 | −1 | 0 | 11 | 11·39 | 11·49 |
| 1 | 0 | 8 | 27·96 | 26·55 | 5 | 0 | 4 | 34·55 | 33·24 | 9 | 0 | 10 | 1·10 | 1·43 | −1 | 0 | 12 | 3·00 | 0·92 |
| 1 | 0 | 9 | 14·78 | 15·03 | 5 | 0 | 5 | 40·45 | 38·85 | 10 | 0 | 1 | 20·37 | 17·08 | −1 | 0 | 13 | 11·48 | 10·94 |
| 1 | 0 | 10 | 19·97 | 21·07 | 5 | 0 | 6 | 13·78 | 10·33 | 10 | 0 | 2 | 3·40 | 0·52 | −1 | 0 | 14 | 4·69 | 4·03 |
| 1 | 0 | 11 | 4·59 | 4·28 | 5 | 0 | 7 | 11·48 | 13·19 | 10 | 0 | 3 | 14·98 | 14·87 | −2 | 0 | 1 | 20·37 | 20·30 |
| 1 | 0 | 12 | 5·59 | 7·33 | 5 | 0 | 8 | 8·09 | 8·06 | 10 | 0 | 4 | 5·59 | 2·96 | −2 | 0 | 2 | 50·53 | 53·35 |
| 1 | 0 | 13 | 4·19 | 5·59 | 5 | 0 | 9 | 10·89 | 9·46 | 10 | 0 | 5 | 10·89 | 8·73 | −2 | 0 | 3 | 17·58 | 21·54 |
| 2 | 0 | 1 | 17·28 | 14·25 | 5 | 0 | 10 | 14·58 | 10·97 | 10 | 0 | 6 | 7·89 | 6·76 | −2 | 0 | 4 | 61·22 | 60·23 |
| 2 | 0 | 2 | 19·37 | 20·40 | 5 | 0 | 11 | 2·80 | 2·78 | 10 | 0 | 7 | 9·39 | 7·10 | −2 | 0 | 5 | 23·07 | 20·13 |

| H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| −2 | 0 | 6 | 34·26 | 36·19 | −5 | 0 | 11 | 18·38 | 17·19 | −9 | 0 | 6 | 18·08 | 16·25 | 4 | 1 | 0 | 45·44 | 48·53 |
| −2 | 0 | 7 | 27·16 | 27·58 | −5 | 0 | 12 | 2·00 | 0·86 | −9 | 0 | 7 | 19·47 | 20·73 | 5 | 1 | 0 | 17·28 | 17·49 |
| −2 | 0 | 8 | 16·48 | 18·10 | −5 | 0 | 13 | 13·68 | 14·36 | −9 | 0 | 8 | 10·69 | 11·84 | 6 | 1 | 0 | 15·78 | 17·42 |
| −2 | 0 | 9 | 12·98 | 13·59 | −6 | 0 | 1 | 33·76 | 33·35 | −9 | 0 | 9 | 7·19 | 8·26 | 7 | 1 | 0 | 23·07 | 24·82 |
| −2 | 0 | 10 | 3·40 | 3·57 | −6 | 0 | 2 | 7·49 | 7·42 | −9 | 0 | 10 | 4·89 | 5·47 | 8 | 1 | 0 | 29·26 | 27·91 |
| −2 | 0 | 11 | 14·78 | 13·23 | −6 | 0 | 3 | 57·22 | 55·20 | −9 | 0 | 11 | 1·40 | 1·49 | 0 | 1 | 11 | 5·79 | 6·94 |
| −2 | 0 | 12 | 5·99 | 5·52 | −6 | 0 | 4 | 5·49 | 3·70 | −10 | 0 | 1 | 18·18 | 15·67 | 0 | 1 | 12 | 5·09 | 5·14 |
| −2 | 0 | 13 | 9·59 | 11·33 | −6 | 0 | 5 | 25·17 | 21·26 | −10 | 0 | 2 | 8·59 | 6·73 | 1 | 1 | 0 | 38·95 | 38·66 |
| −3 | 0 | 1 | 45·94 | 45·85 | −6 | 0 | 7 | 7·79 | 10·28 | −10 | 0 | 3 | 4·79 | 5·95 | 2 | 1 | 0 | 32·46 | 32·87 |
| −3 | 0 | 2 | 15·88 | 17·67 | −6 | 0 | 8 | 9·99 | 9·81 | −10 | 0 | 4 | 11·78 | 11·01 | 3 | 1 | 0 | 35·85 | 38·06 |
| −3 | 0 | 3 | 41·85 | 41·19 | −6 | 0 | 9 | 4·69 | 6·53 | −10 | 0 | 5 | 9·29 | 7·74 | 9 | 1 | 0 | 28·36 | 28·27 |
| −3 | 0 | 4 | 33·36 | 34·80 | −6 | 0 | 11 | 12·38 | 13·46 | −10 | 0 | 6 | 15·28 | 14·44 | 10 | 1 | 0 | 16·68 | 17·56 |
| −3 | 0 | 5 | 48·94 | 48·08 | −6 | 0 | 12 | 7·89 | 8·01 | −10 | 0 | 7 | 13·88 | 12·48 | 11 | 1 | 0 | 9·09 | 8·53 |
| −3 | 0 | 6 | 26·96 | 27·04 | −6 | 0 | 13 | 9·29 | 10·32 | −10 | 0 | 9 | 7·19 | 7·68 | 12 | 1 | 0 | 4·99 | 5·42 |
| −3 | 0 | 7 | 43·84 | 45·69 | −7 | 0 | 1 | 25·37 | 22·93 | −10 | 0 | 10 | 9·39 | 7·11 | 1 | 1 | 1 | 23·67 | 22·92 |
| −3 | 0 | 8 | 5·39 | 4·90 | −7 | 0 | 2 | 8·19 | 5·58 | −11 | 0 | 1 | 10·79 | 10·14 | 1 | 1 | 2 | 20·77 | 23·28 |
| −3 | 0 | 9 | 17·48 | 16·91 | −7 | 0 | 3 | 51·53 | 48·77 | −11 | 0 | 2 | 4·59 | 2·28 | 1 | 1 | 3 | 71·91 | 67·11 |
| −3 | 0 | 10 | 2·60 | 1·99 | −7 | 0 | 4 | 10·29 | 8·53 | −11 | 0 | 3 | 7·89 | 7·44 | 1 | 1 | 4 | 11·48 | 13·81 |
| −3 | 0 | 11 | 10·49 | 10·05 | −7 | 0 | 5 | 18·58 | 20·87 | −11 | 0 | 4 | 9·19 | 7·49 | 1 | 1 | 5 | 42·64 | 41·92 |
| −3 | 0 | 12 | 4·09 | 4·29 | −7 | 0 | 6 | 12·38 | 12·20 | −11 | 0 | 5 | 2·40 | 2·22 | 1 | 1 | 6 | 11·19 | 12·50 |
| −3 | 0 | 13 | 8·29 | 8·81 | −7 | 0 | 7 | 2·60 | 5·06 | −11 | 0 | 6 | 6·99 | 7·44 | 1 | 1 | 7 | 25·47 | 28·36 |
| −4 | 0 | 2 | 19·67 | 20·57 | −7 | 0 | 9 | 6·49 | 8·38 | −11 | 0 | 7 | 4·49 | 5·08 | 1 | 1 | 8 | 7·69 | 8·38 |
| −4 | 0 | 3 | 21·97 | 20·35 | −7 | 0 | 11 | 7·19 | 8·45 | −11 | 0 | 8 | 11·88 | 12·32 | 1 | 1 | 9 | 20·17 | 22·60 |
| −4 | 0 | 4 | 18·18 | 18·69 | −7 | 0 | 12 | 7·29 | 6·58 | −11 | 0 | 9 | 4·49 | 5·31 | 1 | 1 | 10 | 7·39 | 8·92 |
| −4 | 0 | 5 | 47·94 | 49·69 | −8 | 0 | 1 | 23·97 | 22·45 | −12 | 0 | 4 | 2·10 | 3·48 | 1 | 1 | 11 | 5·69 | 8·56 |
| −4 | 0 | 6 | 2·10 | 0·81 | −8 | 0 | 2 | 6·09 | 6·19 | −12 | 0 | 5 | 3·60 | 3·84 | 1 | 1 | 12 | 3·89 | 6·26 |
| −4 | 0 | 7 | 14·88 | 16·88 | −8 | 0 | 3 | 32·26 | 30·82 | −12 | 0 | 6 | 8·19 | 10·24 | 2 | 1 | 1 | 72·90 | 72·66 |
| −4 | 0 | 8 | 14·48 | 12·64 | −8 | 0 | 4 | 10·99 | 10·21 | −12 | 0 | 8 | 9·19 | 10·42 | 2 | 1 | 2 | 54·53 | 52·57 |
| −4 | 0 | 9 | 5·59 | 6·66 | −8 | 0 | 5 | 27·26 | 24·91 | −13 | 0 | 1 | 2·50 | 2·40 | 2 | 1 | 3 | 53·53 | 57·42 |
| −4 | 0 | 10 | 3·40 | 6·40 | −8 | 0 | 6 | 6·59 | 7·06 | −13 | 0 | 2 | 7·99 | 7·71 | 2 | 1 | 4 | 10·59 | 10·49 |
| −4 | 0 | 11 | 16·38 | 14·87 | −8 | 0 | 7 | 30·86 | 28·30 | −13 | 0 | 4 | 7·39 | 7·19 | 2 | 1 | 5 | 24·67 | 25·07 |
| −4 | 0 | 13 | 9·99 | 9·71 | −8 | 0 | 8 | 5·59 | 7·66 | −13 | 0 | 6 | 6·49 | 8·90 | 2 | 1 | 6 | 9·49 | 10·87 |
| −5 | 0 | 1 | 39·05 | 40·18 | −8 | 0 | 9 | 7·59 | 10·87 | −14 | 0 | 2 | 5·29 | 5·66 | 2 | 1 | 7 | 14·28 | 14·08 |
| −5 | 0 | 2 | 20·67 | 20 37 | −8 | 0 | 10 | 8·09 | 8·16 | −14 | 0 | 3 | 3·00 | 1·90 | 2 | 1 | 9 | 20·17 | 20·73 |
| −5 | 0 | 3 | 34·95 | 37·55 | −8 | 0 | 11 | 2·40 | 1·95 | −10 | 0 | 8 | 14·98 | 12·60 | 3 | 1 | 1 | 75·00 | 77·59 |
| −5 | 0 | 4 | 6·59 | 2·78 | −9 | 0 | 1 | 6·49 | 8·57 | 0 | 1 | 1 | 7·69 | 10·75 | 3 | 1 | 2 | 22·27 | 20·87 |
| −5 | 0 | 5 | 28·96 | 28·90 | −9 | 0 | 2 | 4·59 | 5·20 | 0 | 1 | 2 | 46·14 | 43·66 | 3 | 1 | 3 | 47·44 | 45·67 |
| −5 | 0 | 6 | 19·97 | 19·35 | −9 | 0 | 3 | 19·67 | 18·17 | 0 | 1 | 3 | 21·57 | 22·51 | 3 | 1 | 4 | 18·78 | 20·04 |
| −5 | 0 | 9 | 9·39 | 9·88 | −9 | 0 | 4 | 8·09 | 7·88 | 0 | 1 | 4 | 18·18 | 18·84 | 3 | 1 | 5 | 28·06 | 27·14 |
| −5 | 0 | 10 | 4·69 | 3·39 | −9 | 0 | 5 | 30·86 | 28·39 | 0 | 1 | 5 | 39·05 | 38·50 | 3 | 1 | 6 | 21·97 | 20·26 |

| H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 1 | 7 | 7·49 | 8·08 | 9 | 1 | 2 | 16·58 | 19·33 | −4 | 1 | 1 | 15·28 | 15·32 | −8 | 1 | 1 | 4·29 | 2·87 |
| 3 | 1 | 8 | 5·79 | 4·51 | 9 | 1 | 3 | 8·29 | 7·81 | −4 | 1 | 2 | 35·85 | 32·95 | −8 | 1 | 2 | 33·16 | 27·17 |
| 3 | 1 | 9 | 7·39 | 8·72 | 9 | 1 | 6 | 15·88 | 11·55 | −4 | 1 | 3 | 42·74 | 38·86 | −8 | 1 | 3 | 13·68 | 12·63 |
| 3 | 1 | 10 | 4·49 | 5·92 | 10 | 1 | 1 | 4·49 | 6·79 | −4 | 1 | 4 | 54·43 | 53·25 | −8 | 1 | 4 | 9·89 | 9·14 |
| 4 | 1 | 1 | 40·95 | 40·82 | 10 | 1 | 2 | 14·38 | 14·49 | −4 | 1 | 5 | 23·47 | 20·79 | −9 | 1 | 1 | 8·19 | 7·33 |
| 4 | 1 | 2 | 48·84 | 47·23 | 10 | 1 | 3 | 9·99 | 12·36 | −4 | 1 | 6 | 27·06 | 23·68 | −9 | 1 | 2 | 21·47 | 18·06 |
| 4 | 1 | 3 | 49·24 | 50·11 | 12 | 1 | 1 | 3·80 | 7·19 | −4 | 1 | 7 | 5·39 | 2·98 | −9 | 1 | 3 | 4·49 | 6·29 |
| 4 | 1 | 4 | 23·07 | 25·00 | 12 | 1 | 2 | 4·69 | 5·01 | −4 | 1 | 8 | 11·39 | 14·14 | −9 | 1 | 4 | 8·29 | 9·98 |
| 4 | 1 | 5 | 23·57 | 23·91 | −1 | 1 | 1 | 40·45 | 37·83 | −4 | 1 | 9 | 13·18 | 11·07 | −9 | 1 | 5 | 5·89 | 7·76 |
| 4 | 1 | 6 | 17·98 | 21·83 | −1 | 1 | 2 | 24·97 | 23·91 | −4 | 1 | 10 | 11·68 | 14·12 | −9 | 1 | 6 | 4·59 | 4·63 |
| 4 | 1 | 8 | 5·79 | 8·72 | −1 | 1 | 3 | 39·65 | 37·06 | −4 | 1 | 11 | 1·90 | 1·98 | −9 | 1 | 7 | 9·69 | 9·74 |
| 4 | 1 | 9 | 11·09 | 11·83 | −1 | 1 | 4 | 12·88 | 10·53 | −5 | 1 | 1 | 9·99 | 7·44 | −9 | 1 | 8 | 5·29 | 7·01 |
| 5 | 1 | 1 | 15·98 | 16·61 | −1 | 1 | 5 | 22·97 | 24·61 | −5 | 1 | 2 | 39·95 | 39·27 | −10 | 1 | 1 | 8·29 | 8·46 |
| 5 | 1 | 2 | 19·97 | 22·90 | −1 | 1 | 6 | 27·16 | 26·50 | −5 | 1 | 3 | 18·98 | 18·80 | −10 | 1 | 2 | 11·09 | 10·97 |
| 5 | 1 | 3 | 6·39 | 4·89 | −1 | 1 | 7 | 30·56 | 28·48 | −5 | 1 | 4 | 27·76 | 25·81 | −10 | 1 | 3 | 16·08 | 13·89 |
| 5 | 1 | 4 | 29·96 | 29·90 | −1 | 1 | 8 | 15·98 | 15·36 | −5 | 1 | 5 | 18·88 | 16·39 | −11 | 1 | 4 | 10·19 | 9·42 |
| 5 | 1 | 5 | 17·78 | 20·43 | −1 | 1 | 9 | 17·88 | 17·95 | −5 | 1 | 6 | 28·16 | 27·32 | −11 | 1 | 5 | 7·29 | 8·97 |
| 5 | 1 | 6 | 13·38 | 14·17 | −1 | 1 | 10 | 15·08 | 14·20 | −5 | 1 | 7 | 9·59 | 7·94 | −12 | 1 | 1 | 9·99 | 10·73 |
| 5 | 1 | 7 | 9·99 | 11·95 | −1 | 1 | 11 | 9·89 | 10·92 | −5 | 1 | 8 | 26·67 | 25·28 | −12 | 1 | 4 | 3·60 | 6·65 |
| 5 | 1 | 8 | 11·09 | 10·21 | −2 | 1 | 1 | 37·95 | 37·78 | −5 | 1 | 10 | 9·29 | 9·56 | −12 | 1 | 5 | 9·59 | 12·35 |
| 5 | 1 | 9 | 5·79 | 3·65 | −2 | 1 | 2 | 13·48 | 12·66 | −6 | 1 | 1 | 9·09 | 10·01 | 0 | 2 | 1 | 22·07 | 22·97 |
| 6 | 1 | 1 | 6·49 | 6·56 | −2 | 1 | 3 | 29·96 | 29·04 | −6 | 1 | 2 | 28·46 | 29·09 | 0 | 2 | 2 | 30·56 | 30·64 |
| 6 | 1 | 2 | 20·07 | 22·99 | −2 | 1 | 4 | 35·95 | 35·71 | −6 | 1 | 3 | 23·17 | 20·47 | 0 | 2 | 3 | 4·99 | 4·72 |
| 6 | 1 | 3 | 9·89 | 10·03 | −2 | 1 | 5 | 26·96 | 23·20 | −6 | 1 | 4 | 32·66 | 30·11 | 0 | 2 | 4 | 41·45 | 37·20 |
| 6 | 1 | 4 | 27·76 | 27·20 | −2 | 1 | 6 | 28·76 | 27·18 | −6 | 1 | 6 | 35·25 | 34·62 | −10 | 2 | 5 | 18·68 | 18·13 |
| 6 | 1 | 5 | 14·48 | 10·23 | −2 | 1 | 7 | 18·98 | 17·54 | −6 | 1 | 7 | 4·49 | 5·38 | −10 | 1 | 4 | 7·99 | 7·68 |
| 6 | 1 | 6 | 7·19 | 8·07 | −2 | 1 | 8 | 23·27 | 23·34 | −6 | 1 | 8 | 24·97 | 22·55 | −11 | 1 | 5 | 5·69 | 8·37 |
| 6 | 1 | 7 | 9·99 | 12·17 | −2 | 1 | 9 | 9·29 | 8·23 | −6 | 1 | 9 | 9·29 | 8·79 | −11 | 1 | 1 | 7·99 | 9·91 |
| 7 | 1 | 1 | 3·99 | 5·74 | −2 | 1 | 10 | 4·49 | 7·40 | −6 | 1 | 10 | 10·99 | 14·22 | −11 | 1 | 2 | 13·68 | 12·65 |
| 7 | 1 | 2 | 22·07 | 21·24 | −2 | 1 | 11 | 5·69 | 5·55 | −7 | 1 | 1 | 3·89 | 5·70 | 0 | 1 | 3 | 17·18 | 14·07 |
| 7 | 1 | 3 | 11·29 | 13·02 | −3 | 1 | 1 | 45·44 | 45·28 | −7 | 1 | 2 | 21·67 | 17·80 | 0 | 2 | 6 | 40·55 | 37·54 |
| 7 | 1 | 4 | 17·98 | 16·10 | −3 | 1 | 2 | 28·96 | 28·28 | −7 | 1 | 3 | 12·88 | 10·92 | 0 | 2 | 7 | 17·98 | 15·67 |
| 7 | 1 | 5 | 2·00 | 3·90 | −3 | 1 | 3 | 37·95 | 36·87 | −7 | 1 | 4 | 27·36 | 23·91 | 0 | 2 | 8 | 20·07 | 21·38 |
| 7 | 1 | 6 | 14·38 | 14·45 | −3 | 1 | 4 | 46·74 | 44·27 | −7 | 1 | 5 | 7·89 | 8·65 | 0 | 2 | 9 | 2·90 | 2·56 |
| 8 | 1 | 1 | 11·09 | 10·57 | −3 | 1 | 5 | 32·06 | 26·98 | −7 | 1 | 6 | 20·87 | 19·61 | 0 | 2 | 10 | 12·98 | 11·61 |
| 8 | 1 | 4 | 15·98 | 19·00 | −3 | 1 | 6 | 20·27 | 16·56 | −7 | 1 | 7 | 9·49 | 9·97 | 1 | 2 | 12 | 5·89 | 5·96 |
| 8 | 1 | 5 | 10·19 | 9·15 | −3 | 1 | 7 | 19·17 | 19·15 | −7 | 1 | 8 | 8·29 | 13·14 | 1 | 2 | 0 | 16·68 | 21·01 |
| 8 | 1 | 6 | 14·38 | 14·73 | −3 | 1 | 8 | 11·09 | 11·36 | −7 | 1 | 9 | 9·69 | 12·87 | 1 | 2 | 1 | 6·69 | 9·22 |
| 8 | 1 | 7 | 5·79 | 4·08 | −3 | 1 | 9 | 22·57 | 18·66 | −7 | 1 | 10 | 12·68 | 15·72 | 1 | 2 | 2 | 28·26 | 29·96 |
| 9 | 1 | 1 | 14·88 | 12·79 | −3 | 1 | 10 | 5·79 | 6.29 | −7 | 1 | 11 | 7·39 | 7·03 | 1 | 2 | 3 | 24·37 | 28·13 |

| H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 4 | 42·34 | 43·39 | 4 | 2 | 11 | 4·19 | 5·29 | 10 | 2 | 0 | 7·39 | 8·48 | −3 | 2 | 10 | 12·78 | 12·21 |
| 1 | 2 | 6 | 17·18 | 13·99 | 5 | 2 | 12 | 4·99 | 6·77 | 10 | 2 | 1 | 5·19 | 5·47 | −3 | 2 | 11 | 14·28 | 12·06 |
| 1 | 2 | 7 | 10·49 | 9·33 | 5 | 2 | 0 | 16·68 | 18·08 | 10 | 2 | 5 | 6·39 | 6·36 | −4 | 2 | 1 | 27·26 | 20·98 |
| 1 | 2 | 8 | 11·19 | 9·56 | 5 | 2 | 1 | 20·47 | 24·49 | 11 | 2 | 0 | 6·49 | 7·88 | −4 | 2 | 2 | 17·38 | 18·61 |
| 1 | 2 | 10 | 7·39 | 7·37 | 5 | 2 | 2 | 28·36 | 31·02 | 11 | 2 | 2 | 4·69 | 6·41 | −4 | 2 | 3 | 5·79 | 7·04 |
| 2 | 2 | 11 | 2·70 | 4·04 | 5 | 2 | 3 | 27·96 | 32·55 | 12 | 2 | 0 | 6·99 | 9·74 | −4 | 2 | 4 | 8·59 | 9·87 |
| 2 | 2 | 0 | 29·96 | 33·65 | 5 | 2 | 4 | 17·28 | 19·36 | 12 | 2 | 1 | 3·89 | 4·31 | −4 | 2 | 5 | 19·97 | 21·58 |
| 2 | 2 | 1 | 17·38 | 18·02 | 5 | 2 | 5 | 10·59 | 12·68 | 12 | 2 | 2 | 3·80 | 4·16 | −4 | 2 | 6 | 19·17 | 18·15 |
| 2 | 2 | 2 | 49·73 | 50·77 | 5 | 2 | 6 | 15·68 | 19·46 | −1 | 2 | 1 | 16·18 | 15·90 | −4 | 2 | 7 | 19·67 | 19·85 |
| 2 | 2 | 3 | 34·35 | 34·16 | 5 | 2 | 7 | 9·29 | 9·01 | −1 | 2 | 2 | 32·36 | 32·72 | −4 | 2 | 8 | 5·39 | 6·89 |
| 2 | 2 | 4 | 31·46 | 34·60 | 5 | 2 | 8 | 13·58 | 13·90 | −1 | 2 | 3 | 29·46 | 27·10 | −4 | 2 | 9 | 19·97 | 18·08 |
| 2 | 2 | 5 | 5·99 | 7·71 | 5 | 2 | 9 | 2·70 | 3·55 | −1 | 2 | 4 | 32·96 | 35·80 | −4 | 2 | 10 | 11·68 | 12·81 |
| 2 | 2 | 6 | 19·87 | 20·85 | 5 | 2 | 10 | 9·59 | 8·86 | −1 | 2 | 5 | 39·95 | 37·56 | −4 | 2 | 11 | 13·68 | 11·51 |
| 2 | 2 | 7 | 12·88 | 14·32 | 5 | 2 | 11 | 3·80 | 5·43 | −1 | 2 | 6 | 30·66 | 31·79 | −5 | 2 | 1 | 27·06 | 29·79 |
| 2 | 2 | 8 | 5·29 | 5·86 | 6 | 2 | 0 | 7·89 | 6·31 | −1 | 2 | 7 | 18·98 | 16·32 | −5 | 2 | 2 | 17·88 | 18·92 |
| 2 | 2 | 9 | 13·18 | 11·92 | 6 | 2 | 1 | 19·47 | 22·22 | −1 | 2 | 8 | 20·27 | 18·84 | −5 | 2 | 3 | 20·97 | 22·35 |
| 2 | 2 | 10 | 7·29 | 7·49 | 6 | 2 | 2 | 8·09 | 10·47 | −1 | 2 | 9 | 10·39 | 8·67 | −5 | 2 | 5 | 21·47 | 20·47 |
| 2 | 2 | 11 | 5·79 | 5·83 | 6 | 2 | 3 | 23·17 | 26·83 | −1 | 2 | 10 | 12·68 | 9·99 | −5 | 2 | 6 | 15·38 | 10·56 |
| 3 | 2 | 12 | 7·89 | 6·91 | 6 | 2 | 4 | 15·18 | 17·40 | −1 | 2 | 11 | 4·89 | 4·52 | −5 | 2 | 7 | 23·07 | 24·09 |
| 3 | 2 | 0 | 34·75 | 35·60 | 6 | 2 | 5 | 13·18 | 13·68 | −1 | 2 | 12 | 3·00 | 2·28 | −5 | 2 | 8 | 3·80 | 1·17 |
| 3 | 2 | 1 | 17·28 | 17·33 | 6 | 2 | 6 | 9·19 | 8·40 | −2 | 2 | 1 | 27·56 | 23·98 | −5 | 2 | 9 | 22·37 | 14·93 |
| 3 | 2 | 2 | 18·38 | 19·60 | 6 | 2 | 7 | 9·19 | 10·99 | −2 | 2 | 2 | 22·87 | 19·96 | −5 | 2 | 11 | 6·09 | 8·44 |
| 3 | 2 | 3 | 37·15 | 40·77 | 6 | 2 | 8 | 7·29 | 6·84 | −2 | 2 | 3 | 23·67 | 20·69 | −6 | 2 | 1 | 29·76 | 23·87 |
| 3 | 2 | 4 | 24·77 | 23·90 | 6 | 2 | 9 | 8·29 | 7·53 | −2 | 2 | 4 | 34·75 | 37·52 | −6 | 2 | 2 | 16·98 | 15·43 |
| 3 | 2 | 5 | 16·18 | 19·08 | 6 | 2 | 10 | 5·09 | 5·36 | −2 | 2 | 5 | 19·07 | 20·61 | −6 | 2 | 3 | 19·97 | 19·90 |
| 3 | 2 | 6 | 21·47 | 22·63 | 7 | 2 | 10 | 5·69 | 6·56 | −2 | 2 | 6 | 23·77 | 24·65 | −6 | 2 | 10 | 4·69 | 3·51 |
| 3 | 2 | 7 | 11·29 | 12·59 | 7 | 2 | 1 | 34·75 | 33·77 | −2 | 2 | 7 | 18·48 | 19·52 | −7 | 2 | 11 | 7·29 | 9·06 |
| 3 | 2 | 8 | 12·88 | 12·08 | 7 | 2 | 2 | 8·09 | 10·35 | −2 | 2 | 8 | 14·38 | 12·17 | −7 | 2 | 1 | 27·96 | 27·43 |
| 3 | 2 | 10 | 8·79 | 8·34 | 7 | 2 | 3 | 13·18 | 14·36 | −2 | 2 | 9 | 11·98 | 11·07 | −7 | 2 | 2 | 14·98 | 13·07 |
| 4 | 2 | 12 | 11·09 | 9·17 | 7 | 2 | 4 | 5·29 | 6·42 | −2 | 2 | 10 | 12·88 | 10·06 | −6 | 2 | 3 | 15·88 | 13·38 |
| 4 | 2 | 0 | 21·97 | 20·73 | 7 | 2 | 5 | 9·29 | 9·70 | −2 | 2 | 11 | 6·89 | 5·63 | −6 | 2 | 4 | 6·99 | 6·95 |
| 4 | 2 | 1 | 19·47 | 23·69 | 7 | 2 | 7 | 8·19 | 10·58 | −2 | 2 | 12 | 4·09 | 5·26 | −6 | 2 | 5 | 11·88 | 13·13 |
| 4 | 2 | 2 | 18·68 | 20·46 | 8 | 2 | 0 | 15·28 | 13·24 | −3 | 2 | 1 | 24·17 | 23·43 | −6 | 2 | 6 | 10·59 | 8·23 |
| 4 | 2 | 3 | 17·68 | 18·73 | 8 | 2 | 1 | 27·36 | 30·12 | −3 | 2 | 3 | 16·68 | 15·24 | −6 | 2 | 7 | 22·77 | 16·87 |
| 4 | 2 | 4 | 19·67 | 19·03 | 8 | 2 | 3 | 18·38 | 19·73 | −3 | 2 | 4 | 13·68 | 11·24 | −6 | 2 | 9 | 17·38 | 14·94 |
| 4 | 2 | 6 | 12·38 | 12·24 | 8 | 2 | 5 | 7·59 | 6·81 | −3 | 2 | 5 | 6·19 | 8·32 | −7 | 2 | 4 | 9·19 | 7·99 |
| 4 | 2 | 7 | 9·19 | 9·61 | 8 | 2 | 7 | 8·99 | 7·82 | −3 | 2 | 6 | 16·08 | 13·12 | −7 | 2 | 5 | 19·97 | 17·70 |
| 4 | 2 | 8 | 14·68 | 14·37 | 9 | 2 | 0 | 7·59 | 8·73 | −3 | 2 | 7 | 21·47 | 20·83 | −7 | 2 | 6 | 9·19 | 8·10 |
| 4 | 2 | 9 | 5·19 | 3·71 | 9 | 2 | 1 | 12·98 | 13·75 | −3 | 2 | 8 | 15·88 | 12·68 | −7 | 2 | 7 | 18·18 | 16·64 |
| 4 | 2 | 10 | 12·48 | 11·83 | 9 | 2 | 3 | 11·68 | 13·09 | −3 | 2 | 9 | 22·77 | 21·03 | −7 | 2 | 8 | 5·19 | 6·50 |

| H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| −7 | 2 | 9 | 12·28 | 12·63 | −12 | 2 | 6 | 5·99 | 6·19 | 2 | 3 | 10 | 4·69 | 2·82 | 6 | 3 | 9 | 8·29 | 9·12 |
| −8 | 2 | 1 | 38·45 | 29·61 | −13 | 2 | 1 | 2·90 | 3·61 | 2 | 2 | 11 | 4·89 | 4·95 | 7 | 3 | 0 | 9·29 | 10·56 |
| −8 | 2 | 2 | 3·80 | 2·55 | −13 | 2 | 2 | 8·49 | 7·50 | 3 | 3 | 1 | 9·79 | 9·93 | 7 | 3 | 1 | 5·39 | 4·21 |
| −8 | 2 | 3 | 15·78 | 18·44 | −13 | 2 | 3 | 1·80 | 1·79 | 3 | 3 | 2 | 5·99 | 8·15 | 7 | 3 | 2 | 10·79 | 13·64 |
| −8 | 2 | 4 | 13·98 | 13·29 | −13 | 2 | 4 | 5·09 | 6·88 | 3 | 3 | 3 | 9·49 | 11·44 | 7 | 3 | 4 | 7·59 | 10·66 |
| −8 | 2 | 5 | 7·59 | 9·74 | 0 | 3 | 1 | 33·46 | 37·47 | 3 | 3 | 4 | 11·29 | 10·45 | 7 | 3 | 6 | 8·19 | 8·52 |
| −8 | 2 | 6 | 11·88 | 8·62 | 0 | 3 | 2 | 7·09 | 6·59 | 3 | 3 | 5 | 19·27 | 22·62 | 7 | 3 | 7 | 8·29 | 5·25 |
| −8 | 2 | 7 | 12·58 | 9·87 | 0 | 3 | 3 | 20·17 | 19·49 | 3 | 3 | 0 | 10·57 | 21·62 | 7 | 3 | 8 | 5·99 | 5·25 |
| −8 | 2 | 8 | 8·89 | 8·61 | 0 | 3 | 4 | 11·78 | 12·18 | 3 | 3 | 9 | 1·19 | 10·40 | 7 | 3 | 9 | 8·49 | 6·88 |
| −8 | 2 | 9 | 6·19 | 7·21 | 0 | 3 | 5 | 20·07 | 15·46 | 3 | 3 | 17 | 3·20 | 1·96 | 8 | 3 | 0 | 3·00 | 3·12 |
| −8 | 2 | 10 | 5·19 | 6·29 | 0 | 3 | 6 | 19·27 | 16·00 | 4 | 3 | 0 | 18·48 | 21·14 | 8 | 3 | 2 | 6·69 | 8·19 |
| −9 | 2 | 1 | 18·28 | 14·29 | 0 | 3 | 7 | 3·80 | 3·22 | 4 | 3 | 1 | 11·09 | 14·07 | 8 | 3 | 3 | 7·59 | 5·87 |
| −9 | 2 | 2 | 7·59 | 6·87 | 0 | 3 | 8 | 3·80 | 5·55 | 4 | 3 | 2 | 10·79 | 9·17 | 8 | 3 | 4 | 14·08 | 14·32 |
| −9 | 2 | 3 | 16·08 | 14·17 | 0 | 3 | 9 | 10·99 | 9·69 | 4 | 3 | 3 | 12·48 | 12·35 | 8 | 3 | 5 | 5·09 | 5·10 |
| −9 | 2 | 4 | 4·79 | 5·30 | 0 | 3 | 10 | 10·19 | 10·22 | 4 | 3 | 4 | 12·38 | 13·50 | 8 | 3 | 6 | 8·19 | 9·74 |
| −9 | 2 | 5 | 12·98 | 9·86 | 0 | 3 | 11 | 10·39 | 10·96 | 4 | 3 | 5 | 11·58 | 14·36 | 8 | 3 | 7 | 5·99 | 6·98 |
| −9 | 2 | 6 | 7·19 | 6·74 | 0 | 3 | 12 | 8·39 | 7·82 | 4 | 3 | 6 | 9·39 | 9·96 | 8 | 3 | 8 | 4·39 | 6·56 |
| −9 | 2 | 7 | 4·79 | 3·89 | 1 | 3 | 0 | 2·00 | 4·13 | 4 | 3 | 7 | 11·39 | 14·44 | 9 | 3 | 1 | 6·39 | 6·56 |
| −9 | 2 | 8 | 4·39 | 4·93 | 1 | 3 | 1 | 21·97 | 23·88 | 4 | 3 | 8 | 6·49 | 8·62 | 9 | 3 | 2 | 11·39 | 12·79 |
| −10 | 2 | 1 | 12·78 | 12·62 | 1 | 3 | 2 | 9·19 | 9·74 | 4 | 3 | 9 | 6·89 | 7·01 | 9 | 3 | 4 | 13·18 | 15·26 |
| −10 | 2 | 2 | 9·29 | 9·13 | 1 | 3 | 3 | 14·18 | 12·07 | 5 | 3 | 0 | 32·16 | 34·99 | 9 | 3 | 5 | 3·20 | 3·86 |
| −10 | 2 | 3 | 14·18 | 12·91 | 1 | 3 | 4 | 7·59 | 7·19 | 5 | 3 | 1 | 14·48 | 18·43 | 9 | 3 | 6 | 7·09 | 7·05 |
| −10 | 2 | 4 | 12·38 | 9·17 | 1 | 3 | 5 | 22·77 | 23·86 | 5 | 3 | 2 | 4·99 | 4·54 | 9 | 3 | 7 | 2·40 | 2·84 |
| −10 | 2 | 5 | 11·19 | 11·03 | 1 | 3 | 6 | 12·58 | 13·53 | 5 | 3 | 3 | 5·19 | 5·91 | 10 | 3 | 0 | 8·39 | 7·89 |
| −10 | 2 | 6 | 6·49 | 7·33 | 1 | 3 | 7 | 18·48 | 17·26 | 5 | 3 | 4 | 4·69 | 4·10 | 10 | 3 | 2 | 10·19 | 10·65 |
| −10 | 2 | 7 | 4·19 | 6·15 | 1 | 3 | 8 | 6·69 | 6·92 | 5 | 3 | 5 | 2·90 | 1·66 | 10 | 3 | 4 | 10·19 | 11·89 |
| −10 | 2 | 8 | 9·39 | 9·57 | 1 | 3 | 9 | 11·19 | 10·69 | 5 | 3 | 6 | 11·39 | 14·04 | 10 | 3 | 5 | 2·70 | 4·22 |
| −10 | 2 | 9 | 4·59 | 4·99 | 1 | 3 | 10 | 4·89 | 4·19 | 5 | 3 | 7 | 6·59 | 8·79 | 11 | 3 | 0 | 9·19 | 8·18 |
| −11 | 2 | 1 | 6·79 | 6·37 | 1 | 3 | 11 | 11·98 | 11·42 | 5 | 3 | 8 | 6·19 | 6·06 | 11 | 3 | 1 | 4·59 | 5·03 |
| −11 | 2 | 2 | 14·38 | 11·13 | 1 | 3 | 12 | 3·10 | 3·76 | 5 | 3 | 9 | 6·49 | 7·64 | 11 | 3 | 2 | 9·69 | 8·50 |
| −11 | 2 | 3 | 11·39 | 9·25 | 2 | 3 | 0 | 16·98 | 18·42 | 5 | 3 | 10 | 2·70 | 4·03 | 11 | 3 | 3 | 4·79 | 4·73 |
| −11 | 2 | 4 | 16·98 | 14·06 | 2 | 3 | 1 | 15·38 | 17·81 | 6 | 3 | 0 | 17·38 | 17·57 | 11 | 3 | 4 | 10·69 | 9·72 |
| −11 | 2 | 5 | 4·19 | 5·66 | 2 | 3 | 2 | 3·80 | 5·76 | 6 | 3 | 1 | 8·89 | 9·72 | 12 | 3 | 0 | 5·19 | 3·77 |
| −11 | 2 | 6 | 8·99 | 9·50 | 2 | 3 | 3 | 10·59 | 10·31 | 6 | 3 | 2 | 15·68 | 10·10 | 12 | 3 | 1 | 6·19 | 6·47 |
| −11 | 2 | 7 | 4·79 | 4·75 | 2 | 3 | 4 | 5·59 | 6·57 | 6 | 3 | 3 | 7·59 | 6·59 | −1 | 3 | 1 | 42·44 | 43·25 |
| −12 | 2 | 1 | 2·90 | 4·03 | 2 | 3 | 5 | 18·78 | 18·24 | 6 | 3 | 4 | 6·69 | 7·06 | −1 | 3 | 2 | 20·97 | 19·72 |
| −12 | 2 | 2 | 8·99 | 8·56 | 2 | 3 | 6 | 11·09 | 8·87 | 6 | 3 | 5 | 7·69 | 7·06 | −1 | 3 | 3 | 40·85 | 38·29 |
| −12 | 2 | 3 | 2·70 | 2·94 | 2 | 3 | 7 | 28·16 | 30·12 | 6 | 3 | 6 | 6·59 | 8·03 | −1 | 3 | 4 | 10·69 | 8·40 |
| −12 | 2 | 4 | 10·99 | 9·87 | 2 | 3 | 8 | 6·69 | 4·99 | 6 | 3 | 7 | 5·19 | 4·71 | −1 | 3 | 5 | 4·79 | 6·12 |
| −12 | 2 | 5 | 4·69 | 5·02 | 2 | 3 | 9 | 13·78 | 13·16 | 6 | 3 | 8 | 5·79 | 5·79 | −1 | 3 | 6 | 11·39 | 11·06 |

| H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL | H | K | L | KFOB | FCAL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| − 1 | 3 | 7 | 7·59 | 5·00 | − 4 | 3 | 8 | 13·48 | 12·95 | − 8 | 3 | 6 | 18·98 | 18·70 |
| − 1 | 3 | 8 | 6·99 | 6·80 | − 4 | 3 | 10 | 9·19 | 9·21 | − 8 | 3 | 7 | 8·09 | 6·16 |
| − 1 | 3 | 9 | 12·28 | 11·77 | − 5 | 3 | 1 | 28·16 | 26·55 | − 8 | 3 | 8 | 8·39 | 7·62 |
| − 1 | 3 | 10 | 12·08 | 10·85 | − 5 | 3 | 2 | 19·97 | 22·01 | − 8 | 3 | 9 | 3·50 | 3·75 |
| − 1 | 3 | 11 | 9·29 | 7·90 | − 5 | 3 | 3 | 4·99 | 4 91 | − 9 | 3 | 1 | 6·49 | 5·02 |
| − 1 | 3 | 12 | 12·18 | 11·99 | − 5 | 3 | 4 | 15·58 | 13·14 | − 9 | 3 | 2 | 7·49 | 5·91 |
| − 2 | 3 | 1 | 25·77 | 23·33 | − 5 | 3 | 5 | 9·19 | 6·29 | − 9 | 3 | 3 | 3·60 | 3·82 |
| − 2 | 3 | 2 | 19·57 | 18·82 | − 5 | 3 | 6 | 16·38 | 14·58 | − 9 | 3 | 4 | 15·18 | 14·08 |
| − 2 | 3 | 3 | 26·67 | 30·68 | − 5 | 3 | 8 | 10·89 | 9·78 | − 9 | 3 | 5 | 10·29 | 10·60 |
| − 2 | 3 | 4 | 13·08 | 9·11 | − 5 | 3 | 10 | 7·39 | 8·99 | − 9 | 3 | 6 | 13·58 | 12·89 |
| − 2 | 3 | 5 | 10·69 | 12·70 | − 6 | 3 | 1 | 17·78 | 18·06 | − 9 | 3 | 7 | 8·69 | 8·52 |
| − 2 | 3 | 6 | 12·58 | 12·61 | − 6 | 3 | 2 | 19·57 | 21 16 | − 9 | 3 | 8 | 5399 | 6·47 |
| − 2 | 3 | 7 | 2·90 | 2·44 | − 6 | 3 | 4 | 27·86 | 23·11 | − 9 | 3 | 9 | 3·50 | 5·13 |
| − 2 | 3 | 8 | 6·69 | 4·86 | − 6 | 3 | 6 | 13·28 | 11·28 | −10 | 3 | 1 | 4·89 | 3·36 |
| − 2 | 3 | 9 | 7·49 | 7·30 | − 6 | 3 | 8 | 12·38 | 11·93 | −10 | 3 | 2 | 5·89 | 5·32 |
| − 2 | 3 | 10 | 10·89 | 9·49 | − 6 | 3 | 10 | 7·69 | 7·85 | −10 | 3 | 3 | 4·69 | 5·50 |
| − 2 | 3 | 11 | 5·19 | 4·85 | − 7 | 3 | 1 | 9·99 | 9·78 | −10 | 3 | 4 | 6·39 | 5·92 |
| − 2 | 3 | 12 | 10·69 | 10·86 | − 7 | 3 | 2 | 16·18 | 13·05 | −10 | 3 | 5 | 10·29 | 8·84 |
| − 3 | 3 | 1 | 28·96 | 28·18 | − 7 | 3 | 3 | 8·89 | 8·29 | −10 | 3 | 6 | 10·39 | 8·02 |
| − 3 | 3 | 2 | 26·96 | 23·48 | − 7 | 3 | 4 | 20·57 | 18·07 | −10 | 3 | 7 | 6·79 | 7·41 |
| − 3 | 3 | 3 | 22·47 | 23·67 | − 7 | 3 | 5 | 3·80 | 3·64 | −11 | 3 | 2 | 9·99 | 6·69 |
| − 3 | 3 | 4 | 24·37 | 21·50 | − 7 | 3 | 6 | 18·08 | 18·57 | −11 | 3 | 3 | 9·59 | 7·12 |
| − 3 | 3 | 5 | 11·98 | 9·77 | − 7 | 3 | 7 | 7·19 | 6·20 | −11 | 3 | 4 | 6·29 | 5·33 |
| − 3 | 3 | 6 | 13·18 | 10·73 | − 7 | 3 | 8 | 10·09 | 9·46 | −11 | 3 | 5 | 7·99 | 7·67 |
| − 3 | 3 | 7 | 14·78 | 11·70 | − 7 | 3 | 9 | 2·90 | 3·06 | −12 | 3 | 1 | 6·39 | 5·27 |
| − 3 | 3 | 8 | 12·18 | 10·62 | − 7 | 3 | 10 | 3·00 | 2·45 | −12 | 3 | 2 | 3·60 | 4·64 |
| − 3 | 3 | 9 | 5·19 | 5·29 | − 8 | 3 | 1 | 9·09 | 7·75 | −12 | 3 | 3 | 6·49 | 6·69 |
| − 3 | 3 | 10 | 12·18 | 10·17 | − 8 | 3 | 2 | 8·89 | 6·97 | − 6 | 0 | 6 | 2·40 | 2·95 |
| − 3 | 3 | 11 | 3·99 | 4·07 | − 8 | 3 | 3 | 2·90 | 1·58 | 4 | 0 | 7 | 11·88 | 11·21 |
| − 3 | 3 | 12 | 4·09 | 4·33 | − 8 | 3 | 4 | 20·27 | 17·15 | 6 | 0 | 6 | 19·07 | 18·60 |
| − 4 | 3 | 6 | 16·88 | 17.43 | − 8 | 3 | 5 | 5·19 | 4·86 | −12 | 3 | 4 | 2·90 | 3·80 |
| − 4 | 3 | 7 | 7·69 | 6·40 | | | | | | | | | | |

**Table 3.** Least square planes.

The equations of the planes are of the form $Ax + By + Cz = D$ x, y, z are orthogonal coordinates in Å

| Plane | Atoms | *A* | *B* | *C* | *D* |
|---|---|---|---|---|---|
| 1 | 01, 04, N1, N2 | 0·748 | 0·563 | 0·350 | 5·731 |
| 2 | 01, 02, C1, C2 | 0·765 | 0·424 | 0·485 | 5·554 |
| 3 | 04, 05, C5, C6 | 0·577 | 0·511 | 0·637 | 5·838 |

Deviation of atoms from planes

| Plane 1 | | Plane 2 | | Plane 3 | |
|---|---|---|---|---|---|
| *Cu | −0·08Å | 01 | +0·003Å | 04 | +0·007Å |
| 01 | −0·06 | 02 | +0·003 | 05 | +0·008 |
| 04 | −0·06 | C1 | −0·008 | C5 | −0·021 |
| N1 | +0·06 | C2 | +0·002 | C6 | +0·006 |
| N2 | +0·06 | *N1 | +0·548 | *N2 | −0·723 |

* atoms not included in plane fitting.

**Table 4.** Torsion angle

| Angle | Description | Value | Values in $L_s$-threonine* |
|---|---|---|---|
| $\psi^1$ (1) | $N_1-C_1-C_2-O_1$ | − 22 (1)° | − 25·6 (4)° |
| $\psi^2$ (1) | $N_1-C_1-C_2-O_2$ | +156 (1)° | +155·8 (3)° |
| $\chi^{1,1}$ (1) | $N_1-C_2-C_3-O_3$ | − 53 (1)° | − 54·8 (3)° |
| $\chi^{1,2}$ (1) | $N_1-C_2-C_3-C_4$ | −177 (1)° | −175·9 (3)° |
| $\psi^1$ (2) | $N_2-C_5-C_6-O_4$ | + 34 (1)° | |
| $\psi^2$ (2) | $N_2-C_5-C_6-O_5$ | −150 (1)° | |
| $\chi^{1,1}$ (2) | $N_2-C_6-C_7-O_6$ | + 43 (1)° | |
| $\chi^{1,2}$ (2) | $N_2-C_6-C_7-C_8$ | − 74 (1)° | |

* (Ramanadham *et al* 1973)

**Table 5.** Intermolecular contacts less than 3·5 Å

| | | | | | |
|---|---|---|---|---|---|
| Cu–C5 (I) | 3·30Å | 06–N2 (VI) | 3·30Å | Cu–02 (II) | 2·48Å |
| Cu–05 (I) | 2·94 | Cu–C1 (I) | 3·00 | C1–N2 (I) | 3·45 |
| C2–04 (I) | 3·09 | C1–C5 (I) | 3·30 | C5–01 (II) | 3·10 |
| C5–N1 (II) | 3·48 | C3–07 (V) | 3·47 | C6–05 (I) | 3·48 |
| 01–02 (II) | 3·23 | C5–N1 (VII) | 3·34 | 01–N2 (IV) | 3·42 |
| 01–06 (IV) | 3·30 | 01–05 (I) | 3·48 | 02–N2 (I) | 3·18 |
| 01–06 (I) | 3·15 | 01–N2 (I) | 3·35 | *07–03 (VII) | 2·69 |
| 01–04 (I) | 3·12 | N2–05 (I) | 3·48 | *06–N2 (II) | 2·80 |
| 02–04 (I) | 3·13 | 02–N1 (I) | 3·35 | N1–05 (V) | 3·25 |
| 04–N1 (II) | 3·13 | *07–03 (III) | 2·87 | | |
| 04–N1 (VII) | 2·97 | *06–N2 (VIII) | 2·78 | | |
| 07–05 (I) | 2·86 | N1–05 (I) | 3·35 | | |

Key to symmetry operations

| | | |
|---|---|---|
| (I) $x, 1+y, z$ | (IV) $1-x, \frac{1}{2}+y, -z$ | (VII) $1-x, -\frac{1}{2}+y, 1-z$ |
| (II) $x, -1+y, z$ | (V) $1-x, \frac{1}{2}+y, 1-z$ | (VIII) $1-x, -3/2+y, -z$ |
| (III) $1+x, y, z$ | (VI) $1-x, -\frac{1}{2}+y, -z$ | |

*Possible hydrogen bonds.

H-bond. However, the value of $\chi^{1,2} = -74\ (1)^\circ$ is close to 60°, one of the allowed conformations (Ramachandran and Sasisekaran 1968).

The molecules are held by a system of hydrogen bonds. The water molecules act both as donor and acceptor (see figure 1). The other possible hydrogen bonds are listed in table 5, where intermolecular distances less than 3·5 Å are given.

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