

## **Table and text relating to A-type DNA referenced as "A Residuals"**

### **Contributors**

Fuller, Watson, 1935-

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Values of the residuals  $R_1$  and  $R_2$  on various layer planes for the

DNA A conformation.  $R_1$  is defined as  $\sum_{hkl} \frac{|F_o - F_c|}{F_o}$  and  $R_2$  as

$\sum_{hkl} \frac{|I_o - I_c|}{I_o}$ , where  $F_o$  and  $F_c$  are the observed and calculated

structure amplitudes for reflection with indices  $hkl$  and  $I_o$  and  $I_c$  are

the observed and calculated intensities.

All reflections for which  $\xi \leq 0.34 \text{ \AA}^{-1}$  and  $p \leq 0.40 \text{ \AA}^{-1}$  were

included in the sums. However, in those sums indicated by \* the

reflections included were only those for which  $I_c$  changed by more

than 2% when the molecular orientation was changed from  $8.2^\circ$  to

$24.6^\circ$ .

Residual	Layer lines included	Value of residual for $\phi = 8.2^\circ$	Value of residual for $\phi = 24.6^\circ$
$R_1$	1 to 11 inclusive		0.39
$R_2$	1 to 11 inclusive		0.60
* $R_2$	1	0.68	0.72
* $R_2$	2	0.63	0.56
* $R_2$	3	0.82	0.68
* $R_2$	4	0.95	0.74
* $R_2$	5	0.91	0.76
* $R_2$	1 to 5 inclusive	0.75	0.66