

Table 3. Comparing alternate models (by standard R factor, R_{sim} , and R_w)

Min. Confidence and d.f.		Comparison Net. d.f = 1			Comparison Net. d.f = 1			Comparison Net. d.f = 2			Comparison Net. d.f = 2			Comparison Net. d.f = 2			
Model identifier	1	2 to 1	2		3 to 1	3		4 to 1	4		5 to 1	5		6 to 1	6		
Prerefinement																	
R_{sim}^*	21.10	n/a	n/a	22.70	n/a	n/a	32.20	n/a	n/a	33.50	n/a	n/a	27.20	n/a	n/a	25.10	n/a
R factor type/ confidence	R	R_w	Conf.	R	R_w	Conf.	R	R_w	Conf.	R	R_w	Conf.	R	R_w	Conf.	R	R_w
All 414 reflections	28.63	75.05	0.91	28.79	76.19	0.52	45.99	117.16	0.81	47.61	116.26	0.79	42.44	123.31	0.77	43.27	127.66
Only meridional	32.24	80.19	0.65	39.80	100.38	0.33	68.89	176.74	0.65	80.62	164.93	0.82	45.95	120.10	0.74	45.38	141.22
Postrefinement																	
Overall	10.73	22.99	0.62	20.43	47.28												
Group 1	13.35	27.74	0.73	19.39	39.88												
Group 2	6.87	14.39	0.86	8.51	17.47												
Group 3	8.19	16.76	0.66	17.11	35.92												
Group 4	9.61	21.62	0.62	17.54	46.03												
Meridional	17.68	38.12	0.59	28.15	66.64												
Nonoverlapping	15.43	33.33	0.66	23.11	53.05												

All R factors are expressed as percentages; confidence interval (Conf.) as minimum fraction. A high probability/confidence value shows a high degree of similarity/dependence between compared models. The lower confidence interval for model 2 with 1 for meridional subset highlights the difference in chain direction, the meridional series being the subset of the data most susceptible to this difference. d.f., degree of freedom; n/a, not applicable; R_{sim} = rms of observed and simulated diffraction pattern. R factor = $\Sigma(|F_o| - |F_c|)/\Sigma|F_o|$.

$R_w = [\Sigma\omega(|F_o|^2 - |F_c|^2)^2/\Sigma\omega(F_o^2)^2]^{1/2}$. All models are fundamentally similar since they have all been fitted to the observed electron density but contain some significant differences:

1. Most logical fit, N- and C-terminal location and chain direction agrees with heavy atom labeling sites.
2. As above, except chain direction reversed, contrary to evidence from labeling sites. (Models 2-4 could be discounted as viable models on this basis alone). Models 1 and 2 were further refined using CNS (see *Methods*).
3. N- and C-terminal ends of molecule swapped in lateral plane, contrary to heavy atom labeling data.
4. Combines 2 and 3.
5. As 1 except small deviation from electron density (see Fig. 11, no. 1).
6. As 1 except small deviation from electron density (see Fig. 11, no. 2).

*Lowest possible R factor for some types of random fiber diffraction structure has been estimated at $\approx 50\%$ [Welsh, L. C., Symmons, M. F., Sturtevant, J. M., Marvin, D. A. & Perham, R. N. (1998) *J. Mol. Biol.* **283**, 155–177], although this was applied to a structure that produced overlapping Bessel functions rather than the type of overlapping Bragg peaks observed in collagens' low-angle diffraction pattern. R_{sim} here only provides comparison of equatorial reflections; it does not assess the accuracy/error of the meridional series.