Closure of a tyrosine/tryptophan aromatic gate leads to a compact fold in apo flavodoxin

Carlos G. Genzor[2], Aurea Perales-Alcón[1], Javier Sancho[2] and Antonio Romero[1]
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Table 1 was misprinted. The version below is as it should have appeared in the April 1996 issue.

Table 1 Details of hydrogen bonds and structure determination

a, New hydrogen bonds formed by residues in the FMN binding region of apo flavdoxin

Thr 56	N	Thr 88	$O\gamma^1$	2.9(Å)	SO_4	01	Thr 10	$O\gamma^1$	2.8 (Å)
SO_4	01	Thr 15	N	2.8(Å)	SO_4	01	Thr 15	$O\gamma^1$	2.9 (Å)
SO_4	02	Thr 12	N	3.2(Å)	SO_4	02	Thr 12	$O\gamma^1$	2.7 (Å)
SO_4	02	Lys 14	N	2.8(Å)	SO_4	03	Trp 57	$N\varepsilon^1$	3.0 (Å)
SO_4	03	Thr 88	$O\gamma^1$	2.8(Å)	SO_4	04	Gln 11	N	2.9 (Å)
SO_4	04	Thr 12	N	3.1(Å)	SO_4	04	Trp 57	$N\varepsilon^1$	3.1 (Å)
Lys 14	Nε	Asp 146	$O\sigma^1$	3.5(Å)					

b, Data collection and refinement statistics

Data collection			
Space group		$P2_12_12_1$	
maximum resolution		2.0Å	
Number of measured reflections		56,317	
Number of unique reflections		8,437	
R_{merge}[1]		7.4%	
Completeness (%) ($I>2\sigma$)			
	resolution range: ∞–2.0 Å	92	
	2.1–2.0 Å	74	
Refinement			
Resolution range		6–2Å	
Number of protein atoms		1,326	
Number of reflections used in the refinement		7,823	
Crystallographic *R*-factor[2] (%)		18.2	
R.m.s.d. from ideal bond lengths (Å)		0.009	
R.m.s.d. from ideal bond angles (°)		1.482	
R.m.s.d. from ideal dihedral angles (°)		26.0	
R.m.s.d. from ideal improper angles (°)		1.371	
Average temperature factors (Å^2)		apo	holo
	Protein atoms	15.2	8.7
	peptide segment Pro 55–Leu 62	28.2	5.0
	Trp 57	13.1	3.3
	Phe 94	15.2	2.3

[1] $R_{merge} = \Sigma j(|I_j - \langle I \rangle|)/\Sigma \langle I \rangle$, I_j is the observed scaled intensity of each unique reflection j and $\langle I \rangle$ is the mean value of multiple observations.
[2] Crystallographic *R*-factor, $R = \Sigma \, | \, |\boldsymbol{F}_o| - |\boldsymbol{F}_c| \, | / \Sigma |\boldsymbol{F}_o|$.