

Corrections

Crystal Structure of a Molybdopterin Synthase—Precursor Z Complex: Insight into Its Sulfur Transfer Mechanism and Its Role in Molybdenum Cofactor Deficiency, by Juma N. Daniels, Margot M. Wuebbens, K. V. Rajagopalan, and Hermann Schindelin,* Volume 47, Number 2, January 15, 2008, pages 615–626.

Page 618. Below is the corrected version of Table 1, which was originally published on the Web 12/20/07 (ASAP) and in the January 15, 2008, issue (Vol. 47, No. 2, pp 615–626). The correct electronic version was published 02/08/08.

Table 1: Crystallographic Data^a

	apoenzyme	precursor Z complex
	Data Collection Statistics	
space group	C2	P222 ₁
unit cell dimensions	$a = 133.9 \text{ \AA}, b = 45.8 \text{ \AA}, c = 41.8 \text{ \AA},$ $\alpha = 90^\circ, \beta = 93.4^\circ, \gamma = 90^\circ$	$a = 56.6 \text{ \AA}, b = 58.1 \text{ \AA}, c = 331.8 \text{ \AA},$ $\alpha = 90^\circ, \beta = 90^\circ, \gamma = 90^\circ$
resolution limits	50–2.0	50–2.5
completeness	0.948 (0.714)	0.969 (0.830)
R_{sym}^b	0.033 (0.065)	0.071 (0.632)
$\langle I/\sigma I \rangle^c$	42.0 (15.4)	22.2 (2.4)
redundancy	3.3 (2.1)	5.3 (3.6)
no. of reflections	54634	200513
no. of unique reflections	16442	38004
	Refinement Statistics	
no. reflections used	15541	36033
resolution limits	30–2.0	30–2.5
no. of protein/solvent/substrate atoms	1751/152	7004/78/92
R_{factor}^d	0.149	0.206
R_{free}^e	0.193	0.255
rms deviation from ideal values		
bond distances (Å)	0.017	0.009
bond angles (deg)	1.55	1.21
chiral centers (Å ³)	0.10	0.071
average <i>B</i> -factors (Å ²) of		
protein/solvent/substrate atoms	28.0/30.9/–	61.7/66.6/87.0
average <i>B</i> -factors (Å ²) of cofactors and	–	73/79/94/109
surrounding atoms within a 5 Å radius	–	64/65/70/71
Ramachandran statistics ^f	97.6/0.0	97.8/0.0

^a Numbers in parentheses apply to the respective highest-resolution shell. ^b $R_{\text{sym}} = \sum_{hkl} \sum_i |I_i - \langle I \rangle| / \sum_{hkl} \sum_i I_i$, where I_i is the i th measurement and $\langle I \rangle$ is the weighted mean of all measurements of I . ^c $\langle I/\sigma I \rangle$ indicates the average of the intensity divided by its standard deviation. ^d $R_{\text{factor}} = \sum ||F_o| - |F_c|| / \sum |F_o|$, where F_o and F_c are the observed and calculated structure factor amplitudes, respectively. ^e R_{free} is the same as R_{factor} for 5% of the data randomly omitted from the refinement. ^f Ramachandran statistics indicate the fraction of residues in the most favored and disallowed regions of the Ramachandran diagram as defined by the program MOLPROBITY (43).

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