

ERRATUM

Erratum to “Structure and Function of an Archaeal Homolog of Survival Protein E (SurE α): An Acid Phosphatase with Purine Nucleotide Specificity”[☆]

J. Mol. Biol. (2003) 326, 1559–1575

Cameron Mura, Jonathan E. Katz, Steven G. Clarke and David Eisenberg

It is regretted that there is an error in Table 1 and the corrected version follows:

Table 1. Crystallographic statistics for *Pae* SurE α

Data set	Data collection and MAD phasing			Model refinement	
	Inflection	Peak	High-energy remote	Resolution range (Å)	20.0–2.0
Wavelength (Å)	0.97870	0.97860	0.96485	No. reflections (working/test set)	38,377/2033
Resolution range (Å)	100.0–2.40	100.0–2.00	100.0–2.85	No. protein residues (A/B) ^a	276/278
No. reflections (total/unique)	242,223/ 47,599	297,069/ 42,129	206,830/ 28,846	$\langle B \rangle$ (protein atoms, Å ²)	35.73
Completeness (%) ^b	100.0 [100.0]	99.9 [100.0]	99.9 [100.0]	$\langle B \rangle$ (Wilson plot, Å ²)	28.79
$I/\sigma(I)$	15.9 [2.3]	17.4 [2.5]	14.0 [3.3]	No. solvent molecules ($\langle B \rangle$, Å ²)	
R_{merge} (%) ^c	9.8 [77.8]	9.9 [78.1]	14.7 [94.1]	Water	287 (44.8)
Anomalous signal ($\langle \chi^2 \rangle$) ^d	–	4.3 [1.9]	–	Glycerol	7 (73.9)
No. Se sites per a.u. (used/expected) ^e	–	8/12	–	Acetate	2 (59.8)
Phasing resolution range (Å)	38.0–2.85	38.0–2.85	38.0–2.85	No. Ramachandran violations	2/560 residues
R_{cullis} ^f	Acentric	0.94/0.65	0.96/0.95	RMSDs (bonds (Å)/angles (deg.))	0.014/1.79
	Centric	0.90	0.93	$R_{\text{cryst}}/R_{\text{free}}$ (%) ^g	18.5/22.3
Figure of merit ^h	0.43/0.59	–	–	PDB submission code	1L5X

^a Number of SurE α residues built in monomers A and B, out of 280 residues per monomer of recombinant protein (the His-tag and linker add 14 residues to the wild-type sequence).

^b Statistics for the highest-resolution shell are given in square brackets.

^c $R_{\text{merge}}(I) = \sum_{hkl} (\sum_i |I_{hkl,i}| - \langle I_{hkl} \rangle) / \sum_i |I_{hkl,i}|$.

^d Anomalous signal as measured by the normalized χ^2 for merging Bijvoet pairs I^+ , I^- . That is, $\chi^2 = \sum_{1+1} ((I - \langle I \rangle)^2 / \sigma^2(n/n - 1))$. Values > 2 suggest a usefully strong anomalous signal.

^e Number of Se sites calculated by SHELXD and used for phasing (out of 12 sites expected per a.u.).

^f $R_{\text{cullis}} = (\sum_{hkl} ||F_{\text{PH}}| - |F_{\text{P}}| - F_{\text{H,calc}}|) / \sum_{hkl} |F_{\text{PH}}|$. Statistics for acentric reflections are given as isomorphous/anomalous.

^g $R_{\text{cryst}} = \sum_{hkl} ||F_{\text{obs}}| - |F_{\text{calc}}|| / \sum_{hkl} |F_{\text{obs}}|$. R_{free} was computed identically, except that 4.6% of the reflections were omitted as a test set.

^h Values are given before/after density modification and phase extension to 2.0 Å.

[☆] DOI of original article 10.1016/S0022-2836(03)00056-1