

(Supplementary table) Coordinates for HEWL sulfur atoms located by Shake 'n Bake at resolution 3 Å compared with the sulfur atom positions deposited by Dauter et al., (1999) (PDB code:1LZ8).

SnB solution	Atom type	x	y	z	In 1LZ8 equivalent to			Residue type	number	x	y	z
1	S	-1.136	29.642	12.981			CYS A	30	-1.439	29.699	12.121	
											CYS A	115
2	S	-9.129	21.329	3.949			CYS A	6	-8.657	21.198	3.128	
											CYS A	127
3	S	-0.971	16.121	27.302			CYS A	94	-0.571	16.371	26.862	
											CYS A	76
4	S	6.128	13.572	26.837			CYS A	64	5.752	14.107	26.550	
											CYS A	80
5	S	-5.538	27.628	20.164			MET A	105	-5.180	27.521	19.909	
											MET A	12
6	S	-5.990	20.264	14.492								