

Table S2 Data collection, phasing and refinement statistics

	PDLP5 <i>sulfur SAD*</i>	PDLP5 <i>native*</i>	PDLP8 <i>native*</i>
Data collection			
Space group	<i>P1</i>	<i>P1</i>	<i>P3₂ 2 1</i>
Cell dimensions			
<i>a, b, c</i> (Å)	41.81, 48.05, 62.24	41.76, 47.97, 62.19	143.86, 143.86, 59.72
α, β, γ (°)	97.68, 102.74, 99.90	97.70, 102.72, 99.86	90, 90, 120
Resolution (Å)	48.91 – 2.3 (2.36 – 2.30)	37.77 – 1.29 (1.32 – 1.29)	19.91 – 1.95 (2.02 – 1.95)
<i>R</i> _{meas} [#]	0.004 (0.10)	0.049 (1.29)	0.319 (3.62)
<i>I</i> / σ [#]	77.5 (33.5)	12.5 (1.1)	8.82 (1.0)
<i>CC</i> (1/2) [#]	99.9 (99.9)	99.9 (55.7)	99.8 (64.7)
Completeness (%) [#]	91.2 (83.6)	94.5 (89.4)	100.0 (99.9)
Redundancy [#]	28.2 (28.5)	3.6 (3.7)	20.1 (20.1)
Refinement			
Resolution (Å)		37.77 – 1.29	19.91 – 1.95
No. reflections		103,379	49,227
<i>R</i> _{work} / <i>R</i> _{free} [§]		0.18/0.21	0.23/0.26
No. atoms			
protein		3,201	4,821
ligands		153	28
solvent		310	193
Res. B-factors [§]			
protein		23.1	42.7
ligands		47.5	70.1
solvent		32.3	43.6
R.m.s deviations [§]			
Bond lengths (Å)		0.012	0.015
Bond angles (°)		1.58	1.36
Ramachandran favored (%)		98.5	97.24
Ramachandran allowed (%)		1.23	2.76
Ramachandran outliers (%)		0.25	0
PDB - ID		6GRE	6GRF

[#]as defined XDS¹¹ or [§]in Refmac5¹⁷, respectively. *Data were collected from one crystal per experiment.