

Supplementary material

Table S1 X-ray diffraction data-collection and processing statistics

	StSOD 4YIO	SmSOD 4YIP
Space group	C222 ₁	P2 ₁
a (Å)	98.52	67.96
b (Å)	100.23	82.88
c (Å)	118.12	72.78
α (°)	90.00	90.00
β (°)	90.00	94.24
γ (°)	90.00	90.00
Resolution limits (Å)	70.0 –1.60 (1.68-1.60)	50.0-2.15 (2.23-2.15)
No. of observations	289970	246773
No. of unique reflection	81739	43458
Completeness (%)	97.1 (88.4)	99.7 (99.7)
I/ σ (I)	10.8 (2.9)	8.4 (2.6)
Average multiplicity	4.0	5.7
Rmerge (%)	4.7 (31.6)	13.5 (64.7)
Mosaicity	0.4	0.6
V _M (Å ³ Da ⁻¹)	3.13	2.38
Solvent content (%)	60.7	48.3

Table S2 Summary of refinement statistics

	StSOD 4YIO	SmSOD 4YIP
Resolution limits (Å)	27.89-1.60	31.39-2.15
Number of reflections used in the refinement	69916	41189
No. of reflections in working set	66175	39008
No. of reflections in test set	3741	2181
R/R _{free}	0.156/0.175	0.193/0.259
No. of protein atoms	3256	6417
No. of ion and ligand atoms	74	4
No. of water molecules	561	278
RMSD from ideal values		
Bond lengths (Å)	0.027	0.015
Bond angles (°)	2.41	1.718
Average B-factors (Å²)		
All atoms	23.0	32.0
Protein main chains	19.2	31.4
Protein side chains	22.8	33.3
Solvent atoms	33.8	33.0
Ion and ligand atoms	38.1	34.1
Ramachandran plot statistics		
Residues in the most favoured regions (%)	97	95
Residues in the allowed regions (%)	12	5
Residues in the forbidden regions (%)	0	0