Supporting Information

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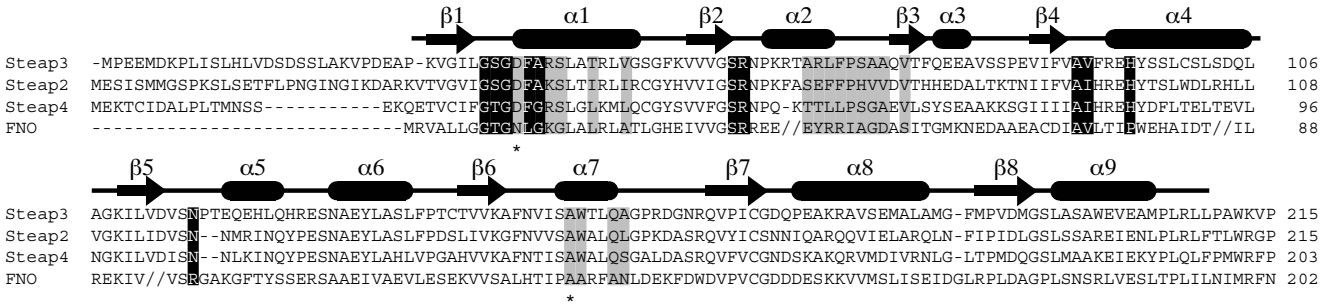

Fig. S1. Sequence alignments with Steap3 homologues. Secondary structural elements in Steap3 are indicated above the sequence. Residues interacting with NADPH are highlighted in white on black background, whereas residues at the putative dimer interface are highlighted in black on gray background. Asp[38] and Ala[151] (asterisks) serve dual roles; while present at the dimer interface, they also interact with NADPH. The Steap2, Steap3, and Steap4 sequences were aligned with ClustalW (1). The FNO sequence represents a structural alignment to Steap3, using SSM (2).

1. Higgins DG (1994) CLUSTAL W: Multiple alignment of DNA and protein sequences. *Methods Mol Biol* 25:307–318.
2. Krissinel E, Henrick K (2004) Secondary-structure matching (SSM), a new tool for fast protein structure alignment in three dimensions. *Acta Crystallogr D* 60:2256–2268.

Table S1. Data collection

Dataset	Apo-Steap3	Steap3-NADPH	Steap3-$Pt(CN)_4^{2-}$ inflection	Steap3 $Pt(CN)_4^{2-}$ peak	Steap3-$Pt(CN)_4^{2-}$ remote	Steap3-mersalyl acid, peak*
Wavelength, Å	1.12709	1.12709	1.07199	1.07149	0.82654	1.00545
Space group			$P2_12_12_1$			
Cell constants [$\alpha = \beta = \gamma = 90°$, Å]						
a	37.69	37.68	37.59	37.56	37.58	37.46
b	66.81	67.00	66.70	66.63	66.67	67.03
c	143.37	143.35	143.47	143.29	143.41	143.28
Resolution range, Å	50–1.98 (2.05–1.98)	50–1.92 (1.99–1.92)	50–2.4 (2.49–2.40)	50–2.10 (2.18–2.10)	50–2.60 (2.69–2.60)	50–3.10 (3.21–3.10)
Unique reflections	25,300 (2,473)	27,874 (2,382)	14,193 (1,395)	21,232 (2,091)	11,135 (1,125)	7,068 (682)
Average redundancy	3.8 (3.7)	3.9 (3.6)	4.2 (4.2)	8.3 (8.2)	4.2 (4.2)	7.8 (7.9)
I/σ	16.10 (3.3)	19.1 (2.8)	15.7 (5.3)	12.8 (3.4)	9.0 (3.0)	12.0 (3.8)
Completeness, %	96.8 (98.3)	97.5 (85.1)	95.6 (97.4)	96.6 (98.3)	93.9 (95.6)	99.7 (100)
R_{sym}, %	5.0 (23.6)	3.4 (27.4)	5.2 (15.4)	7.1 (27.3)	8.5 (29.1)	9.7 (28.4)

Data were integrated, scaled, and reduced by using the HKL-2000 software package. Numbers in parenthesis refer to the highest-resolution shell.
*Mersalyl acid, $HOHgCH_2CH(OCH_3)CH_2NHCOC_6H_4OCH_2CO_2H$.
$R_{sym} = 100 \times \Sigma_h\Sigma_i|I_i(h) - \langle I(h)\rangle|/\Sigma_h I(h)$, where $I_i(h)$ is the *i*th measurement of reflection *h* and $\langle I(h)\rangle$ is the average value of the reflection intensity.

Table S2. Model refinement

Model	apo-Steap3	Steap3-NADPH
R_{cryst}, %	20.3	20.0
R_{free}, %	24.3	24.0
Real space CC, %	93.0	92.8
Mean B value (overall), Å^2	18.3	19.1
Coordinate error (based on maximum likelihood), Å	0.124	0.117
rmsd from ideality		
Bonds, Å	0.013	0.012
Angles, deg.	1.464	1.833
Ramachandran plot		
Most favored, %	96.6	95.53
Additional allowed, %	3.4	4.5
PDB ID code	2VNS	2VQ3

$R_{cryst} = \Sigma||F_o| - F_c||/\Sigma F_o|$, where F_o and F_c are the observed and calculated structure factor amplitudes used in refinement. R_{free} is calculated as R_{cryst} but using the ″test″ set of structure factor amplitudes that were withheld from refinement. Correlation coefficient (CC) is agreement between the model and $2mF_o - DF_c$ electron density map. The Ramachandran plot was calculated by using Molprobity.