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Supplemental materials and methods

Sequence analysis of Sfi1 repeats

The sequences (numbers are GenBank accession nos.) used in an analysis of Sfi1 repeats were *Saccharomyces cerevisiae* (Kilmartin, 2003); *Saccharomyces kluyveri* (a partial sequence available by BLAST using Sfi1p at http://www.genome.wustl.edu/blast/yeast_client.cgi); *Saccharomyces castelli* (available from http://db.yeastgenome.org/fungi/YLL003W.html); *Ashbya gossypii* (*Eremothecium gossypii*; NP 982371); *Kluyveromyces waltii* (contig AAD01000211.1 bases 47388–50072); *Kluyveromyces lactis* (XP 455663); *Candida glabrata* (XP 445660); *Yarrowia lipolytica* (XP 505430); *Candida albicans* (EAK97935); *Schizosaccharomyces pombe* (T40750); *Aspergillus fumigatus* (CAD29603); *Neurospora crassa* (CAD70302); *Ustilago maydis* (XP 401869); *Cryptococcus neoformans* (EAL19270); *Coccoidioides immitis* (contig AAEC 01000149.1 bases 92948–94633); *Magnaporte grisea* (XP 360679); *Chlamydomonas reinhardtii* (JGI assembly release 2.0 predicted proteins from http://genome.jgi-psf.org/chlre2/chlre2.home.html, no. 40135, JGI identifier 166256); *Giardia lamblia* (EAA38349); *Ciona intestinalis* (DNA sequence AK114377, together with ESTs BW035212, AV992885, BW084712, and AV881101); chicken Sfi1 (from ESTs BU284607, BU334263, AI981470, BU325836, BU269267, CD215007, and BU269267, not the database entry XP 425281, which did seem to be a good homologue); dog (XP 543493); mouse (CAI 35196), and human (Kilmartin, 2003). Sfi1 repeats (454) were aligned around the conserved LLX_3F/LX_2W motif, and a logo (Crooks et al., 2004) was calculated (http://weblogo.berkeley.edu/logo.cgi). In addition to the features of the Sfi1 repeat described in Fig. 1 A, there are three positions where there is very little aspartic acid (D): only two in position 19, none at position 27, and one at position 29, compared with a mean of 13.4 D for each position.

Table S1. **Data collection, structure determination, and refinement statistics**

MAD data collection, phasing, and refinement statistics					
Complex	Crystal 1: Cdc31p/Sfi1p (K643-E710)			Crystal 2: Cdc31p/Sfi1p (N218-H306)	
Space group	$P2_12_12_1$			$C222_1$	
Unit cell dimension (Å)	a = 74.78, b = 104.74, c = 184.90			a = 87.28, b = 92.96, c = 189.36	
Data set	Peak[c]	Inflection[c]	Remote[c]	Peak[c]	Remote[c]
Resolution	3.0Å	3.3Å	3.3Å	3.25Å	3.5Å
Completeness (last shell)	99.9 (100)	100 (100)	100 (100)	99.7(99.7)	99.9 (99.9)
R_{merge}[a] (last shell)	0.097 (0.47)	0.14 (0.56)	0.12 (0.49)	0.11 (0.48)	0.067 (0.32)
Redundancy (last shell)	7.3 (7.4)	7.2 (7.3)	7.2 (7.3)	6.8 (6.8)	3.5 (3.5)
<I/s> (last shell)	5.4 (1.6)	4.2 (1.2)	5.0 (1.4)	3.8 (1.3)	5.8 (2.3)
Phasing statistics					
Phasing power (iso)[b]	N/A	0.52	0.25	N/A	1.3
Phasing power (anom)[b]	0.072	0.39	0.32	2.6	1.5
Se sites found/expected	25/28			16/17	
FOM after SHARP	0.26/0.23 (acentric/centric)			0.42/0.27 (acentric/centric)	
Refinement statistics					
Resolution (number of reflections)	2.8 Å (34711)			3.0 Å (14942)	
Protein atoms	6175			4230	
Waters	53			4	
R_{cryst}[d]	0.2531			0.2586	
R_{free}[d] (% data used)	0.2965 (5%)			0.2990 (5%)	
rmsd from ideality[e] bonds/angles/dihedrals	0.008/1.059/4.591			0.01/1.253/5.951	
Average B (Wilson B factor)	70.434 (60.180)			114.140 (113.205)	
rmsd B for bonded main (side) chain atoms	0.478 (1.151)			0.626 (1.290)	

[a] $R_{merge} = \Sigma_{hkl}\Sigma_i|I_i(hkl) - \langle I(hkl)\rangle|/\Sigma_{hkl}\Sigma_i I_i(hkl)$.
[b] The phasing power is defined as the ratio of the rms value of the heavy atom structure factor amplitudes to the rms value of the lack-of-closure error.
[c] Data sets were collected at ESRF, Beamline ID23-1 (crystal 1) at wavelengths 0.9797, 0.9799, and 0.9184 Å for the peak, inflection, and remote data sets, and Beamline ID-144 (crystal 2) at 0.9794 and 0.9393 for the peak and the remote data sets, respectively.
[d] R_{cryst} and $R_{free} = \Sigma(F_{obs} - F_{calc})\Sigma F_{obs}$; R_{free} calculated with the percentage of the data shown in parentheses.
[e] rmsd's for bond angles and lengths in regard to Engh and Huber parameters.

Data collection

MAD datasets were collected at Beamline ID23 and ID14 ESRF (Grenoble). The datasets were processed with Mosflm (Leslie, 1992) and CCP4 (Collaborative Computational Project, No. 4, 1994). Selenium sites were identified with SnB (Smith et al., 1998; Weeks and Miller, 1999; Howell et al., 2000) and refined with SHARP (De La Fortelle and Bricogne, 1997). The initial atomic model was built with the program O (Jones et al., 1991). Manual rebuilding was alternated with Refmac (Murshudov et al., 1997) refinement.

Interhelical angles for the closed and open N- and C-terminal domains of centrin

The change from the closed to the open form in calmodulin is characterized by a change in the angle between the I/II, III/IV, V/VI, and VII/VIII helices from 130–144° in the apo or closed form to 86–100° in the Ca^{2+} bound or open form (Slupsky and Sykes, 1999; Yap et al., 1999). For the closed N-terminal domains in centrins A and B and centrins C–E, these angles were 124–149° and 128–144°, respectively, and for the open C-terminal domains in centrins A and B and centrins C and D, these angles were 95–108° and 94–99°, respectively.

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