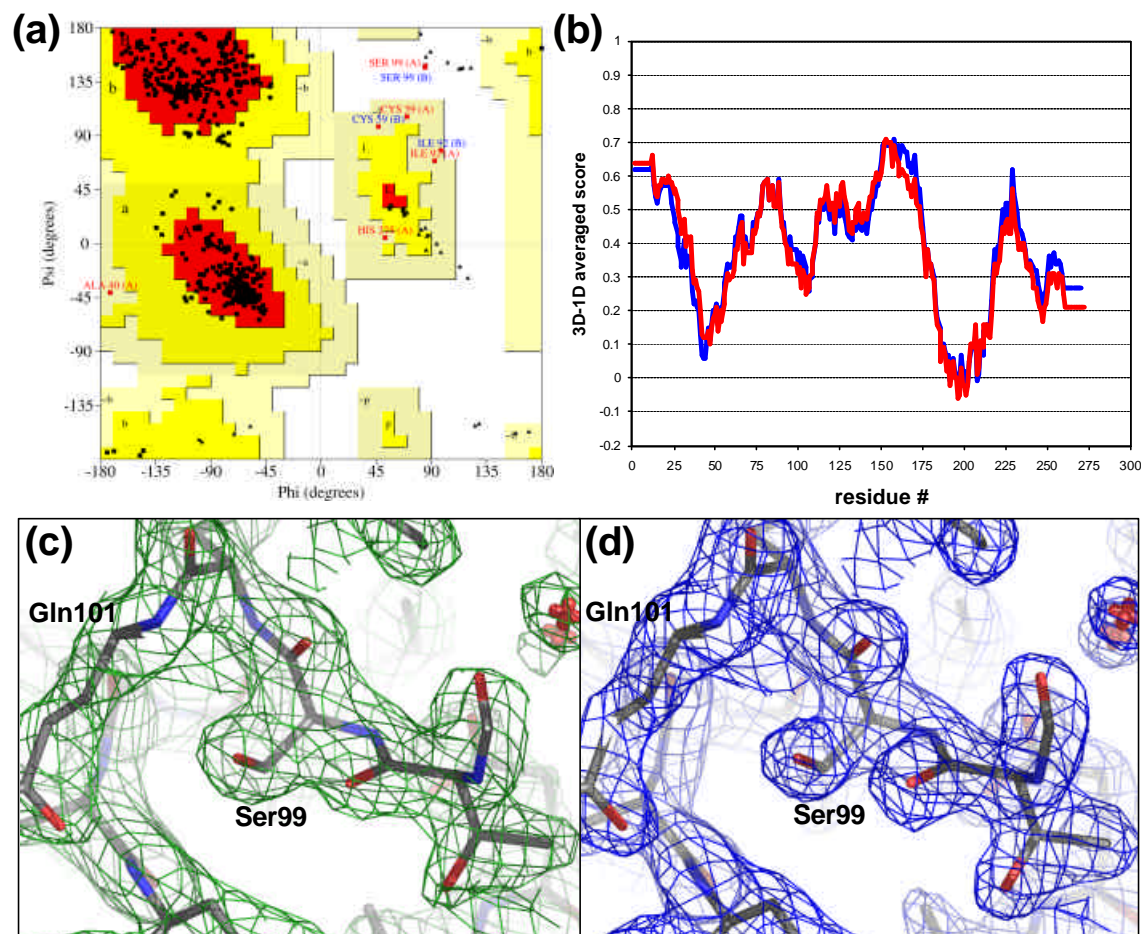


## Supplementary Material

Mura *et al.*, Structure of an archaeal survival protein E



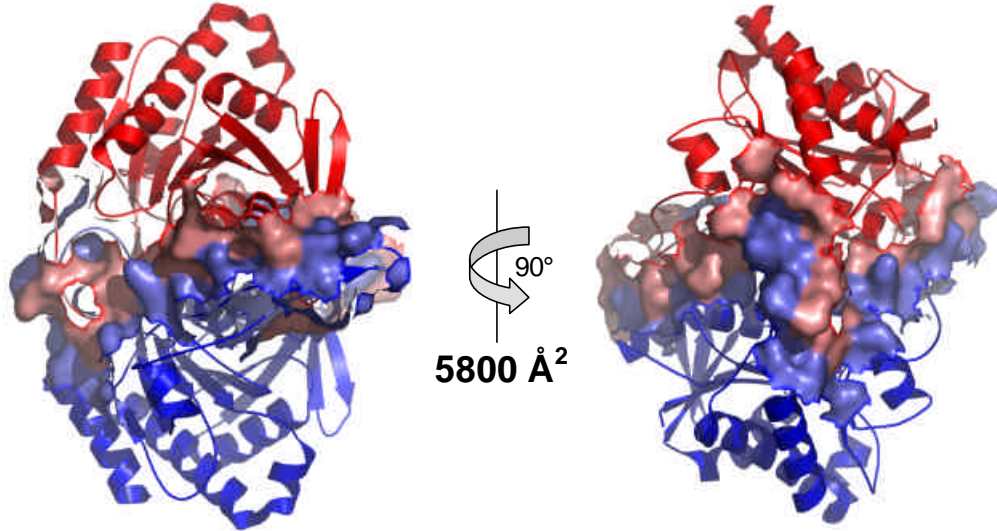
**Supplementary Figure 1: Structure validation and sample electron density for the refined *Pae SurEa* model.** A Ramachandran plot for the refined model is shown in (a), and Verify3D scores for each of the two monomers (A in red and B in blue) are plotted in (b). Out of 560 residues per dimer, only 2 are disallowed (Ser99 in chains A, B) and an additional 6 are generously allowed. Similarly, most of the profile scores in (b) are significantly greater than zero; the poorest-scoring region (near residue 200) is near the C-terminal  $\beta$ -hairpin, and the positive scores for the putative hinge loop (near residue 245) suggest that this region is correctly modeled (in a non-DS conformation). Representative examples of electron density (contoured at  $+1.4\sigma$ ) illustrate the close agreement between maps calculated from experimental MAD phases  $\{F_{\text{obs}}, \Phi_{\text{MAD}}\}$  (c) and those calculated from final model phases  $\{2F_o - F_c, \Phi_{\text{model}}\}$  (d). Together with the lack of significant positive or negative  $F_o - F_c$  density in this region, these maps show that Ser99 – the only strong outlier in the Ramachandran plot – is modeled correctly.

## Supplementary Material

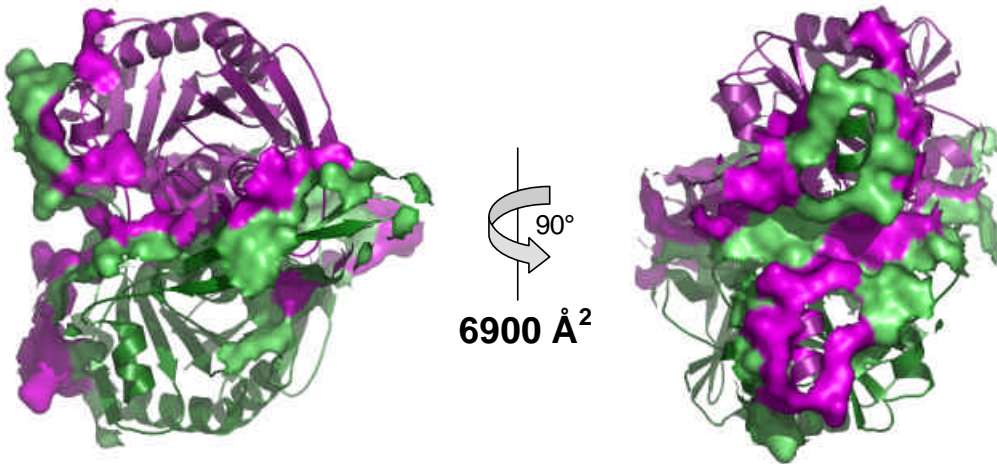
Mura *et al.*, *Structure of an archaeal survival protein E*

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### (a) *Pae* SurE $\alpha$



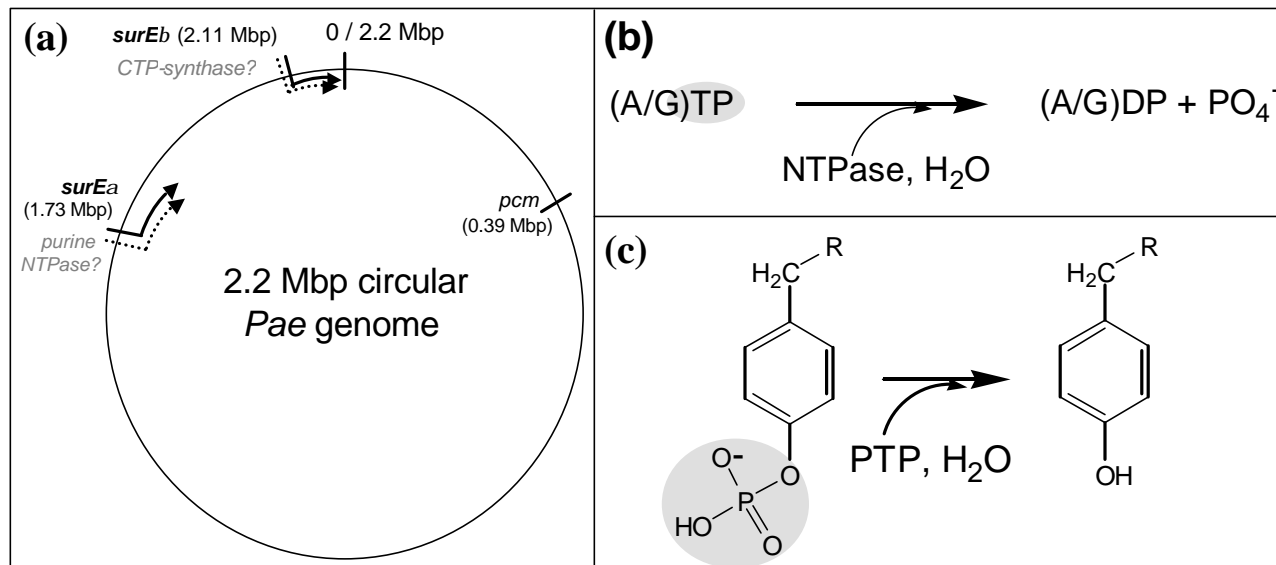
### (b) *Tma* SurE



**Supplementary Figure 2: *Pae* SurE $\alpha$  has a much less extensive dimer interface than domain swapped *Tma* SurE.** Orthogonal views of ribbon diagrams for the *Pae* (a) and *Tma* (b) SurE dimers are shown, with the monomeric subunits colored red and blue (*Pae*) or green and magenta (*Tma*). The total buried surface area in the *Tma* dimer interface is  $6892 \pm 43 \text{ \AA}^2$ , while in the *Pae* interface this value is  $5835 \text{ \AA}^2$ . Comparison of panels (a) and (b) shows that this large difference is primarily due to swapping of the C-terminal  $\alpha$ -helix in *Tma* but not in *Pae* SurE $\alpha$ , *i.e.*, *Tma* SurE forms *open monomers* that exchange helices whereas in *Pae* SurE $\alpha$  *closed monomers* form the less extensive (unswapped) dimer interface.

## Supplementary Material

Mura *et al.*, Structure of an archaeal survival protein E



**Supplementary Figure 3: Genomic organization of *Pae surE* genes and reactions catalyzed by homologs of *surE* gene neighbors.** A cartoon of the circular, 2.2 Mbp genome of *Pae* is shown in (a), with the relative locations of its two *surE* genes marked: *surEa* at 1.73 Mbp and *surEb* at 2.11 Mbp. The two nearest ORFs to these *surEs* are homologs of a purine NTPase ( $\approx 1500$  nt upstream of *surEa*), and a CTP-synthase ( $\approx 1200$  nt upstream of *surEb*). These two ORFs are encoded in the same reading frame as their respective *surE* neighbors. Representative reactions catalyzed by homologs of *surE* gene neighbors in *Pae* (NTPase) and *M. thermautotrophicum* (PTP) are shown in (b) and (c), respectively (see text for details). Although these reactions are not closely related, each enzyme is clearly involved in some form of phosphate hydrolysis (gray-shaded).

## Supplementary Material

Mura *et al.*, Structure of an archaeal survival protein E

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**Supplementary Table 1: Buried surface area statistics for *Pae* and *Tma* SurEs.**

	Molecular species	Total surface area (Å <sup>2</sup> )
<i>Pae</i> SurE $\alpha$	<i>Pae</i> (1L5X) monomer sa	13215.4, 13199.3
	<i>Pae</i> (1L5X) dimer sa	20579.6
	<i>Pae</i> (1L5X) tetramer sa	37451.6
	<b><i>Pae</i> (1L5X) dimer interface</b>	5835.1
	<b><i>Pae</i> (1L5X) tetramer interface</b>	3716.0
<i>Tma</i> SurE (Lee <i>et al.</i> )	1J9J monomer sa	13515.4, 13533.5
	1J9J dimer sa	20113.9
	1J9J tetramer sa	38614.1
	<b>1J9J dimer interface</b>	6935.0
	<b>1J9J tetramer interface</b>	2422.0
<i>Tma</i> SurE (Zhang <i>et al.</i> )	1ILV monomer sa	13446.1, 13429.4
	1ILV dimer sa	20025.6
	1ILV tetramer sa	37896.9
	<b>1ILV dimer interface</b>	6849.9
	<b>1ILV tetramer interface</b>	2006.6

Note 1: An “sa” entry indicates the surface area of that molecular species and the “**interface**” entries indicate the total buried surface area in that type of interface (e.g., counting both subunits of a dimer). The Lee *et al.* (1J9J)<sup>7</sup> and Zhang *et al.* (1ILV)<sup>8</sup> structures are distinguished by their PDB codes.

Note 2: Only two values are given for monomer surface areas and only one value for the dimer surface area (and dimer interface), even though in a tetramer there are four independent monomers and two independent values for a particular type of dimer interface. This is because only one SurE $\alpha$  dimer is in the crystallographic asymmetric unit, and, therefore, any other calculated numbers would almost certainly be artificially identical (due to crystalline symmetry).

Note 3: The difference between buried surface areas in the two *Tma* dimer structures (6935.0 vs. 6849.9 Å<sup>2</sup>) is due to minor variations in crystal packing, and probably is not biochemically significant.

**Supplementary Table 2: All 43 known SurE homologs.**

A comprehensive list of all 43 known SurE homologs as of March 2002 is provided, along with the species abbreviations, GenPept IDs, and phylogenetic kingdom [P = prokaryote/eubacterium, E = eukaryote (green), A = archaeon (red)]. Asterisks denote extremophiles, and genomes with paralogous SurE $\alpha$ / $\beta$  pairs are boldfaced.

Species abbreviation	GenPept ID	Kingdom	Species
Ther_mari_SurE	gi15644410	P*	<i>Thermotoga maritima</i>
Aqui_aeol_SurE	gi15606188	P*	<i>Aquifex aeolicus</i>
Yers_pest_SurE	gi16123508	P	<i>Yersinia pestis</i>
Xyle_fast_SurE	gi15837460	P	<i>Xylella fastidiosa 9a5c</i>
Vibr_chol_SurE	gi15640553	P	<i>Vibrio cholerae</i>
Trep_pall_SurE	gi15639410	P	<i>Treponema pallidum</i>
<b>Syne_sp._SurEa</b>	<b>gi16332288</b>	<b>P</b>	<b><i>Synechocystis sp. PCC 6803</i></b>
<b>Syne_sp._SurEb</b>	<b>gi16330072</b>	<b>P</b>	<b><i>Synechocystis sp. PCC 6803</i></b>
Sino_meli_SurE	gi1754720	P	<i>Sinorhizobium meliloti</i>
Salm_ente_SurE	gi16761699	P	<i>Salmonella enterica</i>
Rubr_gela_SurE	gi11280179	P	<i>Rubrivivax gelatinosus</i>
Rals_sola_SurE	gi17545923	P	<i>Ralstonia solanacearum</i>
Pseu_aeru_SurE	gi15598821	P	<i>Pseudomonas aeruginosa</i>
Past_mult_SurE	gi15603477	P	<i>Pasteurella multocida</i>
<b>Nost_sp._SurEa</b>	<b>gi17232338</b>	<b>P</b>	<b><i>Nostoc sp. PCC 7120</i></b>
<b>Nost_sp._SurEb</b>	<b>gi17230631</b>	<b>P</b>	<b><i>Nostoc sp. PCC 7120</i></b>
Neis_meni_SurE	gi15794586	P	<i>Neisseria meningitidis Z2491</i>
Meso_loti_SurE	gi13471179	P	<i>Mesorhizobium loti</i>
Legi_pneu_SurE	gi5771428	P	<i>Legionella pneumophila</i>
He_pylJ99_SurE	gi15611932	P	<i>Helicobacter pylori J99</i>
He_pyl26695_SurE	gi15645546	P	<i>Helicobacter pylori 26695</i>
Haem_infl_SurE	gi16272643	P	<i>Haemophilus influenzae Rd</i>
Esch_coli_SurE	gi15803261	P	<i>Escherichia coli O157</i>
Dein_radi_SurE	gi15807387	P	<i>Deinococcus radiodurans</i>
Coxi_burn_SurE	gi8141682	P	<i>Coxiella burnetii</i>
Chla_pneu_SurE	gi15618182	P	<i>Chlamydophila pneumoniae</i>
Chla_trac_SurE	gi15604938	P	<i>Chlamydia trachomatis</i>
Chla_muri_SurE	gi14195226	P	<i>Chlamydia muridarum</i>
Caul_cres_SurE	gi16126241	P	<i>Caulobacter crescentus</i>
Camp_jeju_SurE	gi15791661	P	<i>Campylobacter jejuni</i>
Bruc_meli_SurE	gi17987364	P	<i>Brucella melitensis</i>
Agro_tume_SurE	gi15889009	P	<i>Agrobacterium tumefaciens</i>
Yarr_lipo_SurE	gi400781	E	<i>Yarrowia lipolytica</i>
Sacc_cere_SurE	gi6319570	E	<i>Saccharomyces cerevisiae</i>
<b>Arab_thal_SurEa</b>	<b>gi7485145</b>	<b>E</b>	<b><i>Arabidopsis thaliana</i></b>
<b>Arab_thal_SurEb</b>	<b>gi15218620</b>	<b>E</b>	<b><i>Arabidopsis thaliana</i></b>

**Continued:**

Species abbreviation	GenPept ID	Kingdom	Species
Pyro_aero_SurEa	gi18313680	A*	<i>Pyrobaculum aerophilum</i>
Pyro_aero_SurEb	gi18314130	A*	<i>Pyrobaculum aerophilum</i>
Meth_ther_SurE	gi15679432	A*	<i>Methanobacterium thermautotrophicum</i>
Meth_jann_SurE	gi15668739	A*	<i>Methanococcus jannaschii</i>
Halo_sp._SurE	gi15790299	A*	<i>Halobacterium sp. NRC</i>
Arch_fulg_SurE	gi11498547	A*	<i>Archaeoglobus fulgidus</i>
Aero_pern_SurE	gi14600980	A*	<i>Aeropyrum pernix</i>