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Supporting information for article:

Insights into stabilizing interactions in the distorted domain swapped dimer of *Salmonella typhimurium* survival protein

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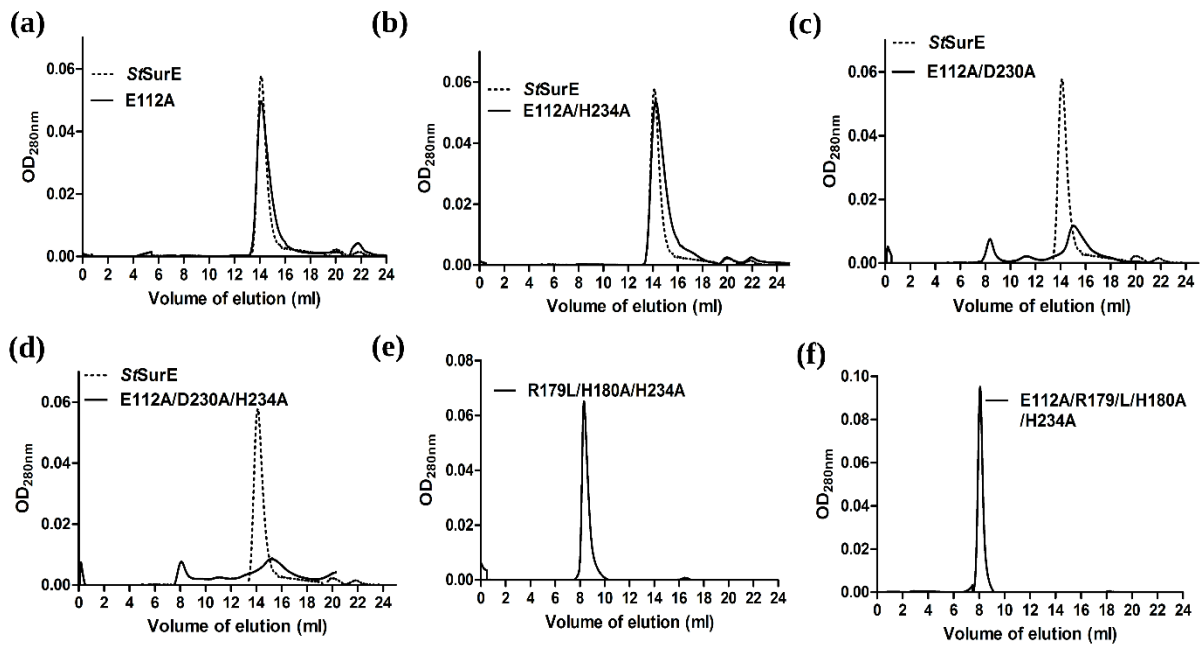


Figure S1 Size exclusion chromatography profile of mutants (a) E112A, (b) E112A/H234A, (c) E112A/D230A, (d) E112A/D230A/H234A, (e) R179L/H180A/H234A and (f) E112A/R179L/H180A/H234A.

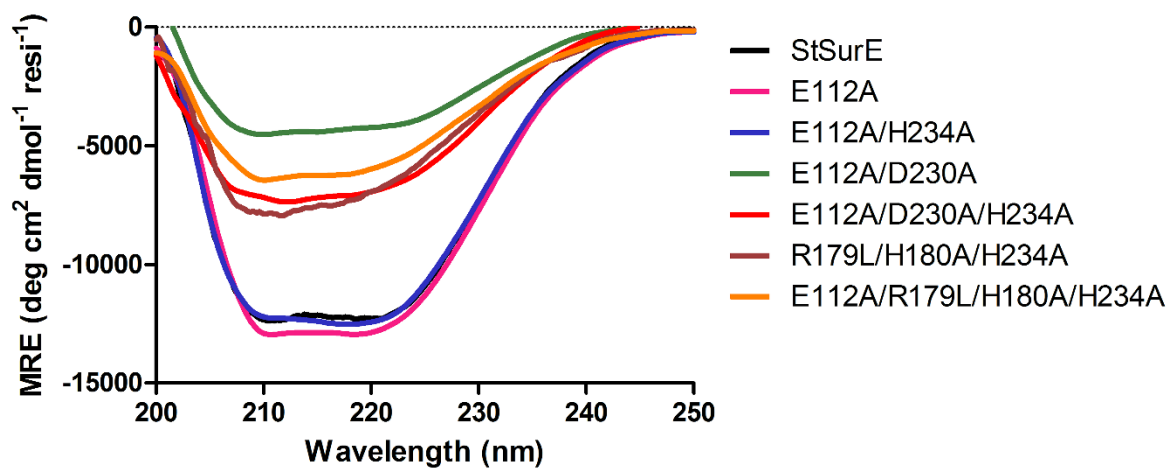


Figure S2 CD spectra of salt bridge mutants. The spectra had minima at 208 and 222 nm.

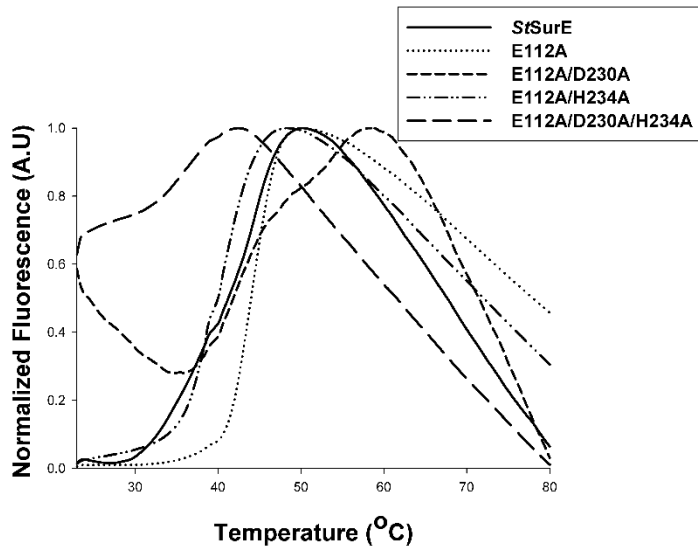


Figure S3 Melting profiles monitored by recording the fluorescence emitted by SYPRO Orange dye on binding with hydrophobic patches that get exposed on protein unfolding. T_m of native, E112A, E112A/D230A, E112A/H234A and E112A/D230A/H234A in 5 mM HEPES buffer (pH 7.5) were 41 °C, 44 °C, 41 °C, 41 °C and 37 °C, respectively.

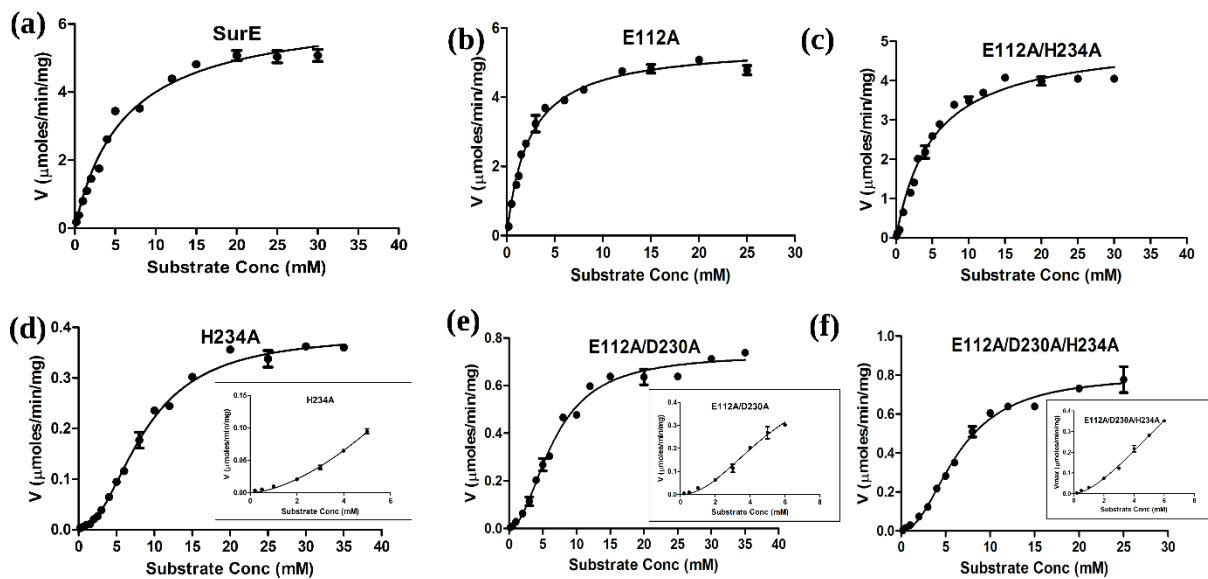


Figure S4 Enzyme activity (V) versus substrate concentration plot for (a) *StSurE*, (b) E112A, (c) E112A/H234A, (d) H234A, (e) E112A/D230A and (f) E112A/D230A/H234A.

Table S1 Template, primer sequences and the restriction enzymes used for PCR amplification and screening of mutants.

| Mutant | Template | Primers (bold letters indicate mutation, underlined sequence shows restriction site) | Restriction enzyme |
|--------------------------------|---------------------------|--|---------------------------|
| E112A | <i>St</i> SurE | Sense 5' - 3' | NaeI |
| E112A/D230A | D230A | GCCGCGGCGATGG <u>C</u> CGG <u>C</u> CGTCATC | |
| E112A/H234A | H234A | TC | |
| E112A/D230A/H234A | D230A/ H234A | Antisense 5'-3' GAGATGACGGCCGGCCATCGCCGCG GC | |
| R179L/H180A/H234A | H234A | Sense 5' - 3' CTCGCTGT <u>G</u> GAT <u>C</u> CCTCGCTCCAGC GGAT Antisense 5'-3' ATCCGCTGGAGCGAGGGATCCACAG CGAG | BamHI |
| E112A/R179L/H180A/H234A | R179L/ H180A/ H234A | Sense 5' - 3' GCCGCGGCGATGG <u>C</u> CGG <u>C</u> CGTCATC TC Antisense 5'-3' GAGATGACGGCCGGCCATCGCCGCG GC | NaeI |

Table S2 Inter-chain hydrogen bonds formed by the segment 39-45 in *St*SurE native and mutant dimers (A/B).

| | Hydrogen bonds (length in Å) |
|--|--|
| <i>St</i>SurE (PDB code: 2V4N) | 45 LEU N/A - 40 GLY O/B (2.9) 45 LEU N/B - 40 GLY O/A (2.9) 43 ASN N/A - 42 SER OG/B (3.2) 43 ASN N/B - 42 SER OG/A (3.2) 42 SER OG/A - 42 SER OG/B (3.1) |
| H234A (PDB code: 4G9O) | 42 SER N/A - 40 GLY O/B (2.9) 42 SER N/B - 40 GLY O/A (2.8) 42 SER OG/A - 39 SER O/B (3.0) 45 LEU N/A - 100 ASP OD1/B (3.4) |
| D230A/H234A (PDB code: 4GAD) | 42 SER N/A - 40 GLY O/B (2.9) 42 SER N/B - 40 GLY O/A (2.7) 42 SER OG/A - 39 SER O/B (3.3) 45 LEU N/A - 100 ASP OD1/B (3.2) 42 SER OG/B - 103 TYR O/A (3.4) |
| E112A (PDB code: 4RYU) | 45 LEU N/A - 40 GLY O/B (2.9) 45 LEU N/B - 40 GLY O/A (2.9) 43 ASN N/B - 42 SER OG/A (3.4) 42 SER OG/A - 42 SER OG/B (3.4) |
| E112A soaked with AMP (PDB code: 4XJ7) | 45 LEU N/A - 40 GLY O/B (3.0) 45 LEU N/B - 40 GLY O/A (2.9) 43 ASN N/A - 42 SER OG/B (3.3) 43 ASN N/B - 42 SER OG/A (3.3) 42 SER OG/A - 42 SER OG/B (3.1) |
| E112A/H234A (PDB code: 4XER) | 45 LEU N/A - 40 GLY O/B (2.9) 45 LEU N/B - 40 GLY O/A (2.9) 43 ASN ND2/B - 102 ILE O/A (3.0) 42 SER OG/A - 43 ASN OD1/B (2.7) 42 SER OG/A - 43 ASN ND2/B (3.5) |
| E112A/H234A form I (PDB code: 4XGB) | 45 LEU N/A - 40 GLY O/B (2.9) 45 LEU N/B - 40 GLY O/A (2.9) |

| | |
|---|--|
| | 43 ASN N/A - 42 SER OG/B (3.2) 43 ASN N/B - 42 SER OG/A (3.3) 42 SER OG/A - 42 SER OG/B (3.0) |
| E112A/H234A form II (PDB code: 4XGP) | 45 LEU N /A – 40 GLY O/B (2.8) 45 LEU N/B - 40 GLY O/A (2.9) 43 ASN OD1/B - 102 ILE O/A (3.1) 42 SER OG/A - 43 ASN OD1/B (2.3) |
| E112A/D230A (PDB code: 4XH8) | 45 LEU N/A - 40 GLY O/B (2.8) 45 LEU N/B - 40 GLY O/A (2.9) 44 SER OG/A - 40 GLY O/B (3.3) 44 SER OG/A - 41 ALA O/B (3.3) 43 ASN ND2/B - 102 ILE O/A (3.3) 44 SER OG/B - 40 GLY O/A (3.4) 44 SER OG/B - 41 ALA O/A (3.5) |