STRUCTURAL BIOLOGY COMMUNICATIONS

Volume 72 (2016)

Supporting information for article:

Structural and functional insights into the stationary phase survival protein SurE, an important virulence factor of *Brucella abortus*

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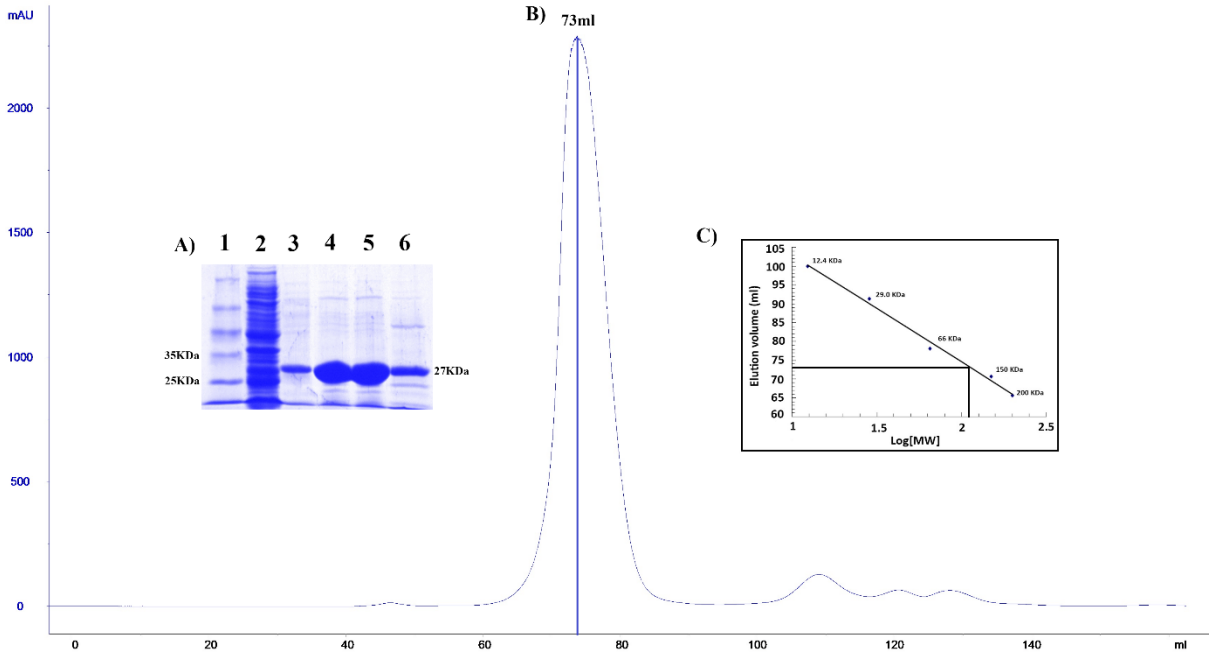

Figure S1 Gel filtration profile **(A)** SDS-PAGE showing fraction purified by gel filtration. The proteins were separated on 12.5 % SDS-PAGE and stained with Coomassie Brilliant Blue. Lane M shows the molecular markers; lane 1 is flow-through while lanes 2, 3, 4 and 5 are fraction from the Ni^{+} affinity purification. **(B)** BaSurE is a tetramer (~108kDa) in solution according to size-exclusion chromatography. The protein was collected after being passed through a HiLoad 16/60 Superdex 200 column. The elution volume (73 ml) and elution pattern of the protein are displayed. **(C)** The monomeric form of BaSurE as shown on SDS-PAGE has a molecular weight of about ~27kDa.

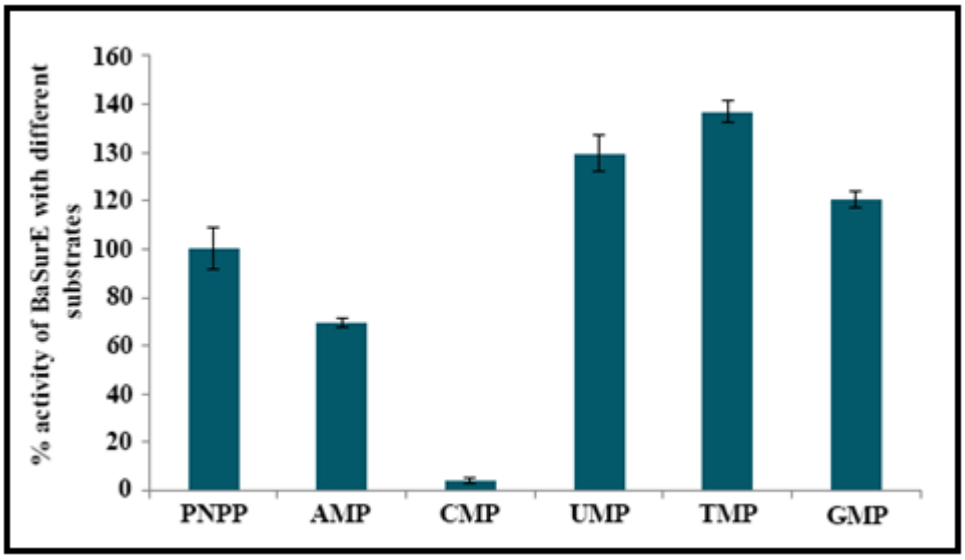

Figure S2 Activity of BaSurE with different substrates as a percentage of the activity with PNPP. The phosphatase activity was found to be maximum with TMP followed by UMP, GMP, AMP and CMP.

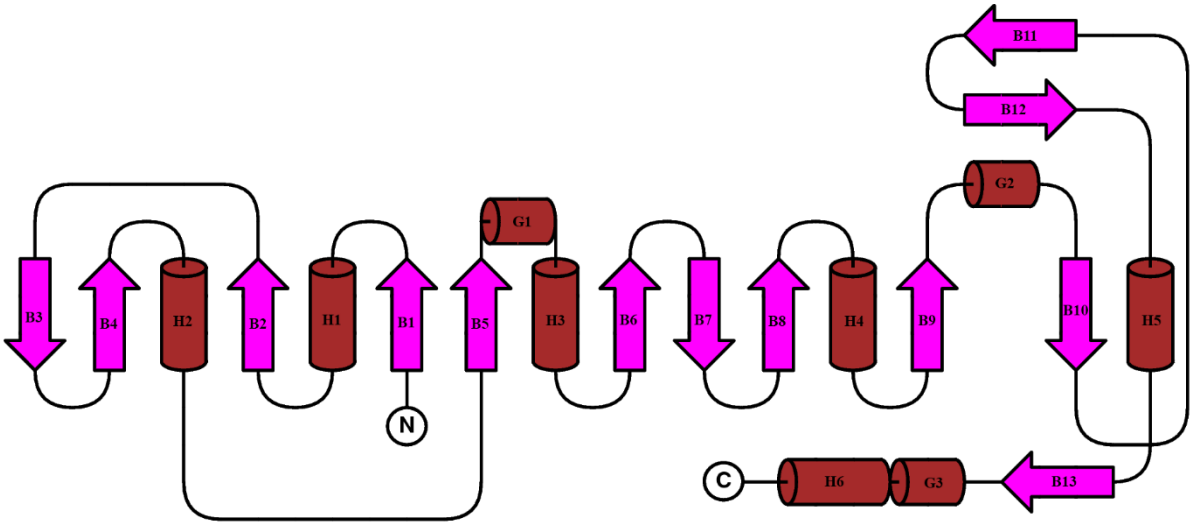

Figure S3 Topology of the secondary structural elements of BaSurE. The N-terminal domain forms an approximate α + ß fold, while the C-terminal domain belongs to the α/ß class. Pink arrows represent ß strands, brown cylinders represent α helices and short brown cylinders labelled with a "G" are 3_{10} helices. The topology diagram was prepared using TopDraw (Bond, 2003).

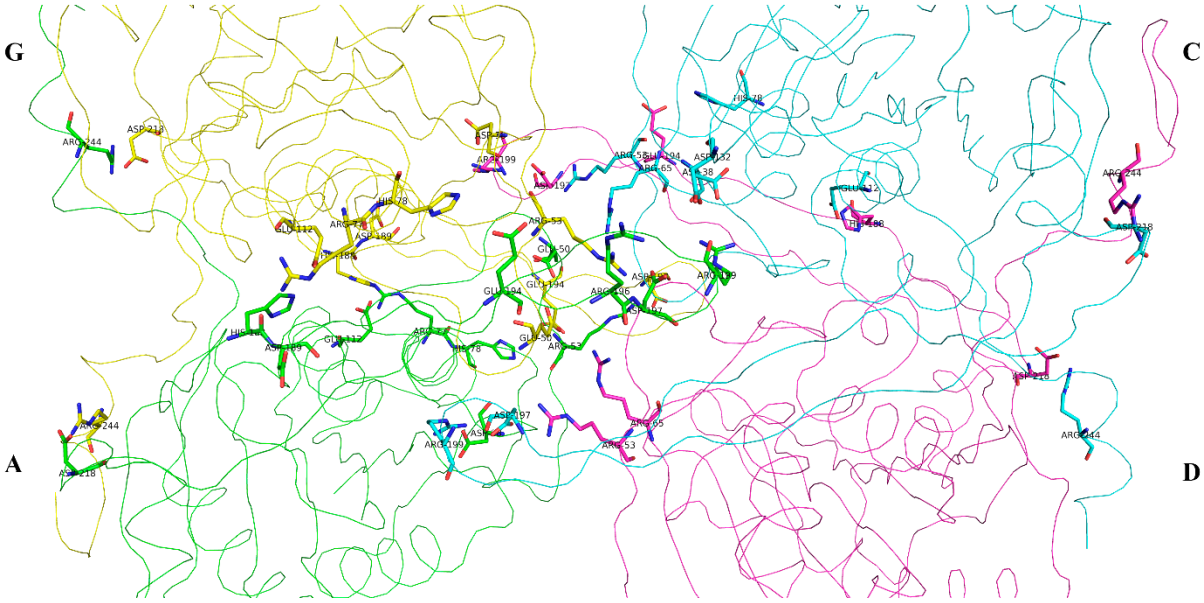

Figure S4 Stabilizing ionic interactions. Schematic representations of important inter subunit ionic interactions between various amino acid residues of BaSurE.

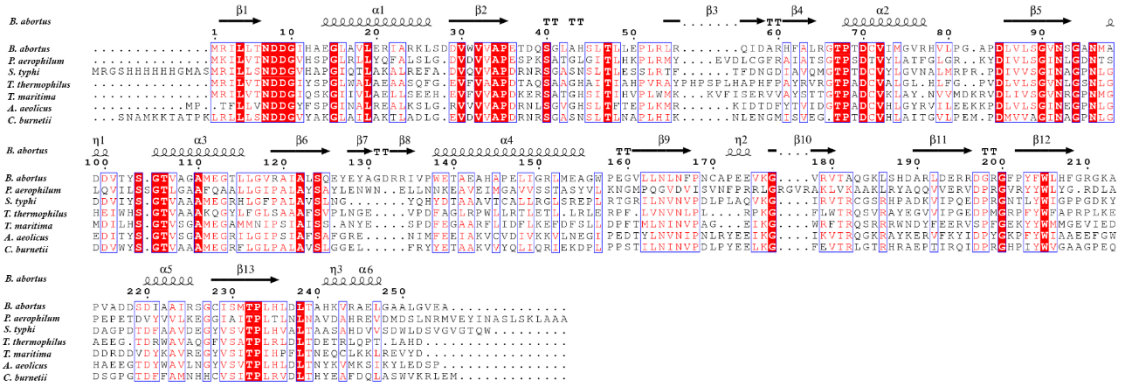

Figure S5 Multiple sequence alignment. Multiple sequence alignment of BaSurE with other members of the SurE family taken from the PDB. The alignment was generated by ESPript (Gouet *et al.*, 2003) with clustalW (McWilliam *et al.*, 2013). Secondary structural elements of BaSurE as determined by "Defined Secondary Structure Prediction" (DSSP) are shown above the sequences (α-helices, ß-strands, η-3_{10} helices and TT- ß turn). All members of this superfamily share a similar core structure and conserved residues essential for metal binding and substrate hydrolysis, in particular NDD just following beta strand 1. (red: totally conserved and pink: partially conserved).

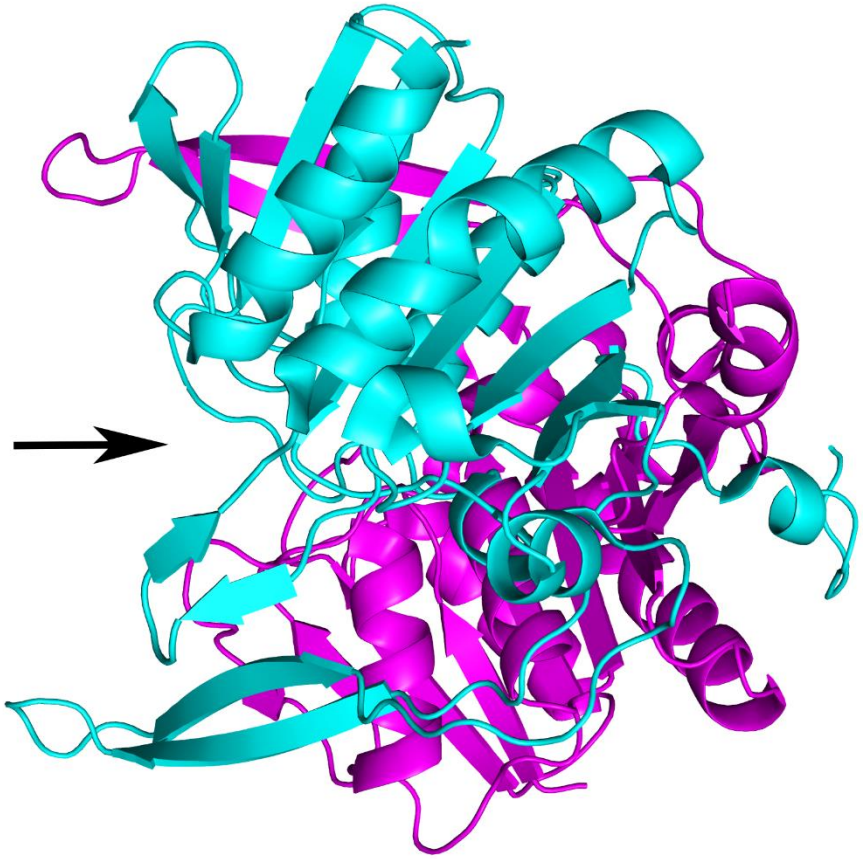

Figure S6 Active site. View of the dimeric portion of the structure rotated by an angle of negative 90^0 about the vertical axis of Figure 2C. The arrow points towards the active site area of the dimeric interface.

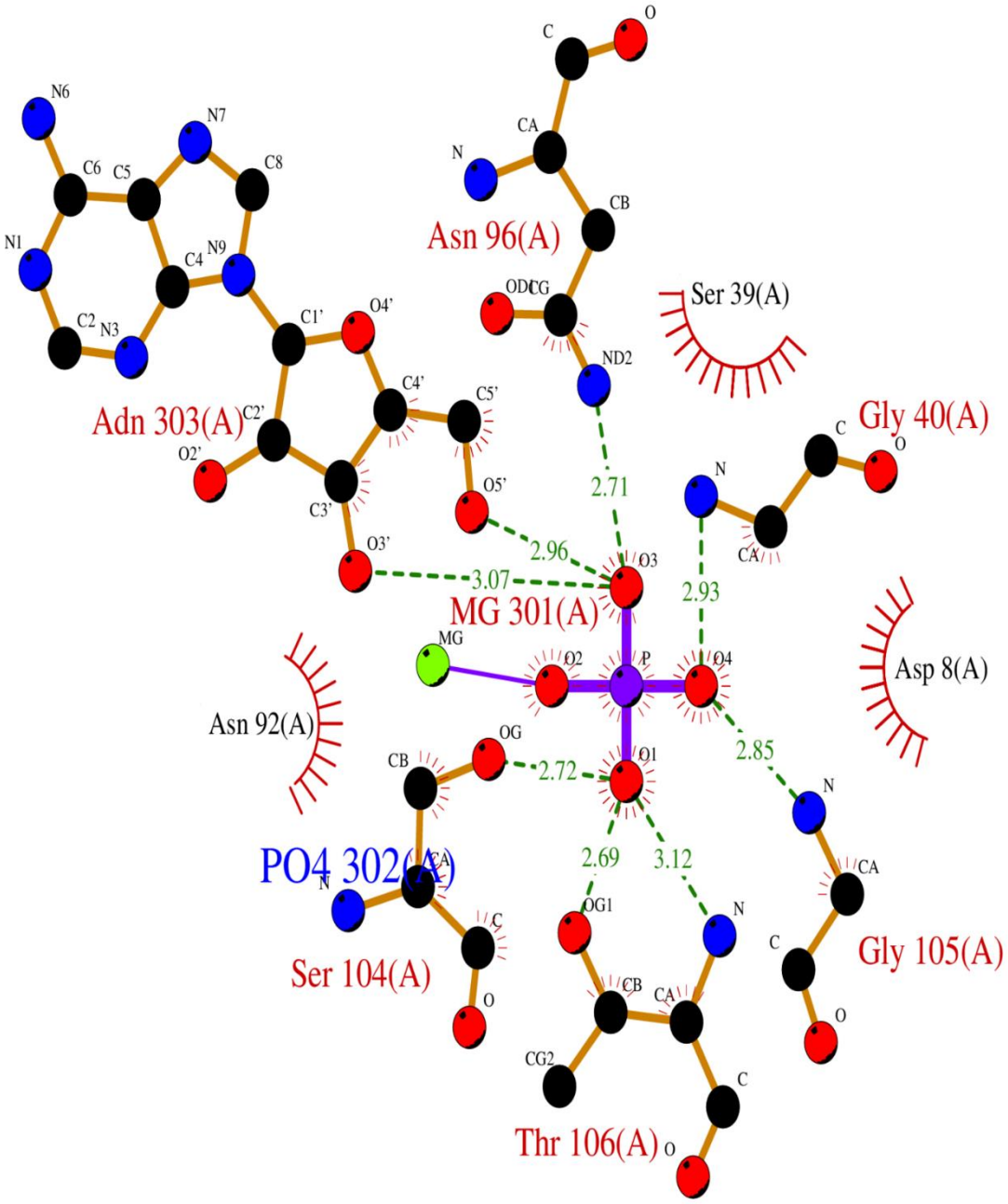

Figure S7 Ligplot interaction of PO_4^{3-} in the crystal structure of stationary phase survival protein from *S. typhimurium*

Table S1 Intermolecular ionic interactions within 6 Angstroms as determined by the PIC server (Tina *et al.*, 2007)

Position	Residue	Chain	Position	Residue	Chain
38	ASP	A	199	ARG	C
38	ASP	D	199	ARG	G
50	GLU	A	65	ARG	C
50	GLU	D	65	ARG	G
53	ARG	A	197	ASP	G
53	ARG	D	197	ASP	C
65	ARG	D	50	GLU	G
77	ARG	A	189	ASP	G
78	HIS	A	194	GLU	G
78	HIS	D	194	GLU	C
112	GLU	A	188	HIS	G
132	ASP	D	196	ARG	G
188	HIS	A	112	GLU	G
188	HIS	D	112	GLU	C
189	ASP	A	77	ARG	G
189	ASP	D	77	ARG	C
194	GLU	A	78	HIS	G
194	GLU	D	78	HIS	C
196	ARG	A	132	ASP	C
197	ASP	A	53	ARG	G
197	ASP	D	53	ARG	C
199	ARG	A	38	ASP	C
199	ARG	D	38	ASP	G
218	ASP	A	244	ARG	G
218	ASP	D	244	ARG	C
244	ARG	A	218	ASP	G
244	ARG	D	218	ASP	C

Table S2 Area and volume of the active site of respective SurE homologues.

Area and volume of the active site were calculated using CASTp (Dundas *et al.*, 2006). The numbers are rounded to the nearest 10th of the total value.

SurE homologues	**Area of the active site**	**Volume of the active site**
4ZG5	660Å^2	1380Å^3
1L5X	1770Å^2	3280Å^3
2V4O	580Å^2	1050Å^3
3TY2	500Å^2	990Å^3
2WQK	2110Å^2	3700Å^3
2E6C	1410Å^2	3060Å^3