



STRUCTURAL
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Supporting information for article:

Crystal structure of bacteriophage T4 Spackle as determined by native SAD phasing

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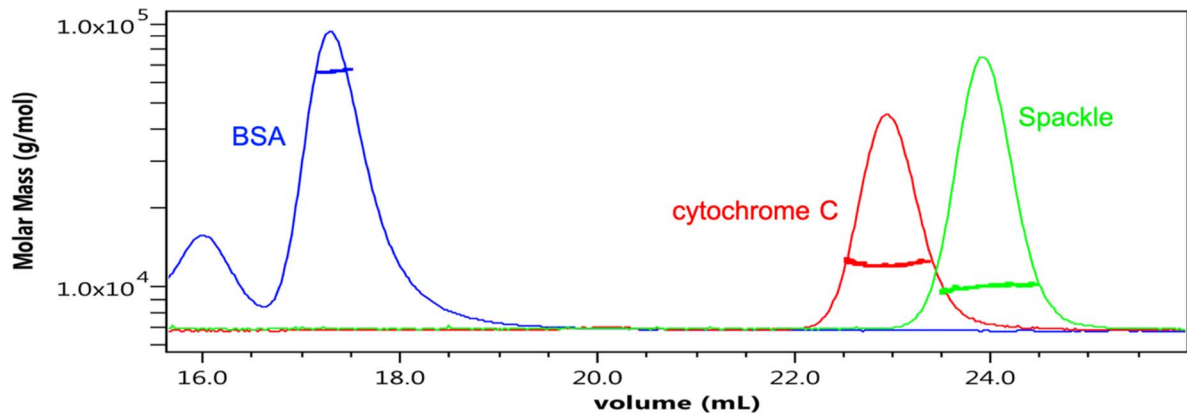


Figure S1 Molar mass distribution plot from the SEC-MALS experiment. Solid lines: Light scattering intensity in arbitrary units; Dots: Weight average molecular masses (Mw) measured across the eluting peaks. Results collected for two protein standards: BSA, 66 kDa (blue) and cytochrome C, 12.3 kDa (red) are overlaid on the Spackle (green) traces.

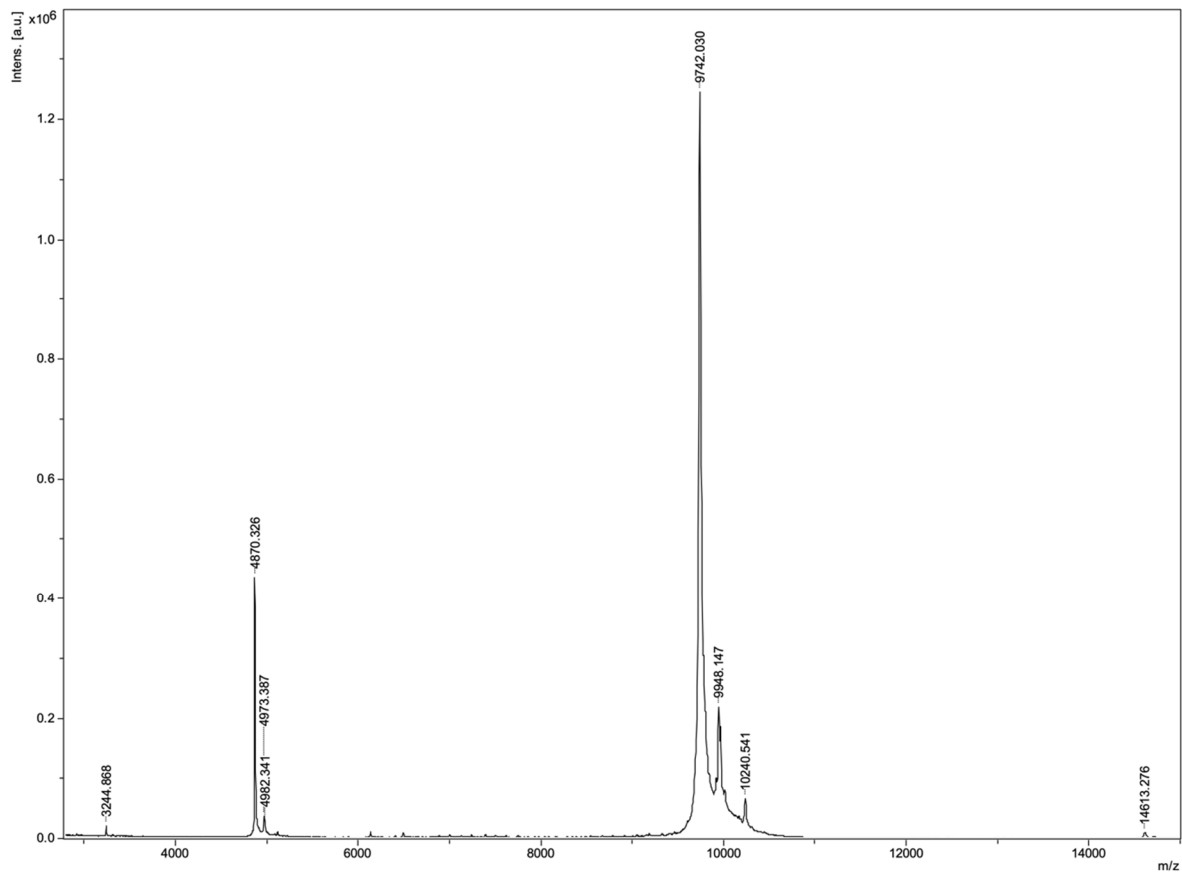


Figure S2 MALDI-TOF mass-spectrum for the purified T4 Spackle protein. The theoretical mass of Spackle with the C-terminal His-tag used in this study is 9,742.9 Da.

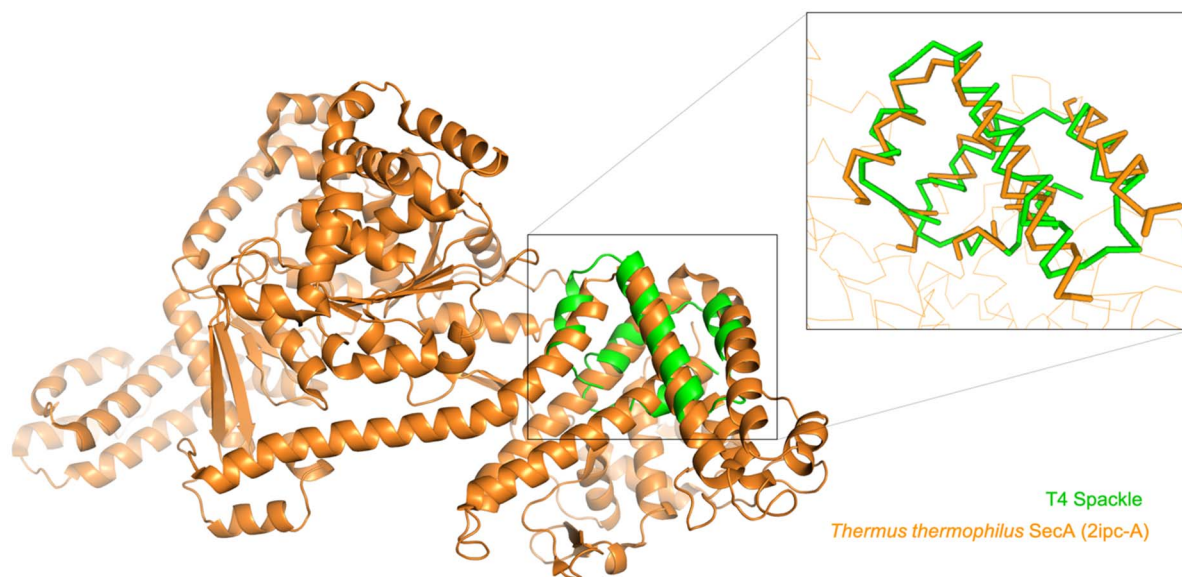


Figure S3 Superposition of T4 Spackle (green) on *Thermus thermophilus* SecA (orange), the top hit obtained in the DALI search (see Supplementary Table S1).

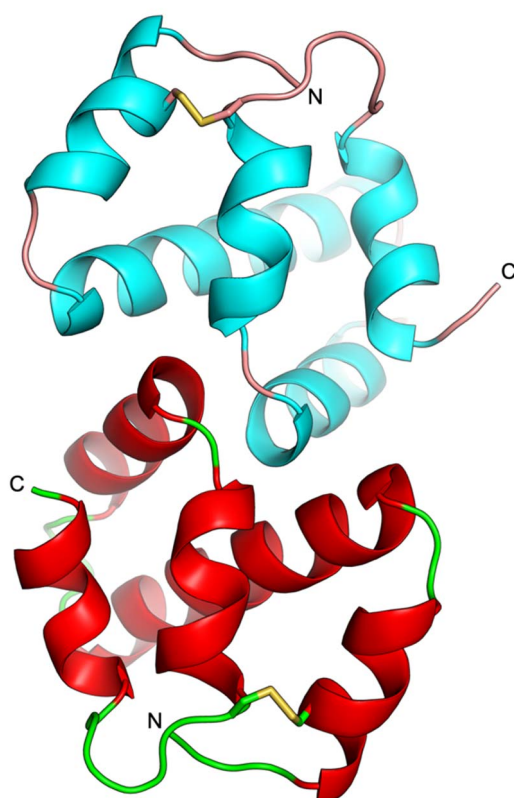


Figure S4 A head-to-head homodimer of Spackle as observed in the asymmetric unit of the crystal. The N and C-terminus of each molecule is labeled.

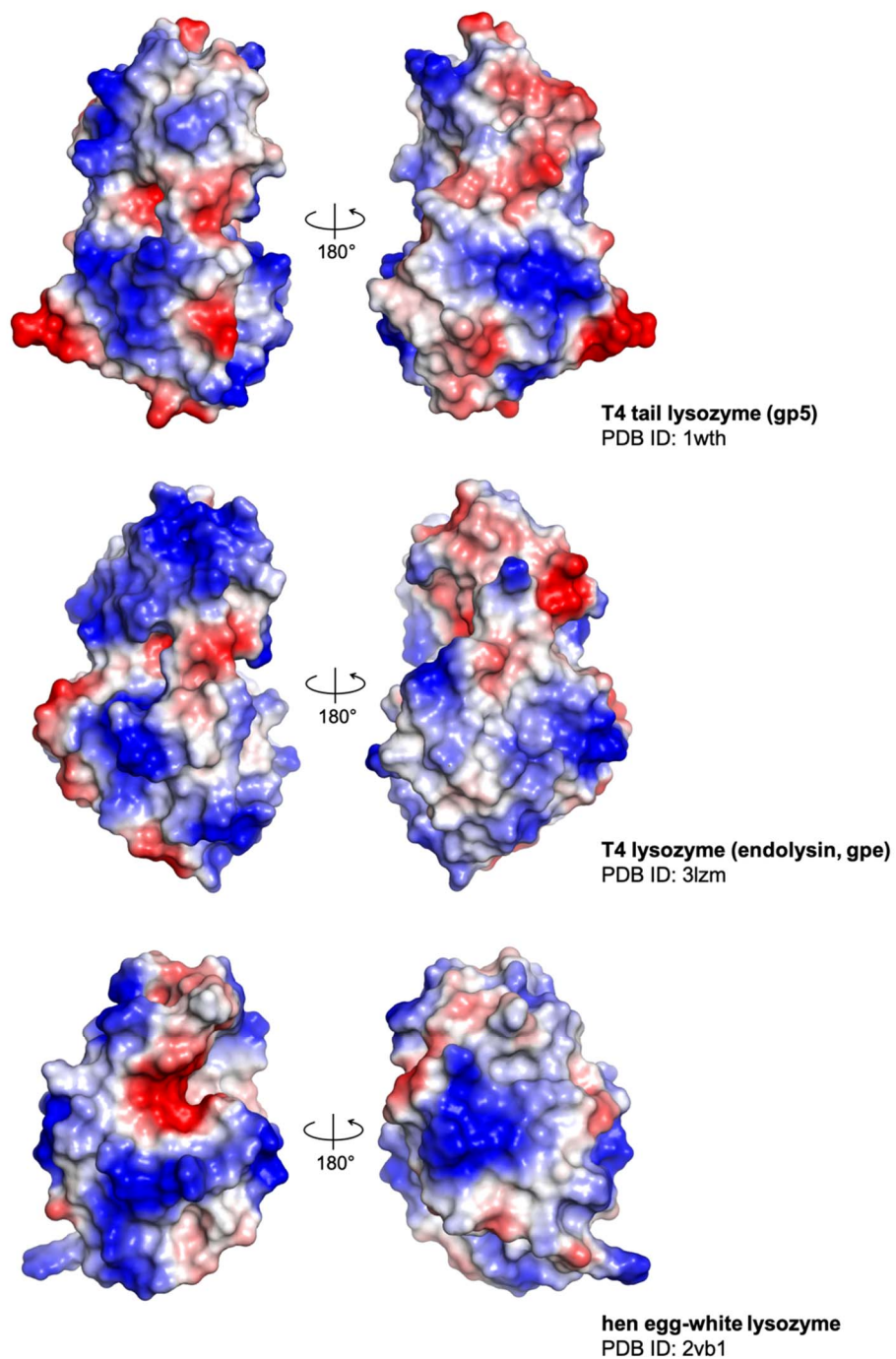


Figure S5 Surface potentials of the T4 and hen egg-white lysozyme proteins (blue: positive, red: negative). Qualitative electrostatic representations were generated using PyMOL.

Table S1 Structural neighbours for Spackle identified by the Dali server (Z score 3.0 or higher)

No:	Chain	Z	rmsd	lali	nres	%id	PDB	Description
1:	2ipc-A	5.1	2.8	68	939	9		MOLECULE: PREPROTEIN TRANSLOCASE SECA SUBUNIT;
2:	5y6o-D	4.1	3.0	57	108	12		MOLECULE: DEATH DOMAIN-ASSOCIATED PROTEIN
6, TRANSCRIPTIONAL								
3:	6hpn-A	4.1	3.2	58	212	10		MOLECULE: ANTIGEN, P35;
4:	2qq8-A	3.8	3.0	63	288	13		MOLECULE: TBC1 DOMAIN FAMILY MEMBER 14;
5:	2lrm-A	3.7	2.8	58	84	16		MOLECULE: UNCHARACTERIZED PROTEIN YMGD;
6:	2o7g-A	3.5	3.0	56	88	11		MOLECULE: PROBABLE RNA POLYMERASE SIGMA-C FACTOR;
7:	6cgh-A	3.5	2.9	56	89	5		MOLECULE: DNAJ HOMOLOG SUBFAMILY C MEMBER 2;
8:	6rf0-C	3.5	3.4	52	275	2		MOLECULE: SODIUM PUMPING RHODOPSIN;
9:	2ff1-A	3.4	4.3	69	732	10		MOLECULE: DICER;
10:	5xtc-p	3.4	2.6	50	172	0		MOLECULE: NADH DEHYDROGENASE [UBIQUINONE] IRON-SULFUR PROTE
11:	2lwx-A	3.3	2.5	54	88	11		MOLECULE: ZUOTIN;
12:	3n6s-A	3.3	3.9	53	344	15		MOLECULE: TRANSCRIPTION TERMINATION FACTOR,
MITOCHONDRIAL;								
13:	6dgc-A	3.3	2.8	43	147	9		MOLECULE: ISC1926 TNPA C-TERMINAL CATALYTIC DOMAIN;
14:	6ql-d-N	3.3	3.0	50	371	6		MOLECULE: INNER KINETOCHORE SUBUNIT MIF2;
15:	2juw-A	3.3	3.2	48	80	10		MOLECULE: UPF0352 PROTEIN SO_2176;
16:	6181-A	3.2	2.5	45	96	4		MOLECULE: GAMMA-TUBULIN COMPLEX COMPONENT 5;
17:	3b42-B	3.2	4.1	44	129	7		MOLECULE: METHYL-ACCEPTING CHEMOTAXIS PROTEIN,
PUTATIVE;								
18:	6ep3-B	3.2	3.5	53	218	9		MOLECULE: LMO0651 PROTEIN;
19:	5xo7-F	3.2	3.3	59	264	10		MOLECULE: LACTONASE FOR PROTEIN;
20:	5xmw-A	3.2	3.3	56	270	9		MOLECULE: ZEARALENONE LACTONASE;
21:	2jppq-A	3.2	3.0	48	83	4		MOLECULE: UPF0352 PROTEIN VP2129;
22:	617r-A	3.2	2.0	43	105	5		MOLECULE: PUTATIVE SPINDLE POLE BODY COMPONENT ALP6
PROTEIN								
23:	4v2o-B	3.2	3.3	56	81	5		MOLECULE: SAPOSIN-B;
24:	6hmj-A	3.2	3.4	54	359	11		MOLECULE: PUTATIVE PAS/PAC SENSOR PROTEIN;
25:	2o31-A	3.2	2.4	47	83	13		MOLECULE: HYPOTHETICAL PROTEIN;
26:	lyz6-A	3.2	3.5	53	261	4		MOLECULE: PROBABLE TRANSLATION INITIATION FACTOR 2
ALPHA								
27:	4xvw-A	3.1	2.6	43	222	7		MOLECULE: DSBA-LIKE PROTEIN;
28:	5zdz-C	3.1	3.2	46	623	11		MOLECULE: MOUSE RAG1;
29:	4v1a-h	3.1	4.1	66	289	8		MOLECULE: MITORIBOSOMAL PROTEIN ML37, MRPL37;
30:	3f46-A	3.1	3.9	47	345	11		MOLECULE: 5,10-METHENYLTETRAHYDROMETHANOPTERIN
HYDROGENASE;								
31:	3nwz-A	3.1	4.7	46	155	17		MOLECULE: BH2602 PROTEIN;
32:	6fxa-A	3.1	2.1	34	35	3		MOLECULE: CI;
33:	5imj-A	3.0	3.3	56	246	9		MOLECULE: CELL DIVISION PROTEIN ZAPD;
34:	4oo8-D	3.0	3.5	54	1163	15		MOLECULE: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1;
35:	4mlp-A	3.0	2.3	49	96	16		MOLECULE: COPPER-SENSITIVE OPERON REPRESSOR (CSOR);
36:	5vvr-B	3.0	7.2	44	1207	5		MOLECULE: DNA-DIRECTED RNA POLYMERASE II SUBUNIT
RPB1;								
37:	5b16-A	3.0	3.2	62	722	3		MOLECULE: RIBONUCLEASE 3, DROSHA, RIBONUCLEASE
3, DROSHA, RIBON								
38:	4gxb-A	3.0	3.6	56	263	4		MOLECULE: SORTING NEXIN-17;
39:	5j5u-B	3.0	3.1	52	452	6		MOLECULE: RAGE/SUSD DOMAIN PROTEIN;
40:	6qph-F	3.0	3.5	51	163	6		MOLECULE: CHLOROPHYLL A-B BINDING PROTEIN,
CHLOROPLASTIC;								