

Supporting Information

Crystal structure of the *Shigella flexneri* SF173 reveals a dimeric helical bundle conformation

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Table S1. Summary of data collection and refinement statistics.

	Native SF173 [12]	Sel-Met SF173
Data collection		
Beamline	PAL 5C SBII	PAL 7A SBI
Wavelength (Å)	1.00000	0.97935
Temperature (K)	100	100
Detector	ADSC Q315r	ADSC Q270
Rotation range per image (°)	1	1
Total rotation range	300	400
Exposure time per image (s)	1	0.5
Space group	I432	I23
Unit-cell parameters (Å)	110.245, 110.245, 110.245	110.310, 110.310, 110.310
Unit-cell parameters (°)	90, 90, 90	90, 90, 90
Mosaicity	0.487	0.229
Resolution range	50.00–1.47 (1.50–1.47)	50.00–1.76(1.79–1.76)
Total No. of reflections	230509	797330
No. of unique reflections	19783	8814(853)
Completeness (%)	96.8 (87.5)	100.0 (100.0)
Multiplicity	5.8 (5.2)	3.6 (3.7)
<I/σ(I)>	49.7 (3.2)	29.1 (13.1)
R _{merge} (%)	6.4 (65.1)	5.1 (10.3)

Overall B factor from Wilson plot	18.0	12.5
CC1/2	99.6 (76.6)	99.8 (99.0)
Refinement		
Resolution	27.56–1.47 (1.52–1.47)	29.48–2.40 (2.49–2.40)
No. reflection	35662 (3408)	8814 (853)
R _{work} (%)	0.2069 (0.2661)	0.2223 (0.2257)
R _{free} (%)	0.2192 (0.3115)	0.2687 (0.3155)
No. of atoms		
Total	1296	1137
Protein	1080	1062
Water	216	72
Ligands	-	3
B-factor (Å ²)		
Protein	24.50	12.79
Water	37.04	18.08
Ligand	-	82.65
R.m.s.deviation		
Bond lengths (Å)	0.015	0.009
Bond angles (°)	1.52	1.32
Ramachandran plot (%)		
Preferred region	100	99.24
Allowed region	0	0.76
Disallowed region	0	0
PDB code	5H1N	

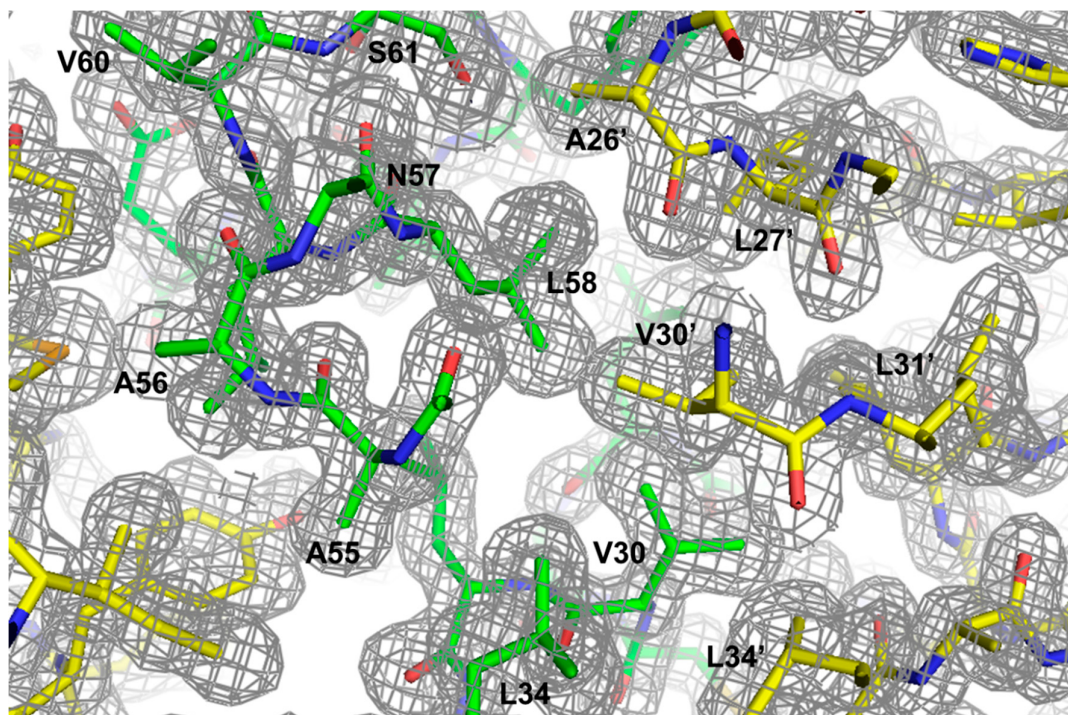


Figure S1. 2F_o-F_c electron density map of SF173 (contoured at 1.0σ). Structural model of SF173 are depicted by sticks, and chain A and B are colored green and yellow, respectively.

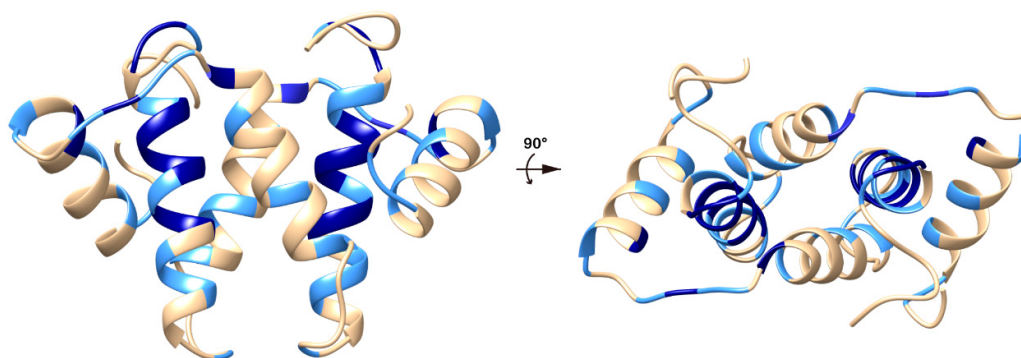


Figure S2. Positions of conserved residues in the SF173 structure. The conserved residues, corresponding to the blue-colored residues in Figure 2a are indicated here

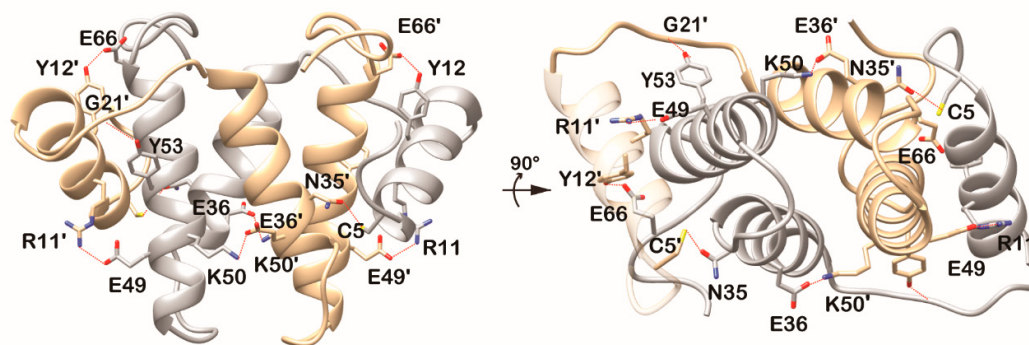


Figure S3. Interchain electrostatic interactions in the SF173 structure. Hydrogen bonds and salt bridges are represented by red dotted lines. Interacting sidechains are shown in a stick presentation with atom-dependent coloring (blue, red, and yellow for N, O, and S, respectively).

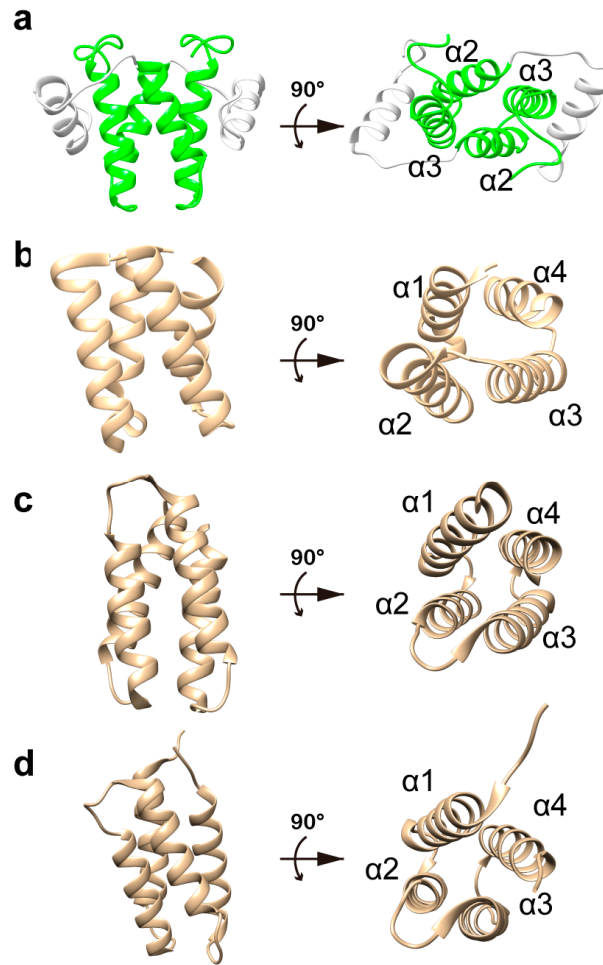


Figure S4. Structural homology of SF173 (A) to UPF0147-family proteins (B, PDB ID 2FU2; C, 2QSB; D, 2QZG). The central interchain four-helix bundle in the SF173 structure is colored green.