Supplementary Material

Crystal structure of the CFA/III major pilin subunit CofA from human enterotoxigenic *Escherichia coli* determined at 0.90 Å by sulfur-SAD phasing

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Table S1 Summary of SAD data collection statistics for each wavelength datasets.

Data collection statistics of each wavelength

Wavelength (Å)	1.3000	1.5000	1.7000
Beamline	SPring-8 BL38B1	SPring-8 BL38B1	SPring-8 BL38B1
Detector	ADSC Quantum 315	ADSC Quantum 315	ADSC Quantum 315r
Exposure time (s)	2.0	3.0	13.5
Crystal to camera distance (mm)	75.0	75.0	75.0
Oscillation angle (º)	1.0	1.0	1.0
Total oscillation range (º)	720	720	720
Resolution (Å)	40.62–1.22 (1.25–1.22)	47.64–1.38 (1.42–1.38)	47.85–1.60 (1.69–1.60)
Space group	$P2_1$	$P2_1$	$P2_1$
Unit-cell parameters (Å, º)	a = 33.87, b = 47.83, c = 42.58, β = 107.44	a = 33.82, b = 47.64, c = 42.53, β = 107.57	a = 33.82, b = 47.85, c = 42.59, β = 107.39
No. of unique reflections	72665	51931	33046
R_{merge} †	0.049 (0.231)	0.041 (0.226)	0.052 (0.098)
Completeness (%)	95.9 (89.5)	99.5 (99.6)	97.6 (97.4)
Wilson B factor	5.8	8.2	12.9
$<I/\sigma(I)>$	28.3 (8.7)	32.1 (6.3)	26.7 (14.4)
Multiplicity	7.1 (6.7)	6.8 (4.7)	6.7 (6.4)
Anomalous signal to noise‡	0.79 (0.74)	1.06 (0.79)	0.86 (0.60)

Values in parentheses are for the highest resolution shell.

†$R_{merge} = \sum_{hkl}\sum_i |Ii(hkl) - \langle I(hkl)\rangle| / \sum_{hkl}\sum_i Ii|Ii(hkl)|$, where I$i$($hkl$) is the observed intensity of the ith measurement of reflection hkl, and (I(hkl)) is the mean intensity of reflection hkl calculated after scaling. ‡ Anomalous signal to noise, $<F^{\pm}>/<\sigma(F)>$, is the ratio of the anomalous differences to the noise. ¶ R_{free} was calculated for a random set of 5% of reflections that were not used in the refinement.

Table S2 Data collection statistics of high-resolution (0.90 Å) dataset in each resolution shell.

Resolution shell	No. of reflections			Completeness (%)	R_{merge} †	<*I*/σ (*I*) >
	Observed	Unique	Possible			
30.86–3.50	5742	1641	1690	97.1	0.054	31.7
3.50–3.00	3485	966	979	98.7	0.052	31.9
3.00–2.60	5111	1376	1399	98.4	0.046	32.1
2.30–2.30	6547	1739	1783	97.5	0.042	32.0
2.30–2.00	10978	2919	2976	98.1	0.038	31.6
2.00–1.70	20202	5354	5487	97.6	0.036	29.7
1.70–1.50	23479	6307	6464	97.6	0.038	27.0
1.50–1.30	38349	10706	11024	97.1	0.045	23.5
1.30–1.00	131036	36360	37759	96.3	0.058	17.7
1.00–0.95	39102	10968	11497	95.4	0.117	10.0
0.95–0.90	47647	13473	14193	94.9	0.170	7.1
Total	331678	91809	95251	96.4	0.050	18.6

†$R_{merge} = \sum_{hkl}\sum_i |Ii(hkl) - \langle I(hkl)\rangle| / \sum_{hkl}\sum_i Ii|Ii(hkl)|$, where *Ii*(*hkl*) is the observed intensity of the *i*th measurement of reflection *hkl*, and (*I*(*hkl*)) is the mean intensity of reflection *hkl* calculated after scaling.

Figure S1 Amount of anomalous signal in the diffraction data. Anomalous signal is plotted as a function of resolution for three SAD datasets (wavelengths of 1.3–1.7 Å).

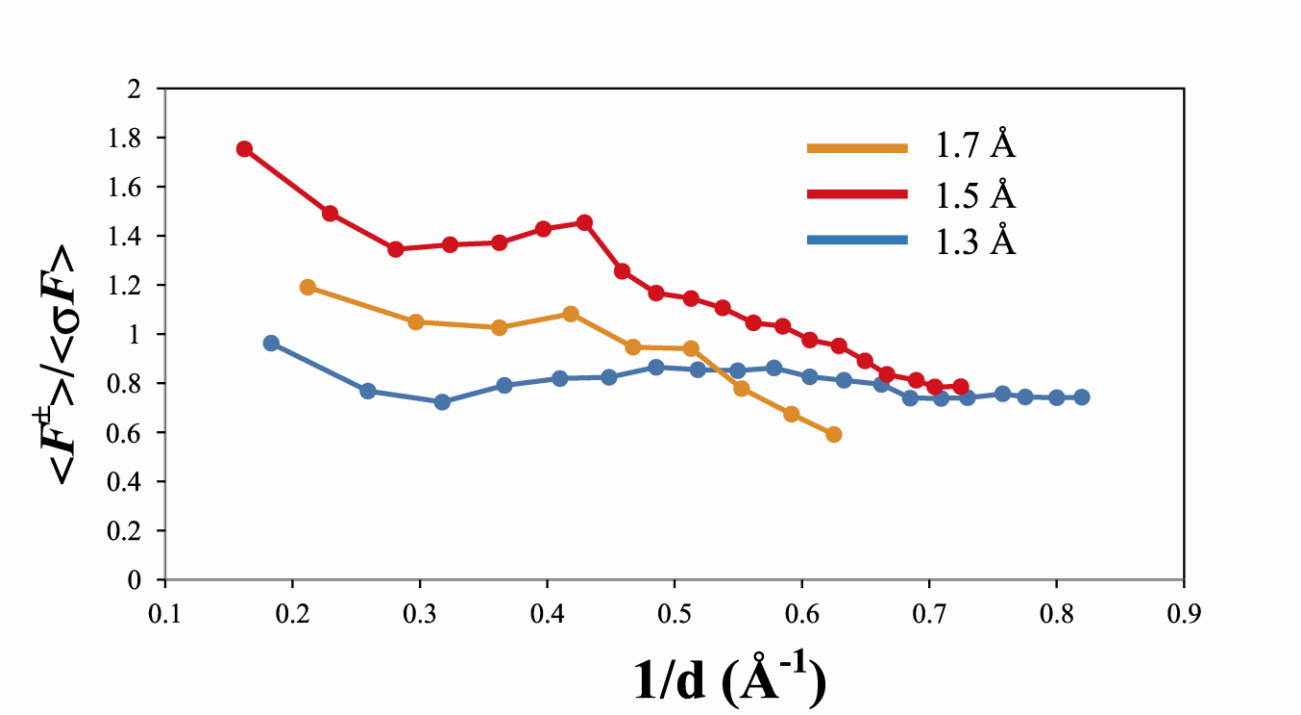

Figure S2 Histograms of the calculated distances of interatomic contacts between subunits in the initial (A) and refined (B) filament models of CofA. In the histograms, the number of contacts within the van der Waals (vdW) interaction distance (defined by the sum of vdW radii of each atom - 0.4) is shown in red.