Supporting Information

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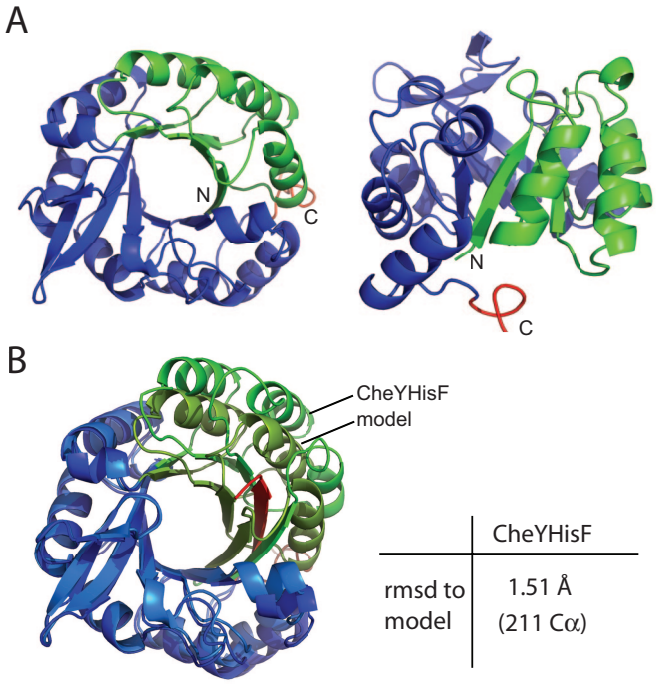

Fig. S1. Model of the originally expected $(\beta\alpha)_8$-barrel structure of CheYHisF. (*A*) Ribbon diagram of the model top and side view. The model was generated with the program Modeller (1), using an alignment of CheY and HisF from *T. maritima* and the structures with the Protein Data Bank identifiers 1TMY (CheY) and 1THF (HisF). The part originating from CheY is shown in green and the part originating from HisF is shown in blue, the residues forming the new β-strand in the crystal structure are shown in red. (*B*) Comparison of the model (lighter colors) with the x-ray structure (darker colors). The two structures superimpose with an rmsd of 1.51 Å over 211 Cα-atoms. The superposition was generated with the program STAMP (2).

1. Sali A, Blundell TL (1993) Comparative protein modeling by satisfaction of spatial restraints. *J Mol Biol* 234:779–815.
2. Russell RB, Barton GJ (1992) Multiple protein sequence alignment from tertiary structure comparison: assignment of global and residue confidence levels. *Proteins* 14:309–323.

Table S1. Secondary structural content calculated from FT-IR data, using multivariant pattern recognition (1) and from the DSSP patterns of the crystal structures (2)

Protein	Calculated from IR-data	Deduced from x-ray structure
CheYHisF		
α-Helix	29.2%	37.6% (40.1%)
β-Sheet	23.8%	24.5% (23.2%)
HisF		
α-Helix	38.0%	36.8%
β-Sheet	20.4%	24.1%
CheY		
α-Helix	51.4%	48.7%
β-Sheet	22.0%	21.0%

The CheYHisF values in brackets are the sum of the DSSP patterns of the parental fragments.

1. Fabian H, Schultz CP (2000) in *Encyclopedia of Anal Chem*, ed Meyers RA (Wiley, Chichester, UK), pp 5799.
2. Kabsch W, Sander C (1983) Dictionary of protein secondary structure; pattern recognition of hydrogen-bonded and geometrical features. Biopolymers 22, 2577–637.

Table S2. Summary of data collection and refinement statistics

Data collection	
Wavelength, Å	1.071
Space group	$P4_12_12$
Resolution, Å	40–3.1 (3.27–3.1)
Unique reflections	8,681 (1,386)
Redundancy	13.4 (13.6)
Completeness, %	92.3 (94.8)
R_{merge}, %	9.3 (54.9)
$I/\sigma(I)$	18.5 (2.4)
Wilson B factor	95.9
Refinement statistics	
Space group	$P4_12_12$
Resolution, Å	30–3.1 (3.18–3.1)
R_{cryst}, %	0.22 (0.35)
R_{free}, %	0.25 (0.37)
Nonhydrogen atoms	1,854
Waters	32
Ligand (sulfate)	2
Mean B-value, Å^2	102
rmsd of bond length, Å^2	0.01
rmsd of angle, °	1.43
Model quality	
Residues in most favored region	200 (86%)
Residues in most allowed region	24 (10.3%)
Residues in outlier region	9 (3.7%)