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Supporting information for article:

Multitasking in the gut: the X-ray structure of the multidomain BbgIII from *Bifidobacterium bifidum* offers possible explanations for its alternative functions

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(a) (b)

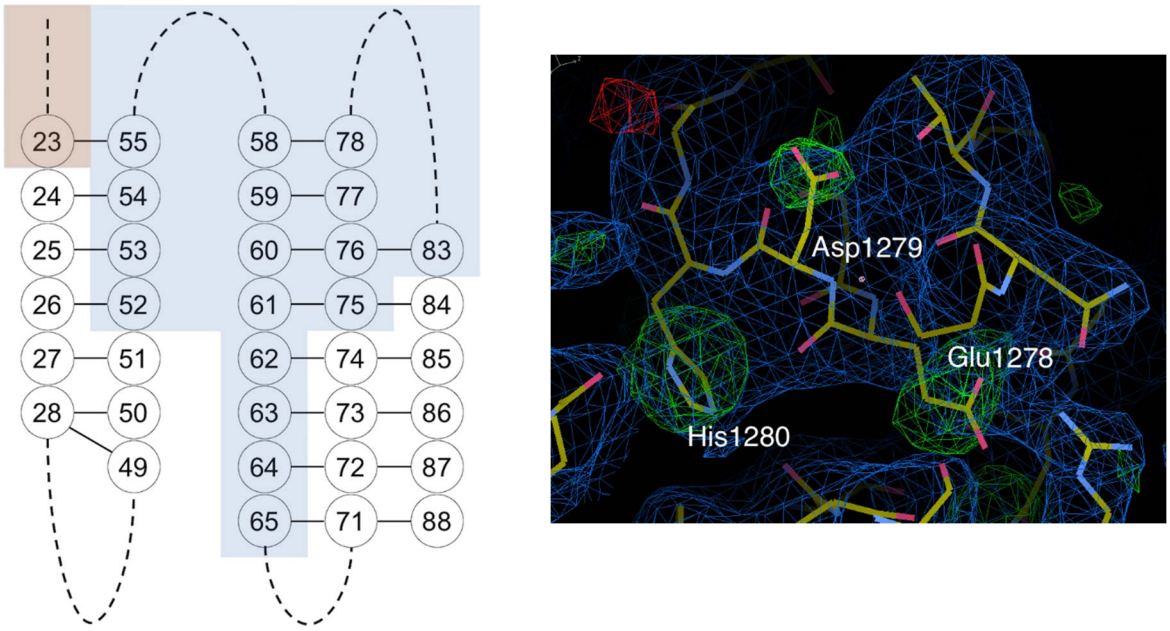

Figure S1 Residue number assignment in two disconnected fragments using contact predictions. (a) A scheme of the secondary structure for residues 1223-1288 derived from the contact map shown in Fig. 5 with two first digits in the residue numbers dropped. Residues up to and including Ser 1223 have been previously assigned residue number and type (orange background) while two disconnected fragments were initially modeled as polyalanine chains (blue background). The contact 1223-1255 led to numbering of residues 1252-1265, then the residues 1275-1278 were identified based on their contacts with residues 1258-1261, then numbering was extended to residue 1283, and finally the contact 1276-1283 observed in both renumbered model and contact map confirmed the consistency of renumbering. (b) Loop 1277-1281 after renumbering and addition of side chains (and before the next round of refinement) showed a good match with weighted 2Fo–Fc (blue) and Fo–Fc (green) electron density maps from the initial model where this loop was a part of a polyalanine chain. Figure 3b was generated by Coot.(Emsley *et al.*, 2010)

(a) (b)

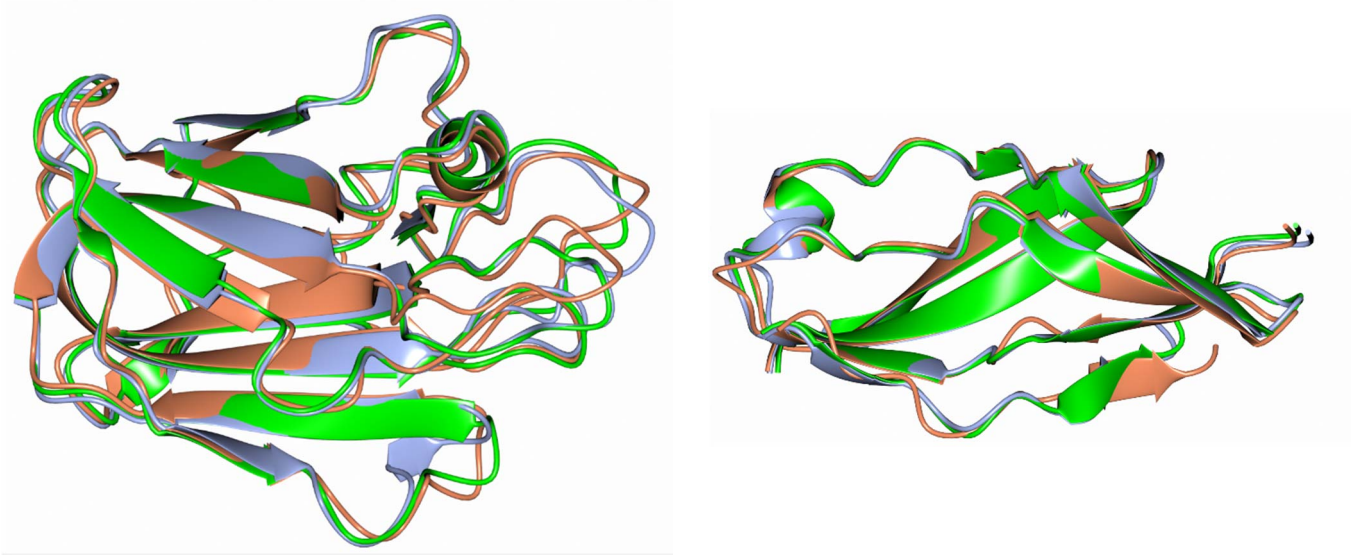

Figure S2 Superposition of the best rank AI models on CBM32 and Big_4-1 domains of the X-ray structure, chain A. The X-ray structure is in ice-blue, AF2 model is in green and ROseTTAFold model is in coral. The figure was prepared by CCP4mg (McNicholas *et al.*, 2011), and structure superposition was carried out using SSM (Krissinel, 2012) as incorporated in CCP4mg.

Table S1 Superposition of the AI models, ordered by rank, on the chain A of the X-ray structure, by different methods and fragments.

Column sub-headers indicate the fragments of chain A (full length or reference name used in the main text), corresponding residue range, and atoms (Cα or all) used in superposition. Values in brackets for SSM superposition show the number of residues automatically selected for alignment and used in r.m.s.d. calculations.

AI models	r.m.s.d., Å					
	SSM[1)]	LSQKab[2)]				
	Full length 1-1304 Cα	Full length 1-1304 Cα	Core domains 30-878 Cα/All	Big_4-1 886-959 Cα/All	Big_4-2 (first half) 962-1038 Cα/All	CBM32 1044-1210 Cα/All
AF 1	2.66 (1061)	6.13	0.38/0.66	0.61/1.26	0.68/0.99	0.84/1.14
AF 2	2.52 (1094)	5.07	0.38/0.71	0.55/1.12	0.61/0.97	0.81/1.20
AF 3	1.50 (1115)	2.36	0.72/1.06	0.54/1.12	0.49/0.90	1.00/1.33
AF 4	1.56 (989)	12.19	0.78/1.07	0.64/1.19	0.91/1.18	0.77/1.14
AF 5	2.63 (1062)	4.53	0.77/1.08	0.54/1.11	0.56/0.94	1.20/1.55
RF 1	1.87 (867)	10.93	1.21/1.76	0.77/1.52	0.92/1.41	1.40/1.87
RF 2	1.64 (850)	13.47	1.18/1.76	0.69/1.56	0.93/1.52	1.33/1.97
RF 3	1.46 (866)	18.68	1.23/1.76	0.91/1.55	0.92/1.42	1.27/1.93
RF 4	1.26 (835)	24.36	1.18/1.81	1.01/2.22	0.92/1.48	1.29/1.79
RF 5	1.25 (831)	30.54	1.19/1.77	0.85/1.65	1.05/1.57	1.34/1.93

[1)] SSM (Krissinel, 2012), incorporated in Coot (Emsley *et al.*, 2010)

[2)] LSQKab (Kabsch, 1976), incorporated in Coot (Emsley *et al.*, 2010)

Emsley, P., Lohkamp, B., Scott, W. G. & Cowtan, K. (2010). *Acta Crystallogr D Biol Crystallogr* **66**, 486-501.

Kabsch, W. (1976). *Acta Crystallographica Section A* **32**, 922-923.

Krissinel, E. (2012). *J Mol Biochem* **1**, 76-85.

McNicholas, S., Potterton, E., Wilson, K. S. & Noble, M. E. (2011). *Acta Crystallogr D Biol Crystallogr* **67**, 386-394.