Daniel Schlatter, Simon Brack, David W. Banner, Sarah Batey, Jörg Benz, Julian Bertschinger, et al. Generation, characterization and structural data of chymase-binding proteins based on the human Fyn kinase SH3 domain. mAbs 2012; 4(4);
http://dx.doi.org/10.4161/mabs.20452
http://www.landesbioscience.com/journals/mabs/article/20452/

Supplementary Materials and Methods

Dataset	1	2	3	4	5	6
PDB accession code	4afq	4afs	4afu	4afz	4ag1	4ag2
Fynomer	4C_A4	4C_A4	4C_A4	4C_E4	4C_E4	3C_B5
Data collection Resolution range (Å)^1	50.0-1.51 (1.61-1.51)	50.0-1.75 (1.84-1.75)	50.0-1.82 (1.91-1.82)	50.0-2.19 (2.28-2.19)	50.0-1.40 (1.49-1.40)	50.0-1.78 (1.87-1.78)
Space group	$P2_12_12_1$	$P2_12_12$	$P2_12_12_1$	$P2_1$	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions (Å/°)	a=59.63, b=92.79, c=116.26	a=78.58, b=89.07, c=48.49	a=58.99, b=59.06, c=158.1	a=60.27, b=58.34, c=93.03 β=103.8	a=59.00, b=59.85, c=89.71	a=56.94, b=64.12, c=175.0
Unique reflections	101765 (17578)	35077 (4764)	50464 (6690)	32077 (3262)	63158 (10573)	62210 (8333)
# complexes / a.u.	2	1	2	2	1	2
Multiplicity	6.64 (6.50)	6.43 (6.35)	6.13 (5.48)	3.38 (3.16)	6.54 (6.62)	6.19 (5.62)
Completeness (%)	99.9 (99.9)	99.6 (97.5)	99.9 (99.7)	98.9 (92.7)	99.7 (99.5)	99.7 (99.0)
R_{sym} (%)^3	6.55 (71.2)	7.11 (67.3)	8.73 (63.1)	9.62 (69.3)	9.94 (77.1)	9.44 (67.1)
Average I/σ(I)	13.6 (1.6)	10.7 (1.5)	9.7 (1.5)	22.3 (1.5)	10.5 (1.6)	10.9 (1.5)
Wilson B value (Å^2)	27.9	38.5	42.6	48.3	22.4	32.0
Refinement Resolution range (Å)	49.26-1.51 (1.55-1.51)	48.49-1.90 (1.95-1.90)	47.3-1.82 (1.86-1.82)	45.2-2.25 (2.31-2.25)	42.0-1.40 (1.49-1.40)	43.7-1.80 (1.85-1.80)
R_{cryst} (%)^{3,4}	19.0 (36.4)	18.9 (28.9)	19.0 (38.3)	18.1 (32.5)	14.0 (31.4)	18.0 (32.0)
R_{free} (%)^{3,4}	21.5 (39.1)	23.8 (33.3)	22.5 (37.9)	24.1 (43.3)	17.0 (34.9)	21.2 (32.5)
# of residues / waters	622 / 547	311 / 185	622 / 52	620 / 180	310 / 273	620 / 514
rmsd Bonds / Angles (Å/°)	0.012 / 1.38	0.011 / 1.51	0.006 / 1.00	0.011 / 1.42	0.010 / 1.36	0.012 / 1.36
Ramachandran plot (%)^5	96.7 / 2.9 / 0.4	96.5 / 2.8 / 0.7	93.0 / 6.3 / 0.7	97.2 / 2.8 / 0	97.2 / 2.8 / 0	96.7 / 2.9 / 0.4
Mean B value (Å^2)	27.5	39.0	37.5	51.0	19.3	28.5
Chain A (chymase)	25.3	37.5	35.4	30.2^5	18.0	25.2
Chain C (fynomer)	25.4	41.9	45.7	26.6^5	18.9	25.3
Chain B (chymase)	29.7		36.5	31.9^5		29.7
Chain D (fynomer)	27.2		41.5	30.9^5		27.2

Table S1

Data collection, analysis and structure refinement. $^{1)}$ Values in parentheses correspond to the highest resolution shell. $^{2)}$ R-factor definitions as collected in Einspahr, H. M. & Weiss, M. S. (2011). *International Tables for Crystallography Vol. F, Crystallography of Biological Macromolecules, 2nd ed.* 64-74. $^{3)}$ R_{free} is R_{cryst} with 5% of test set structure factors. $^{4)}$ The percentage of amino acid residues in preferred regions, allowed regions and outliers as calculated in Coot (Emsley, P. & Cowtan, K.

(2004). Coot: model-building tools for molecular graphics. *Acta Crystallogr., Sect. D: Biol. Crystallogr.* **D60**, 2126-2132). 5) Without TLS component.

Primer	**Sequence (5'- 3')**
1.ba	GAA AAG TGC CAC CTG ACG TCT AA
14.fo	TTC TCC TTT GTG AAA ACT CAG GTC MNN MNN MNN MNN MNN MNN ATA GTC ATA AAG GGC CAC AAA GAG
16.fo	GGA GCG GGC TTC CCA CCA ATC TCC MNN MNN MNN MNN MNN MNN CAA TAT TTG AAA TTT TTC TCC TTT
67.fo	GGA GCG GGC TTC CCA CCA ATC TCC MNN MNN MNN MNN MNN CAA TAT TTG AAA TTT TTC TCC TTT
68.fo	GGA GCG GGC TTC CCA CCA ATC TCC MNN MNN MNN MNN CAA TAT TTG AAA TTT TTC TCC TTT
13.ba	GAC CTG AGT TTT CAC AAA GGA GAA
15.ba	GGA GAT TGG TGG GAA GCC CGC T
2.fo	CGG TCT GGT TAT AGG TAC ATT GAG C
60.fo	TTC TCC TTT GTG AAA ACT CAG GTC MNN MNN MNN MNN MNN MNN CCG AGC TTC ATA GTC ATA AAG GGC CAC AAA GAG
65 fo	TTC TCC TTT GTG AAA ACT CAG GTC MNN MNN MNN MNN CCG AGC TTC ATA GTC ATA AAG GGC CAC AAA GAG
66.fo	TTC TCC TTT GTG AAA ACT CAG GTC MNN MNN MNN MNN CCG AGC TTC ATA GTC ATA AAG GGC CAC AAA GAG
69.fo	TTT TTC TCC TTT GTG AAA ACT CAG MNN MNN MNN MNN MNN MNN MNN TGC TTC ATA GTC ATA AAG GGC CAC AAA GAG
70.fo	TTT TTC TCC TTT GTG AAA ACT CAG MNN MNN MNN MNN MNN MNN TGC TTC ATA GTC ATA AAG GGC CAC AAA GAG
71.fo	TTT TTC TCC TTT GTG AAA ACT CAG MNN MNN MNN MNN MNN TGC TTC ATA GTC ATA AAG GGC CAC AAA GAG
72.ba	CTG AGT TTT CAC AAA GGA GAA AAA
73.fo	CC AGT TGT CAA GGA GCG GGC TTC CCA MNN MNN TCC TTC CGA GCT GTT CAA TA
33.ba	GCC CGC TCC TTG ACA ACT GGA GAG ACA GGT NNK ATT CCC AGC AAT
20b.ba	CAT GCC ATG GGC GGA GTG ACA CTC TTT GTG GCC CTT TAT
21.fo	TTT TCC TTT TGC GGC CGC CTG GAT AGA GTC AAC TGG AGC CAC ATA

Table S2

Primers used for cloning the naïve Fynomer libraries.