

Supplementary information for:

The N-terminal domain of *Staphylothermus marinus* McrB shares structural homology with PUA-like RNA binding proteins

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Supplementary Tables

Supplementary Table 1. X-ray data collection and refinement statistics for Sm3-180.

Supplementary Table 2. Oligo nucleotide substrates used in filter binding.

Supplementary Figures

Supplementary Figure 1. PUA-like domain topologies.

Supplementary Table 1. X-ray data collection and refinement statistics for Sm3-180.

Data collection	
PDB code	6N0S
X-ray Source	NECAT 24-ID-C
Wavelength (Å)	0.9791
Space group	P4 ₃ 2 ₁ 2
Unit cell	$a = 62.41, b = 62.41, c = 118.63 \text{ \AA}$ $\alpha = 90.00^\circ, \beta = 90.00^\circ, \gamma = 90.00^\circ$
Resolution, Å ^a	55.26 – 1.92 (2.09 – 1.92)
No. measured reflections ^a	1224297 (199786)
No. unique reflections ^a	29031 (8197)
Completeness (%) ^a	99.9 (100.0)
Multiplicity ^a	42.2 (24.4)
R _{merge} ^a	0.111 (1.068)
Mean I/σ _I ^a	19.9 (3.63)
CC _{1/2} ^a	0.999 (0.964)
Refinement	
R _{work} /R _{free}	0.1964 / 0.2356
RMSD	
Bond lengths (Å)	0.013
Bond angles (°)	1.029
Ramachandran plot	
Favored (%)	96.65
Allowed (%)	3.35
Outliers (%)	0.00
Average B-Factor	45.72
Clashscore	4.88
No. Atoms	
Macromolecule	1522
Solvent	94
Sulfate	10

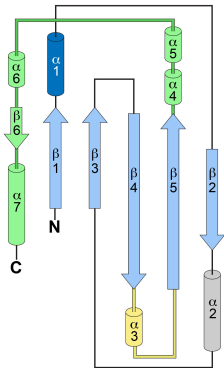
^a Parentheses indicate values for highest resolution shell

Supplementary Table 2. Oligo nucleotide substrates used in binding experiments*.

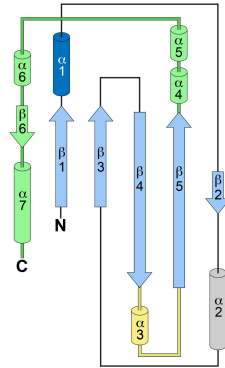
Filter binding substrates	
m ⁶ A ssRNA 7mer	5' -CGG (m ⁶ A) CUG-3'
nmA ssRNA 7mer	5' -CGGACUG-3'
m ⁶ A DNA US	5' -AGATCTA (m ⁶ A) CGTTAGAGCTT-3'
m ⁶ A DNA LS	5' -TAAGCTCTA (m ⁶ A) CGTTAGATC-3'
5mC DNA US	5' -AGATCTA (5mC) CGGTAGAGCTT-3'
5mC DNA LS	5' -TAAGCTCTA (5mC) CGGTAGATC-3'
nm DNA US	5' -AGATCTAACGTTAGAGCTT-3'
nm DNA LS	5' -TAAGCTCTAACGTTAGATC-3'
MST substrates	
Rm6A DNA US	5' - (6-FAM) ATCATCAG (m ⁶ A) TTCAGCGTAT-3'
Rm6A DNA LS	5' -ATACGCTG (m ⁶ A) ATCTGATGAT-3'
RA DNA US	5' - (6-FAM) ATCATCAGATTCAGCGTAT-3'
RA DNA LS	5' -ATACGCTGAATCTGATGAT-3'
Ym6A DNA US	5' - (6-FAM) ATCATCAC (m ⁶ A) TTGAGCGTAT-3'
Ym6A DNA LS	5' -ATACGCTC (m ⁶ A) ATGTGATGAT-3'
YA DNA US	5' - (6-FAM) ATCATCACATTGAGCGTAT-3'
YA DNA LS	5' -ATACGCTCAATGTGATGAT-3'
Rm5C DNA US	5' - (6-FAM) ATCATCAA (m ⁵ C) TGTAGCGTAT-3'
Rm5C DNA LS	5' -ATACGCTA (m ⁵ C) AGTTGATGAT-3'
RC DNA US	5' - (6-FAM) ATCATCAACTGTAGCGTAT-3'
RC DNA LS	5' -ATACGCTACAGTTGATGAT-3'
Ym5C DNA US	5' - (6-FAM) ATCATCAT (m ⁵ C) TGAAGCGTAT-3'
Ym5C DNA LS	5' -ATACGCTT (m ⁵ C) AGATGATGAT-3'
YC DNA US	5' -ATCATCATCTGAAGCGTAT-3'
YC DNA LS	5' -ATACGCTTCAGATGATGAT-3'

* 'US' and 'LS' denote complementary 'upper strand' and 'lower strand' oligos that were annealed to make double stranded DNA substrates. All upper strand MST oligos are 5' end-labeled with 6-carboxyfluorescein (6-FAM). Underlined base denotes the nucleotide position adjacent to the modification site that is varied as either a purine (R) or pyrimidine (Y).

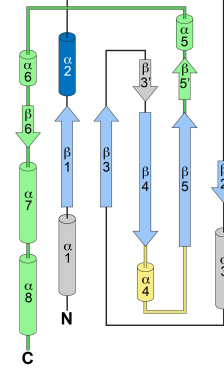
PSPTO5229 (PDB: 2eve)
EVE domain



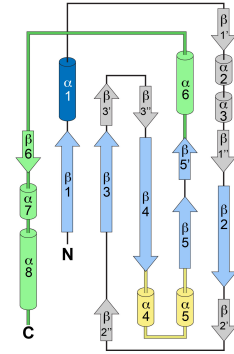
ZrMRB1 (PDB: 4u8t)
YTH domain



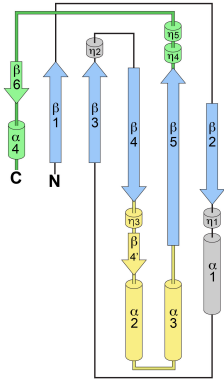
YTHDC1 (PDB: 4r3i)
YTH domain



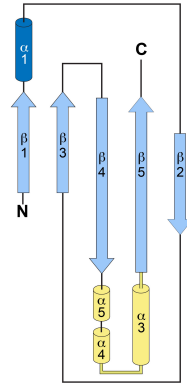
Tg McrB Δ185 (PDB: 6p0g)
YTH domain



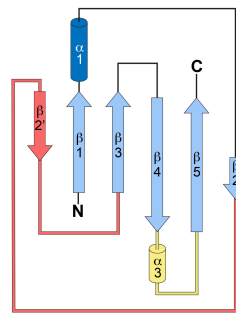
SmMcrB 3-180
EVE domain



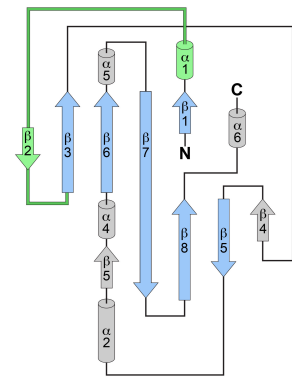
TTHA0113 (PDB: 2dp9)
ASCH domain



ArcTGT (PDB: 1j2b)
PUA domain



Mm UHRF1 (PDB: 2zkd, 3clz, 2zo)
SRA domain



Supplementary Figure 1. PUA-like domain topologies. Topology diagrams of representative EVE, YTH, ASCH, PUA, and SRA domains. Secondary structure elements are colored according to the numbering and nomenclature established by Rost and colleagues (Bertonati et al., 2009): core 5-stranded pseudobarrel present in all folds, light blue; conserved α helix between $\beta 1$ and $\beta 2$, dark blue; Insert 0, red; Insert 1, yellow; Insert 2, green. Additional structural elements are colored gray. Spatially conserved segments in SRA domains are colored similarly.