Supplementary Information for:

Symmetry Breaking and Structural Polymorphism in a Bacterial Microcompartment Shell Protein for Choline Utilization

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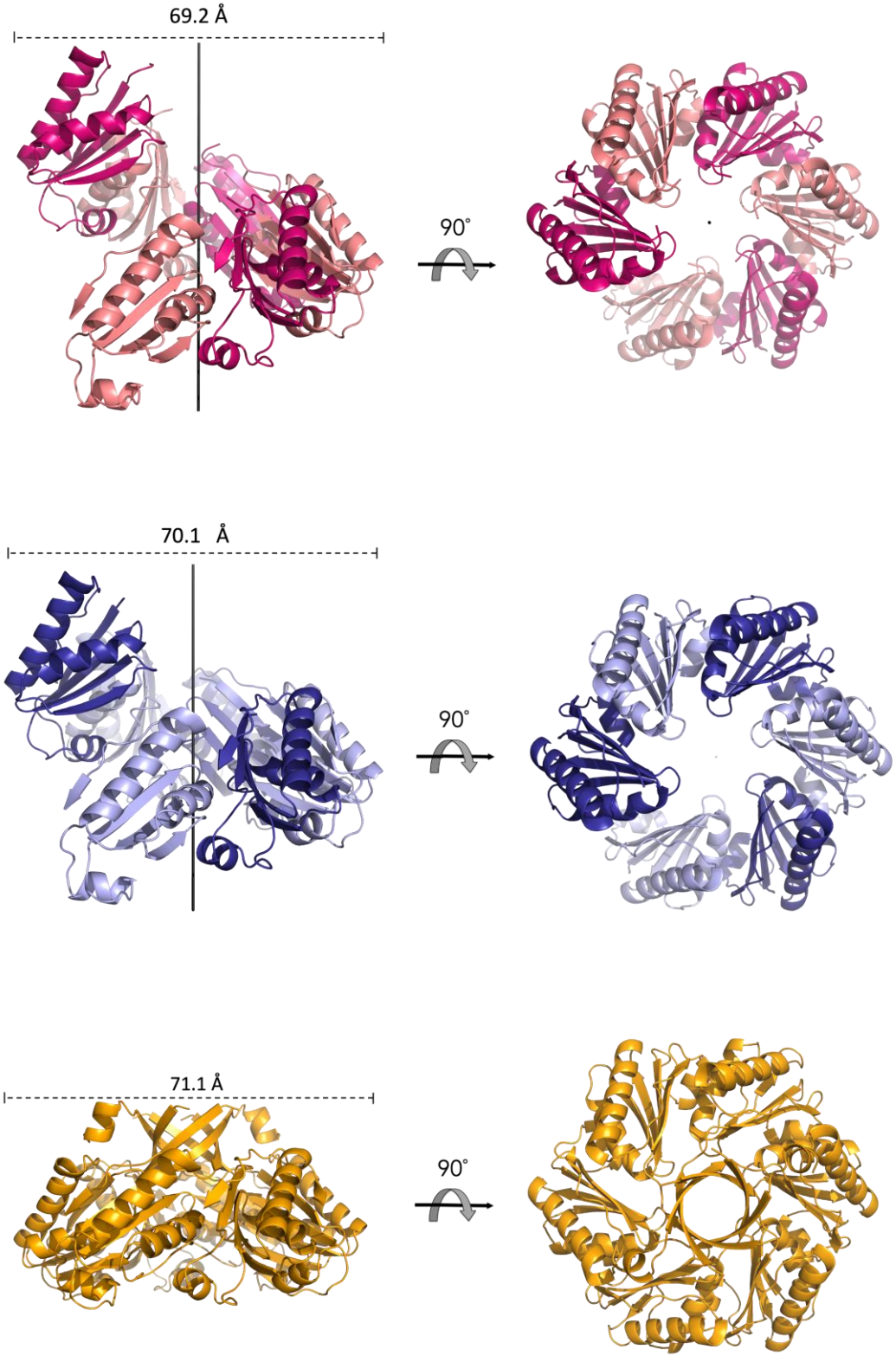
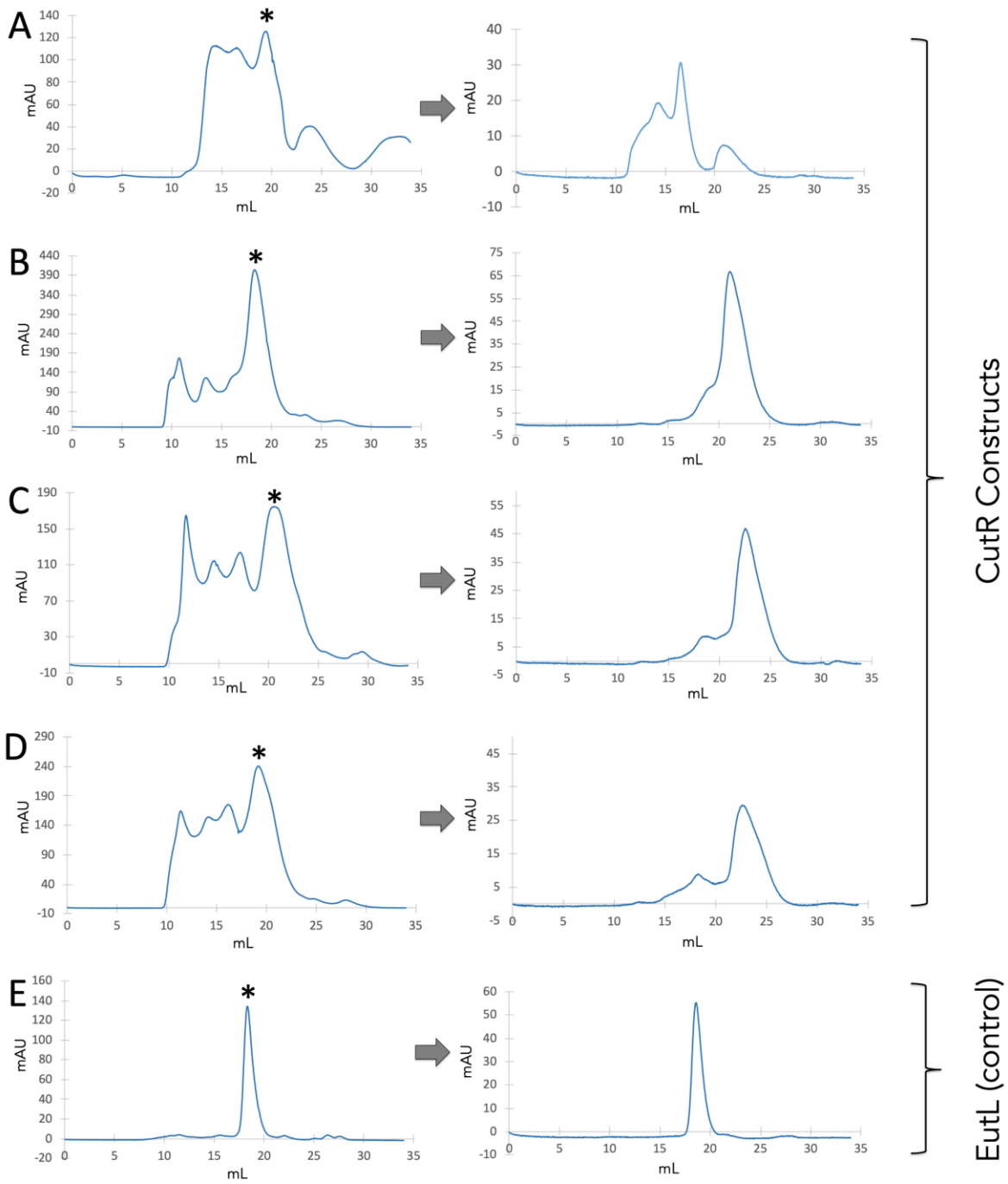


Supplementary Figure 1. Comparison of the screw and flat polymorphs of CutR. When looking down the six-fold axis of symmetry of Screw 1 (magenta) and Screw 2 (purple), CutR forms a similar architecture to the traditional flat hexamer (orange), possessing similar diameters.



Supplementary Figure 2. Size exclusion profiles and recursive runs for the CutR polymorphs and EutL, a natural tandem BMC-domain construct used as a control. After initial size exclusion chromatography (SEC) (left panels), hexameric peaks (denoted by an asterisk) of CutR_K66D (A), CutR_K66A (B), CutR_C37A (C), CutR_TEV (D) and for EutL (E) were concentrated and subject to an additional round of SEC. SEC profiles of those asterisk-denoted peaks are shown in the corresponding right panels.

Supplementary Table 1. CutR and polymorph sequences

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CutR                    -------MIEELGKIDRIIQESVPGKQITLAHVIAAPIEAVYECLGVDHEGAIGVVSLTP 53
Hexamer2(CutR_TEV)      ------GMIEELGKIDRIIQESVPGKQITLAHVIAAPIEAVYECLGVDHEGAIGVVSLTP 54
Hexamer1(CutR_C37A)     MHHHHHHMIEELGKIDRIIQESVPGKQITLAHVIAAPIEAVYEALGVDHEGAIGVVSLTP 60
Dimer(CutR_K66D)        MHHHHHHMIEELGKIDRIIQESVPGKQITLAHVIAAPIEAVYECLGVDHEGAIGVVSLTP 60
Screw1(CutR_K66D)       MHHHHHHMIEELGKIDRIIQESVPGKQITLAHVIAAPIEAVYECLGVDHEGAIGVVSLTP 60
Screw2(CutR_K66A)       MHHHHHHMIEELGKIDRIIQESVPGKQITLAHVIAAPIEAVYECLGVDHEGAIGVVSLTP 60
                               ***********************************.****************

CutR                    NETAIIAADIAGKAANIDICFVDRFTGSVMFSGDIQSVETSLEDILEYFKNSLGFSTVPL 113
Hexamer2(CutR_TEV)      NETAIIAADIAGAAANIDICFVDRFTGSVMFSGDIQSVETSLEDILEYFKNSLGFSTVPL 114
Hexamer1(CutR_C37A)     NETAIIAADIAGAAANIDICFVDRFTGSVMFSGDIQSVETSLEDILEYFKNSLGFSTVPL 120
Dimer(CutR_K66D)        NETAIIAADIAGDAANIDICFVDRFTGSVMFSGDIQSVETSLEDILEYFKNSLGFSTVPL 120
Screw1(CutR_K66D)       NETAIIAADIAGDAANIDICFVDRFTGSVMFSGDIQSVETSLEDILEYFKNSLGFSTVPL 120
Screw2(CutR_K66A)       NETAIIAADIAGAAANIDICFVDRFTGSVMFSGDIQSVETSLEDILEYFKNSLGFSTVPL 120
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CutR                    TKS 116
Hexamer2(CutR_TEV)      TKS 117
Hexamer1(CutR_C37A)     TKS 123
Dimer(CutR_K66D)        TKS 123
Screw1(CutR_K66D)       TKS 123
Screw2(CutR_K66A)       TKS 123
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Supplementary Table 2. X-ray Diffraction and Atomic Refinement Statistics

PDB ID	6XPH	6XPI	6XPJ	6XPK	6XPL
Paper name	Dimer	Hexamer 1	Hexamer 2	Screw 1	Screw 2
Data collection					
Space group	$P4_332$	C2	$P4_22_12$	$P6_1$	$P6_1$
Cell dimensions					
a, *b*, *c* (Å)	109.66, 109.66, 109.66	135.36, 76.14, 67.81	79.29, 79.29, 100.79	61.83, 61.83, 41.93	64.91, 64.91, 33.78
α, β, γ (°)	90.00, 90.00, 90.00	90.00, 119.71, 90.00	90.00, 90.00, 90.00	90.00, 90.00, 120.00	90.00, 90.00, 120.00
Resolution (Å)	77.54-1.80 (1.85-1.80)	63.91-2.60 (2.67-2.60)	62.32-1.50 (1.54-1.50)	53.55-2.80 (2.87-2.80)	56.21-3.30 (3.50-3.30)
R_{merge}	0.079 (1.39)	0.073 (1.44)	0.059 (0.855)	0.113 (0.954)	0.234 (1.34)
I / σ (I)	49.24 (4.71)	10.31 (1.04)	23.7 (3.08)	15.46 (2.22)	4.63 (0.98)
$CC_{1/2}$	100.0 (94.9)	99.9 (74.7)	99.9 (86.0)	99.9 (72.2)	99.2 (51.1)
Completeness (%)	100.0 (100.0)	92.3 (83.1)	99.9 (99.3)	99.4 (95.8)	99.3 (99.5)
Redundancy	75.7 (75.2)	4.02 (4.14)	13.0 (12.7)	9.51 (9.38)	4.68 (4.54)
Refinement					
Resolution (Å)	1.80	2.60	1.50	2.80	3.30
No. reflections	19336 (1386)	17276 (311)	46821 (3373)	2074 (145)	1129 (79)
R_{work} / R_{free}	0.176/0.210 (0.237/0.273)	0.201/0.242 (0.286/0.492)	0.161/0.184 (0.207/0.245)	0.231/0.267 (0.293/0.284)	0.219/0.265 (0.334/0.296)
Molecules per asymmetric unit	2	6	3	1	1
No. atoms					
Protein	1506	4808	2536	734	720
Ligand/ion	21	0	20	0	0
Water	128	0	201	2	0
B-factors					
Protein	35.9	105.5	21.8	67.4	134.5
Ligand/ion	56.1	-	58.0	-	-
Water	41.5	-	29.8	77.5	-
R.m.s. deviations					
Bond lengths (Å)	0.014	0.008	0.010	0.002	0.005
Bond angles (°)	1.8	1.1	1.6	1.2	1.3
Ramachandran statistics (%)					
Most favorable	100	98.3	99.7	93.9	96.9
Allowed	0	1.4	0.3	6.1	3.1
Outliers	0	0.3	0	0	0

Data for each structure were collected from a single crystal. *Values in parentheses are for the highest-resolution shell.

Supplementary citation

S1. Sievers F, Higgins DG (2014) Clustal Omega. Current Protocols in Bioinformatics 48:3.13.1-3.13.16.