STRUCTURAL BIOLOGY

Volume 75 (2019)

Supporting information for article:

Combining rMMS and the Magic Triangle for the efficient structure solution of a potential lysin from bacteriophage P68

Jia Quyen Truong, Santosh Panjikar, Linda Shearwin, John Bruning and Keith Shearwin

Table S1 Crystallization conditions

Below are the formulations for the crystallization conditions where hits appeared.

IndexHT

Well	**Crystallization condition**
A1	0.1 M Citric acid pH 3.5, 2.0 M Ammonium sulfate
A2	0.1 M Sodium acetate trihydrate pH 4.5, 2.0 M Ammonium sulfate
A3	0.1 M BIS-TRIS pH 5.5, 2.0 M Ammonium sulfate
A4	0.1 M BIS-TRIS pH 6.5, 2.0 M Ammonium sulfate
A5	0.1 M HEPES pH 7.5, 2.0 M Ammonium sulfate
A6	0.1 M Tris pH 8.5, 2.0 M Ammonium sulfate
A7	0.1 M Citric acid pH 3.5, 3.0 M Sodium chloride
A9	0.1 M BIS-TRIS pH 5.5, 3.0 M Sodium chloride
A11	0.1 M HEPES pH 7.5, 3.0 M Sodium chloride
A12	0.1 M Tris pH 8.5, 3.0 M Sodium chloride
B1	0.1 M BIS-TRIS pH 5.5, 0.3 M Magnesium formate dihydrate
B2	0.1 M BIS-TRIS pH 6.5, 0.5 M Magnesium formate dihydrate
B3	0.1 M HEPES pH 7.5, 0.5 M Magnesium formate dihydrate
B4	0.1 M Tris pH 8.5, 0.3 M Magnesium formate dihydrate
B5	1.4 M Sodium phosphate monobasic monohydrate/Potassium phosphate dibasic pH 5.6
B6	1.4 M Sodium phosphate monobasic monohydrate/Potassium phosphate dibasic pH 6.9
B7	1.4 M Sodium phosphate monobasic monohydrate/Potassium phosphate dibasic pH 8.2
B10	0.8 M Succinic acid pH 7.0
B12	2.8 M Sodium acetate trihydrate pH 7.0
C1	3.5 M Sodium formate pH 7.0
C2	1.1 M Ammonium tartrate dibasic pH 7.0
C4	35% v/v Tacsimate pH 7.0
C6	0.1 M Sodium chloride, 0.1 M BIS-TRIS pH 6.5, 1.5 M Ammonium sulfate
C7	0.8 M Potassium sodium tartrate tetrahydrate, 0.1 M Tris pH 8.5, 0.5% w/v Polyethylene glycol monomethyl ether 5,000
C9	1.1 M Sodium malonate pH 7.0, 0.1 M HEPES pH 7.0, 0.5% v/v Jeffamine ED-2001 pH 7.0
C10	1.0 M Succinic acid pH 7.0, 0.1 M HEPES pH 7.0, 1% w/v Polyethylene glycol monomethyl ether 2,000
C11	1.0 M Ammonium sulfate , 0.1 M HEPES pH 7.0, 0.5% w/v Polyethylene glycol 8,000
C12	15% v/v Tacsimate pH 7.0, 0.1 M HEPES pH 7.0, 2% w/v Polyethylene glycol 3,350

D1	25% w/v Polyethylene glycol 1,500
D2	0.1 M HEPES pH 7.0, 30% v/v Jeffamine M-600 pH 7.0
D3	0.1 M HEPES pH 7.0, 30% v/v Jeffamine ED-2001 pH 7.0
D4	0.1 M Citric acid pH 3.5, 25% w/v Polyethylene glycol 3,350
D5	0.1 M Sodium acetate trihydrate pH 4.5, 25% w/v Polyethylene glycol 3,350
D6	0.1 M BIS-TRIS pH 5.5, 25% w/v Polyethylene glycol 3,350
D7	0.1 M BIS-TRIS pH 6.5, 25% w/v Polyethylene glycol 3,350
D8	0.1 M HEPES pH 7.5, 25% w/v Polyethylene glycol 3,350
D9	0.1 M Tris pH 8.5, 25% w/v Polyethylene glycol 3,350
D10	0.1 M BIS-TRIS pH 6.5, 20% w/v Polyethylene glycol monomethyl ether 5,000
D11	0.1 M BIS-TRIS pH 6.5, 28% w/v Polyethylene glycol monomethyl ether 2,000
E5	0.2 M Ammonium acetate, 0.1 M Tris pH 8.5, 45% v/v (+/-)-2-Methyl-2,4-pentanediol
E6	0.05 M Calcium chloride dihydrate, 0.1 M BIS-TRIS pH 6.5, 30% v/v Polyethylene glycol monomethyl ether 550
E7	0.05 M Magnesium chloride hexahydrate, 0.1 M HEPES pH 7.5, 30% v/v Polyethylene glycol monomethyl ether 550
E9	0.05 M Ammonium sulfate , 0.05 M BIS-TRIS pH 6.5, 30% v/v Pentaerythritol ethoxylate (15/4 EO/OH)
E11	0.02 M Magnesium chloride hexahydrate, 0.1 M HEPES pH 7.5, 22% w/v Polyacrylic acid sodium salt 5,100
F1	0.2 M L-Proline, 0.1 M HEPES pH 7.5, 10% w/v Polyethylene glycol 3,350
F2	0.2 M Trimethylamine N-oxide dihydrate, 0.1 M Tris pH 8.5, 20% w/v Polyethylene glycol monomethyl ether 2,000
F3	5% v/v Tacsimate pH 7.0, 0.1 M HEPES pH 7.0, 10% w/v Polyethylene glycol monomethyl ether 5,000
F4	0.005 M Cobalt(II) chloride hexahydrate, 0.005 M Nickel(II) chloride hexahydrate, 0.005 M Cadmium chloride hydrate, 0.005 M Magnesium chloride hexahydrate, 0.1 M HEPES pH 7.5, 12% w/v Polyethylene glycol 3,350
F5	0.1 M Ammonium acetate, 0.1 M BIS-TRIS pH 5.5, 17% w/v Polyethylene glycol 10,000
F6	0.2 M Ammonium sulfate, 0.1 M BIS-TRIS pH 5.5, 25% w/v Polyethylene glycol 3,350
F7	0.2 M Ammonium sulfate, 0.1 M BIS-TRIS pH 6.5, 25% w/v Polyethylene glycol 3,350
F8	0.2 M Ammonium sulfate, 0.1 M HEPES pH 7.5, 25% w/v Polyethylene glycol 3,350
F9	0.2 M Ammonium sulfate, 0.1 M Tris pH 8.5, 25% w/v Polyethylene glycol 3,350
F10	0.2 M Sodium chloride, 0.1 M BIS-TRIS pH 5.5, 25% w/v Polyethylene glycol 3,350
F11	0.2 M Sodium chloride, 0.1 M BIS-TRIS pH 6.5, 25% w/v Polyethylene glycol 3,350
F12	0.2 M Sodium chloride, 0.1 M HEPES pH 7.5, 25% w/v Polyethylene glycol 3,350

G1	0.2 M Sodium chloride, 0.1 M Tris pH 8.5, 25% w/v Polyethylene glycol 3,350
G2	0.2 M Lithium sulfate monohydrate, 0.1 M BIS-TRIS pH 5.5, 25% w/v Polyethylene glycol 3,350
G3	0.2 M Lithium sulfate monohydrate, 0.1 M BIS-TRIS pH 6.5, 25% w/v Polyethylene glycol 3,350
G4	0.2 M Lithium sulfate monohydrate, 0.1 M HEPES pH 7.5, 25% w/v Polyethylene glycol 3,350
G5	0.2 M Lithium sulfate monohydrate, 0.1 M Tris pH 8.5, 25% w/v Polyethylene glycol 3,350
G6	0.2 M Ammonium acetate, 0.1 M BIS-TRIS pH 5.5, 25% w/v Polyethylene glycol 3,350
G7	0.2 M Ammonium acetate, 0.1 M BIS-TRIS pH 6.5, 25% w/v Polyethylene glycol 3,350
G8	0.2 M Ammonium acetate, 0.1 M HEPES pH 7.5, 25% w/v Polyethylene glycol 3,350
G9	0.2 M Ammonium acetate, 0.1 M Tris pH 8.5, 25% w/v Polyethylene glycol 3,350
G10	0.2 M Magnesium chloride hexahydrate, 0.1 M BIS-TRIS pH 5.5, 25% w/v Polyethylene glycol 3,350
G11	0.2 M Magnesium chloride hexahydrate, 0.1 M BIS-TRIS pH 6.5, 25% w/v Polyethylene glycol 3,350
G12	0.2 M Magnesium chloride hexahydrate, 0.1 M HEPES pH 7.5, 25% w/v Polyethylene glycol 3,350
H1	0.2 M Magnesium chloride hexahydrate, 0.1 M Tris pH 8.5, 25% w/v Polyethylene glycol 3,350
H2	0.2 M Potassium sodium tartrate tetrahydrate, 20% w/v Polyethylene glycol 3,350
H3	0.2 M Sodium malonate pH 7.0, 20% w/v Polyethylene glycol 3,350
H4	0.2 M Ammonium citrate tribasic pH 7.0, 20% w/v Polyethylene glycol 3,350
H5	0.1 M Succinic acid pH 7.0, 15% w/v Polyethylene glycol 3,350
H6	0.2 M Sodium formate, 20% w/v Polyethylene glycol 3,350
H7	0.15 M DL-Malic acid pH 7.0, 20% w/v Polyethylene glycol 3,350
H8	0.1 M Magnesium formate dihydrate, 15% w/v Polyethylene glycol 3,350
H10	0.2 M Sodium citrate tribasic dihydrate, 20% w/v Polyethylene glycol 3,350
H11	0.1 M Potassium thiocyanate, 30% w/v Polyethylene glycol monomethyl ether 2,000
H12	0.15 M Potassium bromide, 30% w/v Polyethylene glycol monomethyl ether 2,000

PEG/ION HT

Well	**Crystallization condition**
B5	0.2 M Sodium nitrate, 20% w/v Polyethylene glycol 3,350
F5	4% v/v Tacsimate pH 8.0, 12% w/v Polyethylene glycol 3,350
G5	0.1 M Ammonium tartrate dibasic pH 7.0, 12% w/v Polyethylene glycol 3,350
G12	(0.07 M Citric acid, 0.03 M BIS-TRIS propane)/pH 3.4, 16% w/v Polyethylene glycol 3,350
H1	(0.06 M Citric acid, 0.04 M BIS-TRIS propane)/pH 4.1, 16% w/v Polyethylene glycol 3,350
H2	(0.05 M Citric acid, 0.05 M BIS-TRIS propane)/pH 5.0, 16% w/v Polyethylene glycol 3,350
H3	(0.04 M Citric acid, 0.06 M BIS-TRIS propane)/pH 6.4, 20% w/v Polyethylene glycol 3,350
H4	(0.03 M Citric acid, 0.07 M BIS-TRIS propane)/pH 7.6, 20% w/v Polyethylene glycol 3,350
H12	1% w/v Tryptone, 0.001 M Sodium azide, 0.05 M HEPES sodium pH 7.0, 20% w/v Polyethylene glycol 3,350