Table A

Crystallization of *E. coli* KARI. The crystallization conditions are grouped by protein (C-KARI, N-KARI and SeMet-N-KARI), by the ligand present, then sorted by pH.

Condition[a]	Protein	Ligands[b]	Composition of crystallization solution[c]
1 CS2 13	C-KARI	nil	30% (w/v) PEG MME 2000, 0.2 M $(NH_4)_2SO_4$, 0.1 M Na-acetate pH 4.6
2 CSL 10	C-KARI	nil	15% (w/v) PEG 4000, 0.2 M NH_4-acetate, 0.1 M Na-acetate pH 4.6
3 CS1 47	C-KARI	nil	2.0 M $(NH_4)_2SO_4$, 0.1 M Na-acetate pH 4.6
4 P6 A2	C-KARI	nil	5% (w/v) PEG 6000, 0.1 M Na-citrate pH 5.0
5 WI 6	C-KARI	nil	20% (w/v) PEG 3000, 0.1 M Na-citrate pH 5.5
6 CSL 40	C-KARI	nil	10% (v/v) iso-propanol, 10% (w/v) PEG 4000, 0.1 M Na-citrate pH 5.6
7 CS2 14	C-KARI	nil	2.0 M $(NH_4)_2SO_4$, 0.2 M Na/K-tartrate, 0.1 M Na-citrate pH 5.6
8 CS1 40	C-KARI	nil	20% (v/v) iso-propanol, 20% (w/v) PEG 4000, 0.1 M Na-citrate pH 5.6
9 WII 8	C-KARI	nil	10% (w/v) PEG 8000, 0.2 M NaCl, 0.1 M Na/K-phosphate pH 6.2
10 WI 42	C-KARI	nil	15% (v/v) ethanol, 0.1 M Tris-HCl pH 7.0
11 CS2 31	C-KARI	nil	20% (v/v) Jeffamine M-600, 0.1 M Na-HEPES pH 7.5
12 WI 28	C-KARI	nil	20% (w/v) PEG 3000, 0.2 M NaCl, 0.1 M Na-HEPES pH 7.5
13 CSL 22	C-KARI	nil	15% (w/v) PEG 4000, 0.2 M Na-acetate, 0.1 M Tris-HCl pH 8.5
14 AS A6	C-KARI	nil	0.8 M $(NH_4)_2SO_4$, 0.1 M Na-bicine pH 9.0
15 AS B6	C-KARI	nil	1.6 M $(NH_4)_2SO_4$, 0.1 M Na-bicine pH 9.0
16 P6 C6	C-KARI	nil	20% (w/v) PEG 6000, 0.1 M Na-bicine pH 9.0
17 P6 D6	C-KARI	nil	30% (w/v) PEG 6000, 0.1 M Na-bicine pH 9.0
18 CS1 32	C-KARI	nil	2.0 M $(NH_4)_2SO_4$
19 WII 27	C-KARI	(Mg^{2+})	10% (w/v) PEG 3000, 0.2 M $MgCl_2$, 0.1 M Na-cacodylate pH 6.5
20 WII 44	C-KARI	(Mg^{2+})	20% (w/v) PEG 1000, 0.2 M $MgCl_2$, 0.1 M Na-cacodylate pH 6.5
21 CSL 6	C-KARI	(Mg^{2+})	15% (w/v) PEG 4000, 0.2 M $MgCl_2$, 0.1 M Tris-HCl pH 8.5
22 WII 8	C-KARI	NADPH	10% (w/v) PEG 8000, 0.2 M NaCl, 0.1 M Na/K-phosphate pH 6.2
23 AS B6	C-KARI	NADPH	1.6 M $(NH_4)_2SO_4$, 0.1 M Na-bicine pH 9.0

24 WII 27	C-KARI	NADPH, (Mg^{2+})	10% (w/v) PEG 3000, 0.2 M $MgCl_2$, 0.1 M Na-cacodylate pH 6.5
25 PL C4	N-KARI	nil	20% (w/v) PEG 6000, 1.0 M LiCl, 0.1 M Na-HEPES pH 7.0
26 CS2 30*	N-KARI	nil	10% (w/v) PEG 6000, 4.8% (v/v) MPD, 0.1 M Na-HEPES pH 7.5
27 CSL 22	N-KARI	nil	15% (w/v) PEG 4000, 0.2 M Na-acetate, 0.1 M Tris-HCl pH 8.5
28 CS2 13	N-KARI	Mg^{2+}	30% (w/v) PEG MME 2000, 0.2 M $(NH_4)_2SO_4$, 0.1 M Na-acetate pH 4.6
29 NTX 15	N-KARI	(Mg^{2+})	5% (w/v) MPD, 0.04 M $MgCl_2$, 0.05 M Na-cacodylate pH 6.0
30 CS2 43	N-KARI	Mg^{2+}	50% (v/v) MPD, 0.2 M H_2NH_4-phosphate, 0.1 M Tris-HCl pH 8.5
31 CSL 40	N-KARI	NADPH	10% (v/v) iso-propanol, 10% (w/v) PEG 4000, 0.1 M Na-citrate pH 5.6
32 CSL 38	N-KARI	NADPH	0.7 M Na_3-citrate, 0.1 M Na-HEPES pH 7.5
33 CSL 38*	N-KARI	NADPH	0.68 M Na_3-citrate, 0.1 M Tris-HCl pH 8.5
34 CSL 22	N-KARI	NADPH	15% (w/v) PEG 4000, 0.2 M Na-acetate, 0.1 M Tris-HCl pH 8.5
35 CS2 46*	N-KARI	NADPH	30% (v/v) PEG MME 550, 0.1 M NaCl, 0.1 M Na-bicine pH 9.0
36 CS2 13	N-KARI	NADPH, Mg^{2+}	35% (v/v) tert-butanol, 0.1 M Na-citrate pH 5.6
37 PL B3	N-KARI	NADPH, Mg^{2+}	10% (w/v) PEG 6000, 1.0 M LiCl, 0.1 M Na-MES pH 6.0
38 CSL 18	N-KARI	NADPH, (Mg^{2+})	10% (w/v) PEG 8000, 0.2 M Mg-acetate, 0.1 M Na-cacodylate pH 6.5
39 CSL 15	N-KARI	NADPH, Mg^{2+}	15% (w/v) PEG 8000, 0.2 M $(NH_4)_2SO_4$, 0.1 M Na-cacodylate pH 6.5
40 PL C5	N-KARI	NADPH, Mg^{2+}	20% (w/v) PEG 6000, 1.0 M LiCl, 0.1 M Tris-HCl pH 8.0
41 CS2 41	N-KARI	NADPH, Mg^{2+}	1 M Li_2SO_4, 0.01 M $NiCl_2$, 0.1 M Tris-HCl pH 8.5
42 CSL 40	N-KARI	$NADP^+$	10% (v/v) iso-propanol, 10% (w/v) PEG 4000, 0.1 M Na-citrate pH 5.6
43 CSL 38	N-KARI	$NADP^+$	0.7 M Na_3-citrate, 0.1 M Na-HEPES pH 7.5
44 CSL 18	N-KARI	$NADP^+$, (Mg^{2+})	10% (w/v) PEG 8000, 0.2 M Mg-acetate, 0.1 M Na-cacodylate pH 6.5
45 WI 6	SeMet-N-KARI	nil	20% (w/v) PEG 3000, 0.1 M Na-citrate pH 5.5
46 CSL 40	SeMet-N-KARI	nil	10% (v/v) iso-propanol, 10% (w/v) PEG 4000, 0.1 M Na-citrate pH 5.6
47 CSL 15	SeMet-N-KARI	nil	15% (w/v) PEG 8000, 0.2 M $(NH_4)_2SO_4$, 0.1 M Na-cacodylate pH 6.5
48 CSL 28	SeMet-N-KARI	nil	15% (w/v) PEG 8000, 0.2 M Na-acetate, 0.1 M Na-cacodylate pH 6.5
49 WII 12	SeMet-N-KARI	nil	30% (v/v) PEG 400, 0.2 M Li_2SO_4, 0.1 M Na-cacodylate pH 6.5
50 WII 31	SeMet-N-KARI	nil	1.0 M Na_3-citrate, 0.2 M NaCl, 0.1 M Tris-HCl pH 7.0
51 CSL 41	SeMet-N-KARI	nil	5% (v/v) iso-propanol, 10% (w/v) PEG 4000, 0.1 M Na-HEPES pH 7.5
52 CSL 38	SeMet-N-KARI	nil	0.7 M Na_3-citrate, 0.1 M Na-HEPES pH 7.5
53 WI 18	SeMet-N-KARI	nil	1.0 M Na/K-tartrate, 0.2 M NaCl, 0.1 M imidazole-HCl pH 8.0
54 CSL 17	SeMet-N-KARI	nil	15% (w/v) PEG 4000, 0.2 M Li_2SO_4, 0.1 M Tris-HCl pH 8.5

55 CSL 22	SeMet-N-KARI	nil	15% (w/v) PEG 4000, 0.2 M Na-acetate, 0.1 M Tris-HCl pH 8.5
56 CS1 17	SeMet-N-KARI	nil	30% (w/v) PEG 4000, 0.2 M Li_2SO_4, 0.1 M Tris-HCl pH 8.5
57 CSL 33	SeMet-N-KARI	nil	2.0 M Na-formate
58 CSL 18	SeMet-N-KARI	(Mg^{2+})	10% (w/v) PEG 8000, 0.2 M Mg-acetate, 0.1 M Na-cacodylate pH 6.5
59 CSL 44	SeMet-N-KARI	(Mg^{2+})	0.1 M Mg-formate

a. Commercial screen compositions are abbreviated as follows: Hampton Research Crystal Screen (CS1), Crystal Screen 2 (CS2), Crystal Screen Lite (CSL), Grid Screen Ammonium Sulfate (AS), Grid Screen PEG/LiCl (PL), Grid Screen PEG 6000 (P6) and Natrix (NTX), and Emerald Biostructures Wizard I (WI) and Wizard II (WII). The code that follows is the particular condition within each screen as specified by the manufacturers. Variations of these compositions used to improve the crystals are indicated by "*".

b. Ligands were added at a concentration of 4 mM for Mg^{2+}, 2.5 mM for $NADP^{+}$ and 1.7 mM for NADPH. In all cases this represents at least a 10-fold molar excess over the subunit concentration. When Mg^{2+} is shown in parentheses, it is derived from the crystallization solution and is at the concentration shown.

c. MME = monomethyl ether; MPD = 2-methyl-2,4-pentanediol.

Table B.

Preliminary crystallographic data for some crystals of *E. coli* KARI.

Condition	23	27	33.1[a]	33.2[a]	55
Unit cell					
a, *b*, *c* (Å)	226.9, 226.9, 118.9	150.3, 150.3, 207.8	158.9, 274.5, 206.5	154.3, 265.5, 416.1	148.2, 148.2, 211.2
α, β, γ (°)	90, 90, 120	90, 90, 120	90, 90, 90	90, 90, 90	90, 90, 120
Space group	$P6_3$	$P3_121$	$C222_1$	$C222_1$	$P3_121$
Volume/asymmetric unit (Å^3)	883,584	677,552	1,125,890	2,130,777	669,529
Predicted number of monomers/asymmetric unit[b]	6	4	6	12	4
Matthews coefficient (Å^3/Da)	2.6	2.8	3.2	3.0	2.8

a Two crystal types with the same morphology but with different unit cell dimensions are observed in condition 33.

b The predicted number of monomers is that which gives a Matthews coefficient closest to 2.6 Å^3/Da while being consistent with molecular symmetry constraints.