

Well	Precipitant class	Parent screen	JCSG Core Suite	Crystallization solution	JCSG Top96 Cryo	JCSG PDB
A01	Organic	W2cryo #10	JCSG-II F05	40% (v/v) 1,2-Propanediol, 0.1M Sodium acetate pH 4.5	None	6
A02	Organic	H2 #03	JCSG-II H03	25% (v/v) Ethylene glycol	10% EG	5
A03	Organic	MPD #01	JCSG-II H11	10% (v/v) MPD, 0.1 M Citric acid pH 2.5, final pH 4	15% MPD	4
A04	Organic	MPD #02	JCSG-II F07	10% (v/v) MPD, 0.1 M Sodium acetate pH 5.0, final pH 5	10% MPD	5
A05	Organic	MPD #16	JCSG-III D02	40% (v/v) MPD, 0.1 M HEPES pH 6.5, final pH 7	None	5
A06	Organic	MPD #24	JCSG-IV B04	65% (v/v) MPD, 0.1 M Bicine pH 8.5, final pH 9	None	4
A07	Organic/PEG/Salt	W1cryo #14	JCSG-II GI2	0.2 M Ammonium sulfate, 20% (v/v) PEG 300, 10% Glycerol, 0.1M Phosphate-citrate pH 4.2	None	8
A08	Organic/PEG/Salt	H1cryo #39	JCSG-IV D10	1.7 M Ammonium sulfate, 1.7% (v/v) PEG 400, 15% (v/v) Glycerol, 0.085 M HEPES pH 7.5	None	8
A09	Organic/PEG/Salt	H1cryo #20	JCSG-II G08	0.16 M Ammonium sulfate, 20% (w/v) PEG 4000, 20% (v/v) Glycerol, 0.08 M Sodium acetate pH 4.6	None	6
A10	Organic/PEG/Salt	H1cryo #09	JCSG-III F11	0.17 M Ammonium acetate, 25.5% (w/v) PEG 4000, 15% (v/v) Glycerol, 0.085 M Sodium citrate pH 5.6	None	10
A11	Organic/PEG/Salt	H1cryo #22	JCSG-IV C03	0.17 M Sodium acetate, 25.5% (w/v) PEG 4000, 15% (v/v) Glycerol, 0.085 M Tris pH 8.5	None	12
A12	Organic/PEG/Salt	H1cryo #18	JCSG-III E07	0.16 M Magnesium acetate, 16% (w/v) PEG 8000, 20% (v/v) Glycerol, 0.08 M Sodium cacodylate pH 6.5	None	5
B01	Organic/PEG	W2cryo #29	JCSG-III C09	10% (v/v) Glycerol, 5% (w/v) PEG 3000, 30% (v/v) PEG 400, 0.1 M HEPES pH 7.5	None	7
B02	Organic/PEG	W1cryo #16	JCSG-IV F11	30% (v/v) PEG 600, 5% (w/v) PEG 1000, 10% (v/v) Glycerol, 0.1M MES pH 6.0	None	7
B03	Organic/PEG	H1cryo #37	JCSG-II G06	5.6% (w/v) PEG 4000, 30% (v/v) Glycerol, 0.07 M Sodium acetate pH 4.6	None	4
B04	Organic/PEG	H1cryo #41	JCSG-II B11	17% (w/v) PEG 4000, 15% (v/v) Glycerol, 8.5% (v/v) Isopropanol, 0.085 M Sodium HEPES pH 7.5	10% EG	5
B05	Organic/PEG	H1cryo #40	JCSG-I F06	19% (v/v) Isopropanol, 19% (w/v) PEG 4000, 5% (v/v) Glycerol, 0.095 M Sodium citrate pH 5.6	None	9
B06	Organic/PEG	H1 #41	JCSG-I B05	20% (w/v) PEG 4000, 10% (v/v) Isopropanol, 0.1 M HEPES pH 7.5	10% G	12
B07	Organic/PEG	H1 #40	JCSG-I F07	20% (v/v) Isopropanol, 20% (w/v) PEG 4000, 0.1 M Sodium citrate pH 5.6	10% EG	10
B08	Organic/PEG	W2cryo #01	JCSG-I C03+	5% (w/v) PEG 8000, 40% (v/v) MPD, 0.1M Sodium cacodylate pH 6.5	None	7
B09	Organic/Salt	H1cryo #47	JCSG-II G05	1.6 M Ammonium sulfate, 20% (v/v) Glycerol, 0.08 M Sodium acetate pH 4.6	None	4
B10	Organic/Salt	H2 #10	JCSG-III GI1	0.2 M Sodium chloride, 30% (v/v) MPD, 0.1 M Sodium acetate pH 4.6	None†	5
B11	Organic/Salt	H1 #26	JCSG-IV G08	0.2 M Ammonium acetate, 30% (v/v) MPD, 0.1 M Sodium citrate pH 5.6	5% MPD†	4
B12	Organic/Salt	W2 #02	JCSG-I E08	0.2 M Lithium sulfate, 35% (v/v) MPD, 0.1 M MES pH 6.0	None	4
C01	PEG	W2cryo #27	JCSG-III D10	50% (v/v) PEG 200, 0.1 M Tris pH 7.0	None	4
C02	PEG	W1cryo #46	JCSG-III F01	40% (v/v) PEG 400, 5% (w/v) PEG 3000, 0.1M MES pH 6.0	None	5
C03	PEG	W2cryo #31	JCSG-III A02	40% (v/v) PEG 600, 0.1M CHES pH 9.5	None	4
C04	PEG	W1 #06	JCSG-I F08+	20% (w/v) PEG 3000, 0.1 M Sodium citrate pH 5.5	10% EG	5
C05	PEG	P6K #01	JCSG-I H12	5% (w/v) PEG 6000, 0.1 M Citric acid pH 4.0, final pH 4	25% P200	4
C06	PEG	P6K #14	JCSG-I G04+	20% (w/v) PEG 6000, 0.1 M Citric acid pH 4.0, final pH 5	15% G	6
C07	PEG	P6K #18	JCSG-I A02+	20% (w/v) PEG 6000, 0.1 M Bicine pH 8.5, final pH 9	10% EG	4
C08	PEG	P6K #21	JCSG-IV G06	30% (w/v) PEG 6000, 0.1 M MES pH 5.0, final 6	10% P200	7
C09	PEG	P6K #24	JCSG-IV B03	30% (w/v) PEG 6000, 0.1 M Bicine pH 8.5, final pH 9	5% EG	6
C10	PEG	W1 #21	JCSG-I B02	20% (w/v) PEG 8000, 0.1 M HEPES pH 7.5	10% EG	6
C11	PEG	W1 #01	JCSG-I A01+	20% (w/v) PEG 8000, 0.1 M CHES pH 9.5	12% P200	5
C12	Salt	AmSO4 #01	JCSG-I H09+	0.8 M Ammonium sulfate, 0.1 M Citric acid pH 3.5, final pH 4	20% G	5
D01	Salt	AmSO4 #08	JCSG-II F09	1.6 M Ammonium sulfate, 0.1 M Citric acid pH 4.0, final pH 5	20% G	7
D02	Salt	AmSO4 #09	JCSG-IV G05	1.6 M Ammonium sulfate, 0.1 M MES pH 5.0, final 6	20% G	6
D03	Salt	AmSO4 #12	JCSG-IV A10	1.6 M Ammonium sulfate, 0.1 M Bicine pH 9.0, final 9	15% G	4
D04	Salt	W2 #04	JCSG-II D10+	0.2 M Sodium chloride, 2.0 M Ammonium sulfate, 0.1 M Sodium cacodylate pH 6.5	15% EG	7
D05	Salt	H1 #04	JCSG-II B01	2.0 M Ammonium sulfate, 0.1 M Tris pH 8.5	15% EG	7
D06	Salt	W1 #33	JCSG-IV A01	0.2 M Lithium sulfate, 2.0 M Ammonium sulfate, 0.1 M CAPS pH 10.5	15% EG	5
D07	Salt	AmSO4 #17	JCSG-III B10	2.4 M Ammonium sulfate, 0.1 M Tris pH 8.5, final pH 8	15% G	5
D08	Salt	AmSO4 #18	JCSG-IV A12	2.4 M Ammonium sulfate, 0.1 M Bicine pH 9.0, final 9	20% G	9
D09	Salt	W2 #38	JCSG-III H03	0.2 M Lithium sulfate, 2.5 M Sodium chloride, 0.1 M Sodium acetate pH 4.5	10% EG	4
D10	Salt	W1 #14	JCSG-III D12+	1.0 M Sodium citrate, 0.1 M Sodium cacodylate pH 6.5	15% G	8
D11	Salt	W2 #31	JCSG-III C10	0.2 M Sodium chloride, 1.0 M Sodium citrate, 0.1 M Tris pH 7.0	10% EG	6
D12	Salt	W2 #16	JCSG-II A03	1.0 M Sodium citrate, 0.1 M CHES pH 9.5	10% EG	4

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E01	Salt	H1 #38	JCSG-III C05	1.4 M tri-Sodium citrate, 0.1 M Sodium HEPES pH 7.5	10% EG	10
E02	Salt	W1 #27	JCSG-IV A02Δ	0.2 M Lithium sulfate, 1.2 M Sodium dihydrogen phosphate/0.8 M di-Potassium hydrogen phosphate, 0.1M CAPS pH 10.5	25% G	5
E03	Salt/PEG	W2cryo #48	JCSG-I F09	0.2 M Sodium chloride, 50% (v/v) PEG 200, 0.1M Phosphate-citrate pH 4.2	None	5
E04	Salt/PEG	W1cryo #37	JCSG-II C07+	0.2 M Calcium acetate, 40% (v/v) PEG 300, 0.1M Sodium cacodylate pH 6.5	None	4
E05	Salt/PEG	H1 #14	JCSG-III C06	0.2 M Calcium chloride, 28% (v/v) PEG 400, 0.1 M Sodium HEPES pH 7.5	10% EG	6
E06	Salt/PEG	W1 #44	JCSG-II H01	0.2 M Calcium acetate, 30% (v/v) PEG 400, 0.1 M Sodium acetate pH 4.5	None	4
E07	Salt/PEG	W1cryo #38	JCSG-II B02+	0.2 M Lithium sulfate, 40% (v/v) PEG 400, 0.1M Tris pH 8.5	5% P400	4
E08	Salt/PEG	W1cryo #05	JCSG-II G03	0.2 M Magnesium chloride, 40% (v/v) PEG 400, 0.1M MES pH 5.5	None	4
E09	Salt/PEG	W2 #27	JCSG-II D08	0.2 M Magnesium chloride, 10% (w/v) PEG 3000, 0.1 M Sodium cacodylate pH 6.5	15% EG	5
E10	Salt/PEG	W1 #28	JCSG-I B01	0.2 M Sodium chloride, 20% (w/v) PEG 3000, 0.1 M HEPES pH 7.5	10% EG	4
E11	Salt/PEG	W2 #07	JCSG-IV E07	0.2 M Sodium chloride, 30% (w/v) PEG 3000, 0.1 M Tris pH 7.0	None	6
E12	Salt/PEG	PEG/ion #03	JCSG-I E05	0.2 M Ammonium fluoride, 20% (w/v) PEG 3350	15% EG	6
F01	Salt/PEG	PEG/ion #23	JCSG-I D09+	0.2 M Ammonium formate, 20% (w/v) PEG 3350	10% EG	5
F02	Salt/PEG	PEG/ion #35	JCSG-I E09	0.2 M Ammonium sulfate, 20% (w/v) PEG 3350	10% EG	5
F03	Salt/PEG	PEG/ion #28	JCSG-I B08	0.2 M Calcium acetate hydrate, 20% (w/v) PEG 3350	10% EG	14
F04	Salt/PEG	PEG/ion #07	JCSG-III G05	0.2 M Calcium chloride, 20% (w/v) PEG 3350	10% EG	9
F05	Salt/PEG	PEG/ion #44	JCSG-III B11	0.2 M di-Ammonium hydrogen phosphate, 20% (w/v) PEG 3350	10% EG	9
F06	Salt/PEG	PEG/ion #38	JCSG-I D07	0.2 M di-Ammonium tartrate, 20% (w/v) PEG 3350	15% EG	10
F07	Salt/PEG	PEG/ion #40	JCSG-III A07	0.2 M di-Sodium hydrogen phosphate, 20% (w/v) PEG 3350	15% EG	5
F08	Salt/PEG	PEG/ion #25	JCSG-I A12	20% (w/v) PEG 3350, 0.2 M Magnesium acetate	10% EG	12
F09	Salt/PEG	PEG/ion #05	JCSG-I F05	0.2 M Magnesium chloride, 20% (w/v) PEG 3350	10% EG	11
F10	Salt/PEG	PEG/ion #20	JCSG-I F03+	0.2 M Magnesium formate, 20% (w/v) PEG 3350	10% EG	5
F11	Salt/PEG	PEG/ion #16	JCSG-I F04	0.2 M Magnesium nitrate, 20% (w/v) PEG 3350	15% EG	6
F12	Salt/PEG	PEG/ion #22	JCSG-I B09+	0.2 M Potassium formate, 20% (w/v) PEG 3350	10% EG	5
G01	Salt/PEG	PEG/ion #18	JCSG-I C11+	0.2 M Potassium nitrate, 20% (w/v) PEG 3350	10% EG	12
G02	Salt/PEG	PEG/ion #27	JCSG-I C08	0.2 M Sodium acetate, 20% (w/v) PEG 3350	10% P200	4
G03	Salt/PEG	PEG/ion #01	JCSG-II C05	0.2 M Sodium fluoride, 20% (w/v) PEG 3350	15% P200	6
G04	Salt/PEG	PEG/ion #21	JCSG-I B11	0.2 M Sodium formate, 20% (w/v) PEG 3350	10% EG	6
G05	Salt/PEG	PEG/ion #17	JCSG-II D02	0.2 M Sodium nitrate, 20% (w/v) PEG 3350	10% EG	5
G06	Salt/PEG	PEG/ion #13	JCSG-I C12+	0.2 M Sodium thiocyanate, 20% (w/v) PEG 3350	10% EG	6
G07	Salt/PEG	PEG/ion #48	JCSG-I G01Δ	20% (w/v) PEG-3350, 0.2 M di-Ammonium citrate	10% EG	7
G08	Salt/PEG	PEG/ion #47	JCSG-I A07+	20% (w/v) PEG 3350, 0.2 M tri-Potassium citrate	10% EG	7
G09	Salt/PEG	H1 #20	JCSG-I G11	0.2 M Ammonium sulfate, 25% (w/v) PEG 4000, 0.1 M Sodium acetate pH 4.6	10% EG	6
G10	Salt/PEG	H1 #09	JCSG-II E10	0.2 M Ammonium acetate, 30% (w/v) PEG 4000, 0.1 M Sodium citrate pH 5.6	None	10
G11	Salt/PEG	H1 #17	JCSG-IV B11	0.2 M Lithium sulfate, 30% (w/v) PEG 4000, 0.1 M Tris pH 8.5	10% EG	8
G12	Salt/PEG	H1 #06	JCSG-IV B09	0.2 M Magnesium chloride, 30% (w/v) PEG 4000, 0.1 M Tris pH 8.5	None	13
H01	Salt/PEG	H1 #22	JCSG-III B05	0.2 M Sodium acetate, 30% (w/v) PEG 4000, 0.1 M Tris pH 8.5	None	9
H02	Salt/PEG	P6K/LiCl #08	JCSG-I G03	1.0 M Lithium chloride, 10% (w/v) PEG 6000, 0.1 M Citric acid pH 5.0, final pH 5	15% EG	5
H03	Salt/PEG	P6K/LiCl #11	JCSG-IV C12	1.0 M Lithium chloride, 10% (w/v) PEG 6000, 0.1 M Tris pH 8.5, final pH 8	15% EG	5
H04	Salt/PEG	P6K/LiCl #16	JCSG-III D07	1.0 M Lithium chloride, 20% (w/v) PEG 6000, 0.1 M HEPES pH 7.0, final pH 7	10% EG	8
H05	Salt/PEG	P6K/LiCl #15	JCSG-II E03	1.0 M Lithium chloride, 20% (w/v) PEG 6000, 0.1 M MES pH 6.0, final pH 6	20% G	10
H06	Salt/PEG	P6K/LiCl #14	JCSG-II F11	1.0 M Lithium chloride, 20% (w/v) PEG 6000, 0.1 M Citric acid pH 5.0, final pH 5	20% G	4
H07	Salt/PEG	W1 #46	JCSG-II B03	0.2 M Calcium acetate, 10% (w/v) PEG 8000, 0.1 M Imidazole pH 8.0	20% EG	9
H08	Salt/PEG	W2 #28	JCSG-I E07	0.2 M Calcium acetate, 20% (w/v) PEG 8000, 0.1 M MES pH 6.0	15% G	9
H09	Salt/PEG	H1 #18	JCSG-I D12	0.2 M Magnesium acetate, 20% (w/v) PEG 8000, 0.1 M Sodium cacodylate pH 6.5	15% EG	10
H10	Salt/PEG	W2 #03	JCSG-III B01	0.2 M Magnesium chloride, 20% (w/v) PEG 8000, 0.1 M Tris pH 8.5	10% P200	12
H11	Salt/PEG	W2 # 39	JCSG-II A01	0.2 M Sodium chloride, 20% (w/v) PEG 8000, 0.1 M CAPS pH 10.5	10% EG	7
H12	Salt/PEG	H1 #28	JCSG-III E09	0.2 M Sodium acetate, 30%(w/v) PEG 8000, 0.1 M Sodium cacodylate pH 6.5	15% EG	5

JCSG Top96 Screen

List of the 96 most successful JCSG crystallization conditions with respect to JCSG structures deposited in the PDB (conditions responsible for 631 JCSG PDB depositions between 1/1/2001 and 9/23/2010). Conditions listed in plate order (according to major precipitant class) as currently employed at the JCSG. The parent screen is noted and abbreviated as follows: H1: Crystal Screen (Hampton Research), H2: Crystal Screen 2 (Hampton Research), H1cryo: Crystal Screen Cryo (Hampton Research), H2cryo: Crystal Screen 2 Cryo (Hampton Research), W1: Wizard Classic 1 (Emerald Biosystems), W2: Wizard Classic 2 (Emerald Biosystems), W1cryo: Wizard Cryo 1 (Emerald Biosystems), W2cryo: Wizard Cryo 2 (Emerald Biosystems), MPD: MPD Grid Screen (Hampton Research), PEG/ion: PEG ion screen (Hampton Research), AmSO4: Grid Screen Ammonium sulfate (Hampton Research) and P6K/LiCl: Grid Screen PEG/LiCl (Hampton Research). The corresponding JCSG Core Suite (Qiagen) conditions are listed and those also represented in the "Core Screen" (later JCSG+ screen) are denoted by a plus sign (+) in the JCSG Core Suite column. The top 10 conditions with respect to PDB depositions are highlighted in the PDB column in bold and underline. Due to formulation and manufacturing considerations two conditions (JCSG-IV A02 and JCSG-I G01, highlighted by a triangle (Δ) in the JCSG Core Suite column), were modified in the Qiagen JCSG Core Suite formulation. To ensure consistency with the PDB entries the original screening condition, as used at the JCSG (W1 #27 and PEG/ion #48, respectively), is reported above and not the condition currently reported in the Qiagen formulation of the JCSG Core Suite. For example, JCSG-IV A02: 0.2 M Lithium sulfate, 1.2 M Sodium dihydrogen phosphate/0.8 M di-Potassium hydrogen phosphate, 0.1 M Glycine pH 10.5 vs. W1 #27: 0.2 M Lithium sulfate, 1.2 M Sodium dihydrogen phosphate/0.8 M di-Potassium hydrogen phosphate, 0.1M CAPS pH 10.5 (change in buffer highlighted by underline). JCSG-I G01: 20% (w/v) PEG 3350, 0.18 M tri-Ammonium citrate vs. PEG/ion #48: 20% (w/v) PEG-3350, 0.2 M di-Ammonium citrate (change in salt highlighted by underline). *JCSG Top96 Cryo* conditions are abbreviated as follows: EG: Ethylene glycol, MPD: 2-Methyl-2,4-pentanediol, G: Glycerol, P200: PEG 200 and P400: PEG 400. *JCSG Top96 Cryo* conditions were selected from coarse screen crystallization conditions that produced a clear visual freeze and a score of zero for ice rings during diffraction screening, with the exception of *JCSG Top96* conditions B10 (JCSG-III G11) and B11 (JCSG-IV G08) which resulted from fine-screen conditions and scored 1 for ice rings during diffraction screening, these conditions are denoted with a dagger ($\dagger$) in the Top96 Cryo column.