

Supplementary Material

A Quality Comparison of Protein Crystals Grown under Containerless Conditions Generated by Diamagnetic Levitation, Silicone Oil, and Agarose Gel

Hui-Ling Cao, Li-Hua Sun, Jian Li, Lin Tang, Hui-Meng Lu, Yun-Zhu Guo, Jin He,
 Yong-Ming Liu, Xu-Zhuo Xie, He-Fang Shen, Chen-Yan Zhang , Wei-Hong Guo,
 Lin-Jun Huang, Peng Shang, Jian-Hua He*, Da-Chuan Yin*

Supplementary Tables: X-ray diffraction data statistics of the crystals of seven different proteins from the four crystallization conditions

Supplementary Table S1. X-ray diffraction data statistics of lysozyme crystals

Data set name	Diffraction data statistics of lysozyme crystals from the four conditions			
	Magnetic levitation	Silicone oil	Agarose gel	Control
Wavelength (Å)		0.97946		
Resolution range (Å)	50-0.95 (0.98-0.95)*	50-1.20 (1.22-1.20)	50-1.10 (1.14-1.10)	50-1.20 (1.22-1.20)
Mosaicity (°)	0.17	0.39	0.57	0.27
$R_{\text{merge}}^{\text{a}}$ (%)	5.6 (77.8)	7.4 (51.7)	6.2 (76.9)	9.3 (60.6)
$\langle I \rangle / \langle \sigma(I) \rangle$	73.9 (2.5)	88.5 (8.6)	59.6 (6.6)	54.0 (4.3)
Redundancy	24.9 (9.5)	27.2 (26.8)	24.4 (24.0)	14.3 (13.8)
Completeness (%)	98.3 (86.5)	99.9 (100)	99.4 (100)	99.9 (96.8)
Space group	$P4_32_12$	$P4_32_12$	$P4_32_12$	$P4_32_12$
Cell dimensions	$a = 78.91$	$a = 77.90$	$a = 78.28$	$a = 77.26$
a, b, c (Å)	$b = 78.91$	$b = 77.90$	$b = 78.28$	$b = 77.26$
α, β, γ (°)	$c = 36.95$	$c = 37.02$	$c = 36.91$	$c = 37.18$
$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$

* The numbers in parentheses represent the value for the highest-resolution shell.

^a $R_{\text{merge}} = \sum_{hkl} \sum_i I_{i(hkl)} - \langle I_{(hkl)} \rangle / \sum_{hkl} \sum_i \langle I_{(hkl)} \rangle$, where $\langle I_{(hkl)} \rangle$ is the mean intensity of the i observation of reflection hkl .

Supplementary Table S2. X-ray diffraction data statistics of proteinase K crystals

Data set name	Diffraction data statistics of lysozyme crystals from the four conditions				
	Magnetic levitation	Silicone oil	Agarose gel	Control	
Wavelength (Å)		0.97946			
Resolution range (Å)	50-0.95 (0.98-0.95)*	50-1.12 (1.14-1.12)	50-1.02 (1.06-1.02)	50-1.14 (1.16-1.14)	
Mosaicity (°)	0.13	0.40	0.25	0.19	
$R_{\text{merge}}^{\text{a}}$ (%)	10.9 (50.0)	7.8 (31.7)	11.5 (76.8)	15.3 (78.0)	
$\langle I \rangle / \langle \sigma(I) \rangle$	67.5 (6.8)	59.9 (13.2)	46.7 (7.2)	24.9 (2.5)	
Redundancy	23.8 (10.5)	26.8 (26.1)	25.2 (24.6)	26.4 (14.8)	
Completeness (%)	98.2 (88.3)	100 (100)	98.8 (96.2)	99.9 (99.1)	
Space group	$P4_32_12$	$P4_32_12$	$P4_32_12$	$P4_32_12$	
Cell dimensions	$a = 67.88$	$a = 67.91$	$a = 67.89$	$a = 67.87$	
a, b, c (Å)	$b = 67.88$	$b = 67.91$	$b = 67.89$	$b = 67.87$	
α, β, γ (°)	$c = 102.22$	$c = 102.42$	$c = 102.57$	$c = 102.24$	
$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	

* The numbers in parentheses represent the value for the highest-resolution shell.

^a $R_{\text{merge}} = \sum_{hkl} \sum_i I_{i(hkl)} - \langle I_{(hkl)} \rangle / \sum_{hkl} \sum_i \langle I_{(hkl)} \rangle$, where $\langle I_{(hkl)} \rangle$ is the mean intensity of the i observation of reflection hkl .

Supplementary Table S3. X-ray diffraction data statistics of TCS crystals.

Data set name	Diffraction data statistics of lysozyme crystals from the four conditions				
	Magnetic levitation	Silicone oil	Agarose gel	Control	
Wavelength (Å)		0.97852			
Resolution range (Å)	50-1.12 (1.14-1.12)*	50-1.43 (1.45-1.43)	50-1.15 (1.17-1.15)	50-1.07 (1.09-1.07)	
Mosaicity (°)	0.27	0.38	0.29	0.22	
$R_{\text{merge}}^{\text{a}}$ (%)	5.8 (43.5)	7.4 (47.7)	7.1 (42.9)	6.8 (42.9)	
$\langle I \rangle / \langle \sigma(I) \rangle$	36.4 (4.1)	37.1 (4.0)	52.1 (7.3)	41.8 (5.0)	
Redundancy	6.8 (6.6)	7.1 (7.0)	14.1 (13.8)	6.9 (6.6)	
Completeness (%)	99.8 (99.6)	100 (100)	100 (100)	99.5 (98.8)	
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	
Cell dimensions	$a = 37.72$	$a = 37.74$	$a = 37.90$	$a = 37.73$	
a, b, c (Å)	$b = 74.62$	$b = 74.69$	$b = 75.14$	$b = 74.57$	
α, β, γ (°)	$c = 78.52$	$c = 78.49$	$c = 78.73$	$c = 78.44$	
$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	

* The numbers in parentheses represent the value for the highest-resolution shell.

^a $R_{\text{merge}} = \sum_{hkl} \sum_i I_{i(hkl)} - \langle I_{(hkl)} \rangle / \sum_{hkl} \sum_i \langle I_{(hkl)} \rangle$, where $\langle I_{(hkl)} \rangle$ is the mean intensity of the i observation of reflection hkl .

Supplementary Table S4. X-ray diffraction data statistics of concanavalin A crystals

Data set name	Diffraction data statistics of lysozyme crystals from the four conditions				
	Magnetic levitation	Silicone oil	Agarose gel	Control	
Wavelength (Å)		0.97946			
Resolution range (Å)	50-1.23 (1.25-1.23)*	50-1.76 (1.79-1.76)	50-1.79 (1.82-1.79)	50-1.78 (1.82-1.78)	
Mosaicity (°)	0.34	0.53	0.67	0.77	
$R_{\text{merge}}^{\text{a}}$ (%)	6.6 (90.1)	7.6 (46.8)	4.9 (62.9)	6.6 (94.4)	
$\langle I \rangle / \langle \sigma(I) \rangle$	58.0 (2.4)	51.6 (4.6)	60.7 (5.0)	54.2 (3.3)	
Redundancy	14.0 (11.1)	7.1 (6.3)	14.0 (13.5)	14.2 (13.7)	
Completeness (%)	99.1 (84.7)	99.1 (98.7)	99.7 (99.7)	99.9 (99.9)	
Space group	<i>I</i> 222	<i>I</i> 222	<i>I</i> 222	<i>I</i> 222	
Cell dimensions	$a = 61.73$	$a = 63.77$	$a = 63.79$	$a = 64.14$	
a, b, c (Å)	$b = 86.84$	$b = 87.77$	$b = 89.46$	$b = 88.33$	
α, β, γ (°)	$c = 89.02$	$c = 89.47$	$c = 87.85$	$c = 89.53$	
	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	

* The numbers in parentheses represent the value for the highest-resolution shell.

^a $R_{\text{merge}} = \sum_{hkl} \sum_i I_{i(hkl)} - \langle I_{(hkl)} \rangle / \sum_{hkl} \sum_i \langle I_{(hkl)} \rangle$, where $\langle I_{(hkl)} \rangle$ is the mean intensity of the i observation of reflection hkl .

Supplementary Table S5. X-ray diffraction data statistics of HSP90^N crystals

Data set name	Diffraction data statistics of lysozyme crystals from the four conditions				
	Magnetic levitation	Silicone oil	Agarose gel	Control	
Wavelength (Å)		0.97852			
Resolution range (Å)	50-1.61 (1.64-1.61)*	50-2.13 (2.17-2.13)	50-2.15 (2.19-2.15)	50-2.89 (2.94-2.89)	
Mosaicity (°)	0.14	0.91	1.86	2.26	
$R_{\text{merge}}^{\text{a}}$ (%)	11.3 (52.6)	11.9 (33.8)	8.8 (52.5)	13.5 (53.9)	
$\langle I \rangle / \langle \sigma(I) \rangle$	63.3 (7.4)	77.8 (34.8)	42.3 (6.3)	10.5 (2.5)	
Redundancy	14.6 (14.6)	14.2 (14.2)	14.2 (14.0)	3.1 (3.1)	
Completeness (%)	100 (100)	99.5 (99.5)	100 (100)	88.7 (85.2)	
Space group	<i>I</i> 222	<i>I</i> 222	<i>I</i> 222	<i>I</i> 222	
Cell dimensions	$a = 65.55$	$a = 65.45$	$a = 65.39$	$a = 65.47$	
a, b, c (Å)	$b = 89.08$	$b = 89.10$	$b = 89.10$	$b = 88.62$	
α, β, γ (°)	$c = 99.87$	$c = 99.48$	$c = 99.68$	$c = 99.49$	
	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	

* The numbers in parentheses represent the value for the highest-resolution shell.

^a $R_{\text{merge}} = \sum_{hkl} \sum_i I_{i(hkl)} - \langle I_{(hkl)} \rangle / \sum_{hkl} \sum_i \langle I_{(hkl)} \rangle$, where $\langle I_{(hkl)} \rangle$ is the mean intensity of the i observation of reflection hkl .

Supplementary Table S6. X-ray diffraction data statistics of thaumatin crystals

Data set name	Diffraction data statistics of lysozyme crystals from the four conditions				
	Magnetic levitation	Silicone oil	Agarose gel	Control	
Wavelength (Å)		0.97918			
Resolution range (Å)	50-1.35 (1.37-1.35)*	50-1.60 (1.63-1.60)	50-1.50 (1.53-1.50)	50-2.70 (2.75-2.70)	
Mosaicity (°)	0.21	0.70	0.38	1.18	
$R_{\text{merge}}^{\text{a}}$ (%)	7.9 (53.3)	9.3 (65.5)	6.8 (56.1)	16.6 (42.7)	
$\langle I \rangle / \langle \sigma(I) \rangle$	76.0 (9.6)	78.6 (11.4)	57.6 (6.2)	91.6 (37.4)	
Redundancy	28.2 (28.2)	27.6 (27.6)	14.8 (14.7)	24.8 (24.8)	
Completeness (%)	100 (100)	99.0 (98.6)	100 (100)	99.9 (99.9)	
Space group	$P4_12_12$	$P4_12_12$	$P4_12_12$	$P4_12_12$	
Cell dimensions	$a = 57.80$	$a = 52.81$	$a = 57.61$	$a = 58.04$	
a, b, c (Å)	$b = 57.80$	$b = 52.81$	$b = 57.61$	$b = 58.04$	
α, β, γ (°)	$c = 150.11$	$c = 151.94$	$c = 149.93$	$c = 151.36$	
	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	

* The numbers in parentheses represent the value for the highest-resolution shell.

^a $R_{\text{merge}} = \sum_{hkl} \sum_i I_{i(hkl)} - \langle I_{(hkl)} \rangle / \sum_{hkl} \sum_i \langle I_{(hkl)} \rangle$, where $\langle I_{(hkl)} \rangle$ is the mean intensity of the i observation of reflection hkl .

Supplementary Table S7. X-ray diffraction data statistics of catalase crystals

Data set name	Diffraction data statistics of lysozyme crystals from the four conditions				
	Magnetic levitation	Silicone oil	Agarose gel	Control	
Wavelength (Å)		0.97946			
Resolution range (Å)	50-2.28 (2.32-2.28)*	50-3.59 (3.65-3.59)	50-2.70 (2.75-2.70)	50-4.64 (4.72-4.64)	
Mosaicity (°)	0.77	0.73	0.43	1.35	
$R_{\text{merge}}^{\text{a}}$ (%)	15.3 (94.4)	16.8 (35.1)	12.8 (53.1)	59.7 (95.5)	
$\langle I \rangle / \langle \sigma(I) \rangle$	31.5 (3.8)	29.2 (10.6)	10.4 (2.5)	16.1 (7.8)	
Redundancy	10.3 (10.0)	9.5 (9.5)	10.4 (10.3)	3.9 (3.7)	
Completeness (%)	100 (100)	91.5 (85.6)	85.5 (82.0)	85.5 (82.1)	
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	
Cell dimensions	$a = 130.68$	$a = 139.96$	$a = 127.81$	$a = 122.46$	
a, b, c (Å)	$b = 139.88$	$b = 228.88$	$b = 124.05$	$b = 131.45$	
α, β, γ (°)	$c = 98.35$	$c = 86.65$	$c = 117.04$	$c = 99.10$	
	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$	

* The numbers in parentheses represent the value for the highest-resolution shell.

^a $R_{\text{merge}} = \sum_{hkl} \sum_i I_{i(hkl)} - \langle I_{(hkl)} \rangle / \sum_{hkl} \sum_i \langle I_{(hkl)} \rangle$, where $\langle I_{(hkl)} \rangle$ is the mean intensity of the i observation of reflection hkl .