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Attaining atomic resolution from *in situ* data collection at room temperature using counterdiffusion-based low-cost microchips

Jose A. Gavira, Isaac Rodriguez-Ruiz, Sergio Martinez-Rodriguez, Shibom Basu, Sébastien Teychené, Andrew A. McCarthy and Christoph Mueller-Dieckman

Glucose Isomerase

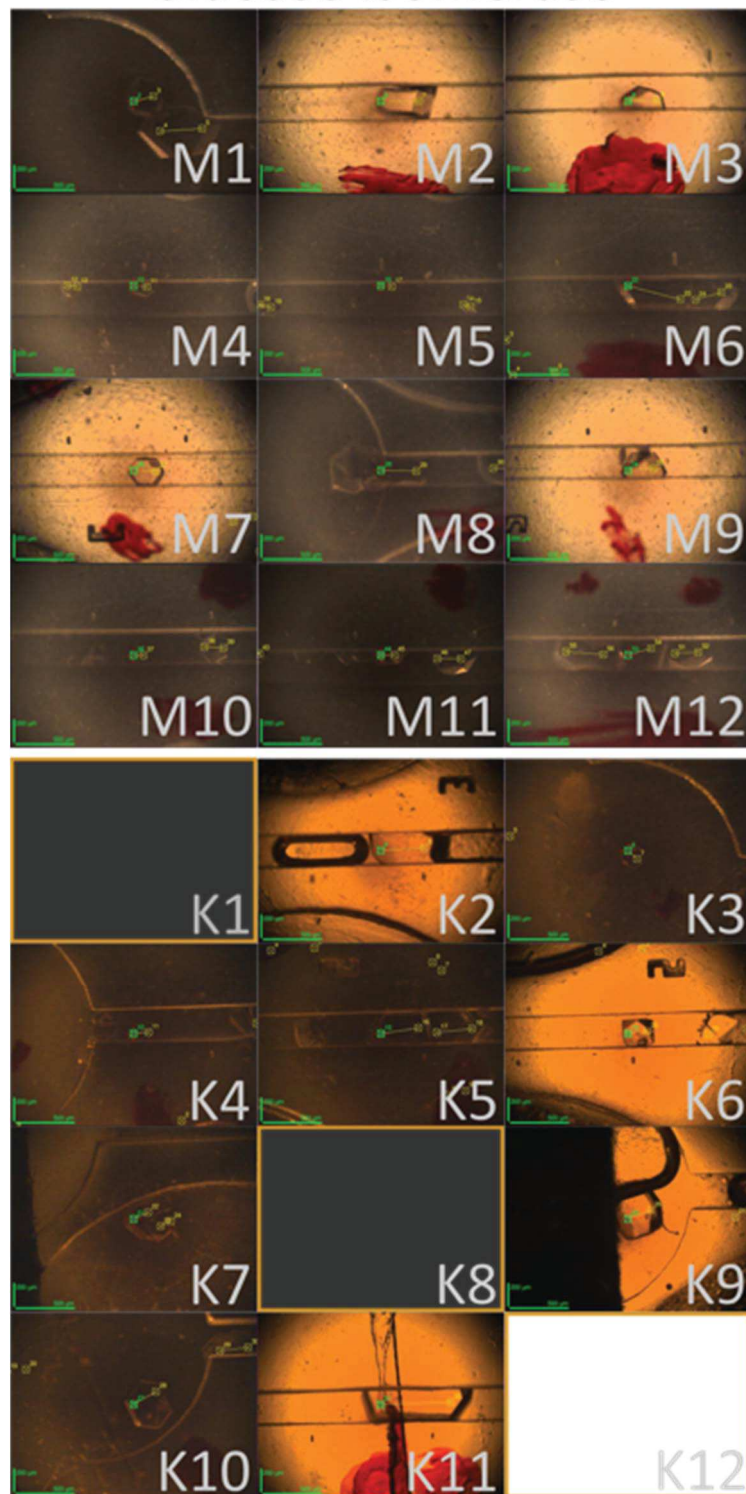


Figure S1 Snapshot pictures of the counter-diffusion crystallization experiments of glucose isomerase implemented in Mylar (M1 to M12) and Kapton (K1 to K12) microchips. Green-path on the crystals shows initial and final points of the helical trajectories followed for data collection.

Lysozyme

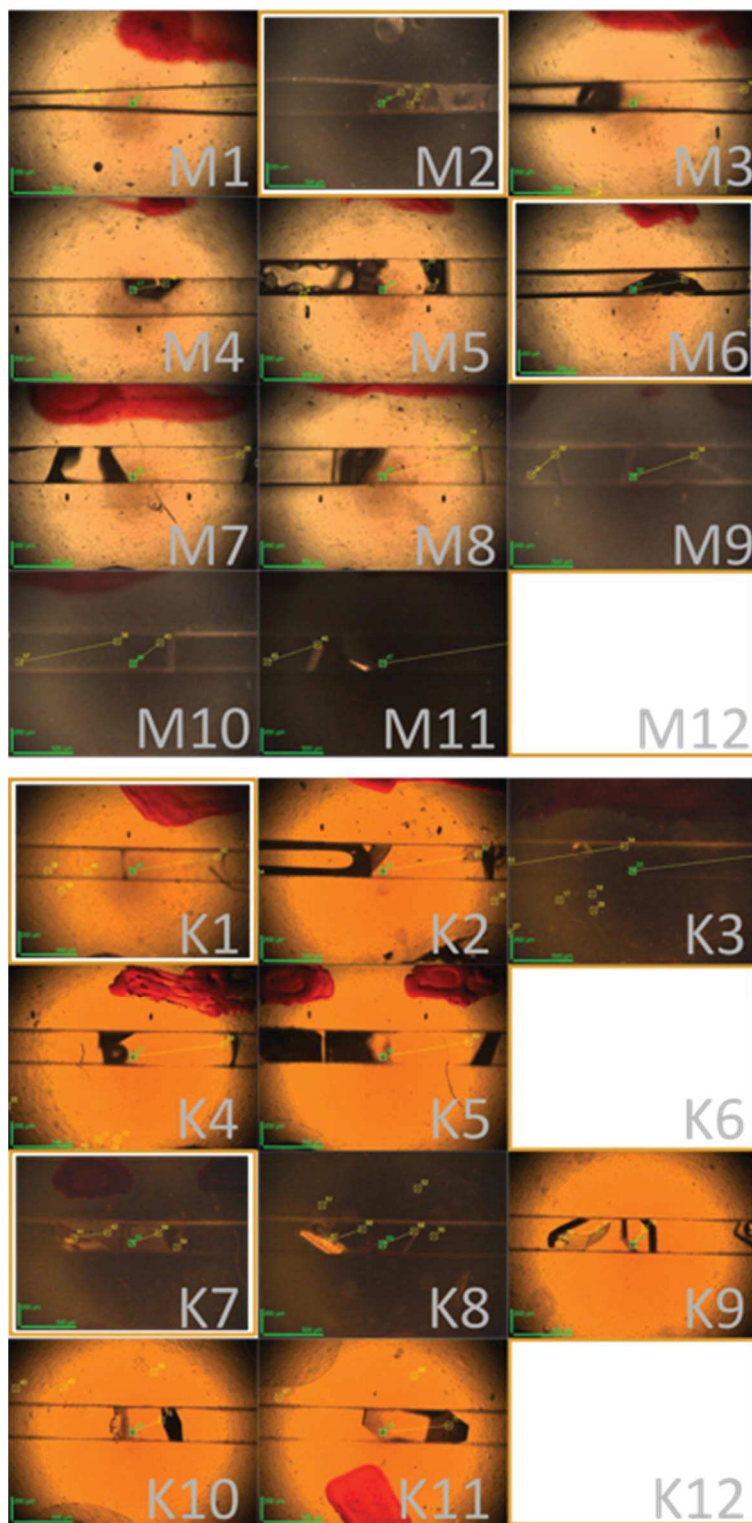


Figure S2 Snapshot pictures of the counter-diffusion crystallization experiments of lysozyme implemented in Mylar (M1 to M12) and Kapton (K1 to K12) microchips. Green-path on the crystals shows initial and final points of the helical trajectories followed for data collection.

Thaumatoin

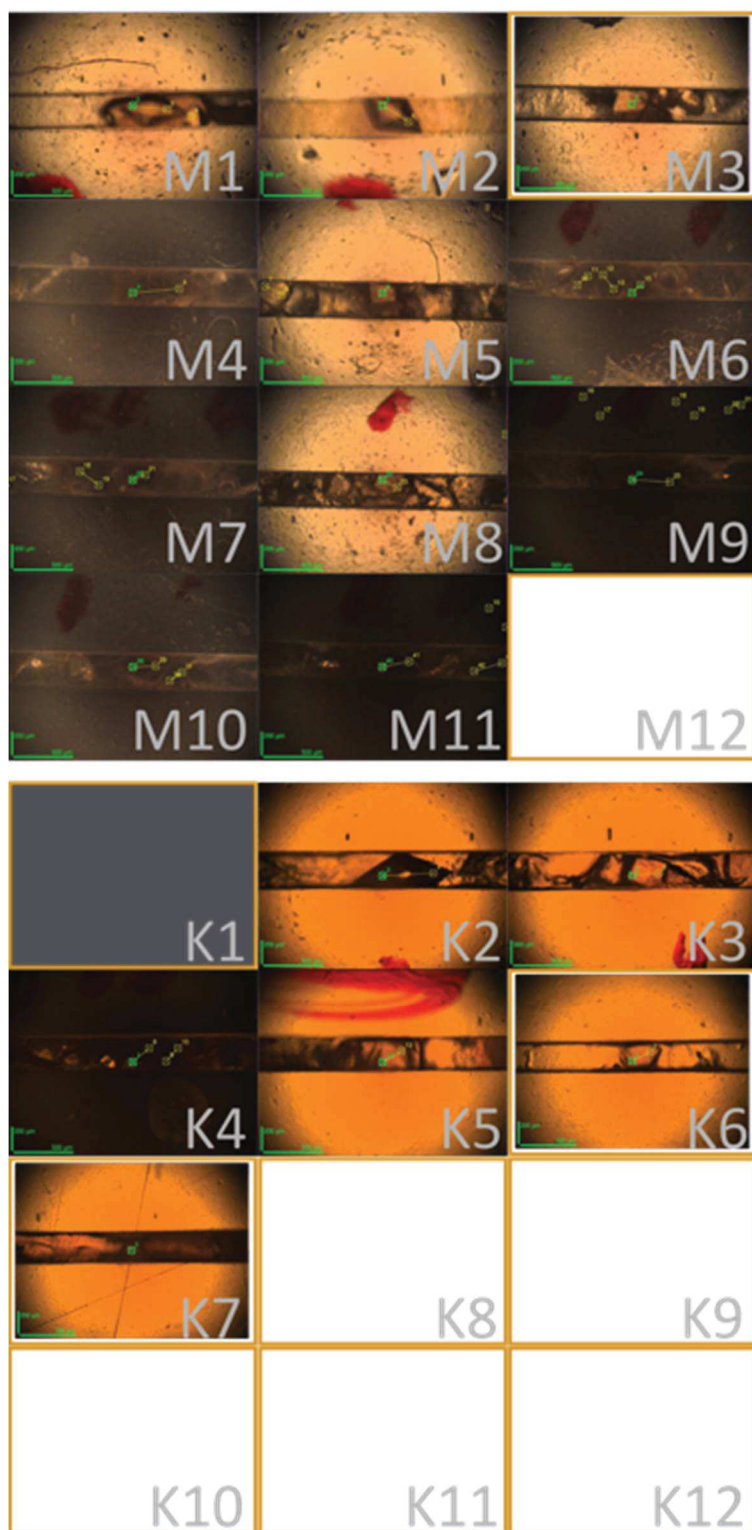


Figure S3 Snapshot pictures of the counter-diffusion crystallization experiments of thaumatoin implemented in Mylar (M1 to M12) and Kapton (K1 to K12) microchips. Green-path on the crystals shows initial and final points of the helical trajectories followed for data collection.

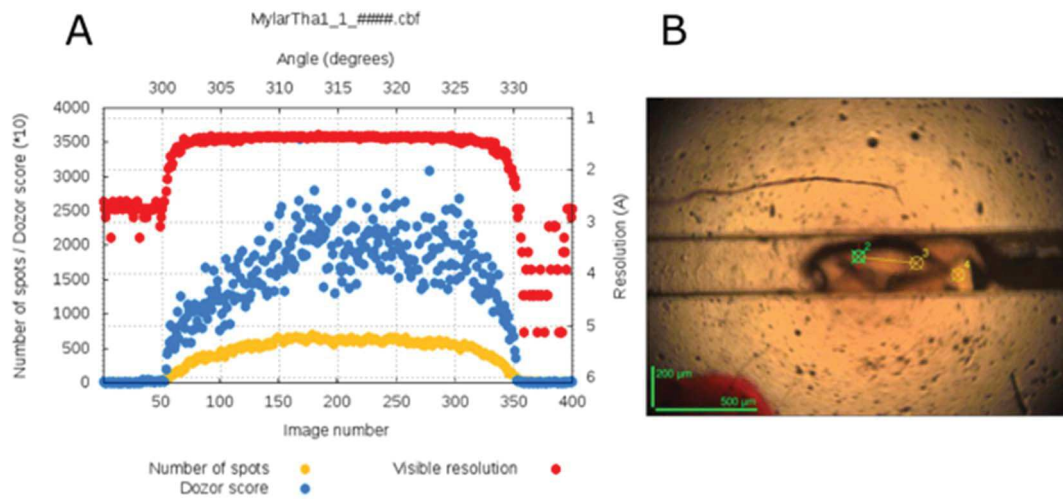


Figure S4 A. Snapshot pictures of the Dozor score output of the data collection of a thaumatin crystal exemplifying the difficulties in properly centering the crystals in the plane perpendicular to the X-ray beam. B. Helical trajectory (2 to 3) followed during data collection.

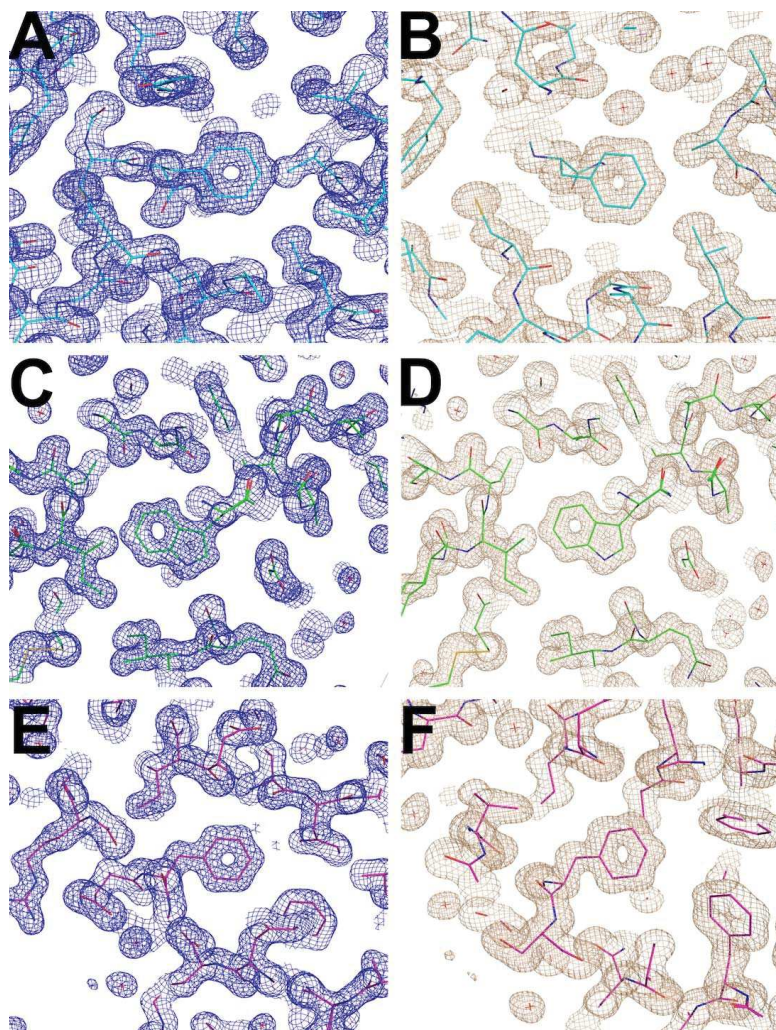


Figure S5 Snapshot of the $|2F_o - F_c|$ electron-density maps contoured at 1.0σ showing the built models of glucose isomerase (cyan), lysozyme (green) and thaumatin (pink). A, C, E (blue) and B, D, E (brownish) maps correspond to crystals grown in Mylar and Kapton chips, respectively.

Supplementary multimedia

Supplementary Movie S1 represents a full dataset collected by rotating 45° .

Table S1 Summary of the data collection conditions and final statistical values for glucose isomerase crystals grown in the Kapton microchips

The final statistical values are from XSDAPP, XIA2, EDNA or aimless (note as ccp4).

Dataset	KGlu2	KGlu3	KGlu4	KGlu5	KGlu6	KGlu7	KGlu9	KGlu10	KGlu11
Data Acquisition									
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	268	188	188	188	188	188	159	159	159
Number of images	400	400	450	450	450	450	450	450	450
Oscillation (°)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Transmission (%)	9.8	9.8	9.8	9.8	9.8	9.8	19.2	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Data Statistics	XDSAPP	XIA2	XIA2	EDNA/XIA2	autoPROC	EDNA/ccp4	EDNA/ccp4	XIA2	XIA2
Space group	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 222	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2
Unit cell a, b, c (Å)	93.95, 99.36, 103.05	94.03, 99.37, 103.07	93.95, 99.37, 103.06	94.03, 99.41, 103.09	94.05, 99.40, 103.06	94.06, 99.42, 103.24	93.97, 99.42, 103.05	94.03, 99.35, 103.07	93.99, 99.36, 103.05
Resolution (Å) (High shell)	41.13-1.50 (1.40-1.50)	40.01-1.23 (1.25-1.23)	40.00-1.08 (1.10-1.08)	41.15-1.12 (1.15-1.12)	51.53-1.35 (1.37-1.35)	41.19-1.30 (1.33-1.30)	41.13-1.15 (1.17-1.15)	39.29-1.16 (1.19-1.16)	41.13-1.11 (1.14-1.11)
Unique reflections	50656	91046	124576	142169	55424	101639	98050	141313	157647
R-merge * (%)	8.7 (9.6)	7.9 (51.8)	7.5 (49.0)	8.2 (35.6)	9.3 (38.5)	6.2 (65.9)	5.1 (18.4)	6.4 (55.0)	10.5 (53.1)
<I/σ(I)>	9.2 (7.5)	5.0 (1.1)	5.4 (1.0)	5.0 (1.1)	5.6 (2.1)	5.2 (0.9)	14.8 (2.3)	5.4 (1.3)	3.7 (0.9)
Completeness (%)	68.3 (70.8)	65.8 (66.9)	61.3 (35.1)	77.7 (65.1)	52.1 (56.7)	86.5 (90.5)	57.9 (47.4)	85.9 (81.7)	84.0 (84.1)
Multiplicity	1.4 (1.4)	2.1 (2.1)	2.3 (1.6)	1.9 (1.4)	2.2 (2.0)	1.9 (1.8)	1.9 (1.4)	1.8 (1.8)	1.9 (1.8)
CC(1/2)	98 (97)	98 (62)	98.9 (66.1)	97.7 (61.5)	98.6 (84.5)	97.5 (61.5)	99.2 (95.3)	98.4 (55.8)	96.1 (62.7)
B-factor (Å ²)	11.7	13.7	13.5	12.6	14.68	13.8	12.5	11.6	11.8
Mosaicity (°)	0.016	0.04	0.11	0.08	0.2	0.08	0.04	0.03	0.01

Dataset	KGlu3b	KGlu4b	KGlu5b	KGlu7b	KGlu10-2
Data Acquisition					
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	188	188	188	188	159
Number of images	400	450	450	450	450
Oscillation (°)	0.1	0.1	0.1	0.1	0.1
Transmission (%)	9.8	9.8	9.8	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02
Data Statistics					
	XIA2	XIA2	EDNA/ccp4	EDNA/ccp4	EDNA/ccp4
Space group	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2
Unit cell a, b, c (Å)	94.04, 99.36, 103.07	94.012, 99.33, 103.045	93.99, 99.38, 103.07	94.01, 99.40, 103.10	94.03, 99.35, 103.07
Resolution (Å) (High shell)	47.02-1.28 (1.31-1.28)	41.13-1.20 (1.22-1.20)	41.14-1.05 (1.07-1.05)	41.14-1.67 (1.70-1.67)	39.29-1.16 (1.17-1.15)
Unique reflections	81005	111428	138864	43838	119599
R-merge * (%)	6.3 (67.4)	7.4 (52.5)	5.8 (59.4)	5.1 (6.6)	5.9 (47.5)
<I/σ(I)>	6.1 (1.0)	5.8 (1.0)	5.9 (1.2)	17.0 (10.8)	4.8 (0.7)
Completeness (%)	66.0 (69.0)	74.4 (81.20)	62.6 (30.1)	78.8 (75.3)	70.7 (61.8)
Multiplicity	2.2 (1.9)	2.1 (1.9)	1.8 (1.0)	1.9 (1.7)	1.7 (1.5)
CC(1/2)	98.6 (55.4)	98.1 (59.1)	99.1 (89.7)	99.2 (98.1)	99.0 (84.6)
B-factor (Å ²)	13.57	13.47	11.6	12.7	12.8
Mosaicity (°)	0.046	0.067	0.03	0.06	0.03

Table S2 Summary of the data collection conditions and final statistical values for glucose isomerase crystals grown in the Mylar microchips.

The final statistical values are from XSDAPP, XIA2, EDNA or aimless (note as ccp4).

Dataset	MylarGlu1	MylarGlu2	MylarGlu3	MylarGlu4	MylarGlu5	MylarGlu6	MylarGlu7	MylarGlu8	MylarGlu9
Data Acquisition									
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	188	188	188	215	215	188	188	188	188
Number of images	450	450	450	450	450	450	450	450	450
Oscillation (°)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Transmission (%)	9.8	9.8	9.8	9.8	9.8	9.8	9.8	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Data Statistics	EDNA/ccp4	EDNA	parallelProc	XIA2	EDNA	autoProc/ccp4	EDNA/ccp4	EDNA/ccp4	autoProc
Space group	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2
Unit cell a, b, c (Å)	93.99, 99.37, 103.10	95.93, 99.40, 104.87	94.01, 99.40, 103.10	94.016, 99.42, 103.09	94.08, 99.40, 103.10	93.94, 99.38, 103.10	93.93, 99.32, 103.01	93.98, 99.35, 103.01	93.93, 99.41, 103.07
Resolution (Å)	39.28-1.10	42.13-1.18	39.29-1.30	68.30-1.26	47.04-1.30	41.14-1.06	47.01-1.20	40.30-1.05	41.13-1.15
(High shell)	(1.12-1.10)	(1.22-1.18)	(1.32-1.30)	(1.29-1.26)	(1.39-1.30)	(1.10-1.06)	(1.22-1.20)	(1.07-1.15)	(1.17-1.15)
Unique reflections	123280	112849	100012	109177	90258	152288	111745	151745	133170
R-merge * (%)	5.6 (25.9)	12.1 (47.0)	7.6 (61.1)	6.5 (59.3)	4.3 (77.7)	7.7 (42.5)	5.6 (66.2)	5.8 (64.5)	6.8 (28.3)
<I/σ(I)>	10.7 (3.0)	3.3 (0.9)	3.7 (1.0)	5.5 (1.1)	8.4 (1.1)	7.3 (1.2)	4.1 (1.1)	12.5 (1.2)	6.8 (2.2)
Completeness (%)	64.0 (33.6)	65.9 (54.5)	85.2 (88.1)	84.8 (87.5)	76.9-79.9	70.9 (31.9)	75.2 (69.0)	68.3 (25.8)	71.8 (70.9)
Multiplicity	1.8 (1.5)	2.2 (2.0)	1.8 (1.8)	1.9 (1.8)	2.1 (2.0)	1.9 (1.5)	1.9 (1.8)	1.7 (1.2)	1.8 (1.6)
CC(1/2)	99.0 (91.6)	96.4 (62.9)	98.4 (67.0)	97.9 (48.0)	99.7 (48.5)	98.3 (64.9)	99.2 (77.5)	99.0 (75.0)	98.9 (88.9)
B-factor (Å ²)	11.4	9.7	12.9	23.78	13.7	18.3	12.8	12.0	13.2
Mosaicity (°)	0.03	0.03	0.00	0.08	0.03	0.02	0.02	0.03	0.06

Dataset	MylarGlu6b	MylarGlu8b	MylarGlu10	MylarGlu11	MylarGlu12
Data Acquisition					
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	188	188	188	242	242
Number of images	450	450	450	450	450
Oscillation (°)	0.1	0.1	0.1	0.1	0.1
Transmission (%)	9.8	9.8	9.8	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02
Data Statistics	autoPROC/ccp4	EDNA/ccp4	EDNA/ccp4	autoProc	EDNA/ccp4
Space group	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2	I 2 2 2
Unit cell a, b, c (Å)	93.94, 99.38, 103.10	93.93, 99.32, 103.01	93.96, 99.39, 103.07	94.03, 99.38, 103.07	93.94, 99.41, 103.09
Resolution (Å) (High shell)	41.14-1.06 (1.10-1.06)	40.39-1.10 (1.12-1.10)	39.27-1.25 (1.27-1.25)	69.46-1.15 (1.17-1.15)	40.42-1.18 (1.21-1.18)
Unique reflections	152288	129386	90696	103887	116638
R-merge * (%)	7.7 (42.5)	4.6 (74.3)	9.1 (59.9)	4.9 (29.4)	8.2(30.9)
<I/σ(I)>	7.3 (1.2)	11.2 (1.4)	7.1 (1.2)	10.2 (2.0)	6.0 (1.0)
Completeness (%)	70.9 (31.9)	67.0 (40.9)	68.9 (69.4)	61.8 (14.8)	74.5 (23.4)
Multiplicity	1.9 (1.5)	2.0 (1.5)	2.3 (2.2)	1.7 (1.1)	1.7 (1.3)
CC(1/2)	98.3 (64.9)	99.4 (79.0)	98.7 (61.6)	99.4 (87.0)	96.9 (86.6)
B-factor (Å ²)	18.3	12.3	13.1	15.18	13.1
Mosaicity (°)	0.02	0.03	0.03	0.03	0.02

Table S3 Summary of the data collection conditions and final statistical values for lysozyme crystals grown in the Mylar microchips.

The final statistical values are from XSDAPP, XIA2, EDNA or aimless (note as ccp4).

Dataset	MylarLzm1	MylarLzm3	MylarLzm4	MylarLzm5	MylarLzm7	MylarLzm8	MylarLzm9	MylarLzm10	MylarLzm11
Data Acquisition									
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	242	242	242	242	242	242	242	242	242
Number of images	400	400	400	400	450	450	450	450	450
Oscillation (°)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Transmission (%)	100	9.8	9.8	9.8	9.8	9.8	9.8	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Data Statistics	XDSAPP/ccp4	autoProc/ccp4	XDSAPP/ccp4	parallel	XDSAPP/ccp4	EDNA/ccp4	XDSAPP	EDNA	autoProc/ccp4
Space group	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2
Unit cell									
a= b, c (Å)	78.48, 37.53	79.15, 37.97	78.85, 38.30	78.82, 38.27	79.08, 37.86	79.18, 37.93	79.19, 37.97	79.17, 37.97	79.18, 37.97
Resolution (Å)	39.24-1.85	34.23-1.20	35.50-1.31	39.40-1.12	39.54-1.27	27.99-1.19	34.24-1.17	37.97-1.12	37.97-1.14
(High shell)	(1.89-1.85)	(1.22-1.20)	(1.33-1.31)	(1.16-1.12)	(1.31-1.27)	(1.21-1.19)	(1.19-1.17)	(1.16-1.12)	(1.16-1.14)
Unique reflections	5729	19568	23567	20612	29621	30310	31586	32304	32079
R-merge * (%)	30.0 (72.5)	6.9 (50.8)	8.0 (47.6)	6.5 (45.0)	7.0 (30.7)	5.5 (31.4)	9.2 (28.7)	6.0 (32.5)	8.2 (33.1)
<I/σ(I)>	4.8 (2.5)	11.5 (2.0)	10.1 (2.2)	15.9 (1.7)	8.1 (1.7)	12.8 (1.1)	8.7 (2.2)	13.1 (1.4)	10.4 (2.2)
Completeness (%)	54.1 (59.5)	52.6 (21.1)	80.6 (74.1)	44.0 (6.3)	92.8 (82.9)	78.0 (42.6)	77.1 (35.0)	70.3 (15.8)	72.3 (17.8)
Multiplicity	4.7 (4.6)	4.3 (3.3)	3.2 (2.4)	4.0 (1.7)	3.1 (2.0)	3.2 (1.6)	3.0 (1.6)	3.1 (1.1)	2.9 (1.2)
CC(1/2)	94.1 (62.0)	99.1 (61.5)	99.1 (72.8)	99.4 (77.4)	99.1 (82.9)	99.3 (82.5)	98.9 (86.8)	99.4 (74.0)	98.6 (84.1)
B-factor (Å ²)	13.9	15.5	14.1	15.1	17.18	14.7	16.7	14.6	15.6
Mosaicity (°)	0.311	0.31	0.02	0.03	0.06	0.04	0.03	0.03	0.02

Dataset	MylarLzm9b	MylarLzm10b	MylarLzm10b	MylarLzm11b	MylarLzm11c
Data Acquisition					
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	242	242	242	242	242
Number of images	450	450	450	450	450
Oscillation (°)	0.1	0.1	0.1	0.1	0.1
Transmission (%)	9.8	9.8	9.8	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02
Data Statistics					
	XDSAPP	EDNA	EDNA	autoProc/ccp4	autoProc/ccp4
Space group	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2
Unit cell					
a= b, c (Å)	79.19, 37.97	79.18, 37.97	79.18, 37.97	79.18, 37.97	79.11, 38.02
Resolution (Å)	34.24-1.15	37.97-1.12	34.25-1.16	34.24-1.14	37.97-1.12
(High shell)	(1.17-1.15)	(1.16-1.12)	(1.18-1.16)	(1.17-1.14)	(1.14-1.12)
Unique reflections	32346	32009	31774	31061	30859
R-merge * (%)	8.5 (43.1)	6.4 (28.4)	8.2 (32.8)	6.8 (31.7)	6.4 (23.2)
<I/σ(I)>	9.4 (2.0)	12.9 (1.6)	9.0 (0.9)	10.0 (0.9)	8.9 (2.0)
Completeness (%)	75.8 (28.8)	69.5 (15.1)	75.1 (30.5)	70.9 (19.1)	67.4 (8.7)
Multiplicity	2.9 (1.1)	3.0 (1.1)	3.1 (1.2)	3.2 (1.3)	3.1 (1.1)
CC(1/2)	98.8 (81.5)	99.2 (69.3)	98.6 (72.4)	98.8 (75.6)	99.1 (82.0)
B-factor (Å ²)	16.2	14.6	14.9	14.8	15.3
Mosaicity (°)	002	0.03	0.08	0.02	0.02

Table S4 Summary of the data collection conditions and final statistical values for lysozyme crystals grown in the Kapton microchips.

The final statistical values are from XSDAPP, XIA2, EDNA or aimless (note as ccp4).

Dataset	K-Lzm2	K-Lzm3	K-Lzm4	K-Lzm5	K-Lzm8	K-Lzm8	K-Lzm9	K-Lzm10	K-Lzm11
Data Acquisition									
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	242	242	188	188	188	188	188	188	188
Number of images	450	450	470	500	500	500	450	450	450
Oscillation (°)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Transmission (%)	9.8	9.8	9.8	19.2	9.8	9.8	9.8	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Data Statistics	EDNA	XIA2	EDNA/ccp4	EDNA/ccp4	EDNA/ccp4	autoProc/ccp4	parallel	EDNA/ccp4	EDNA/ccp4
Space group	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2	P 4 ₃ 2 ₁ 2
Unit cell									
a= b, c (Å)	79.14, 37.97	79.14, 38.99	78.91, 38.01	78.88, 37.96	79.11, 38.02	79.11, 38.03	79.14, 38.03	79.11, 38.03	79.11, 38.05
Resolution (Å)	39.57-1.19	38.00-1.20	39.46-1.10	39.44-1.55	34.27-1.10	55.94-1.13	38.03-1.14	35.28-1.15	34.29-1.15
(High shell)	(1.23-1.19)	(1.23-1.20)	(1.12- 1.10)	(1.58-1.55)	(1.12- 1.10)	(1.15-1.13)	(1.18-1.14)	(1.17-1.15)	(1.17-1.15)
Unique reflections	34031	33642	46282	12437	45994	40888	39675	35695	33808
R-merge * (%)	7.0 (50.8)	8.3 (29.4)	6.5 (82.8)	14.5 (89.5)	6.5 (87.1)	9.7 (40.0)	8.5 (75.4)	7.4 (66.2)	8.8 (65.0)
<I/σ(I)>	8.0 (1.3)	10.1 (1.2)	8.4 (0.8)	8.0 (3.6)	11.5 (1.1)	7.5 (2.2)	7.9 (1.1)	13.0 (1.1)	10.6 (1.3)
Completeness (%)	87.0 (49.6)	58.5 (59.0)	94.7 (68.2)	69.5 (74.1)	93.7 (68.7)	90.4 (70.6)	90.3 (81.6)	82.8 (84.7)	79.2 (71.5)
Multiplicity	2.9 (1.5)	2.0 (1.1)	3.1 (2.2)	4.5 (4.4)	3.2 (2.0)	3.1 (2.6)	3.1 (2.5)	3.4 (2.6)	3.8 (3.2)
CC(1/2)	99.1 (75.5)	98.0 (79.9)	99.1 (45.5)	96.6 (39.8)	99.3 (68.7)	98.8 (84.5)	98.6 (53.4)	99.1 (63.6)	99.1 (68.2)
B-factor (Å ²)	15.4	14.13	14.1	13.4	14.6	16.2	14.3	14.9	14.4
Mosaicity (°)	0.05	0.00	0.05	0.28	0.03	0.02	0.03	0.03	0.03

Dataset	K-Lzm9b
Data Acquisition	
ESRF Beam-line	ID30B
Detector type	Pilatus3 6M
Wavelength (Å)	0.9763
Distance (mm)	188
Number of images	450
Oscillation (°)	0.1
Transmission (%)	9.8
Exposure time (ms)	0.02
Data Statistics	parallel
Space group	P 4 ₃ 2 ₁ 2
Unit cell	
a= b, c (Å)	79.14, 38.03
Resolution (Å)	34.27-1.18
(High shell)	(1.20-1.18)
Unique reflections	34498
R-merge * (%)	9.4 (85.4)
<I/σ(I)>	6.9 (1.4)
Completeness (%)	86.6 (84.9)
Multiplicity	3.5 (3.4)
CC(1/2)	98.6 (5394)
B-factor (Å ²)	15.6
Mosaicity (°)	0.01

Table S5 Summary of the data collection conditions and final statistical values for thaumatin crystals grown in the Kapton microchips.

The final statistical values are from XSDAPP, XIA2, EDNA or aimless (note as ccp4).

Dataset	K-Thau2	K-Thau3	K-Thau4	K-Thau5
Data Acquisition				
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763
Distance (mm)	317	187	267	267
Number of images	400	400	450	450
Oscillation (°)	0.1	0.1	0.1	0.1
Exposure time (ms)	0.02	0.02	0.02	0.02
Transmission (%)	9.8	9.8	9.8	9.8
Data Statistics	autoPro/ccp4	autoPro/ccp4	XIA2	EDNA/ccp4
Space group	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2
Unit cell				
a, b, c (Å)	58.28, 151.45	58.50, 151.44	58.19, 151.35	57.18, 149.04
Resolution (Å)	39.76-1.32	54.57-1.30	54.31-1.43	45.37-2.10
(High shell)	(1.34-1.32)	(1.32-1.30)	(1.45-1.43)	(2.16-2.10)
Unique reflections	40601	45819	46125	9496
R-merge * (%)	4.1 (25.7)	6.1 (45.2)	4.6 (62.7)	7.8 (68.0)
<I/σ(I)>	10.7 (1.6)	7.4 (1.5)	9.8 (1.0)	6.9 (0.9)
Completeness (%)	65.8 (10.9)	71.0 (57.8)	94.0 (89.9)	62.6 (50.1)
Multiplicity	2.5 (1.0)	3.1 (1.4)	2.8 (2.4)	2.6 (2.4)
CC(1/2)	99.7 (84.6)	99.4 (81.4)	98.8 (63.6)	99.6 (62.8)
B-factor (Å ²)	16.7	17.5	18.51	31.7
Mosaicity (°)	0.04	0.03	0.01	0.86

Table S6 Summary of the data collection conditions and final statistical values for lysozyme crystals grown in the Mylar microchips.

The final statistical values are from XSDAPP, XIA2, EDNA or aimless (note as ccp4).

Dataset	MylarThau1	MylarThau2	MylarThau4	MylarThau4b	MylarThau5	MylarThau6	MylarThau7	MylarThau8	MylarThau9
Data Acquisition									
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	267	267	267	267	267	267	188	188	268
Number of images	400/300	400/250	400	400	400	400	400	400	400
Oscillation (°)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Transmission (%)	100	100	100	9.8	9.8	9.8	19.2	19.2	19.2
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Data Statistics	autoPro/ccp4	XDSAPP/ccp4	EDNA/ccp4	XDSAPP/ccp4	XIA2/ccp4	EDNA/ccp4	XIA2	EDNA/ccp4	EDNA/ccp4
Space group	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2
Unit cell									
a, b, c (Å)	58.58, 151.54	58.61, 151.58	58.55, 151.58	58.52, 151.55	58.49, 151.71	58.57, 151.56	58.57, 151.51	58.57, 151.55	58.57, 151.57
Resolution (Å)	38.26-1.40	39.98-1.30	46.34-1.20	54.59-1.35	41.36-1.38	41.41-1.40	54.63-1.30	46.34-1.35	46.34-1.25
(High shell)	(1.42-1.40)	(1.32-1.30)	(1.22-1.20)	(1.39-1.35)	(1.40-1.38)	(1.42-1.40)	(1.33-1.30)	(1.37-1.35)	(1.27-1.25)
Unique reflections	45224	48703	55591	54511	37150	48286	57029	55886	57570
R-merge * (%)	7.6 (60.7)	10.1 (66.8)	5.1 (26.1)	7.8 (42.1)	7.0 (68.8)	8.1 (74.1)	9.8 (80.5)	10.5 (88.5)	8.4 (33.7)
<I/σ(I)>	7.0 (1.5)	6.5 (0.6)	17.3 (0.9)	6.8 (1.3)	8.9 (1.4)	9.5 (1.2)	5.8 (1.2)	6.3 (1.2)	6.0 (1.0)
Completeness (%)	86.7 (75.6)	74.9 (42.6)	67.6 (14.9)	92.8 (66.6)	68.6 (58.8)	92.5 (92.1)	87.4 (89.7)	95.8 (97.4)	79.1 (75.0)
Multiplicity	2.2 (1.9)	2.0 (1.4)	2.5 (1.1)	2.7 (1.9)	3.9 (2.7)	2.9 (2.1)	3.2 (3.2)	2.9 (2.9)	2.8 (2.2)
CC(1/2)	98.5 (47.5)	96.5 (45.5)	99.4 (95.9)	98.4 (71.1)	99.2 (57.9)	98.8 (59.9)	98.2 (52.3)	98.3 (53.4)	98.6 (90.8)
B-factor (Å ²)	16.9	12.9	13.8	14.1	16.4	15.1	14.2	13.1	13.8
Mosaicity (°)	0.13	0.09	0.04	0.01	0.01	0.02	0.02	0.03	0.03

Dataset	MylarThau9b	MylarThau10b	MylarThau11	MylarThau13	MylarThau14b
Data Acquisition					
ESRF Beam-line	ID30B	ID30B	ID30B	ID30B	ID30B
Detector type	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M	Pilatus3 6M
Wavelength (Å)	0.9763	0.9763	0.9763	0.9763	0.9763
Distance (mm)	187	187	188	188	188
Number of images	400	400	400	400	400
Oscillation (°)	0.1	0.1	0.1	0.1	0.1
Transmission (%)	19.2	19.2	9.8	9.8	9.8
Exposure time (ms)	0.02	0.02	0.02	0.02	0.02
Data Statistics	XIA2	XIA2	XIA2/ccp4	XIA2/ccp4	XIA2/ccp4
Space group	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2	P 4 ₁ 2 ₁ 2
Unit cell					
a, b, c (Å)	58.58, 151.55	58.58, 151.56	58.57, 151.55	58.57, 151.55	58.57, 151.55
Resolution (Å)	54.64-1.25	39.95-1.32	54.63-1.32	54.63-1.38	38.25-1.34
(High shell)	(1.28-1.25)	(1.35-1.32)	(1.34-1.32)	(1.40-1.38)	(1.36-1.34)
Unique reflections	72059	60512	51725	49938	53759
R-merge * (%)	7.6 (73.4)	8.8 (91.5)	10.3 (78.4)	10.3 (69.8)	10.3 (65.0)
<I/σ(I)>	5.6 (1.0)	5.2 (1.1)	5.4 (1.1)	5.0 (1.3)	4.8 (1.1)
Completeness (%)	97.9 (95.9)	96.9 (95.6)	83.4 (89.2)	91.8 (90.0)	90.0 (90.8)
Multiplicity	2.8 (2.7)	2.9 (3.0)	3.3 (3.1)	3.0 (3.1)	3.0 (3.1)
CC(1/2)	98.4 (57.4)	98.0 (51.0)	95.1 (50.7)	98.4 (64.7)	98.4 (59.2)
B-factor (Å ²)	14.9	14.6	16.5	15.1	15.5
Mosaicity (°)	0.01	0.01	0.01	0.01	0.01

Table S7 Resolution limit of the three model proteins, lysozyme, thaumatin and glucose isomerase, obtained from microfluidic systems compared with the data obtained in this work.

Material	Resolution limit (Å)			Publication
	Lysozyme	Thaumatin	Glucose Isomerase	
Kapton	1.13	1.35	1.06	This work
Mylar	1.12	1.14	1.20	This work
	1.75	2.00		(Ng <i>et al.</i> , 2008)
COC	1.5	1.65		(Dhouib <i>et al.</i> , 2009)
	1.43	1.55		(Pinker <i>et al.</i> , 2013)
PDMS		1.25		(Hansen <i>et al.</i> , 2006)
		2.80		(Dhouib <i>et al.</i> , 2009)
PMMA		1.85		(Dhouib <i>et al.</i> , 2009)
Droplet system	1.9			(Gerdtts <i>et al.</i> , 2008)*
			2.1	(Heymann <i>et al.</i> , 2014)
Kapton	-	1.89	1.75	(Gicquel <i>et al.</i> , 2018)

*Polycarbonate