

Supplementary Material.

Table 1. Data collection and processing statistics of the seven ConA-Xe diffraction data sets

Data Collection		1.00	1.50	1.70	1.90	2.10	2.30	2.50
λ [Å]		1.00	1.50	1.70	1.90	2.10	2.30	2.50
detector dist. [mm]		120	70	55	40	36	36	36
$d_{\min, \text{obs}}$ [Å]		1.75	1.85	1.85	1.83	1.95	2.14	2.40
$\Delta\phi$ [°]		1	1	1	1	1	1	1
no. images		360	360	360	360	283	360	230
Data Processing		99.0–2.40 (2.46–2.40)	99.0–2.40 (2.46–2.40)	99.0–2.40 (2.46–2.40)	99.0–2.40 (2.46–2.40)	99.0–2.40 (2.46–2.40)	99.0–2.40 (2.46–2.40)	99.0–2.40 (2.46–2.40)
d_{\min} [Å]		125613	126099	123708	117451	87425	100307	58419
total no. reflections		9457	9529	9542	9558	9573	9604	9614
unique reflections		0	0	1	3	1	3	2
rejected reflection		13.3	13.2	13.0	12.3	9.1	10.4	6.1
Redundancy		99.9 (100)	99.9 (100)	99.9 (100)	99.9 (100)	99.9 (100)	99.9 (100)	99.8 (100)
completeness [%]		54.9 (38.8)	62.3 (43.5)	61.4 (39.1)	57.4 (33.1)	46.0 (25.8)	44.3 (22.0)	28.5 (6.9)
$I/\sigma(I)$		0.57	0.58	0.59	0.58	0.60	0.55	0.44
Mosaicity [°]		4.3 (6.8)	4.1 (5.6)	4.4 (6.4)	4.5 (7.2)	4.9 (7.7)	5.3 (9.9)	6.2 (24.0)
R_{merge}		4.4 (7.1)	4.2 (5.8)	4.5 (6.6)	4.7 (7.6)	5.2 (8.3)	5.6 (10.5)	6.8 (26.9)
$R_{\text{p.i.m.}}$		1.2 (1.9)	1.1 (1.6)	1.2 (1.9)	1.3 (2.3)	1.7 (3.0)	1.7 (3.5)	2.6 (11.8)
R_{anom}		1.5 (2.1)	2.4 (3.3)	2.9 (4.0)	3.1 (4.6)	3.6 (5.4)	3.5 (5.5)	3.8 (12.4)
estimated $\Delta F/F$ [%]		1.9	3.8	4.7	5.3	6.1	6.2	5.4

Table 2. Data collection and processing statistics of the nine Adaptin-Xe diffraction data sets

Data Collection		0.80	1.50	1.70	1.90	2.10	2.25	2.40	2.50	2.65
λ [Å]		0.80	1.50	1.70	1.90	2.10	2.25	2.40	2.50	2.65
detector dist. [mm]		150	70	55	40	36	36	36	36	36
$d_{\min, \text{obs}}$ [Å]		1.65	1.82	1.82	1.82	1.94	2.08	2.22	2.30	2.44
$\Delta\phi$ [°]		1	1	1	1	1	1	1	1	1
no. images		360	360	360	360	360	360	360	360	360
Data Processing		99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)
d_{\min} [Å]		57667	56144	52068	50831	51546	50390	50045	47108	45843
total no. reflections		4807	4917	4722	4709	4855	4963	5047	5058	5021
unique reflections		0	4	20	13	13	57	12	213	40
rejected reflection		12.0	11.4	11.0	10.8	10.6	10.2	9.9	9.3	9.1
Redundancy		99.8 (100)	99.0 (100)	94.5* (100)	93.9* (100)	96.3* (100)	98.4* (100)	99.9 (100)	100 (100)	99.2 (89.9)
completeness [%]		60.6 (55.5)	94.0 (83.9)	89.6 (80.7)	77.4 (59.9)	57.6 (40.6)	53.4 (36.2)	39.8 (23.8)	34.7 (16.0)	23.4 (4.3)
$I/\sigma(I)$		0.36	0.30	0.29	0.30	0.24	0.30	0.30	0.31	0.27
Mosaicity [°]		4.4 (4.6)	3.3 (3.7)	3.8 (4.3)	4.2 (5.5)	5.7 (8.6)	6.0 (8.9)	8.5 (12.8)	8.8 (20.2)	11.0 (45.0)
R_{merge}		4.7 (4.8)	3.5 (3.8)	4.0 (4.5)	4.4 (5.7)	6.0 (9.0)	6.4 (9.4)	9.0 (13.6)	9.5 (21.8)	11.9 (50.1)
$R_{\text{p.i.m.}}$		1.3 (1.3)	1.0 (1.1)	1.2 (1.3)	1.3 (1.7)	1.8 (2.7)	2.0 (3.0)	2.9 (4.6)	3.2 (7.9)	4.2 (21.1)
R_{anom}		1.4 (1.6)	2.2 (2.7)	2.8 (3.7)	3.2 (4.4)	4.3 (5.9)	4.3 (6.3)	4.7 (6.5)	5.9 (8.8)	6.1 (18.5)
estimated $\Delta F/F$ [%]		1.2	3.5	4.3	5.2	6.0	6.7	6.6	5.3	2.9

* ice ring formation led to a reduction of the completeness in the 3.64–3.45 resolution bin.

Table 4. Data collection and processing statistics of the nine HEL-Xe diffraction data sets

Data Collection		0.80	1.50	1.70	1.90	2.10	2.25	2.40	2.50	2.65
λ [Å]		0.80	1.50	1.70	1.90	2.10	2.25	2.40	2.50	2.65
detector dist. [mm]		150	70	55	40	36	36	36	36	36
$d_{\min, \text{obs}}$ [Å]		1.65	1.82	1.82	1.82	1.94	2.08	2.22	2.30	2.44
$\Delta\phi$ [°]		1	1	1	1	1	1	1	1	1
no. images		360	360	360	360	360	360	360	360	360
Data Processing		99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.44 (2.50–2.44)	99.0–2.60 (2.67–2.60)
d_{\min} [Å]		108370	107740	112967	111837	110219	104052	96191	90955	66275
total no. reflections		4411	4793	4567	4572	4590	4608	4620	4626	3854
unique reflections		27	1	4	5	1	5	3	12	0
rejected reflection		24.6	22.5	24.7	24.5	24.0	22.6	20.8	19.7	17.2
Redundancy		100 (100)	100 (100)	99.9 (100)	99.9 (100)	99.9 (100)	99.9 (100)	100 (100)	100 (100)	100 (100)
completeness [%]		77.8 (54.4)	80.9 (46.7)	85.0 (61.7)	78.4 (59.6)	71.9 (51.1)	63.4 (39.8)	50.4 (22.5)	43.3 (13.6)	17.2 (14.5)
$I/\sigma(I)$		0.68	0.75	0.75	0.77	0.78	0.78	0.84	0.83	0.77
Mosaicity [°]		4.0 (5.7)	3.7 (5.4)	3.9 (5.5)	4.3 (5.8)	4.7 (6.9)	5.2 (8.6)	6.1 (14.4)	6.6 (23.2)	10.6 (62.0)
R_{merge}		4.1 (5.8)	3.8 (5.7)	3.9 (5.6)	4.4 (5.9)	4.8 (7.0)	5.3 (8.8)	6.2 (14.8)	6.8 (23.9)	10.9 (64.2)
$R_{\text{p.i.m.}}$		0.8 (1.1)	0.8 (1.5)	0.8 (1.1)	0.9 (1.2)	1.0 (1.4)	1.1 (1.9)	1.3 (3.5)	1.5 (5.8)	2.6 (16.6)
R_{anom}		0.8 (1.0)	1.5 (2.2)	1.7 (2.5)	2.1 (2.7)	2.4 (3.4)	2.7 (3.8)	2.9 (5.2)	2.9 (5.2)	3.7 (14.6)
estimated $\Delta F/F$ [%]		1.0	2.9	3.6	4.3	5.0	5.6	5.7	5.1	4.1

Table 6. Data collection and processing statistics of the five HEL diffraction data sets

Data Collection						
λ [Å]	1.50	1.70	1.90	2.10	2.30	
detector dist. [mm]	70	55	40	40	40	
$d_{\min, \text{obs}}$ [Å]	1.85	1.85	1.85	2.04	2.20	
$\Delta\phi$ [°]	1	1	1	1	1	
no. images	360	360	360	360	360	
Data Processing						
d_{\min} [Å]	99.0–2.20 (2.26–2.20)	99.0–2.20 (2.26–2.20)	99.0–2.20 (2.26–2.20)	99.0–2.20 (2.26–2.20)	99.0–2.20 (2.26–2.20)	
total no. reflections	146779	150269	146503	140386	128250	
unique reflections	6290	6309	6324	6331	6187	
rejected reflection	9	49	2	2	0	
Redundancy	23.3	23.8	23.2	22.2	20.7	
completeness [%]	99.5 (100)	99.7 (100)	99.8 (100)	99.9 (100)	99.7 (96.2)	
$I/\sigma(I)$	115.1 (100)	107.3 (88.5)	83.5 (63.8)	73.5 (52.3)	50.0 (23.3)	
Mosaicity [°]	0.39	0.39	0.41	0.43	0.44	
R_{merge}	3.1 (3.7)	3.4 (4.6)	4.3 (6.0)	4.9 (7.9)	7.1 (15.6)	
$R_{\text{r.i.m.}}$	3.2 (3.8)	3.5 (4.7)	4.4 (6.1)	5.1 (8.1)	7.3 (16.3)	
$R_{\text{p.i.m.}}$	0.7 (0.8)	0.7 (1.0)	0.9 (1.3)	1.1 (1.7)	1.5 (4.4)	
R_{anom}	1.2 (1.5)	1.5 (1.8)	1.8 (2.2)	2.1 (2.7)	2.4 (3.7)	
estimated $\Delta F/F$ [%]	1.4	1.8	2.2	2.7	3.1	

Table 7. Data collection and processing statistics of the eight Thermolysin diffraction data sets

	1	2	3	4	5	4	3	5
Data Collection								
Crystal								
λ [Å]	1.28	1.50	1.70	1.80	1.90	2.00	2.10	2.64
detector dist. [mm]	90	70	55	40	40	40	40	40
$d_{\min, \text{obs}}$ [Å]	1.82	1.85	1.82	1.82	1.82	1.94	2.24	2.56
$\Delta\phi$ [°]	0.5	0.5	0.5	0.5	0.5	0.5	0.5	1
no. images	720	720	720	720	720	720	720	360
Data Processing								
d_{\min} [Å]	99.0–2.24 (2.30–2.24)	99.0–2.24 (2.30–2.24)	99.0–2.24 (2.30–2.24)	99.0–2.24 (2.30–2.24)	99.0–2.24 (2.30–2.24)	99.0–2.24 (2.30–2.24)	99.0–2.24 (2.30–2.24)	99.0–2.56 (2.63–2.56)
total no. reflections	582453	630396	660154	649529	648954	629563	588036	398982
unique reflections	16632	16314	16465	16548	16587	16533	16451	11250
rejected reflection	3	108	55	4	7	4	48	25
Redundancy	35.0	38.6	40.1	39.3	39.1	38.1	35.7	35.5
completeness [%]	99.9 (99.9)	99.3 (99.3)	99.8 (99.8)	99.9 (99.9)	100 (100)	99.9 (99.9)	99.7 (99.7)	100(100)
$I/\sigma(I)$	84.3 (70.6)	80.0 (68.7)	112.1 (93.3)	112.6 (85.0)	112.6 (76.5)	97.1 (76.3)	59.0 (45.7)	66.7 (20.6)
Mosaicity [°]	0.27	0.51	0.51	0.33	0.24	0.34	0.55	0.32
R_{merge}	5.5 (6.4)	5.0 (6.6)	3.6 (5.6)	3.5 (5.9)	3.6 (6.1)	4.2 (6.8)	6.8 (11.8)	6.7 (24.3)
$R_{\text{r.i.m.}}$	5.6 (6.4)	5.1 (6.7)	3.7 (5.7)	3.6 (6.0)	3.7 (6.7)	4.3 (6.9)	6.9 (12.0)	6.8 (24.7)
$R_{\text{p.i.m.}}$	0.9 (1.1)	0.8 (1.1)	0.6 (0.9)	0.6 (0.9)	0.6 (1.0)	0.7 (1.1)	1.2 (2.1)	1.1 (4.5)
R_{anom}	2.1 (2.5)	1.2 (1.4)	1.3 (1.7)	1.4 (1.7)	1.6 (1.9)	1.7 (2.0)	2.0 (2.8)	2.8 (4.8)
estimated $\Delta F/F$ [%]	1.9	1.3	1.6	1.8	1.9	2.1	2.3	3.4

Table 8. Data collection and processing statistics of the six Trypsin diffraction data sets

Data Collection		1.00	1.50	1.90	2.10	2.30	2.50
λ [Å]		1.00	1.50	1.90	2.10	2.30	2.50
detector dist. [mm]		150	70	40	36	36	36
$d_{\min, \text{obs}}$ [Å]		2.10	1.84	1.88	1.95	2.15	2.32
$\Delta\phi$ [°]		0.5	0.5	0.5	0.5	0.5	0.5
no. images		720	720	720	720	720	720
Data Processing							
d_{\min} [Å]		99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)
total no. reflections		156412	160120	151076	135981	125089	113416
unique reflections		8258	8340	8378	8411	8438	8453
rejected reflection		2	4	5	3	17	23
Redundancy		18.9	19.2	18.0	16.2	14.8	13.4
completeness [%]		100 (100)	99.9 (100)	99.8 (100)	100 (100)	100 (100)	100 (100)
$I/\sigma(I)$		74.9 (59.6)	73.8 (62.2)	83.6 (66.4)	66.2 (43.2)	57.9 (30.3)	46.8 (18.5)
Mosaicity [°]		0.26	0.26	0.30	0.31	0.29	0.30
R_{merge}		3.3 (4.7)	3.5 (4.4)	32. (4.1)	3.9 (5.4)	4.1 (7.1)	4.6 (12.4)
$R_{\text{f.i.m.}}$		3.4 (4.8)	3.6 (4.5)	3.3 (4.2)	4.0 (5.6)	4.2 (7.5)	4.8 (13.1)
$R_{\text{p.i.m.}}$		0.8 (1.1)	0.8 (1.0)	0.8 (1.0)	1.0 (1.5)	1.0 (2.2)	1.2 (4.1)
R_{anom}		0.7 (0.9)	1.1 (1.4)	1.5 (1.8)	1.7 (2.2)	1.9 (2.9)	2.2 (4.5)
estimated $\Delta F/F$ [%]		0.6	1.3	2.0	2.4	2.8	3.2

Table 9. Data collection and processing statistics of the seven Thaumatin diffraction data sets

Data Collection		1.00	1.50	1.70	1.90	2.10	2.30	2.50*
λ [Å]		1.00	1.50	1.70	1.90	2.10	2.30	2.50*
detector dist. [mm]		120	70	55	40	36	36	36
$d_{\min, \text{obs}}$ [Å]		1.75	1.85	1.85	1.83	1.96	2.15	2.32
$\Delta\varphi$ [°]		0.6	0.6	0.6	0.6	0.6	0.6	0.6
no. images		600	600	600	600	600	600	256
Data Processing		99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)	99.0–2.32 (2.38–2.32)
total no. reflections		294929	303941	297298	272198	279246	249425	95804
unique reflections		11440	11568	11567	11571	11581	11557	11462
rejected reflection		1	6	4	2	6	1	1
Redundancy		25.8	26.3	25.7	23.5	24.1	21.6	8.4
completeness [%]		100 (100)	100 (100)	99.9 (99.8)	99.8 (99.4)	99.6 (98.7)	99.3 (98.0)	98.7 (95.0)
$I/\sigma(I)$		126.8(107.7)	106.4 (79.5)	109.6 (78.7)	77.3 (52.8)	78.3 (46.3)	56.2 (27.5)	30.1 (7.4)
Mosaicity [°]		0.44	0.36	0.45	0.48	0.31	0.40	0.50
R_{merge}		2.4 (3.2)	3.1 (4.3)	2.9 (4.3)	4.3 (6.1)	4.2 (7.4)	5.5 (13.5)	5.8 (27.5)
$R_{\text{f.i.m.}}$		2.4 (3.3)	3.2 (4.3)	3.0 (4.4)	4.3 (6.2)	4.3 (7.6)	5.7 (13.9)	6.1 (30.1)
$R_{\text{p.i.m.}}$		0.5 (0.6)	0.6 (0.8)	0.6 (0.8)	0.9 (1.3)	0.9 (1.7)	1.2 (3.3)	2.0 (11.9)
R_{anom}		0.6 (0.7)	1.0 (1.2)	1.2 (1.5)	1.5 (1.9)	1.6 (2.4)	2.0 (3.5)	2.7 (10.8)
estimated $\Delta F/F$ [%]		0.6	1.2	1.5	1.9	2.3	2.7	3.1

