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Supporting information for article:

On the influence of crystal size and wavelength on native SAD phasing

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Table S1 Experimental parameters for the BphA4 crystals collected at 1.9 and 2.7 Å.

	λ (Å)	¹ data sets	² combined	sweep (°)	exposure time (s)	$\Delta\phi$	camera	crystal dimensions	dose (Mgy)	³ mosaicity	flux 10^9 pho/s
size							distance (mm)	⊥ spindle axis (μm)			
L1	1.9	5	1	360	1	0.5	60	100 x 50	2.8	0.08	3.98
	2.7	5	1	360	1	0.5	60		2.6	0.07	1.99
L2	1.9	5	1	360	1	0.5	60	100 x 50	2.8	0.10	3.98
	2.7	5	1	360	1	0.5	60		2.6	0.08	1.99
L3	1.9	5	1	360	1	0.5	60	100 x 50	2.8	0.09	3.98
	2.7	5	1	360	1	0.5	60		2.6	0.07	1.99
M1	1.9	5	5	360	1	0.5	60	150 x 30	5.2	0.10	4.75
	2.7	5	5	360	1	0.5	60		5.0	0.08	2.30
M2	1.9	5	5	360	1	0.5	60	150 x 30	5.2	0.10	4.75
	2.7	5	5	360	1	0.5	60		5.0	0.08	2.30
S1	1.9	5	4	50 + 50	0.1	0.5	60	20 x 10	1.0	0.15	28.0
	2.7	5	4	50 + 50	0.13	0.5	60		1.1	0.10	10.5
S2	1.9	5	4	50 + 50	0.1	0.5	60	20 x 10	1.0	0.10	28.0
	2.7	5	4	50 + 50	0.13	0.5	60		1.1	0.07	10.5
S3	1.9	5	4	50 + 50	0.1	0.5	60	20 x 10	1.0	0.09	28.0
	2.7	5	4	50 + 50	0.13	0.5	60		1.1	0.09	10.5
S4	1.9	5	4	50 + 50	0.1	0.5	60	20 x 10	1.0	0.08	28.0
	2.7	5	4	50 + 50	0.13	0.5	60		1.1	0.09	10.5
S5	1.9	5	4	50 + 50	0.1	0.5	60	20 x 10	1.0	0.16	28.0
	2.7	5	4	50 + 50	0.13	0.5	60		1.1	0.15	10.5
S6	1.9	5	4	50 + 50	0.1	0.5	60	20 x 10	1.0	0.14	28.0
S7	2.7	5	4	50 + 50	0.13	0.5	60	20 x 10	1.1	0.20	10.5

¹number of data sets collected²number of data sets used³mosaicity of first sweep, if multiple sweep data collection was performed

Table S2 Experimental parameters for all lysozyme crystals collected at 1.9 and 2.7 Å. Same annotations as in table S1.

size	λ (Å)	data sets	combined	sweep (°)	exposure time (s)	$\Delta\phi$ (°)	camera distance (mm)	crystal dimensions \perp spindle axis (μm)	dose (MGy)	mosaicty	flux 10^9 pho/s
L1	1.9	5	1	360	0.1	0.5	62	150 100	0.9	0.14	15.0
	2.7	5	1	360	0.1	0.5	62		0.7	0.14	7.6
L2	1.9	5	1	360	0.1	0.5	62	150 100	0.9	0.14	15.0
	2.7	5	1	360	0.1	0.5	62		0.7	0.14	7.6
L3	1.9	5	1	360	0.1	0.5	62	200 120	0.7	0.15	15.0
	2.7	5	1	360	0.1	0.5	62		0.5	0.16	7.6
L4	1.9	5	1	360	0.1	0.5	62	250 110	2.4	0.11	48.0
	2.7	5	1	360	0.1	0.5	62		1.7	0.11	26.0
L5	1.9	5	1	360	0.1	0.5	62	170 110	2.6	0.12	48.0
	2.7	5	1	360	0.1	0.5	62		2.0	0.14	26.0
L6	1.9	5	1	360	0.1	0.5	62	250 110	2.4	0.14	48.0
	2.7	5	1	360	0.1	0.5	62		1.7	0.14	26.0
M1	1.9	5	1	360	0.1	0.5	62	150 40	4.5	0.23	48.0
	2.7	5	1	360	0.1	0.5	62		4.1	0.19	26.0
M2	1.9	5	1	360	0.1	0.5	62	150 60	3.8	0.18	48.0
	2.7	5	1	360	0.1	0.5	62		3.2	0.18	26.0
M3	1.9	5	1	360	0.1	0.5	62	150 50	4.1	0.15	48.0
	2.7	5	1	360	0.1	0.5	62		3.6	0.14	26.0
S1	1.9	5	5	360	0.1	0.5	62	50 25	8.1	0.20	57.0
S2	1.9	5	5	360	0.1	0.5	62	50 25	8.1	0.20	57.0
S3	1.9	5	5	360	0.12	0.5	62	30 15	9.3	0.20	48.0
S4	1.9	5	5	360	0.12	0.5	62	30 20	9.0	0.23	48.0
S5	2.7	5	5	360	0.1	0.5	62	50 25	8.1	0.15	31.0
S6	2.7	5	5	360	0.1	0.5	62	50 25	8.1	0.19	31.0
S7	2.7	5	5	360	0.12	0.5	62	25 15	9.9	0.28	26.0
S8	2.7	5	5	360	0.12	0.5	62	50 20	8.0	0.31	26.0

Table S3 Experimental parameters for all BphA4 crystals collected at 3.0 and 3.3 Å.

size	λ (Å)	data sets	combined	sweep (°)	exposure time (s)	$\Delta\phi$ (°)	camera distance (mm)	crystal dimensions \perp spindle axis (μm)	dose (MGy)	mosaicity	flux 10^9 pho/s
L1	3.0	5	1	100 + 100	1	0.5	60	100 50	0.8	0.07	0.72
	3.3	5	1	100 + 100	1	0.5	60		0.8	0.07	0.62
L2	3.0	5	1	100 + 100	0.45	0.5	60	150 100	0.6	0.10	2.2
	3.3	5	1	100 + 100	0.3	0.5	60		0.6	0.10	2.3
L3	3.0	5	1	100 + 100	0.3	0.5	60	150 100	0.4	0.07	2.2
	3.3	5	1	100 + 100	0.4	0.5	60		0.8	0.08	2.3
M1	3.0	5	1	100 + 100	1	0.5	60	75 50	0.8	0.10	0.72
	3.3	5	1	100 + 100	1	0.5	60		0.8	0.16	0.62
M2	3.0	5	1	100 + 100	1	0.5	60	75 30	0.8	0.13	0.72
	3.3	5	1	100 + 100	1	0.5	60		1.0	0.10	0.62
M3	3.0	5	1	100 + 100	1	0.5	60	75 50	0.8	0.10	0.72
	3.3	5	1	100 + 100	1	0.5	60		0.8	0.10	0.62
S1	3.0	5	5	100 + 100	0.5	0.5	60	30 30	3.6	0.07	5.2
S2	3.0	5	5	100 + 100	0.5	0.5	60	30 30	4.0	0.10	5.2
S3	3.0	5	5	100 + 100	1	0.5	60	25 25	3.6	0.08	2.2
S4	3.3	5	5	100 + 100	2.3	0.5	60	30 25	2.6	0.10	0.62
S5	3.3	5	5	100 + 100	2.3	0.5	60	25 25	2.6	0.06	0.62
S6	3.3	5	5	100 + 100	0.35	0.5	60	60 25	1.2	0.12	2.3

Table S4 Experimental parameters for all lysozyme crystals collected at 3.0 and 3.3 Å.

size	λ (Å)	data sets	combined	sweep (°)	exposure time (s)	delta phi (°)	camera distance (mm)	crystal dimensions \perp spindle axis (μm)	dose (MGy)	mosaicty	flux 10^9 pho/s
L1	3.0	5	1	100 + 100	0.18	0.5	60	100 150	0.2	0.16	2.2
	3.3	5	1	100 + 100	0.3	0.5	60		0.4	0.14	2.3
L2	3.0	5	5	100 + 100	0.41	0.5	60	150 80	0.8	0.11	2.2
	3.3	5	5	100 + 100	0.56	0.5	60		1.4	0.13	2.3
M1	3.0	5	1	100 + 100	0.3	0.5	60	50 50	0.8	0.17	2.2
	3.3	5	1	100 + 100	0.4	0.5	60		1.4	0.16	2.3
M2	3.0	5	5	100 + 100	0.3	0.5	60	100 50	0.8	0.27	2.2
	3.3	5	5	100 + 100	0.4	0.5	60		1.4	0.20	2.3
S1	3.0	5	5	100 + 100	0.3	0.5	60	50 25	1.0	0.20	2.2
S2	3.3	5	5	100 + 100	0.4	0.5	60	75 25	1.8	0.15	2.3

Table S5 Integration statistics for data sets obtained from medium BphA4 crystals, collected at 1.9 and 2.7 Å.

crystal	λ (Å)	data set	highest shell (Å)	I/σ	R_{meas} (%)	multiplicity	CC_{anom}	mosaicity	$^1\text{meas.}$ (Å)	AvI
M1	1.9	1	2.62 - 2.52	28.2 (8.0)	14.6 (62.1)	38.5 (40.4)	4.9	0.10	-	48
		2	2.62 - 2.52	25.7 (6.3)	16.3 (81.5)	38.5 (40.4)	4.4	0.10	-	43
		3	2.62 - 2.52	23.0 (4.4)	19.0 (118.1)	38.5 (40.4)	1.1	0.11	-	37
		4	2.62 - 2.52	19.8 (3.1)	23.0 (172.7)	38.5 (40.4)	-1.1	0.12	-	33
		5	2.62 - 2.52	16.9 (2.1)	27.9 (253.4)	38.5 (40.4)	-2.4	0.13	-	28
	2.7	1	2.62 - 2.52	25.1 (3.4)	16.7 (131.6)	37.0 (35.3)	13	0.08	5.7	50
		2	2.62 - 2.52	22.6 (2.4)	19.3 (190.2)	36.9 (35.0)	8.8	0.09	6.2	43
		3	2.79 - 2.66	21.4 (2.7)	21.1 (168.9)	37.1 (36.2)	5.6	0.10	7.4	42
		4	2.93 - 2.78	19.0 (2.6)	24.4 (188.0)	37.1 (37.4)	3	0.11	12.5	40
		5	3.09 - 2.91	16.8 (2.6)	28.1 (186.7)	36.9 (36.2)	0.8	0.13	12.5	36
M2	1.9	1	2.62 - 2.52	29.4 (8.8)	13.3 (54.5)	37.4 (38.6)	7.7	0.10	6.2	51
		2	2.62 - 2.52	27.6 (7.2)	14.5 (67.8)	37.4 (38.6)	6.5	0.09	20.4	44
		3	2.62 - 2.52	24.7 (5.3)	16.6 (94.7)	37.4 (38.6)	4.6	0.10	7.4	37
		4	2.62 - 2.52	21.8 (3.7)	19.7 (138.0)	37.4 (38.5)	1.1	0.11	8.3	31
		5	2.62 - 2.52	18.7 (2.6)	23.8 (204.3)	37.4 (38.5)	1.3	0.12	12.5	28
	2.7	1	2.62 - 2.52	26.9 (4.8)	13.9 (84.6)	34.4 (30.7)	14.1	0.08	5.4	65
		2	2.65 - 2.54	22.2 (2.4)	18.2 (172.7)	34.3 (30.8)	10.6	0.10	6.2	53
		3	2.94 - 2.79	19.6 (2.5)	22.4 (183.7)	35.0 (33.5)	2.9	0.14	8.3	49
		4	3.25 - 3.04	15.6 (2.7)	29.1 (182.3)	35.2 (34.9)	1.6	0.18	12.5	43
		5	3.55 - 3.29	12.7 (2.9)	36.7 (177.2)	35.1 (36.1)	9.1	0.23	-	36

¹If no value is reported, XTRIAGE did not find anomalous signal in the data.

Table S6 Integration statistics for data sets obtained from small BphA4 crystals, collected at 1.9 and 2.7 Å.

crystal	λ (Å)	data set	highest shell (Å)	I/σ	R_{meas} (%)	multiplicity	CC_{anom}	$^1\text{meas.}$ (Å)
S1	-1.9	1	2.75 -2.63	10.0 (2.2)	23.5 (113.6)	10.3 (10.5)	3.9	-
		2	2.78 -2.65	10.0 (2.2)	23.2 (111.7)	10.3 (10.5)	3.2	-
		3	2.79 -2.66	10.0 (2.2)	23.4 (109.2)	10.3 (10.4)	2.2	-
		4	2.80 -2.67	10.0 (2.2)	23.4 (109.9)	10.3 (10.4)	2.5	12.5
	2.7	1	2.74 -2.62	13.5 (2.3)	15.2 (92.1)	9.6 (8.8)	7.6	9.8
		2	2.75 -2.63	13.5 (2.4)	15.1 (87.5)	9.6 (8.8)	5.7	8.3
		3	2.77 -2.64	13.5 (2.5)	15.1 (84.7)	9.6 (8.9)	6.8	8.3
		4	2.78 -2.65	13.5 (2.4)	15.2 (86.4)	9.6 (8.9)	6.3	9.8
S2	1.9	1	2.60 -2.50	9.7 (2.1)	23.7 (122.8)	10.7 (11.3)	0.9	-
		2	2.64 -2.53	9.8 (2.1)	23.8 (122.1)	10.7 (11.2)	5.1	-
		3	2.67 -2.56	9.7 (2.1)	23.9 (126.4)	10.7 (11.2)	2.4	-
		4	2.71 -2.59	9.8 (2.2)	24.1 (118.3)	10.7 (11.2)	1.9	-
	2.7	1	2.85 -2.72	11.7 (2.4)	18.9 (93.5)	10.6 (11.1)	4	9.8
		2	2.87 -2.74	11.6 (2.4)	18.9 (95.8)	10.5 (11.1)	4.5	9.8
		3	2.87 -2.74	11.5 (2.3)	19.2 (98.9)	10.5 (11.0)	5.4	-
		4	2.91 -2.76	11.6 (2.4)	19.3 (97.7)	10.5 (11.0)	6.2	20.2
S3	1.9	1	2.57 -2.47	10.4 (2.2)	22.2 (117.1)	10.5 (10.9)	4.3	-
		2	2.58 -2.48	10.4 (2.2)	21.8 (117.0)	10.5 (10.9)	2.8	-
		3	2.59 -2.49	10.4 (2.1)	22.0 (119.5)	10.5 (10.8)	3.4	-
		4	2.61 -2.51	10.5 (2.1)	21.7 (118.5)	10.4 (10.8)	3.9	-
	2.7	1	2.97 -2.82	11.6 (2.3)	19.4 (97.9)	10.1 (10.3)	4.4	12.5
		2	2.98 -2.83	11.5 (2.4)	19.5 (96.4)	10.1 (10.3)	6.5	12.5
		3	2.99 -2.84	11.3 (2.3)	19.8 (98.5)	10.1 (10.1)	2.7	20.4
		4	3.03 -2.87	11.3 (2.3)	19.9 (99.4)	10.1 (10.0)	6.5	-
S4	1.9	1	2.51 -2.42	10.2 (2.2)	23.1 (118.2)	10.7 (11.2)	3	12.5
		2	2.54 -2.44	10.2 (2.2)	23.0 (114.3)	10.7 (11.2)	4.7	-
		3	2.56 -2.46	10.1 (2.3)	23.0 (114.0)	10.7 (11.2)	3.4	-
		4	2.58 -2.48	10.2 (2.1)	23.0 (121.8)	10.7 (11.2)	3	20.4
	2.7	1	3.02 -2.86	10.6 (2.4)	22.1 (99.2)	10.3 (10.4)	4.5	9.8
		2	3.03 -2.87	10.8 (2.4)	21.9 (98.2)	10.3 (10.3)	5.8	20.4
		3	3.07 -2.89	10.7 (2.4)	21.9 (95.8)	10.3 (10.0)	4.9	9.8
		4	3.09 -2.91	10.7 (2.4)	22.1 (96.9)	10.3 (10.0)	6.3	9.8
S5	1.9	1	3.16 -2.98	8.1 (2.2)	30.5 (104.5)	10.3 (9.4)	5	-
		2	3.17 -2.99	8.1 (2.2)	30.7 (105.3)	10.4 (9.3)	3.3	-
		3	3.19 -3.01	8.1 (2.2)	30.6 (104.5)	10.4 (9.4)	3.7	-
		4	3.20 -3.02	8.0 (2.2)	31.3 (107.1)	10.4 (9.4)	2.9	-
	2.7	1	3.31 -3.10	9.4 (2.6)	25.7 (90.0)	10.0 (9.6)	0.9	12.5
		2	3.34 -3.12	9.2 (2.6)	26.0 (89.5)	10.0 (9.6)	3.2	12.5
		3	3.35 -3.13	9.1 (2.5)	26.4 (94.6)	10.0 (9.7)	3.2	-
		4	3.37 -3.15	9.0 (2.6)	26.9 (92.2)	10.0 (9.7)	3.1	12.5
S6	1.9	1	3.01 -2.86	8.4 (2.2)	28.4 (109.2)	10.3 (9.9)	3.1	-

	2	3.01 -2.86	8.5 (2.2)	28.3 (111.3)	10.3 (10.0)	4.5	-
	3	3.04 -2.88	8.5 (2.3)	28.1 (108.3)	10.3 (9.9)	1.7	-
	4	3.07 -2.89	8.4 (2.3)	28.1 (104.9)	10.3 (9.7)	1.1	-
	1	3.31 -3.10	9.4 (2.6)	25.3 (90.3)	9.8 (9.5)	4.3	20.2
S7 2.7	2	3.31 -3.10	9.4 (2.6)	25.2 (90.8)	9.9 (9.6)	1.8	-
	3	3.32 -3.11	9.5 (2.7)	25.3 (87.7)	9.9 (9.5)	1.3	-
	4	3.32 -3.11	9.3 (2.6)	25.5 (89.2)	9.9 (9.5)	2.5	20.4

[†]If no value is reported, XTRIAGE did not find anomalous signal in the data.

Table S7 Integration statistics for data sets obtained from small lysozyme crystals, collected at 1.9 and 2.7 Å.

crystal	λ (Å)	data set	highest shell (Å)	I/ σ	R _{meas} (%)	multiplicity	CC _{anom}	mosaicity	¹ meas. (Å)	² Avl
S1	1.9	1	2.62 - 2.52	68.4 (50.3)	4.5 (6.3)	23.2 (24.6)	56.7	0.20	2.52	1457
		2	2.62 - 2.52	65.3 (43.3)	4.6 (7.6)	23.3 (24.7)	57	0.22	2.6	1236
		3	2.62 - 2.52	56.5 (33.8)	5.1 (9.9)	23.2 (24.6)	51.7	0.25	3.3	1022
		4	2.62 - 2.52	48.9 (26.5)	5.8 (12.7)	23.2 (24.7)	44.9	0.26	3.6	824
		5	2.62 - 2.52	41.8 (20.9)	6.7 (16.5)	23.2 (24.7)	32.9	0.27	4.3	669
		1	2.62 - 2.52	69.6 (47.3)	4.4 (6.9)	23.3 (24.8)	57	0.20	2.52	1286
S2	1.9	2	2.62 - 2.52	70.3 (43.7)	4.3 (7.5)	23.5 (24.9)	58.5	0.19	2.8	1020
		3	2.62 - 2.52	64.5 (36.8)	4.6 (9.1)	23.7 (25.0)	55.2	0.20	3.3	813
		4	2.62 - 2.52	57.0 (29.2)	5.2 (11.8)	23.7 (24.9)	50.1	0.21	3.7	657
		5	2.62 - 2.52	48.3 (21.5)	6.1 (17.2)	23.7 (24.9)	40.1	0.23	4.1	538
		1	2.62 - 2.52	49.4 (32.5)	6.0 (9.7)	23.6 (25.0)	44.2	0.20	3.6	697
		2	2.62 - 2.52	42.7 (21.5)	6.7 (16.0)	23.7 (24.9)	42.9	0.25	4.1	532
S3	1.9	3	2.62 - 2.52	31.4 (10.7)	8.8 (34.7)	23.5 (25.0)	26.2	0.32	4.6	368
		4	2.62 - 2.52	22.1 (4.6)	12.4 (83.6)	23.4 (24.8)	14.9	0.38	5.4	243
		5	2.68 - 2.57	16.4 (2.3)	17.1 (170.0)	23.4 (24.5)	9.2	0.44	8.3	168
		1	2.62 - 2.52	55.3 (37.5)	5.4 (8.9)	22.8 (24.4)	56	0.23	3.0	1144
		2	2.62 - 2.52	56.7 (35.3)	5.2 (9.5)	23.0 (24.5)	50	0.24	2.52	961
		3	2.62 - 2.52	54.0 (30.9)	5.3 (10.8)	23.2 (24.6)	46.3	0.24	3.2	813
S4	1.9	4	2.62 - 2.52	50.5 (25.7)	5.6 (13.4)	23.2 (24.8)	47.2	0.25	3.5	676
		5	2.62 - 2.52	46.3 (21.1)	6.0 (16.4)	23.3 (24.9)	43	0.26	4.0	561
		1	2.62 - 2.52	47.9 (24.6)	6.5 (14.7)	23.3 (22.6)	77.1	0.15	2.52	564
		2	2.62 - 2.52	47.7 (21.6)	6.4 (16.3)	23.3 (22.4)	75.4	0.15	2.52	465
		3	2.62 - 2.52	44.4 (16.3)	6.6 (21.6)	23.3 (22.3)	72.1	0.15	3.0	370
		4	2.62 - 2.52	39.5 (10.3)	7.3 (34.8)	23.2 (22.1)	71	0.17	3.4	287
S5	2.7	5	2.62 - 2.52	32.7 (5.7)	8.8 (63.7)	23.1 (22.2)	65.9	0.20	3.6	218
		1	2.62 - 2.52	53.2 (27.2)	5.8 (11.2)	21.8 (19.5)	78.5	0.19	2.6	772
		2	2.62 - 2.52	54.6 (26.2)	5.6 (11.3)	21.9 (19.6)	78.7	0.18	2.5	671
		3	2.62 - 2.52	53.3 (22.9)	5.6 (13.2)	21.8 (19.4)	76.6	0.18	2.6	571
		4	2.62 - 2.52	50.4 (17.5)	5.7 (17.8)	21.8 (19.4)	76.9	0.18	2.9	479
		5	2.62 - 2.52	45.5 (12.4)	6.2 (26.0)	21.8 (19.3)	73.6	0.19	3.1	401
S6	2.7	1	2.62 - 2.52	39.5 (14.1)	7.7 (24.3)	22.4 (20.7)	73.3	0.28	3.0	468
		2	2.62 - 2.52	38.4 (11.2)	7.8 (30.5)	22.5 (20.5)	70.7	0.28	3.2	379
		3	2.62 - 2.52	34.3 (7.8)	8.6 (44.9)	22.5 (20.8)	64.5	0.29	3.5	293
		4	2.62 - 2.52	28.3 (4.6)	10.2 (73.4)	22.5 (20.7)	58.5	0.31	3.9	219
		5	2.62 - 2.52	22.3 (2.6)	12.7 (129.9)	22.5 (21.0)	46.2	0.32	4.4	159
		1	2.62 - 2.52	45.4 (21.1)	6.5 (14.1)	21.5 (19.0)	72.5	0.31	2.6	925
S7	2.7	2	2.62 - 2.52	46.5 (19.8)	6.3 (15.1)	21.5 (19.0)	70.1	0.32	2.9	793
		3	2.62 - 2.52	44.1 (16.4)	6.5 (18.9)	21.5 (19.1)	68.4	0.33	3.1	672
		4	2.62 - 2.52	39.1 (12.3)	7.0 (25.3)	21.5 (18.8)	63.5	0.36	3.4	557
		5	2.62 - 2.52	33.8 (8.7)	7.9 (37.4)	21.5 (18.9)	58.8	0.39	3.7	461

¹measurability based resolution cut-off.

²Average intensity from AIMLESS

Table S8 Integration statistics¹ for data sets obtained from small BphA4 crystals, collected at 3.0 and 3.3 Å.

crystal	λ (Å)	data set	highest shell (Å)	I/σ	R_{meas} (%)	multiplicity	CC_{anom}	² mosaicity	³ meas. (Å)	⁴ AvI
S1	3.0	1	3.29 -3.08	30.7 (13.5)	9.8 (20.9)	19.3 (18.2)	21	0.07	5.4	122
		2	3.29 -3.08	29.1 (11.4)	10.6 (26.0)	19.3 (18.2)	15.6	0.08	5.7	110
		3	3.29 -3.08	26.3 (8.2)	12.4 (37.7)	19.2 (18.1)	9.9	0.09	6.2	99
		4	3.29 -3.08	22.2 (5.7)	15.2 (57.0)	19.2 (18.0)	8.8	0.12	6.7	85
		5	3.29 -3.08	18.9 (3.9)	19.0 (85.2)	19.1 (18.1)	4.8	0.15	8.3	73
		1	3.29 -3.08	42.3 (19.3)	6.9 (13.7)	19.3 (18.6)	33	0.10	4.6	243
S2	3.0	2	3.29 -3.08	39.8 (16.0)	7.6 (17.5)	19.4 (18.6)	28.8	0.11	4.9	214
		3	3.29 -3.08	35.7 (11.3)	9.0 (26.5)	19.3 (18.5)	21.1	0.14	5.4	182
		4	3.29 -3.08	28.4 (7.3)	11.5 (44.3)	19.2 (18.5)	11.9	0.17	6.1	149
		5	3.29 -3.08	23.4 (4.8)	14.9 (70.3)	19.1 (18.4)	9.3	0.20	6.7	119
		1	3.29 -3.08	35.7 (17.6)	8.2 (16.2)	20.0 (19.9)	27.7	0.08	5.4	122
S3	3.0	2	3.29 -3.08	33.9 (15.0)	8.8 (19.1)	20.0 (19.8)	24.2	0.08	5.7	109
		3	3.29 -3.08	31.4 (12.2)	9.6 (24.4)	20.0 (19.9)	21.6	0.08	6.1	93
		4	3.29 -3.08	28.6 (9.4)	10.8 (32.8)	20.0 (19.9)	20.1	0.09	6.1	79
		5	3.29 -3.08	25.8 (6.9)	12.3 (45.9)	20.0 (19.9)	16	0.09	6.7	66
		1	3.29 -3.08	29.2 (11.3)	10.5 (23.9)	18.6 (16.6)	19.9	0.10	5.1	104
S4	3.3	2	3.29 -3.08	27.5 (9.5)	11.6 (30.5)	18.6 (16.6)	16.3	0.09	5.1	97
		3	3.29 -3.08	23.9 (7.1)	13.8 (44.5)	18.6 (16.5)	9.8	0.10	5.7	85
		4	3.29 -3.08	20.8 (4.8)	17.1 (67.5)	18.5 (16.5)	6.2	0.12	6.1	72
		5	3.29 -3.08	17.6 (3.2)	21.6 (102.2)	18.3 (16.4)	-1.7	0.14	7.4	60
		1	3.29 -3.08	15.0 (4.5)	23.4 (69.0)	18.6 (17.0)	5.3	0.06	20.2	39
S5	3.3	2	3.29 -3.08	13.8 (3.6)	26.4 (88.7)	18.5 (17.1)	6	0.07	-	37
		3	3.29 -3.08	12.2 (2.7)	31.0 (118.0)	18.5 (17.0)	2.6	0.08	-	33
		4	3.29 -3.08	10.7 (1.8)	37.2 (172.9)	18.5 (17.1)	1.7	0.09	-	28
		5	3.29 -3.08	9.3 (1.2)	44.9 (265.4)	18.5 (17.1)	1	0.10	-	24
		1	3.27 -3.06	19.8 (4.6)	16.1 (63.0)	19.0 (17.6)	14.6	0.12	6.1	20
S6	3.3	2	3.28 -3.07	19.6 (4.6)	16.4 (63.5)	19.1 (17.8)	15	0.12	5.7	19
		3	3.29 -3.08	19.2 (4.5)	16.7 (66.0)	19.1 (17.7)	11.2	0.12	6.1	19
		4	3.30 -3.09	18.6 (4.2)	17.1 (70.6)	19.1 (17.7)	11	0.12	6.1	18
		5	3.32 -3.11	18.2 (4.3)	17.4 (69.2)	19.1 (17.8)	10.7	0.11	6.7	17

¹The overall statistics are for the combined 100+100° data sets

²Mosaicity is indicated for the first sweep of data (100°)

³Measurability based resolution cut-off. If no value is reported, XTRIAGE did not find anomalous signal in the data.

⁴Average intensity from AIMLESS, from the first sweep of data (100°)

Table S9 Integration statistics¹ for data sets obtained from lysozyme crystals, collected at 3.0 and 3.3 Å.

crystal	λ (Å)	data set	highest shell (Å)	I/σ	R_{meas} (%)	multiplicity	CC_{anom}	² mosaicity	³ meas. (Å)	⁴ AvI
L2	3.0	1	3.29 -3.08	27.6 (23.0)	8.4 (8.8)	10.6 (9.9)	37.7	0.11	3.2	450
		2	3.29 -3.08	27.8 (23.1)	8.3 (8.7)	10.6 (9.9)	40.9	0.11	3.08	452
		3	3.29 -3.08	27.9 (23.3)	8.3 (8.7)	10.6 (9.9)	37.8	0.11	3.2	451
		4	3.29 -3.08	27.6 (22.7)	8.3 (8.7)	10.7 (10.0)	39.3	0.11	3.2	444
	3.3	5	3.29 -3.08	27.4 (22.6)	8.3 (8.8)	10.7 (10.0)	38.8	0.11	3.4	440
		1	3.29 -3.08	27.0 (21.7)	8.5 (9.7)	9.9 (9.3)	51.1	0.13	3.1	417
		2	3.29 -3.08	27.2 (21.7)	8.4 (9.3)	9.9 (9.2)	47.9	0.13	3.1	436
		3	3.29 -3.08	26.8 (21.5)	8.5 (9.5)	9.9 (9.3)	54.7	0.13	3.1	439
		4	3.29 -3.08	26.4 (21.3)	8.6 (9.6)	9.8 (9.3)	51	0.13	3.1	437
		5	3.29 -3.08	26.7 (21.2)	8.4 (9.6)	9.8 (9.2)	45.2	0.13	3.08	431
M2	3.0	1	3.29 -3.08	48.9 (35.9)	5.6 (6.6)	12.0 (11.2)	67.9	0.27	3.08	494
		2	3.29 -3.08	48.5 (35.3)	5.6 (6.5)	12.0 (11.2)	67.2	0.27	3.1	491
		3	3.29 -3.08	48.6 (35.4)	5.6 (6.5)	12.0 (11.2)	69.3	0.27	3.1	486
		4	3.29 -3.08	48.2 (34.8)	5.6 (6.7)	12.0 (11.2)	66.4	0.27	3.2	479
		5	3.29 -3.08	48.1 (34.4)	5.6 (6.7)	12.0 (11.2)	67.4	0.27	3.1	477
	3.3	1	3.29 -3.08	33.8 (21.2)	7.7 (10.4)	11.6 (10.3)	61.9	0.2	3.3	179
		2	3.29 -3.08	31.2 (19.1)	8.3 (11.6)	11.6 (10.3)	55.1	0.19	3.3	149
		3	3.29 -3.08	30.1 (18.1)	8.5 (12.0)	11.6 (10.2)	53.9	0.19	3.3	132
		4	3.29 -3.08	29.1 (17.1)	8.7 (12.6)	11.6 (10.2)	51.8	0.19	3.3	122
		5	3.29 -3.08	28.1 (16.3)	9.0 (13.1)	11.6 (10.2)	50	0.19	3.6	114
S1	3.0	1	3.29 -3.08	56.9 (39.5)	5.1 (5.9)	12.2 (11.9)	80.6	0.2	3.08	728
		2	3.29 -3.08	57.4 (39.5)	5.0 (6.0)	12.2 (11.8)	80.7	0.2	3.08	725
		3	3.29 -3.08	58.4 (39.9)	4.9 (5.9)	12.2 (11.9)	80.4	0.19	3.08	722
		4	3.29 -3.08	58.7 (39.7)	4.9 (6.0)	12.2 (11.9)	83.2	0.19	3.08	709
		5	3.29 -3.08	58.1 (39.1)	5.0 (5.9)	12.3 (11.9)	78.7	0.19	3.08	702
	3.3	1	3.29 -3.08	47.8 (33.2)	5.9 (6.8)	12.0 (10.8)	78.7	0.15	3.08	404
		2	3.29 -3.08	47.5 (32.7)	5.9 (6.9)	12.0 (10.9)	78.4	0.15	3.08	399
		3	3.29 -3.08	47.2 (32.5)	5.9 (6.9)	12.0 (10.9)	77.6	0.15	3.08	392
		4	3.29 -3.08	47.1 (32.1)	5.9 (6.8)	12.0 (10.8)	78	0.15	3.08	387
		5	3.29 -3.08	46.0 (31.0)	6.0 (7.1)	12.0 (10.8)	79.6	0.16	3.08	379

¹The overall statistics are for the combined 100+100° data sets²Mosaicity is indicated for the first sweep of data (100°)³Measurability based resolution cut-off. If no value is reported, XTRIAGE did not find anomalous signal in the data.⁴Average intensity from AIMLESS, from the first sweep of data (100°)

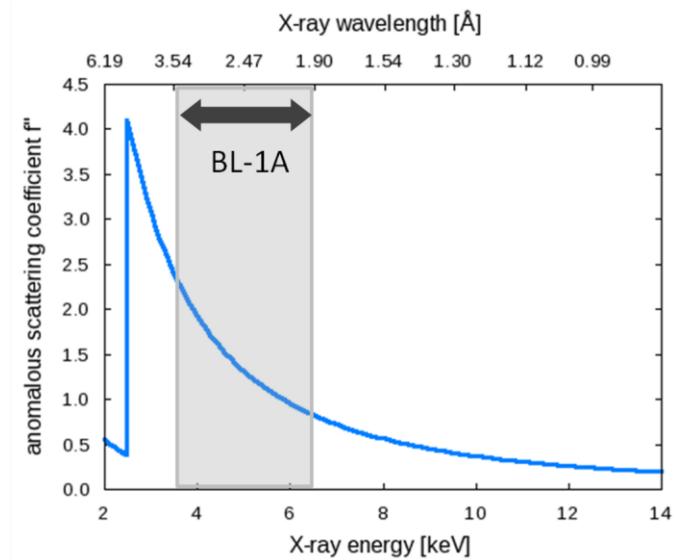


Figure S1 Anomalous scattering coefficient f'' of sulfur. The absorption edge is at 5.016 \AA . The long wavelength range of beamline BL-1A is highlighted in grey. Between 1.9 \AA and 3.5 \AA , f'' increases from 0.8176 to 2.3431 .

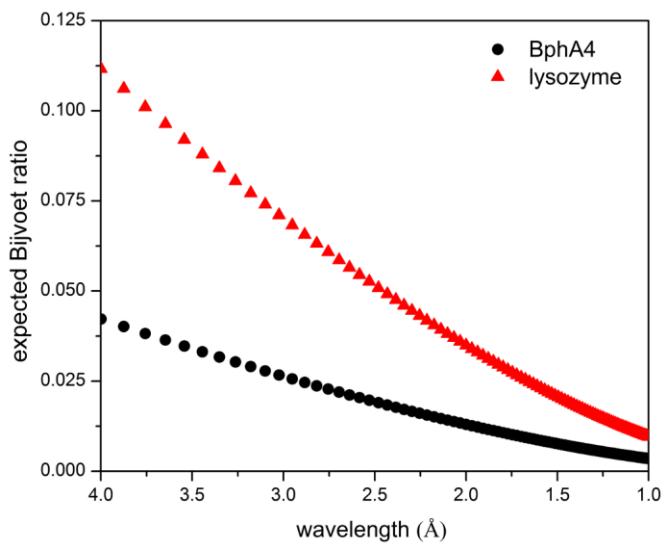


Figure S2 Mean ratio of the Bijvoet difference to the total protein amplitude for BphA4 (black circles) and lysozyme (red triangles), $\frac{\langle \Delta F^{anom} \rangle}{\langle F \rangle} = \sqrt{\frac{2N_A}{N_T}} \cdot \frac{f''_A}{Z_{eff}}$, where N_A is the number of anomalous scatterers, N_T the total number of atoms, f_A'' the imaginary scattering contribution of the anomalous scatterer and Z_{eff} the effective number of electrons (6.7).

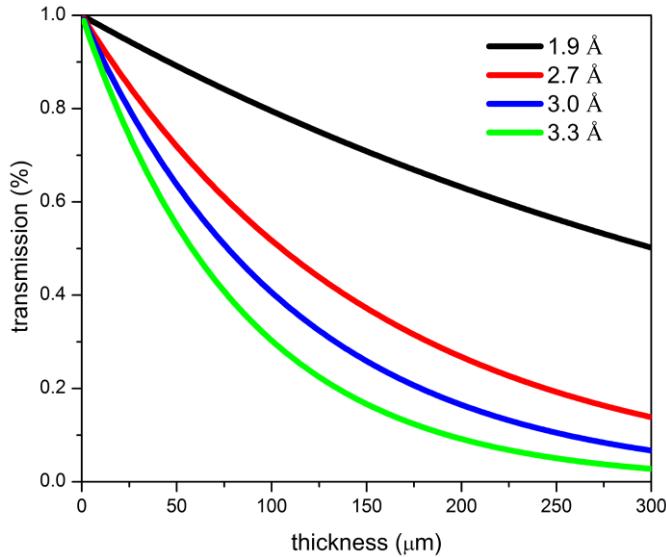


Figure S3 Transmission of X-rays through protein as a function of the wavelength over the range of crystal thicknesses and wavelengths used: 1.9 Å (black), 2.7 Å (red), 3.0 Å (blue) and 3.3 Å (green).

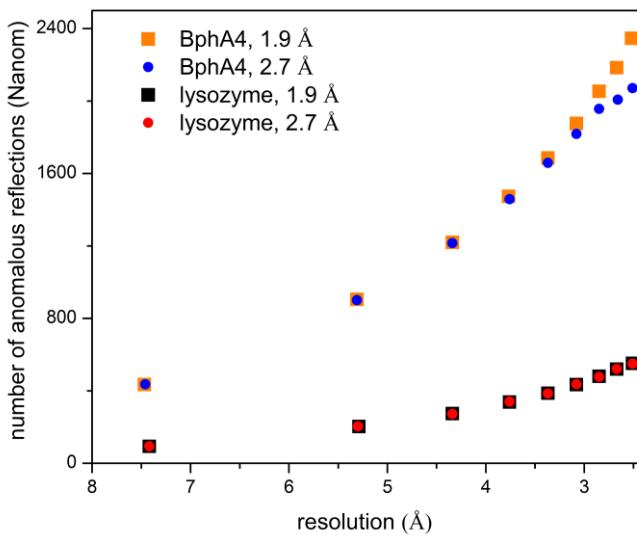


Figure S4 Number of anomalous reflections as a function of resolution for the crystals BphA4_{large-3} and lyso_{large-2}.