Supporting Information

Zeldin et al. 10.1073/pnas.1315879110

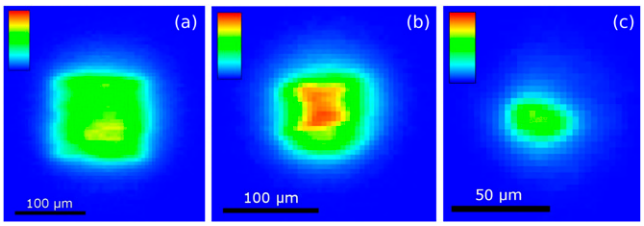

Fig. S1. False color images of the beam profiles used for the experiments presented here. Pixel size is 5×5 μm^2 in all cases. Note the different sizes of scale bars for *A*–*C*. The color scale is from 0 to 255 (blue–red), and is the same for all of the images. Images were subsequently scaled to the full flux, as measured by the in-line calibrated diode. (*A*) Big beam, $\sim 115 \times 115$ μm^2 FWHM, slits set to 120×120 μm^2, dark current value: 21. Dynamic range after dark current (DC) subtraction: 0–185. (*B*) Medium beam, $\sim 60 \times 60$ μm^2 FWHM. DC value: 18. Dynamic range after DC subtraction: 0–237, but only 1 pixel saturated (value after DC subtraction: 237). (*C*) Small beam, $\sim 25 \times 40$ μm^2 FWHM (vertical, horizontal). Dark current value: 21. Dynamic range after DC subtraction: 0–222.

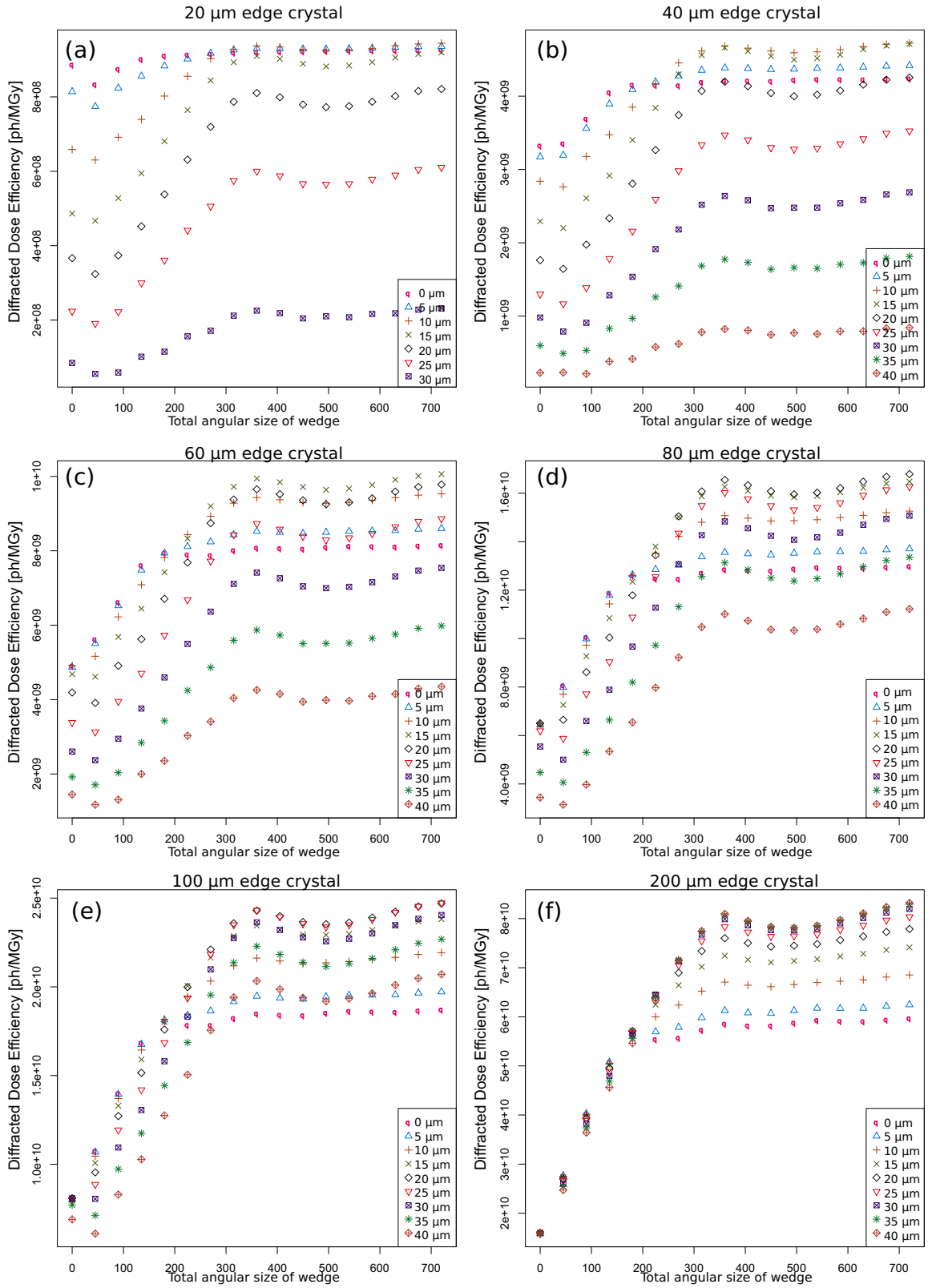

Fig. S2. Simulated offset data for crystals with edges up to 200 µm (*A–F*), using a beam of FWHM 20 × 20 µm^2. In some cases, a bigger offset can lead to a drop of the DDE, because the crystal was unevenly exposed with relatively high damage around the edges.

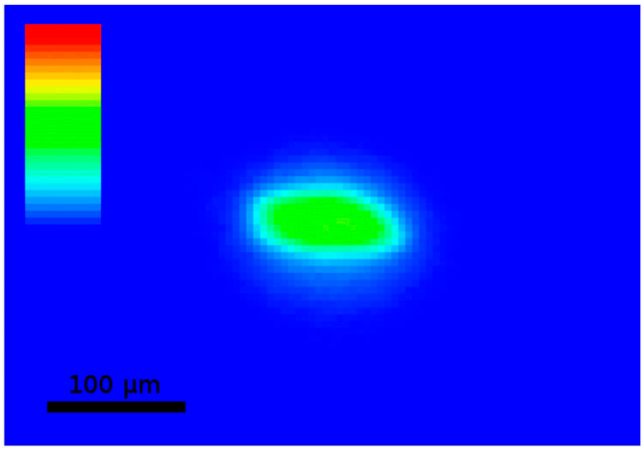

Fig. S3. Beam shape for the offset experiments, with the color bar representing 0–255 intensity units.

Table S1. Statistics for the big beam data collection

Crystal	Probe	I_n/I_1	Unique observations	$CC_{1/2}$	Multiplicity	$I/\sigma(I)$	R_{meas}	Unit cell (Å)	Mosaicity (°)
P2S5	1	1.0	7,513	0.998 (0.985)	7.1 (7.3)	22.3 (10.7)	0.066 (0.176)	78.14	0.13
	2	0.64	7,572	0.998 (0.952)	7.1 (7.3)	17.9 (6.0)	0.072 (0.322)	78.32	0.12
	3	0.4	7,613	0.998 (0.386)	7.1 (7.2)	11.6 (1.2)	0.105 (1.832)	78.46	0.42
	4*	0.088	7,515	0.558 (0.017)	7.1 (7.3)	1.2 (0.1)	1.005 (25.785)	78.14	0.05
	5*	0.075	7,513	0.644 (0.036)	7.0 (7.1)	0.7 (-0.1)	1.254 (-9.990)	78.14	0.05
P3S1	1	1.0	7,469	0.998 (0.971)	7.0 (7.2)	20.2 (7.5)	0.069 (0.250)	78.02	0.49
	2	0.73	7,545	0.998 (0.882)	7.0 (7.2)	15.9 (3.4)	0.080 (0.554)	78.31	0.51
	3	0.51	7,606	0.998 (0.237)	7.0 (7.2)	11.2 (1.0)	0.107 (2.020)	78.56	0.57
	4	0.34	7,616	0.998 (0.071)	6.9 (7.1)	7.6 (0.3)	0.161 (6.710)	78.60	0.65
	5	0.23	7,625	0.997 (0.078)	6.8 (7.0)	5.2 (0.2)	0.253 (9.169)	78.65	0.78
	6	0.16	7,683	0.993 (0.011)	6.7 (6.8)	4.1 (0.1)	0.390 (28.006)	78.77	0.91
	7	0.12	7,689	0.990 (0.098)	6.5 (6.1)	2.5 (-0.4)	0.626 (-3.458)	78.89	0.98
	8	0.034	7,791	0.971 (-0.013)	6.5 (6.5)	1.5 (0.1)	1.072 (58.404)	79.21	1.05
P3S9	1	1.0	7,492	0.999 (0.971)	7.1 (7.2)	21.1 (7.9)	0.061 (0.251)	78.04	0.26
	2	0.74	7,547	0.999 (0.853)	7.1 (7.3)	16.6 (3.3)	0.073 (0.633)	78.24	0.34
	3	0.54	7,569	0.999 (0.211)	7.0 (7.2)	11.1 (0.9)	0.114 (2.499)	78.32	0.49
	4	0.37	7,586	0.998 (0.029)	7.0 (7.1)	8.0 (0.3)	0.181 (7.011)	78.34	0.62
	5	0.21	7,596	0.996 (-0.037)	6.9 (6.9)	4.1 (0.1)	0.311 (20.043)	78.39	0.72
	6	0.14	7,611	0.988 (0.023)	6.1 (5.9)	2.4 (0.0)	0.438 (-9.990)	78.46	0.73
	7*	0.092	7,576	0.932 (0.015)	6.7 (7.3)	1.4 (0.0)	1.228 (34.847)	78.38	0.05
	8*	0.096	7,570	0.972 (-0.001)	6.9 (7.1)	1.6 (0.1)	1.362 (26.384)	78.30	0.20
	9*	0.034	7,580	0.827 (0.063)	6.6 (5.5)	0.9 (-0.4)	3.866 (-1.311)	78.38	0.05
	10*	0.016	7,582	0.826 (0.032)	7.0 (7.1)	0.9 (0.0)	2.382 (-9.990)	78.38	0.05
P3S10	1	1.0	7,516	0.998 (0.875)	7.1 (7.2)	15.3 (3.5)	0.093 (0.560)	78.18	0.53
	2	0.68	7,582	0.997 (0.447)	7.0 (7.2)	11.0 (1.2)	0.129 (1.671)	78.45	0.66
	3	0.47	7,602	0.996 (0.061)	6.9 (7.0)	6.8 (0.3)	0.230 (7.417)	78.53	0.99
	4	0.32	7,599	0.990 (0.052)	6.6 (6.5)	4.4 (-0.1)	0.441 (-9.467)	78.54	1.19
	5	0.23	7,505	0.988 (-0.046)	5.7 (3.5)	2.6 (-1.4)	0.596 (-0.657)	78.32	1.34
	6*	0.076	7,582	0.903 (0.080)	6.5 (5.0)	0.7 (-1.0)	2.004 (-1.050)	78.48	0.05
	7*	0.015	7,577	0.878 (-0.021)	7.0 (7.2)	0.6 (0.0)	2.865 (-9.990)	78.48	0.05
	8*	0.0036	7,576	0.706 (-0.029)	6.9 (6.7)	0.3 (-0.1)	11.254 (-3.461)	78.48	0.05

These crystals were highly damaged as the experiment progressed, and so later datasets exhibit unphysical statistics. The use of the $I_n/I_1 > 0.4$ cutoff for later data analysis ensured that data from crystals that were too damaged to be meaningful were not included. Once the data are sufficiently degraded ($I/\sigma(I) < 1.5$, I_n/I_1 0.1), the mosaicity for the crystal cannot be determined in *MOSFLM*, so the value is reset to its default, indicated by an asterisk in the table. All datasets had completeness >99.2% (98.2% in the highest resolution shell). Average values are shown, with the outer resolution shell (1.8–1.9 Å) in brackets.

Table S2. Statistics for the medium beam data collection

Crystal	Probe	I_n/I_1	Unique observations	$CC_{1/2}$	Multiplicity	$I/\sigma(I)$	R_{meas}	Unit cell (Å)	Mosaicity (°)
191	1	1.0	7,505	0.974 (0.976)	6.9 (7.2)	12.1 (9.7)	0.158 (0.174)	78.26	0.43
	2	0.86	7,550	0.980 (0.974)	6.9 (7.2)	11.9 (8.7)	0.157 (0.179)	78.40	0.43
	3	0.88	7,572	0.980 (0.975)	6.9 (7.1)	12.4 (8.1)	0.145 (0.181)	78.42	0.41
	4	0.85	7,597	0.982 (0.970)	6.9 (7.1)	11.9 (7.2)	0.148 (0.209)	78.51	0.46
	5	0.53	7,597	0.984 (0.963)	6.9 (7.1)	11.3 (7.1)	0.147 (0.232)	78.55	0.43
	6	0.61	7,598	0.985 (0.949)	6.9 (7.1)	10.8 (5.6)	0.143 (0.283)	78.54	0.46
	7	0.51	7,599	0.987 (0.941)	6.9 (7.1)	11.0 (5.9)	0.141 (0.332)	78.58	0.48
	8	0.4	7,609	0.986 (0.908)	6.9 (7.1)	9.9 (5.0)	0.155 (0.426)	78.59	0.47
	9	0.33	7,615	0.987 (0.870)	6.9 (7.1)	9.1 (4.1)	0.165 (0.548)	78.60	0.51
	10	0.3	7,621	0.985 (0.809)	6.9 (7.1)	8.8 (3.7)	0.164 (0.701)	78.62	0.54
	11	0.26	7,632	0.984 (0.761)	6.9 (7.1)	8.5 (3.2)	0.168 (0.828)	78.65	0.49
225	1	1.0	7,465	0.998 (0.994)	6.8 (7.1)	25.6 (16.7)	0.060 (0.097)	78.03	0.34
	2	0.83	7,482	0.996 (0.991)	6.8 (7.1)	21.2 (13.1)	0.075 (0.118)	78.11	0.35
	3	0.98	7,508	0.998 (0.989)	6.8 (7.1)	23.4 (13.6)	0.063 (0.129)	78.25	0.38
	4	0.82	7,551	0.998 (0.984)	6.8 (7.1)	21.6 (11.0)	0.067 (0.163)	78.36	0.43
	5	0.7	7,578	0.997 (0.972)	6.8 (7.1)	19.3 (8.6)	0.072 (0.209)	78.44	0.45
	6	0.61	7,587	0.997 (0.959)	6.8 (7.1)	17.9 (7.1)	0.077 (0.273)	78.47	0.49
	7	0.53	7,607	0.997 (0.930)	6.8 (7.1)	16.4 (5.9)	0.085 (0.351)	78.54	0.51
	8	0.42	7,612	0.996 (0.886)	6.8 (7.1)	14.7 (4.8)	0.092 (0.461)	78.58	0.54
	9	0.38	7,627	0.996 (0.836)	6.8 (7.1)	13.1 (3.7)	0.101 (0.605)	78.62	0.55
	10	0.33	7,625	0.996 (0.756)	6.8 (7.1)	12.2 (3.1)	0.110 (0.772)	78.61	0.57
	11	0.31	7,666	0.996 (0.621)	6.8 (7.1)	11.2 (2.4)	0.120 (1.043)	78.67	0.58
2004	1	1.0	7,483	0.998 (0.994)	7.0 (7.2)	29.7 (16.1)	0.053 (0.110)	78.05	0.41
	2	0.76	7,532	0.998 (0.988)	7.0 (7.2)	27.1 (12.6)	0.057 (0.151)	78.25	0.34
	3	0.61	7,596	0.998 (0.963)	7.0 (7.2)	23.1 (7.1)	0.063 (0.285)	78.45	0.34
	4	0.49	7,632	0.998 (0.856)	7.0 (7.2)	18.2 (3.2)	0.074 (0.624)	78.61	0.40
	5	0.37	7,700	0.998 (0.491)	7.0 (7.2)	13.8 (1.5)	0.087 (1.354)	78.76	0.51
	6	0.31	7,702	0.998 (0.134)	6.9 (7.1)	10.9 (0.7)	0.104 (3.022)	78.80	0.61
	7	0.24	7,709	0.998 (0.014)	6.9 (7.1)	8.6 (0.3)	0.129 (5.384)	78.86	0.72
	8	0.19	7,712	0.998 (-0.029)	6.8 (7.0)	6.9 (0.2)	0.164 (11.106)	78.90	0.83
	9	0.16	7,739	0.998 (0.024)	6.8 (7.0)	5.6 (0.1)	0.211 (20.484)	78.98	0.89
	10*	0.039	7,527	0.749 (-0.015)	7.0 (7.2)	1.0 (0.1)	1.033 (49.363)	78.24	0.05
2012	1	1.0	7,522	0.996 (0.996)	6.9 (7.2)	30.8 (25.0)	0.065 (0.078)	78.20	0.07
	2	0.8	7,545	0.996 (0.994)	7.0 (7.3)	29.7 (19.7)	0.063 (0.095)	78.29	0.14
	3	0.64	7,569	0.997 (0.985)	7.0 (7.2)	25.1 (11.7)	0.064 (0.149)	78.35	0.25
	4	0.5	7,584	0.997 (0.969)	7.0 (7.2)	20.9 (8.6)	0.069 (0.236)	78.41	0.34
	5	0.38	7,601	0.998 (0.932)	7.0 (7.2)	16.4 (5.3)	0.078 (0.374)	78.44	0.42
	6	0.32	7,606	0.997 (0.860)	7.0 (7.2)	13.1 (3.2)	0.089 (0.569)	78.46	0.47
	7	0.27	7,607	0.996 (0.736)	7.0 (7.2)	10.4 (2.3)	0.108 (0.846)	78.48	0.51
	8	0.25	7,611	0.995 (0.614)	7.0 (7.1)	8.3 (1.7)	0.130 (1.185)	78.48	0.51
	9	0.2	7,591	0.993 (0.491)	7.0 (7.2)	6.9 (1.4)	0.156 (1.446)	78.40	0.46
	10*	0.15	7,577	0.969 (0.496)	7.1 (7.3)	4.9 (1.2)	0.248 (1.483)	78.37	0.03
	11*	0.16	7,567	0.984 (0.306)	7.0 (7.2)	5.3 (1.0)	0.212 (2.083)	78.32	0.34
2019	1	1.0	7,429	0.993 (0.996)	6.9 (7.2)	28.4 (23.6)	0.071 (0.079)	77.95	0.07
	2	0.88	7,483	0.996 (0.995)	7.0 (7.2)	30.3 (19.6)	0.063 (0.097)	78.10	0.13
	3	0.74	7,522	0.998 (0.990)	7.0 (7.2)	26.7 (13.7)	0.062 (0.137)	78.23	0.18
	4	0.64	7,547	0.998 (0.982)	7.0 (7.2)	23.3 (9.5)	0.067 (0.199)	78.33	0.20
	5*	0.51	7,568	0.992 (0.957)	7.0 (7.2)	10.9 (5.3)	0.117 (0.300)	78.42	0.02
	6*	0.43	7,553	0.984 (0.915)	6.9 (7.2)	8.2 (3.8)	0.153 (0.434)	78.44	−0.01
	7*	0.38	7,556	0.978 (0.847)	6.9 (7.2)	6.8 (2.7)	0.183 (0.604)	78.43	−0.01
	8*	0.32	7,529	0.969 (0.748)	6.9 (7.2)	5.9 (2.0)	0.203 (0.842)	78.35	0.00
2024	1	1.0	7,419	0.996 (0.996)	6.6 (7.1)	29.8 (22.4)	0.060 (0.078)	78.04	0.23
	2	0.81	7,486	0.996 (0.993)	6.6 (7.2)	26.8 (17.0)	0.064 (0.104)	78.18	0.25
	3	0.73	7,518	0.996 (0.989)	6.8 (7.2)	23.5 (12.6)	0.068 (0.138)	78.26	0.29
	4	0.65	7,547	0.997 (0.982)	6.8 (7.2)	20.8 (10.0)	0.071 (0.184)	78.35	0.31
	5	0.53	7,559	0.997 (0.967)	6.9 (7.2)	18.5 (6.7)	0.077 (0.259)	78.41	0.32
	6	0.48	7,581	0.996 (0.933)	6.8 (7.2)	15.7 (5.6)	0.087 (0.368)	78.50	0.32
	7	0.38	7,578	0.995 (0.890)	6.9 (7.2)	12.4 (4.6)	0.106 (0.479)	78.49	0.20
	8	0.34	7,611	0.995 (0.801)	6.9 (7.2)	11.6 (3.4)	0.112 (0.709)	78.62	0.28
	9*	0.29	7,617	0.985 (0.687)	6.9 (7.2)	6.8 (2.5)	0.180 (0.953)	78.65	0.09
	10*	0.23	7,642	0.979 (0.562)	6.9 (7.2)	5.9 (2.0)	0.199 (1.253)	78.68	0.08
	11*	0.21	7,659	0.992 (0.419)	6.9 (7.1)	7.7 (1.8)	0.154 (1.601)	78.68	0.32

An asterisk indicates unreliable data, a consequence of the high levels of damage. All datasets had >99.3% completeness. Average values are shown, with the outer resolution shell (1.8–1.9 Å) in brackets.

Table S3. Statistics for the small beam data collection

Crystal	Probe	I_n/I_1	Unique observations	$CC_{1/2}$	Multiplicity	$I/\sigma(I)$	R_{meas}	Unit cell (Å)	Mosaicity (°)
55	1	1.0	7,498	0.997 (0.986)	7.1 (7.3)	20.0 (10.9)	0.078 (0.171)	78.07	0.03
	2	0.9	7,508	0.997 (0.984)	7.1 (7.3)	19.4 (9.6)	0.074 (0.195)	78.13	0.06
	3	0.89	7,540	0.997 (0.971)	7.1 (7.3)	18.5 (7.6)	0.075 (0.251)	78.19	0.09
	4	0.85	7,560	0.997 (0.948)	7.1 (7.3)	16.8 (5.5)	0.081 (0.350)	78.25	0.12
	5	0.7	7,566	0.997 (0.921)	7.1 (7.3)	15.6 (4.5)	0.087 (0.458)	78.33	0.13
	6	0.69	7,577	0.997 (0.872)	7.1 (7.3)	14.5 (3.6)	0.094 (0.588)	78.35	0.14
	7	0.68	7,576	0.997 (0.824)	7.1 (7.3)	13.3 (2.9)	0.101 (0.732)	78.36	0.16
	8	0.66	7,604	0.997 (0.723)	7.1 (7.3)	12.1 (2.3)	0.111 (0.958)	78.45	0.17
	9	0.58	7,609	0.996 (0.615)	7.1 (7.3)	11.3 (1.9)	0.121 (1.180)	78.49	0.18
	10	0.54	7,571	0.997 (0.629)	7.0 (7.3)	11.4 (1.9)	0.119 (1.150)	78.37	0.19
	11	0.49	7,600	0.997 (0.488)	7.0 (7.3)	10.5 (1.4)	0.131 (1.573)	78.46	0.22
197	1	1.0	7,558	0.993 (0.984)	7.1 (7.3)	17.0 (10.2)	0.099 (0.164)	78.28	0.06
	2	0.87	7,565	0.993 (0.987)	7.1 (7.3)	17.2 (10.6)	0.096 (0.173)	78.32	0.06
	3	0.8	7,580	0.995 (0.979)	7.1 (7.3)	16.8 (9.1)	0.093 (0.200)	78.35	0.07
	4	0.82	7,641	0.990 (0.959)	7.1 (7.4)	10.7 (5.9)	0.124 (0.290)	78.60	0.02
	5	0.79	7,591	0.996 (0.961)	7.1 (7.3)	15.8 (6.8)	0.093 (0.283)	78.38	0.09
	6	0.56	7,590	0.996 (0.953)	7.1 (7.4)	15.5 (6.0)	0.096 (0.332)	78.39	0.10
	7	0.67	7,590	0.996 (0.952)	7.1 (7.3)	16.1 (6.0)	0.092 (0.330)	78.41	0.11
	8	0.57	7,606	0.996 (0.926)	7.1 (7.3)	14.7 (5.0)	0.097 (0.417)	78.43	0.11
	9	0.5	7,606	0.997 (0.892)	7.1 (7.3)	14.2 (4.2)	0.100 (0.510)	78.45	0.12
	10*	0.49	7,640	0.995 (0.857)	7.1 (7.4)	12.4 (3.6)	0.113 (0.593)	78.60	0.06
	11*	0.45	7,640	0.996 (0.831)	7.1 (7.4)	12.2 (3.4)	0.113 (0.655)	78.60	0.07
5185	1	1.0	7,428	0.996 (0.988)	7.1 (7.3)	19.3 (12.4)	0.082 (0.151)	77.92	0.03
	2	0.82	7,428	0.996 (0.982)	7.1 (7.3)	19.5 (11.6)	0.082 (0.173)	77.92	0.03
	3	0.83	7,430	0.996 (0.983)	7.1 (7.3)	18.0 (10.0)	0.084 (0.186)	77.92	0.03
	4	0.83	7,429	0.995 (0.976)	7.1 (7.3)	16.2 (8.7)	0.087 (0.209)	77.92	0.02
	5	0.78	7,429	0.994 (0.974)	7.1 (7.3)	15.0 (7.7)	0.094 (0.238)	77.92	0.02
	6	0.71	7,430	0.992 (0.963)	7.1 (7.3)	13.0 (6.7)	0.102 (0.275)	77.92	0.02
	7	0.69	7,498	0.997 (0.960)	7.1 (7.3)	17.2 (6.8)	0.082 (0.306)	78.15	0.11
	8	0.61	7,530	0.997 (0.947)	7.1 (7.3)	16.2 (5.7)	0.086 (0.363)	78.18	0.12
P1S10	1	1.0	7,445	0.998 (0.986)	7.1 (7.2)	22.4 (11.4)	0.065 (0.164)	77.94	0.14
	2	0.96	7,465	0.998 (0.983)	7.1 (7.2)	22.3 (9.8)	0.062 (0.193)	78.03	0.14
	3	0.89	7,485	0.998 (0.974)	7.1 (7.2)	20.5 (8.2)	0.064 (0.231)	78.10	0.16
	4	0.89	7,485	0.998 (0.965)	7.1 (7.2)	18.7 (6.6)	0.069 (0.283)	78.16	0.21
	5	0.83	7,517	0.998 (0.950)	7.1 (7.2)	17.1 (5.6)	0.076 (0.344)	78.20	0.25
	6	0.77	7,520	0.998 (0.932)	7.1 (7.2)	15.6 (4.9)	0.082 (0.398)	78.24	0.26
	7	0.67	7,536	0.997 (0.905)	7.1 (7.2)	14.5 (4.2)	0.089 (0.475)	78.27	0.28
	8	0.56	7,542	0.997 (0.882)	7.1 (7.2)	13.9 (3.6)	0.094 (0.568)	78.30	0.29
	9	0.55	7,557	0.997 (0.845)	7.1 (7.2)	13.1 (3.2)	0.098 (0.642)	78.34	0.30
P3S2	1	1.0	7,489	0.998 (0.987)	7.0 (7.1)	23.1 (12.2)	0.062 (0.152)	78.03	0.60
	2	0.93	7,500	0.998 (0.986)	7.0 (7.1)	22.7 (11.1)	0.063 (0.168)	78.08	0.61
	3	0.89	7,510	0.998 (0.980)	7.0 (7.1)	21.7 (9.9)	0.063 (0.193)	78.10	0.61
	4	0.82	7,510	0.998 (0.975)	7.0 (7.1)	21.2 (8.8)	0.064 (0.213)	78.15	0.62
	5	0.79	7,510	0.998 (0.973)	7.0 (7.1)	20.4 (8.1)	0.066 (0.234)	78.16	0.63
	6	0.73	7,542	0.998 (0.965)	7.0 (7.1)	19.8 (7.4)	0.068 (0.259)	78.18	0.63
	7	0.73	7,542	0.998 (0.964)	7.0 (7.1)	19.3 (6.7)	0.068 (0.277)	78.20	0.65
	8	0.67	7,545	0.998 (0.954)	7.0 (7.1)	18.3 (6.3)	0.072 (0.310)	78.25	0.65
	9	0.64	7,561	0.998 (0.948)	7.0 (7.1)	17.8 (5.7)	0.074 (0.341)	78.26	0.66

An asterisk indicates that there were very few reflection available for postrefinement, leading to problems in obtaining the correct mosaicity. All datasets had >99.6% completeness. Average values are shown, with the outer resolution shell (1.8–1.9 Å) in brackets.