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Supporting information for article:

**Whole-pattern fitting technique in serial femtosecond
nanocrystallography**

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and Harry M. Quiney**

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Supplementary Information

Table S1. Structure factor moduli of selected Bragg reflections extracted from a merged diffraction pattern from the test protein using the whole-pattern fitting approach, $|F^{WPF}|$, the integration approach, $|F^I|$, and calculated using published data (PDB ID: 4AK8), $|F^C|$. Ω^{WPF} and Ω^I are the relative errors for $|F^{WPF}|$ and $|F^I|$ respectively. The diffraction pattern was calculated in the $(hk0)$ crystallographic plane from a set of 2000 crystallites with a mean of 30 unit-cells along [100] direction and of 10 unit-cells along the [010] direction. The diffraction pattern was simulated on a 340x340 pixel array to 5.0 Å resolution. The average relative errors, $\langle \Omega^{WPF} \rangle = 0.06$ and $\langle \Omega^I \rangle = 0.13$, have been calculated with several weak reflections excluded (indicated in bold).

<i>h</i>	<i>k</i>	<i>l</i>	$ F^C $	$ F^{WPF} $	Ω^{WPF}	$ F^I $	Ω^I	<i>h</i>	<i>k</i>	<i>l</i>	$ F^C $	$ F^{WPF} $	Ω^{WPF}	$ F^I $	Ω^I
15	15	0	1479.44	1387.84	0.06	1392.08	0.06	9	15	0	348.55	334.33	0.04	348.15	0.00
15	14	0	765.45	721.29	0.06	673.07	0.12	9	14	0	1691.03	1580.70	0.07	1653.20	0.02
15	13	0	719.08	667.83	0.07	719.89	0.00	9	13	0	601.14	559.13	0.07	618.65	0.03
15	12	0	119.05	118.77	0.00	61.28	0.49	9	12	0	427.85	413.24	0.03	469.07	0.10
15	11	0	341.29	321.21	0.06	297.45	0.13	9	11	0	718.64	673.14	0.06	739.90	0.03
15	10	0	140.19	137.59	0.02	183.96	0.31	9	10	0	112.06	106.48	0.05	106.82	0.05
15	9	0	175.08	171.20	0.02	147.19	0.16	9	9	0	164.33	152.49	0.07	184.38	0.12
15	8	0	165.56	164.25	0.01	152.63	0.08	9	8	0	552.65	521.81	0.06	458.84	0.17
15	7	0	1122.08	1033.00	0.08	1219.34	0.09	9	7	0	746.68	704.97	0.06	766.41	0.03
15	6	0	885.83	833.21	0.06	925.19	0.04	9	6	0	153.23	148.84	0.03	121.82	0.20
15	5	0	564.17	536.45	0.05	473.25	0.16	9	5	0	276.23	259.15	0.06	284.48	0.03

15	4	0	71.54	63.84	0.11	87.91	0.23	9	4	0	117.62	108.81	0.07	121.12	0.03
14	15	0	167.96	170.06	0.01	118.12	0.30	8	15	0	1812.42	1707.92	0.06	1217.05	0.33
14	14	0	20.86	50.87	1.44	107.26	4.14	8	14	0	407.59	413.67	0.01	379.02	0.07
14	13	0	499.89	478.94	0.04	460.92	0.08	8	13	0	385.09	366.66	0.05	287.63	0.25
14	12	0	292.23	269.80	0.08	300.99	0.03	8	12	0	398.74	367.24	0.08	301.99	0.24
14	11	0	606.21	580.16	0.04	525.56	0.13	8	11	0	722.81	683.22	0.05	518.26	0.28
14	10	0	646.32	601.57	0.07	669.65	0.04	8	10	0	85.76	83.17	0.03	78.79	0.08
14	9	0	860.07	820.86	0.05	787.53	0.08	8	9	0	8.01	27.15	2.39	39.13	3.89
14	8	0	358.53	332.21	0.07	324.87	0.09	8	8	0	896.86	851.94	0.05	589.38	0.34
14	7	0	681.36	668.68	0.02	576.98	0.15	8	7	0	556.19	524.18	0.06	419.52	0.25
14	6	0	106.9	112.57	0.05	84.99	0.20	8	6	0	726.95	686.99	0.05	550.99	0.24
14	5	0	126.26	132.99	0.05	90.37	0.28	8	5	0	801.94	759.75	0.05	588.94	0.27
14	4	0	268.05	263.09	0.02	235.68	0.12	8	4	0	350.58	335.85	0.04	235.91	0.33
13	15	0	485.27	462.25	0.05	405.44	0.16	7	15	0	218.99	234.03	0.07	173.69	0.21
13	14	0	356.15	340.18	0.04	302.92	0.15	7	14	0	1709.09	1606.52	0.06	1708.67	0.00
13	13	0	1149.61	1059.99	0.08	1160.89	0.01	7	13	0	1367.24	1285.66	0.06	1358.00	0.01
13	12	0	216.53	214.50	0.01	174.26	0.20	7	12	0	662.9	625.29	0.06	624.81	0.06
13	11	0	1223.02	1133.39	0.07	1196.68	0.02	7	11	0	1236.52	1145.95	0.07	1323.64	0.07
13	10	0	426.65	403.27	0.05	358.40	0.16	7	10	0	311.26	289.61	0.07	333.50	0.07
13	9	0	918.49	836.41	0.09	1002.50	0.09	7	9	0	378.71	356.56	0.06	351.76	0.07
13	8	0	93.16	97.20	0.04	86.90	0.07	7	8	0	1498.04	1390.75	0.07	1427.53	0.05
13	7	0	146.65	111.93	0.24	370.75	1.53	7	7	0	245.37	228.05	0.07	262.17	0.07
13	6	0	893	824.27	0.08	855.68	0.04	7	6	0	671.73	629.14	0.06	662.50	0.01
13	5	0	257.16	232.58	0.10	311.06	0.21	7	5	0	778.76	724.03	0.07	756.87	0.03

13	4	0	1261.17	1171.24	0.07	1320.11	0.05	7	4	0	1146.02	1054.02	0.08	916.75	0.20
12	15	0	52.75	57.86	0.10	49.83	0.06	6	15	0	940.32	863.88	0.08	1017.66	0.08
12	14	0	848.74	797.85	0.06	738.27	0.13	6	14	0	420.59	401.57	0.05	337.22	0.20
12	13	0	779.71	728.85	0.07	678.33	0.13	6	13	0	76.35	85.81	0.12	117.27	0.54
12	12	0	71.84	99.87	0.39	175.15	1.44	6	12	0	142.85	136.45	0.04	141.40	0.01
12	11	0	33.66	54.62	0.62	110.16	2.27	6	11	0	259.31	246.29	0.05	292.42	0.13
12	10	0	351.8	326.95	0.07	330.60	0.06	6	10	0	226.49	215.36	0.05	268.17	0.18
12	9	0	179.03	170.95	0.05	143.44	0.20	6	9	0	1036.46	962.12	0.07	1047.75	0.01
12	8	0	661.74	598.35	0.10	614.85	0.07	6	8	0	92.91	84.33	0.09	95.98	0.03
12	7	0	1959.28	1801.15	0.08	2000.03	0.02	6	7	0	1658.77	1514.36	0.09	1541.82	0.07
12	6	0	400.67	372.29	0.07	347.30	0.13	6	6	0	1572.69	1466.04	0.07	1701.61	0.08
12	5	0	1451.56	1331.97	0.08	1401.46	0.03	6	5	0	2078.15	1949.36	0.06	2144.43	0.03
12	4	0	117.12	104.85	0.10	136.19	0.16	6	4	0	1193.89	1118.89	0.06	1050.45	0.12
11	15	0	1274.6	1177.02	0.08	1135.88	0.11	5	15	0	641.56	595.28	0.07	642.92	0.00
11	14	0	1310.49	1197.69	0.09	1317.61	0.01	5	14	0	569.29	528.86	0.07	682.76	0.20
11	13	0	155.39	141.02	0.09	147.16	0.05	5	13	0	641.29	595.14	0.07	669.67	0.04
11	12	0	87.11	79.89	0.08	90.34	0.04	5	12	0	385.65	358.87	0.07	415.65	0.08
11	11	0	601.96	551.54	0.08	587.95	0.02	5	11	0	227.69	214.54	0.06	204.94	0.10
11	10	0	267.75	243.51	0.09	260.08	0.03	5	10	0	347.6	326.38	0.06	328.63	0.05
11	9	0	345.26	309.20	0.10	362.41	0.05	5	9	0	20.71	57.53	1.78	114.41	4.52
11	8	0	1239.06	1137.83	0.08	1057.75	0.15	5	8	0	1539.322	1422.43	0.08	1380.10	0.10
11	7	0	963.78	871.50	0.10	885.66	0.08	5	7	0	734.355	675.08	0.08	897.25	0.22
11	6	0	169.48	172.22	0.02	179.56	0.06	5	6	0	1276.226	1172.88	0.08	1542.77	0.21
11	5	0	4.7	75.16	14.99	169.74	35.1	5	5	0	1304.423	1220.63	0.06	1285.38	0.01

11	4	0	232.14	226.63	0.02	294.30	0.27	5	4	0	219.441	215.97	0.02	283.23	0.29
10	15	0	1312.66	1217.34	0.07	1198.69	0.09	4	15	0	740.335	693.27	0.06	718.09	0.03
10	14	0	523.55	476.59	0.09	555.52	0.06	4	14	0	696.137	654.89	0.06	785.23	0.13
10	13	0	937.45	871.30	0.07	838.97	0.11	4	13	0	316.475	298.97	0.06	332.46	0.05
10	12	0	27.12	26.18	0.03	44.19	0.63	4	12	0	248.249	238.62	0.04	183.95	0.26
10	11	0	266.22	251.80	0.05	227.62	0.14	4	11	0	141.391	137.01	0.03	90.99	0.36
10	10	0	44.03	96.23	1.19	176.72	3.01	4	10	0	9.473	12.56	0.33	27.53	1.91
10	9	0	815.12	743.33	0.09	874.84	0.07	4	9	0	132.585	128.05	0.03	107.41	0.19
10	8	0	257.22	260.94	0.01	257.20	0.00	4	8	0	611.249	579.59	0.05	503.28	0.18
10	7	0	641.8	595.20	0.07	700.55	0.09	4	7	0	206.147	190.97	0.07	320.08	0.55
10	6	0	248.37	233.29	0.06	265.64	0.07	4	6	0	437.267	410.74	0.06	591.85	0.35
10	5	0	119.71	111.89	0.07	215.90	0.80	4	5	0	346.362	328.70	0.05	346.36	0.00
10	4	0	617.62	576.90	0.07	650.90	0.05	4	4	0	1473.183	1384.90	0.06	1313.24	0.11