

Supplementary Table 1.

Data statistics versus resolution for Native A.

Resolution Å							
Lower limit	Upper limit	Average I	Average error	Norm. stat	Linear Chi**2	Square R-fac	R-fac
50.00	9.48	3729.4	147.1	119.4	1.097	0.061	0.063
9.48	7.53	1637.8	109.2	105.0	1.022	0.109	0.106
7.53	6.58	955.2	107.7	107.5	0.925	0.180	0.168
6.58	5.98	928.3	120.4	120.2	0.937	0.210	0.180
5.98	5.55	988.1	134.8	134.6	0.888	0.222	0.193
5.55	5.23	1139.8	149.1	148.8	0.922	0.217	0.191
5.23	4.97	1264.5	161.2	160.9	0.876	0.209	0.181
4.97	4.75	1327.9	176.0	175.8	0.841	0.208	0.186
4.75	4.57	1511.1	191.9	191.6	0.885	0.206	0.180
4.57	4.41	1397.2	214.7	214.5	0.889	0.231	0.205
4.41	4.27	1350.8	225.2	224.9	0.862	0.257	0.233
4.27	4.15	1175.1	233.2	233.0	0.829	0.297	0.243
4.15	4.04	1018.2	234.7	234.6	0.866	0.357	0.325
4.04	3.94	891.9	245.1	245.0	0.832	0.394	0.357
3.94	3.85	811.5	262.0	261.9	0.827	0.455	0.419
3.85	3.77	852.1	257.7	257.6	0.798	0.455	0.392
3.77	3.69	708.4	259.8	259.7	0.831	0.527	0.464
3.69	3.63	695.1	273.9	273.8	0.823	0.566	0.490
3.63	3.56	612.6	265.6	265.5	0.869	0.652	0.583
3.56	3.50	616.0	268.8	268.7	0.807	0.650	0.540
All reflections		1203.0	199.3	197.4	0.885	0.250	0.203

In the 3.56-3.50 resolution shell, the average intensity divided by the error (616.0/268.8) is about 2.3. This table is from *SCALEPACK* (Otwinowski, Z. & Minor, W, 1997).