Supplementary material

Reflection data statistics

Resolution range (Å)	Number of unique ref.	<I/σ>	Comp. (%)	Comp. (%) (I > 2σ)	R (all)	R ($I > 2\sigma$)
31.0 > 2.55	3812	25.24	96.38	96.28	0.157	0.157
2.55 > 2.02	3804	25.21	99.71	99.34	0.114	0.113
2.02 > 1.77	3632	27.06	99.75	99.04	0.103	0.103
1.77 > 1.61	3600	23.08	99.20	98.26	0.094	0.094
1.61 > 1.49	3805	22.68	99.71	98.38	0.089	0.088
1.49 > 1.40	3779	21.84	99.74	98.02	0.088	0.086
1.40 > 1.33	3661	20.69	99.78	96.43	0.092	0.088
1.33 > 1.28	3125	19.79	99.68	96.11	0.095	0.091
1.28 > 1.23	3671	18.86	99.73	95.19	0.097	0.091
1.23 > 1.18	4286	17.70	99.95	93.54	0.100	0.092
1.18 > 1.15	2952	16.72	99.80	93.34	0.103	0.094
1.15 > 1.11	4415	14.57	99.70	92.09	0.108	0.096
1.11 > 1.09	2454	13.11	99.96	90.31	0.117	0.100
1.09 > 1.06	4060	10.77	100.00	87.44	0.126	0.106
1.06 > 1.03	4526	8.19	99.98	84.25	0.141	0.113
1.03 > 1.01	3332	6.61	99.97	81.58	0.150	0.116
1.01 > 0.99	3594	5.09	99.89	75.82	0.167	0.121
0.99 > 0.97	3918	3.97	100.00	72.08	0.184	0.130
0.97 > 0.96	2052	3.11	100.00	64.47	0.222	0.141
0.96 > 0.94	3912	2.66	88.63	55.32	0.300	0.210
All data	72390	15.53	98.95	88.51	0.123	0.116

SHELXPRO statistics after the last refinement step. The percentage with I>2σ is expressed relative to the theoretical number of unique reflections. $R = \Sigma (|F_o - F_c|)/ \Sigma(F_o)$.