Supplementary material (OH-APLA2)

Summary of observation redundancies

Shell		% of reflections with given No. of observations										
Lower limit	Upper limit	0	1	2	3	4	5-6	7-8	9-12	13-19	>19	Total
20.00	5.57	8.7	14.4	27.6	26.1	23.2	0.0	0.0	0.0	0.0	0.0	91.3
5.57	4.43	1.8	8.9	28.5	33.7	27.2	0.0	0.0	0.0	0.0	0.0	98.2
4.43	3.88	2.2	7.9	28.1	36.5	25.3	0.0	0.0	0.0	0.0	0.0	97.8
3.88	3.52	1.2	7.7	29.8	38.4	22.9	0.0	0.0	0.0	0.0	0.0	98.8
3.52	3.27	1.9	10.1	27.6	37.5	23.0	0.0	0.0	0.0	0.0	0.0	98.1
3.27	3.08	1.2	7.2	30.6	40.8	20.2	0.0	0.0	0.0	0.0	0.0	98.8
3.08	2.93	0.8	7.2	31.6	40.7	19.7	0.0	0.0	0.0	0.0	0.0	99.2
2.93	2.80	4.7	7.8	31.6	37.7	18.2	0.0	0.0	0.0	0.0	0.0	95.3
2.80	2.69	15.2	5.8	29.1	31.8	18.1	0.0	0.0	0.0	0.0	0.0	84.8
2.69	2.60	25.0	6.2	28.0	25.6	15.2	0.0	0.0	0.0	0.0	0.0	75.0
All *hkl*		6.2	8.3	29.2	34.9	21.3	0.0	0.0	0.0	0.0	0.0	93.8

Summary of reflections intensities and *R* factors by shells

Shell		% of reflections with I/σ											
Lower limit	Upper limit	<0	<1	<2	<3	<5	<10	<20	>20	Total	Norm χ^2	Linear *R* fac	Square *R* fac
20.00	5.57	0.8	2.3	4.3	5.9	9.0	15.7	35.9	55.3	91.3	2.174	0.054	0.059
5.57	4.43	0.9	3.0	5.1	7.5	12.3	22.0	46.2	52.0	98.2	2.118	0.065	0.070
4.43	3.88	1.6	4.2	6.4	9.3	15.3	27.4	52.8	45.0	97.8	2.067	0.072	0.075
3.88	3.52	1.4	5.1	9.5	13.7	20.3	38.2	65.3	33.5	98.8	1.841	0.082	0.084
3.52	3.27	2.3	7.3	13.7	18.3	28.7	48.2	75.0	23.1	98.1	1.601	0.098	0.099
3.27	3.08	4.5	9.2	16.4	24.5	37.2	58.8	84.9	13.9	98.8	1.443	0.118	0.111
3.08	2.93	5.0	13.0	22.0	30.2	43.6	69.5	90.2	9.0	99.2	1.294	0.139	0.125
2.93	2.80	4.8	14.7	23.9	32.7	47.9	72.2	90.4	4.9	95.3	1.266	0.170	0.167
2.80	2.69	5.0	12.8	22.4	31.9	46.5	66.2	82.3	2.5	84.8	1.237	0.184	0.181
2.69	2.60	3.4	13.3	24.5	33.6	45.0	62.2	73.6	1.4	75.0	1.147	0.205	0.193
All *hkl*		3.0	8.4	14.7	20.7	30.4	47.9	69.5	24.3	93.8	1.640	0.087	0.079

R linear = $\Sigma[\mathrm{ABS}(I - \langle I \rangle)]/\Sigma(I)$.
R square = $\Sigma[(I - \langle I \rangle)^2]/\Sigma(I^2)$.
$\chi^2 = \Sigma[(I - \langle I \rangle)^2]/[\mathrm{Error}^2\ N/(N\text{-}1)]$.
In all sums single measurements are excluded.