



Data set	THA_cluster 1	THA_all
Unit-cell parameters (\AA)		
a	58.00	58.00
c	150.35	150.35
Multiplicity	56.0 (54.4)	100.9 (94.7)
Completeness (%)	99.9 (99.9)	100.0 (100.0)
R factor (%)	9.2 (18.7)	12.2 (23.6)
$\langle I/\sigma(I) \rangle$	59.2 (30.9)	57.3 (31.9)
B factor (\AA^2)	12.9	12.8
$\langle \Delta F/\sigma(\Delta F) \rangle$, first shell	4.5	3.9
CC_{map} , first shell (%)	94	96.4
Best CC_{all} (%)	57.6	55.1
Best CC_{weak} (%)	32.3	26.6
No. of solutions	323	181
CC_{map} (%)	83	60