Table. Crystallographic details.

A. Three different crystal forms used in the initial low-resolution phasing.

spacegroup	a × b × c (Å); α, β, γ	AU contents	% solvent
$P3_112$	96 × 96 × 280; 90°, 90°, 120°	monomer	67%
$P4_22_12$	199 × 199 × 75; 90°, 90°, 90°	monomer	67%
$P2_1$	96 × 154 × 104; 90°, 114°, 90°	dimer	65%

B. Data collection- Three individual datasets from one monoclinic ($P2_1$) crystal

data-set	beam line	wave-length		Detector Distance	Detector (mode)	# images	reso-lution	# unique reflections	R-sym
1	SSRL 7-1	1.08	1*	400	mar345(300)	205	21.8 - 3.3	35,658	0.127
2	ALS 5.02	1.10	1*	240	ADSC-Q4	180	20.0 - 3.3	36,140	0.092
3	ALS 5.02	1.10	1*	240	ADSC-Q4	180	59.8 - 3.8	26,460	0.116

C. Data reduction- merged dataset

resolution	3.8	3.5	3.3
unique refln	26,590	33,596	39,079
completeness, (last shell)	98.7% (96%)	97.6% (94%)	95.3 (59%)
redundancy[1]	2.88	2.68	2.51
$<I>/<\sigma>$	9.5 (7.1)	8.5 (3.9)	7.0 (1.1)
R-merge	0.115 (.29)	0.120 (0.28^2)	.122 ($.28^2$)
"optical" resol.[3]	2.69	2.52	2.45
B_{wilson}[4]	-	-	59.0

1. Actual redundancy is higher because three pre-merged sets are combined here.
2. Note last shell has redundancy <2 so R-merge underestimates variability
3. Optical resolution as defined by Vaguine (Acta Cryst. D55, 191-205, 1999) and reported by sfcheck program
4. Wilson plot from truncate program, 4.0 to 3.3 Å

D. Refinement- merged dataset

resolution	59.8 - 3.8	59.8 - 3.5
# atoms	13252	13252
F/σ_F cutoff	0	0
# reflections	26,318	33,264
completeness	98.8%	97.6%
test set (%)	1323 (5.0%)	1661 (5.0%)
R_{crys} (last shell)	0.295 (0.41)	0.302 (0.42)
R_{free} (last shell)	0.345 (0.45)	0.358 (0.53)
iso $B_{overall}$	86.3	88.1
aniso B_{11}	-37	-34
aniso B_{22}	+92	+87
aniso B_{33}	-55	-53
RMSD (angles)	2.6	2.6
RMSD (bonds)	0.031	0.032
RMSD (dihedr)	23.9	23.9
ESD coord error[1]	0.68	0.73
NCS model	strongly restrained	

1. From cross-validated Luzatti plot, low cutoff 5.0 Å