

FIGURE 1 -FIGURE SUPPLEMENT 1

Data collection and refinement statistics (molecular replacement)

	Luciferase/iLH2
Data collection	
Space group	P 2 ₁
Cell dimensions	
<i>a</i> , <i>b</i> , <i>c</i> (Å)	47.509, 114.016, 101.557
α , β , γ (°)	90.00, 98.18, 90.00
Resolution (Å)	22.5- 3.1 (3.21)
<i>R</i> _{sym} or <i>R</i> _{merge}	22.7 (46.0)
<i>I</i> / σI	2.15 (1.1)
Completeness (%)	94.2 (97.2)
Redundancy	2.7 (2.6)
Refinement	
Resolution (Å)	17.85 - 3.1
No. reflections	17435(1328)
<i>R</i> _{work} / <i>R</i> _{free}	27.4/32.0 (0.39/0.42)
No. atoms	
Protein	8428
Ligand/ion	84
Water	0
<i>B</i> -factors	-
Protein	43
Ligand/ion	24
R.m.s. deviations	-
Bond lengths (Å)	0.01
Bond angles (°)	1.417

*Values in parentheses are for highest-resolution shell.

	HJ ₂	HJ ₃
Data collection		
Space group	P 1 2 ₁ 1	P 1 2 ₁ 1
Cell dimensions		
<i>a</i> , <i>b</i> , <i>c</i> (Å)	48.3013, 45.9128, 62.4669	49.937, 45.374, 63.828
α, β, γ (°)	90.00, 99.2863, 90.00	90.00, 101.01, 90.00
Resolution (Å)	24-3.5 () *	49-2.69 (2.74-2.69)
<i>R</i> _{sym} or <i>R</i> _{merge}	10.5 ()	5.4% (64%)
<i>I</i> / σ <i>I</i>	17.4 ()	10.9 (1.6)
Completeness (%)	99.7 ()	99.9 (97.6)
Redundancy	6.1 ()	3.6 (3.7)
Refinement		
Resolution (Å)	30-3.05	49-3.0
No. reflections	5038	5446
<i>R</i> _{work} / <i>R</i> _{free}	23.0/32.3	24.6/28.5
No. atoms		
DNA	1684	1712
Ligand/ion	2	2
<i>B</i> -factors		
Protein	77	50
Ligand/ion		49
R.m.s deviations		
Bond lengths (Å)	0.008	0.008
Bond angles (°)	1.47	1.56

*Values in parentheses are for highest-resolution shell.

Data collection, phasing and refinement statistics for mad (semet) structures

	Native	Crystal 1 name			Crystal 2 name	
Data collection						
Space group		common #			common #	
Cell dimensions						
<i>a</i> , <i>b</i> , <i>c</i> (Å)		common #			common #	
α, β, γ (°)		common #			common #	
		<i>Peak</i>	<i>Inflection</i>	<i>Remote</i>	<i>Peak</i>	<i>Inflection</i>
Wavelength		#	#	#	#	#
Resolution (Å)		#	#	#	#	#
<i>R</i> _{sym} or <i>R</i> _{merge}		#	#	#	#	#
<i>I</i> / σ <i>I</i>		#	#	#	#	#
Completeness (%)		#	#	#	#	#
Redundancy		#	#	#	#	#
Refinement						
Resolution (Å)		common #			common #	
No. reflections						
<i>R</i> _{work} / <i>R</i> _{free}						
No. atoms						
Protein						
Ligand/ion						
Water						
<i>B</i> -factors						
Protein						
Ligand/ion						
Water						
R.m.s deviations						
Bond lengths (Å)						
Bond angles (°)						

*Number of xtals for each structure should be noted in footnote. *Values in parentheses are for highest-resolution shell.