

Table 1 Data collection and refinement statistics (Molecular Replacement)

	Crystal 1 name	Crystal 2 name
Data collection		
Space group		
Cell dimensions		
<i>a</i> , <i>b</i> , <i>c</i> (Å)	42.08, 86.93, 86.24	
α , β , γ (°)	118.11, 99.65, 95.47	
Resolution (Å)	##(high res shell) *	
R_{sym} or R_{merge}	##(high res shell)	
$I / \sigma I$	##(high res shell)	
Completeness (%)	##(high res shell)	
Redundancy	##(high res shell)	
Refinement		
Resolution (Å)		
No. reflections		
$R_{\text{work}} / R_{\text{free}}$		
No. atoms		
Protein		
Ligand/ion		
Water		
<i>B</i> -factors	(Ask for input)	
Protein		
Ligand/ion		
Water		
R.m.s deviations		
Bond lengths (Å)		
Bond angles (°)		

* Number of xtals for each structure should be noted in footnote. *Highest resolution shell is shown in parenthesis.

[AU: Equations defining various R values are standard and hence are no longer defined in the footnotes.]

[AU: Ramachandran statistics should be in methods section at the end of the refinement sub-section.]

[AU: Wavelength of data collection, temperature, beamline should all be in methods section.]

Table 2 Data collection, phasing and refinement statistics (MIR)

	Crystal 1 name	Crystal 2 name
Data collection		
Space group		
Cell dimensions		
<i>a</i> , <i>b</i> , <i>c</i> (Å)		
α , β , γ (°)		
Resolution (Å)	##(high res shell) *	
R_{sym} or R_{merge}	##(high res shell)	
$I / \sigma I$	##(high res shell)	
Completeness (%)	##(high res shell)	
Redundancy	##(high res shell)	
Refinement		
Resolution (Å)		
No. reflections		
$R_{\text{work}} / R_{\text{free}}$		
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. *Highest resolution shell is shown in parenthesis.

[AU: Equations defining various R values are standard and hence are no longer defined in the footnotes.]

[AU: Phasing data should be reported in the methods section]

[AU: Ramachandran statistics should be in methods section at the end of the refinement sub-section.]

[AU: Wavelength of data collection, temperature, beamline should all be in methods section.]

Table 3 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, b, 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>	<i>Remote</i>
Wavelength		#	#	#	#	#	#
Resolution (Å)		#	#	#	#	#	#
R_{sym} or R_{merge}		#	#	#	#	#	#
$I / \sigma I$		#	#	#	#	#	#
Completeness (%)		#	#	#	#	#	#
Redundancy		#	#	#	#	#	#
Refinement							
Resolution (Å)			common #			common #	
No. reflections							
$R_{\text{work}} / R_{\text{free}}$							
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. *Highest resolution shell is shown in parenthesis.

[AU: Equations defining various R values are standard and hence are no longer defined in the footnotes.]

[AU: Phasing data should be reported in the methods section]

[AU: Ramachandran statistics should be in methods section at the end of the refinement sub-section.]

[AU: Wavelength of data collection, temperature, beamline should all be in methods section.]