

**Table S2. Data Collection and Refinement Statistics**

	<i>Dda_ykkC</i> IrHex	<i>Dda_ykkC</i>
<b>Data Collection</b>		
<b>Wavelength</b>	1.1049	.9791
<b>Resolution range</b>	100.63 – 2.25 (2.32 – 2.25)	51.12 - 2.3 (2.382 - 2.3)
<b>Space group</b>	P 2 12 12	I 2 2 2
<b>Unit cell</b>	31.72 74.12 100.63 90 90 90	67.441 78.371 98.844 90 90 90
<b>Total reflections</b>	73599	79395 (7799)
<b>Unique reflections</b>	11858	11977 (1178)
<b>Multiplicity</b>	6.2 (5.9)	6.6 (6.6)
<b>Completeness (%)</b>	99.5 (95.2)	100 (100)
<b>Mean I/sigma(I)</b>	10.8 (0.8)	13.33 (2.05)
<b>Wilson B-factor</b>		54.76
<b>R-merge</b>	0.070 (1.835)	0.07749 (1.033)
<b>R-meas</b>	0.077 (1.998)	0.08472 (1.123)
<b>CC1/2</b>	0.998 (0.536)	0.991 (0.785)
<b>CC*</b>	0.999 (0.687)	0.998 (0.938)
<b>Refinement</b>		
<b>Reflections used in refinement</b>		16941 (1624)
<b>Reflections used for R-free</b>		1693 (163)
<b>R-work</b>		0.2061 (0.4408)
<b>R-free</b>		0.2389 (0.4601)
<b>CC(work)</b>		0.978 (0.662)
<b>CC(free)</b>		0.960 (0.526)
<b>Number of non-hydrogen atoms</b>		1904
macromolecules		1820
ligands		61
waters		23
<b>Protein residues</b>		0
<b>RMS(bonds)</b>		0.014
<b>RMS(angles)</b>		1.28
<b>Clashscore</b>		6.05
<b>Average B-factor</b>		56.54
macromolecules		56.23
ligands		67.17
solvent		53.44