

**Supplementary information, Table S1** Statistics of data sets and structure refinement

	PYL2/AM1/HAB1	PYL2/AM2/HAB1	PYL2/AM3/HAB1
PDB code	4LG5	4LGA	4LGB
<b>Data collection</b>			
Beam line	SSRF-BL17U1	SSRF-BL17U1	SSRF-BL17U1
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Resolution, Å	30-2.88	30-2.70	30-3.15
Cell parameters, Å, °	a=60.83, b=65.90, c=146.23; α=β=γ=90	a=61.03, b=67.16, c=145.35; α=β=γ=90	a=60.96, b=66.17, c=143.84; α=β=γ=90
Total/Unique reflections	51771 /12560	62634/16757	37143/8417
Completeness, %	89.8(92.6)	97.9(99.6)	79.0 (58.2)
I/σ	10.6(2.0)	14.7(2.5)	8.1(2.0)
Redundancy	4.1(4.2)	3.7(3.9)	4.4(3.6)
Rsym	0.149(0.562)	0.103(0.720)	0.168(0.558)
<b>Refinement</b>			
Resolution, Å	30-2.88	30-2.70	30-3.15
No. reflections	9697	13831	6407
No. residues	498	496	495
No. solvent molecules	61	49	47
No. of non-H atoms	3818	3785	3774
Rcryst	22.9%	22.0%	21.5%
Rfree	29.9%	28.8%	31.5%
rmsd bonds, Å	0.011	0.008	0.009
rmsd angles, °	1.62	1.42	1.25
Average Bfactor, Å <sup>2</sup>	16.38	30.61	24.09

Rmsd is the root-mean-square deviation from ideal geometry of protein.