
S3 Table. Crystallographic Table
Data Collection and Refinement Statistics^a

	InIP	Lmo2027
<i>PDB code</i>	5HL3	5KZS
<i>Data Collection</i>		
Resolution range, Å	30.00-1.40 (1.42-1.40)	30.00-2.30 (2.34-2.30)
Space group	P4 ₁ 2 ₁ 2	I ₄
Unit cell dimensions		
a,b,c, Å	a & b = 72.9 c = 179.5	a & b = 157.8 c = 36.3
α , β , γ , degrees	α , β , γ = 90	α , β , γ = 90
Completeness, %	99.8 (100)	98.6 (99.6)
No. reflections	180423 (9031)	20005 (1429)
Redundancy	45.6 (5.3)	6.2 (4.5)
$\langle I/\sigma(I) \rangle$	30.2 (2.6)	79.7 (2.0)
R_{merge} , %	7.9 (65.3)	9.0 (57.1)
<i>Refinement statistics</i>		
R-factor ($R_{\text{work}}/R_{\text{free}}$) ^b	16.0/17.6	22.8/27.9
No. atoms		
Protein	2935	2377
Waters	828	26
Ca ²⁺	8	n/a
R.M.S. deviations		
Bond lengths, Å	0.011	0.009
Bond angles, degrees	1.51	1.47
Ramachandran analysis		
Favored regions, %	96	95
Allowed regions, %	100	99
Disallowed regions, %	0	1

^aHighest resolution shell in parenthesis.

^bDefinition of R_{work} , R_{free} : $R = \sum_{hkl} |F_{\text{obs}} - |F_{\text{calc}}| / \sum_{hkl} |F_{\text{obs}}|$, where hkl are the reflection indices used in refinement for R_{work} , and **5% not used in refinement for R_{free}** . F_{obs} and F_{calc} are structure factors deduced from measured intensities or calculated from the model, respectively.