

Pea and Lentil 7S Globulin Crystal Structures with Comparative Ig Epitope Mapping

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Supplemental Tables and Figures

Supplemental Table T1: Crystallization conditions

	Pis s 1	Pis s 2	Len c 1*
Buffer:	0.075 M sodium fluoride, 0.1 M bis-tris propane pH 5.5, 10% PEG 3350	0.15 M ammonium acetate, 0.05 M bis tris pH 6.0, 25% PEG 3350	0.01 M zinc chloride, 0.1 M sodium acetate trihydrate pH 5.5, 15% PEG 6000
Protein concentration:	8.0-9.8 mg/mL	2.0 mg/mL	2.0-10 mg/mL
Drop ratio:	2 μ L well: 1 μ L protein	1 μ L well: 2 μ L protein	1 μ L well: 2 μ L protein
Cryo-protectant:	none	none	20% glycerol
Time to form:	9-12 days	3 days	1-11 day post microseed

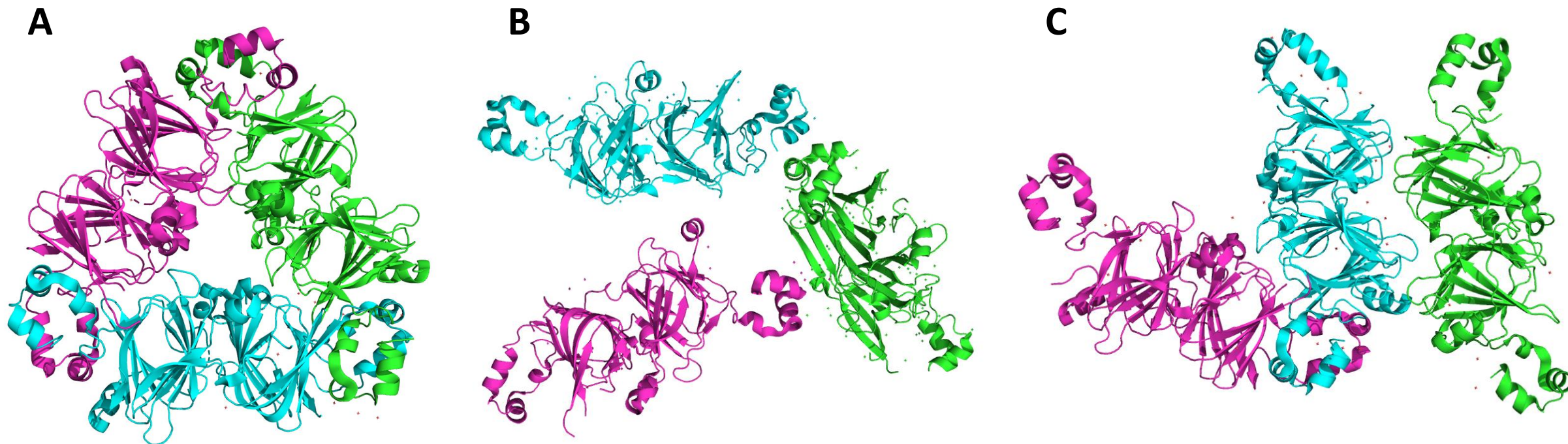
* indicates crystal obtained after microseeding

Supplemental Table T2.

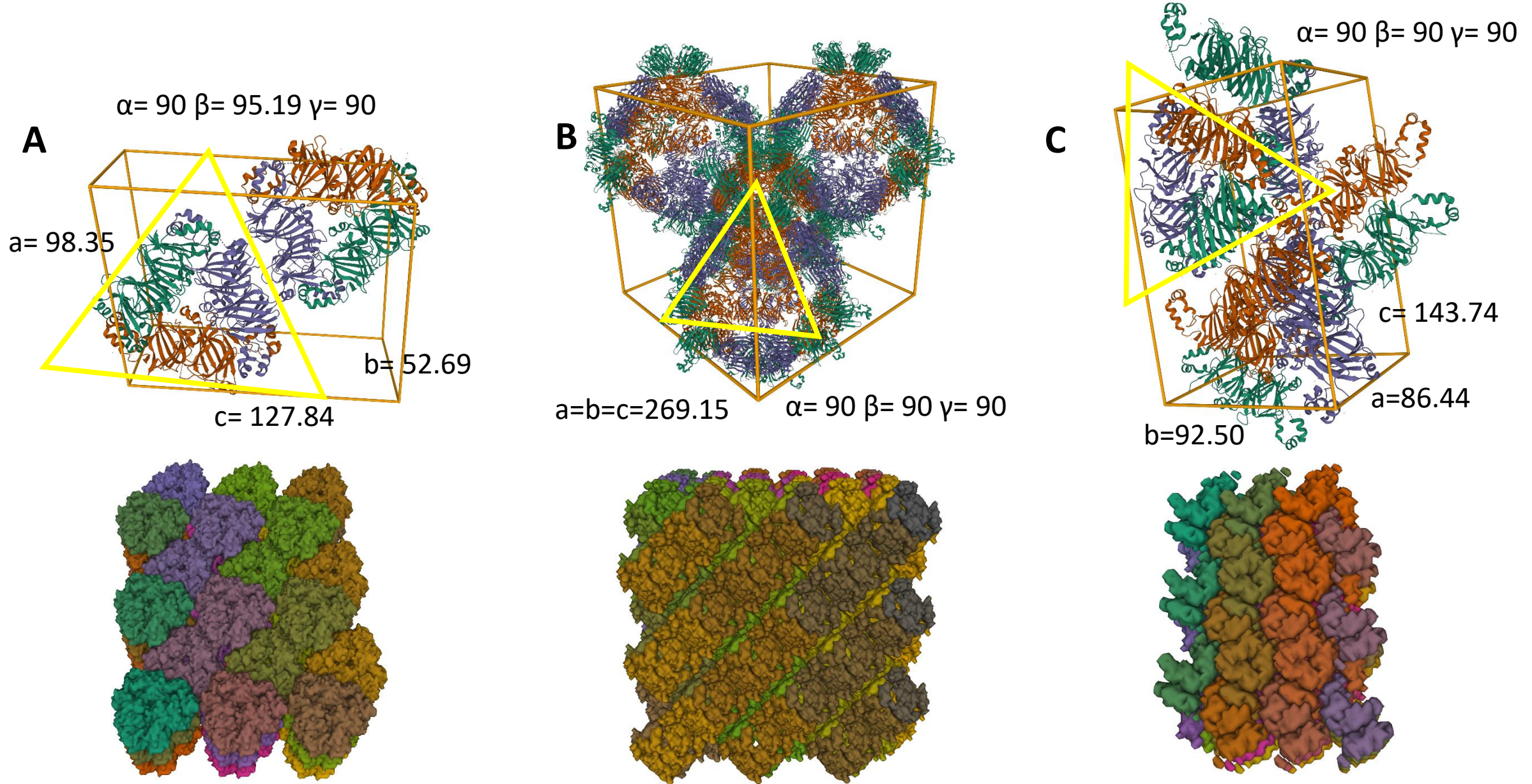
*Epitopes share in position of sequence, but do not share high sequence identity or tertiary structure.

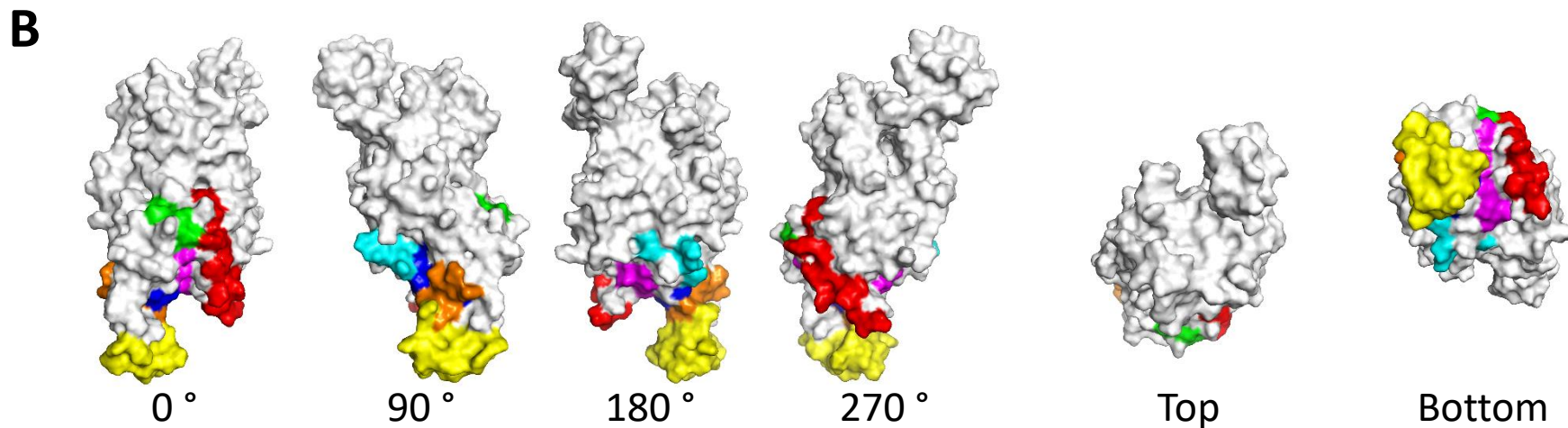
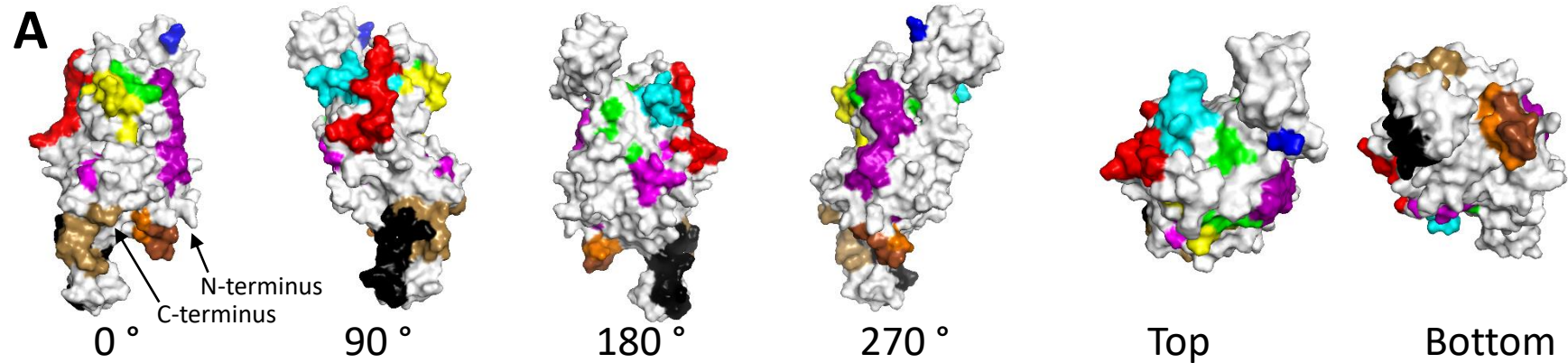
Pis s 1	Len c 1	Ara h 1	Gly m 5.01
3			11,12
14			
20			3,13
28			14
		7	
		8	
		9	
44*		10*	5,6*
53		21	7,15
		11	7, 16
		12	17
64			
74		13	
78	1	14	
	2-3	15	
	3	16	
93	3-4, 4	17	
	4	18	
100		19	18
			4, 18

Supplemental Figure S2: Representative images of the orientation of the monomers included in the asymmetric units of the crystals obtained for A) Pis s 1 (PDB 7U1I), B) Pis s 2 (PDB 7U1J) and C) Len c 1 (PDB 7U1H).



Supplemental Figure S3. Representative images of the crystallographic packing for A) Pis s 1, PDB 7U1I, B) Pis s 2, PDB 7U1J and C) Len c 1, PDB 7U1H. Upper panels depict packing in the unit cells (orange lines), with dimensions indicated with lengths (a, b, c) in Å and angles (α , β , γ) in degrees. Yellow triangles highlight representative trimers in each unit cell. Lower panels depict packing in the super cell. Images were obtained from the RCSB deposition site for each PDB entry.





Supplemental Figure S4. Surface character and mapping of previously identified linear IgE epitopes on the molecular surface of the Pis s 1 and Len c 1 crystal monomeric unit structures. Epitopes were mapped onto the structure of a monomer of (a) Pis s 1 (PDB# 7U1I) and (B) Len c 1 (PDB# 7U1H). For Pis s 1 epitopes (Popp et al. (2020)): 3 purple; 14 green; 20 cyan; P28 yellow; 44 blue; 53 red; 64 magenta; 74 orange; P78 brown; 93 black; 100 sand. For Len c 1 epitopes (Vereda et al. (2010)) : 1 red and magenta; 2 magenta, green, and cyan; 3 cyan, blue, and orange; 4 orange and yellow.