

Supplementary Material

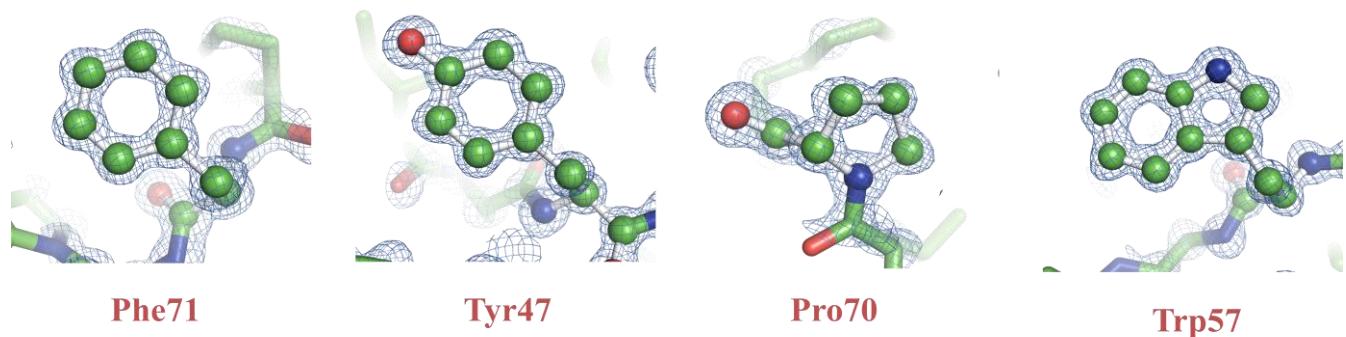


Figure S1. 2Fo-Fc electron density maps contoured at 1σ of representative Geodin residues.

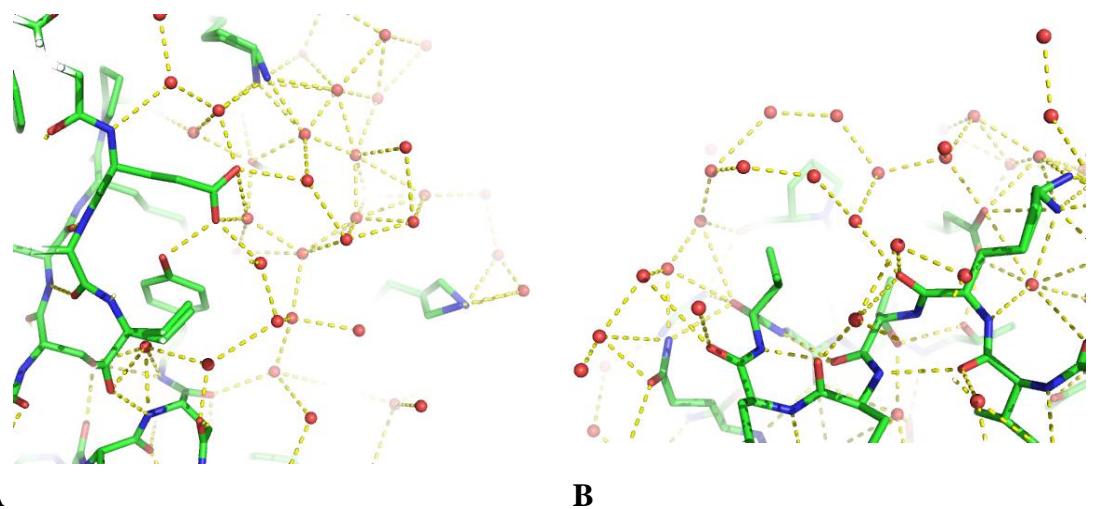


Figure S2. Networks of water molecules observed in the Geodin structure.

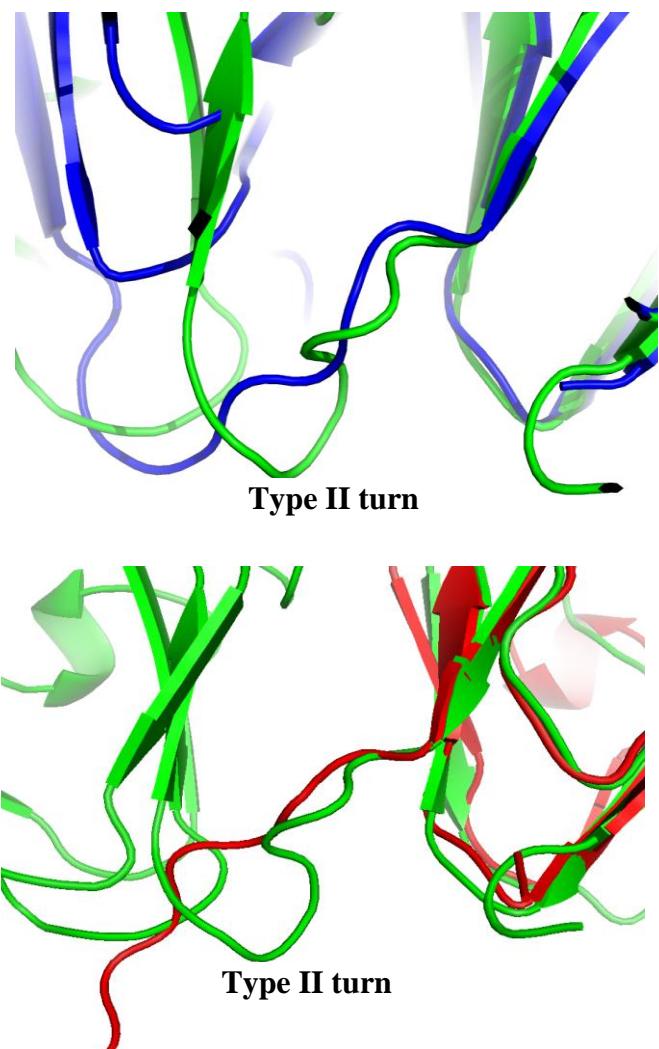


Figure S3. Ribbon representation showing the domain connecting peptide of Geodin (green) as compared to that of γ B bovine crystallin (blue) (a) and of β B2 human crystallin (red) (b), after the superimposition of the N-domain.

Table S1. Geodin and $\beta\gamma$ -cristallin domains: structural relatedness.

RMSD (\AA), Aligned C $^{\alpha}$ residues	Ci- $\beta\gamma$ -crystallin /	γD - human crystallin (2BV2)	γB bovine crystallin (1HK0)	βB2 human crystallin (4GCR)	Protein S (1PRR) (1YTQ)	Geodin N-domain	Geodin C-domain
Ci-$\beta\gamma$-crystallin (2BV2)	-	1.1/81 C $^{\alpha}$	1.1/81 C $^{\alpha}$	1.2/83 C $^{\alpha}$	1.9/79 C $^{\alpha}$	1.7/67 C $^{\alpha}$	1.3/77 C $^{\alpha}$
γD human crystallin (1HK0)	24%	-	0.8/173 C $^{\alpha}$	1.2/86 C $^{\alpha}$	2.0/80 C $^{\alpha}$	1.7/68 C $^{\alpha}$	1.2/77 C $^{\alpha}$
γB bovine crystallin (4GCR)	32%	76%	-	1.1/86 C $^{\alpha}$	1.9/80 C $^{\alpha}$	1.7/70 C $^{\alpha}$	1.2/77 C $^{\alpha}$
βB2 human crystallin (1YTQ)	36%	38%	35%	-	2.2/83 C $^{\alpha}$	1.6/70 C $^{\alpha}$	1.3/77 C $^{\alpha}$
Protein S (1PRR)	23%	20%	16%	25%	-	2.2/68 C $^{\alpha}$	2.1/71 C $^{\alpha}$
Geodin N-domain	15%	29%	17%	21%	21%	-	1.3/58 C $^{\alpha}$
Geodin C-domain	34%	26%	23%	26%	24%	15%	-

All information was obtained by using pairwise structural alignment of Dali server (Holm et al., 2008)

Table S2. Structural features of $\beta\gamma$ -crystallin interdomain interface

	Geodin	γ E murine crystallin (1A5D)	γ F bovine crystallin (1A45)	γ B bovine crystallin (4GCR)	Protein S (1PRR)
Accessible Surface Area (ASA) (\AA^2) (N-C)	685	875	801	745	520
Accessible Surface Area (ASA) (\AA^2) (C-N)	675	801	793	759	537
ASA (N-C) %	15.1	18.5	16.6	16.6	10.1
ASA (C-N) %	16.0	14.6	14.7	13.5	11.0
Planarity (\AA) (N-C)	1.74	2.13	2.37	2.00	1.45
Planarity (\AA) (C-N)	1.65	2.26	2.25	1.99	1.52
Length/ Breadth (N-C)	0.78	0.67	0.69	0.75	0.86
Length / Breadth (C-N)	0.83	0.63	0.65	0.78	0.81
% Polar Atoms at interface (N-C)	37.85	18.46	21.62	23.26	39.71
% Polar Atoms at interface (C-N)	26.65	27.91	27.74	29.50	50.75
% Non Polar Atoms at interface (N-C)	41.80	50.08	49.51	41.95	47.62
% Non Polar Atoms at interface (C-N)	49.93	42.26	36.64	38.24	24.50
Hydrogen bonds	8	2	5	3	3

Data were obtained using the protein–protein interaction server, <http://www.biochem.ucl.ac.uk/bsm/PP/server>. N- and C- refer to N- and C-domains.

Table S3. Ca²⁺ coordination sphere in Geodin and Ci-βγ-crystallin

Ca ²⁺ coordination sphere in Geodin		Ca ²⁺ coordination sphere in Ci-βγ-crystallin (2BV2)	
	Distance from Ca ²⁺ (Å)		Distance from Ca ²⁺ (Å)
Lys90 O	2.29	Glu7 O	2.30
Gly112 O	2.50	Ile33 O	2.40
Ser114 O^γ	2.37	Ser35 O ^γ	2.40
Asp154 O^{δ1}	2.38	Asp75 O ^{δ1}	2.50
Glycerol O	2.51	Glu7 O ^{ε1} (from a symmetry related molecule)	2.20
Glycerol O	2.43	H ₂ O	2.40
H₂O	2.35	H ₂ O	2.30

Table S4. Sequence alignment of Geodin interdomain peptide (underlined residues) with those of γ - and β -type crystallins.

β B2 human crystallin	$_{80}$ P I <u>K V D S Q E</u>
γ B bovine crystallin	$_{80}$ L I <u>P Q H T G T</u>
Geodin	$_{78}$ P V <u>K T F Q V G</u>